

1 Contents

1	Contents	1
2	Remarks Regarding the Labelling of the Geometries	3
3	Catalyst Coordinates	4
4	Uncatalyzed Background Reaction	12
4.1	Educt Complexes 16	12
4.2	Product Complexes 17	14
4.3	Transition States for Product Formation	15
5	Preactivation of Catalyst	17
5.1	Educt Complexes and Intermediates	17
5.2	Product Complexes	25
5.3	Transition States	33
6	Structures of the proposal in the main text of the paper	40
6.1	Educt Complexes 14	40
6.2	Product Complexes 15	72
6.3	Transition States for Product formation	86
7	Other Pathways	102
7.1	Complexes 10, 11, 14 and 15	102
7.1.1	Educt Complexes 10	102
7.1.2	Product Complexes 11	110
7.1.3	Educt Complexes 14	119
7.1.4	Product Complexes 15	162
7.2	Pathways from Complexes 14 to 15	210
7.2.1	Pathways starting from 14d-mi	210
7.2.1.1	to 15d-mi	210
7.2.1.2	to 15r-mi	221
7.2.1.3	to 15s-mi	223
7.2.1.4	to 15l-mi	225
7.2.1.5	to 15a-mi	227
7.2.1.6	to 15j-mi	232
7.2.2	Pathways starting from 14j-mi	235
7.2.2.1	to 15d-mi	235
7.2.2.2	to 15r-mi	246
7.2.2.3	to 15c-mi	259
7.2.2.4	to 15s-mi	260
7.2.2.5	to 15q-mi	263
7.2.2.6	to 15l-mi	265
7.2.2.7	to 15a-mi	266
7.2.2.8	to 15j-mi	272
7.2.2.9	to 15o-mi	274
7.2.3	Pathways starting from 14j-ma	277
7.2.3.1	to 15r-ma and 15r-2-ma	277
7.2.3.2	to 15d-ma and 15d-2-ma	291
7.2.3.3	to 15n-ma	311
7.2.3.4	to 15q-ma	313
7.2.3.5	to 15j-ma	316
7.2.3.6	to 15o-ma	318

7.2.3.7	to 15c-ma	320
7.2.3.8	to 15p-ma	326
7.2.3.9	to 15b-ma	330
7.2.3.10	to 15l-ma	336
7.2.4	Pathways starting from 14d-ma	341
7.2.4.1	to 15r-ma and 15r-2-ma	341
7.2.4.2	to 15d-ma and 15d-2-ma	350
7.2.4.3	to 15n-ma	353
7.2.4.4	to 15j-ma	355
7.2.4.5	to 15o-ma	357
7.2.4.6	to 15c-ma	364
7.2.4.7	to 15p-ma	370
7.2.4.8	to 15b-ma	382
7.2.4.9	to 15l-ma	388
7.3	Complexes 13	389
7.4	Agglomeration to Complexes 13	399
7.4.1	Pathways starting from 13j-ma	399
7.4.2	Pathways starting from 13d-ma	417
7.4.3	Pathways starting from 13d-mi	434
7.5	Interconversion of Complexes 13	452
7.5.1	Pathway 13d-ma ↔ 13d-mi	452
7.5.2	Pathway 13j-ma ↔ 13d-ma	458
7.5.3	Pathway 13j-ma ↔ 13d-mi	464
7.6	Complexes 12	466
7.7	Agglomeration to Complexes 12	474
7.7.1	Pathway 12d-ma → 14d-ma	474
7.7.2	Pathway 12d-mi → 14d-mi	477
7.7.3	Pathway 12j-ma → 14j-ma	479
7.7.4	Pathway 12j-mi → 14j-mi	481
7.8	Interconversion of Complexes 14 - Mechanism 1	483
7.8.1	Pathway 14j-ma ↔ 14d-ma	483
7.8.2	Pathway 14j-ma ↔ 14j-mi	485
7.8.3	Pathway 14j-ma ↔ 14d-mi	492
7.8.4	Pathway 14j-mi ↔ 14d-mi	499
7.8.5	Pathway 14d-ma ↔ 14j-mi	501
7.8.6	Pathway 14d-ma ↔ 14d-mi	512
7.9	Interconversion of Complexes 14 - Mechanism 2	515
7.9.1	Pathway 14j-ma ↔ 14j-mi	515
7.9.2	Pathway 14j-ma ↔ 14d-mi	526
7.9.3	Pathway 14d-ma ↔ 14j-mi	533
7.9.4	Pathway 14d-ma ↔ 14d-mi	562
7.10	Interconversion of Complexes 14 - Mechanism 3	569
7.10.1	Pathway 14j-ma ↔ 14d-mi	569
7.10.2	Pathway 14d-ma ↔ 14j-mi	584
7.10.3	Pathway 14d-ma ↔ 14d-mi	596

2 Remarks Regarding the Labelling of the Geometries

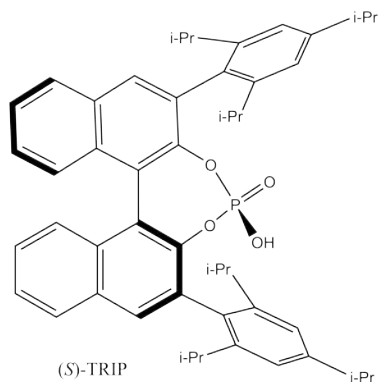
All geometries included in this file were optimized with RI-PBE-D3/def2-SVP. The general labelling follows the one used in the supporting information.

“COSMO” indicates a geometry which was optimized by including the COSMO solvation model. “Woelfling data” indicates that the corresponding transition state has not been fully optimized, but was obtained from TURBOMOLE’s woelfling-program. Energies given are the RI-PBE-D3/def2-SVP(+COSMO) energies.

For gas-phase optimized transition state geometries, we also give the number of remaining imaginary frequencies. These are not stated for the COSMO-optimized geometries, as TURBOMOLE currently does not allow the calculation of vibrational frequencies in an analytical way when the COSMO model is utilized.

3 Catalyst Coordinates

(*S*)-TRIP; COSMO

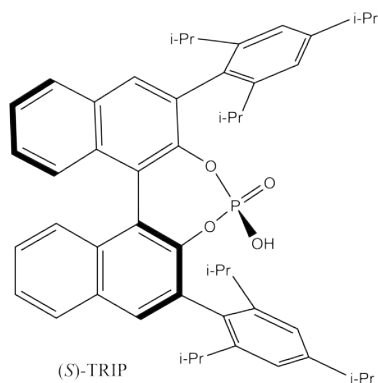


Energy (Hartree) = -2577.437910017

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C	0.3411892	-1.0192079	30.7078899
C	1.1357169	-2.0589155	31.2782417
C	-0.9683999	-0.7772474	31.2667865
C	-1.4500884	-1.6261485	32.3085941
C	-1.7344531	0.3375326	30.8182917
H	-2.7159109	0.5232272	31.2797280
C	-1.2489517	1.2257647	29.8662652
C	4.3486320	0.4685250	28.2982481
C	4.7006741	-0.7938779	27.8355390
H	5.7170652	-0.9580229	27.4462118
C	3.7714764	-1.8724933	27.8112583
C	4.1221818	-3.1360455	27.2468454
C	2.4417119	-1.6791266	28.3381529
C	1.5043296	-2.7489045	28.2131444
C	2.1009402	-0.4087798	28.9334003
C	3.0355472	0.6306850	28.8357399
O	0.4325147	1.7291017	28.2207962
O	2.7166794	1.8948637	29.3366198
P	1.6391626	2.8097977	28.5042828
O	1.1805589	3.7313407	29.7546710
H	0.5003423	4.3820702	29.4773011
O	2.0362357	3.4861755	27.2400365
C	-0.6645947	-2.6505750	32.8153811
C	0.6454650	-2.8539898	32.3055058
H	-2.4557979	-1.4377293	32.7162892
H	-1.0456815	-3.2934683	33.6234033
H	2.1543019	-2.2239187	30.9010736
H	1.2809960	-3.6454739	32.7312687
C	1.8710606	-3.9595099	27.6412570
C	3.1947342	-4.1639108	27.1672897
H	0.4738866	-2.6025965	28.5656457
H	1.1269562	-4.7654123	27.5493028
H	3.4758968	-5.1310210	26.7233283
H	5.1442271	-3.2721861	26.8597537
C	-1.9476892	3.5690115	30.5014590
C	-1.9120634	2.5246363	29.5284986
C	-2.4689184	4.8229779	30.1229020
C	-2.4178770	2.7574707	28.2182930
C	-2.9362331	4.0251381	27.9011226
C	-2.9620484	5.0783633	28.8319945
H	-2.4964843	5.6372357	30.8647793
C	-2.4575577	1.6580429	27.1591908
H	-3.3283168	4.1963350	26.8860331
C	-1.7778049	2.0814015	25.8454587

H	-1.7398349	1.2274171	25.1382968
H	-0.7407921	2.4256044	26.0261345
H	-2.3324133	2.9002610	25.3413679
C	-3.9066631	1.1899490	26.9241827
H	-1.8983571	0.7862721	27.5547098
H	-3.9362678	0.3573819	26.1910856
H	-4.5354934	2.0136428	26.5254948
H	-4.3735880	0.8362130	27.8659196
C	-3.4990099	6.4532318	28.4557915
C	-2.6366393	7.1124568	27.3636994
H	-1.5751897	7.1848456	27.6761506
H	-2.9998548	8.1362874	27.1375945
H	-2.6691599	6.5289618	26.4198331
C	-4.9803985	6.3951101	28.0419343
H	-3.4294866	7.0866531	29.3674642
H	-5.1186882	5.7881879	27.1227441
H	-5.3701807	7.4122741	27.8307734
H	-5.6051475	5.9448899	28.8395837
C	-1.4794050	3.3697940	31.9448446
C	-0.6074912	4.5172400	32.4837931
H	-0.2597269	4.2763231	33.5091404
H	-1.1642787	5.4749919	32.5480123
H	0.2904844	4.6757788	31.8562603
C	-2.6934117	3.1415440	32.8685151
H	-0.8563777	2.4532434	31.9716964
H	-3.3202834	2.2943284	32.5260043
H	-3.3420725	4.0423169	32.8948053
H	-2.3643740	2.9281393	33.9066060
H	8.1740690	5.2685019	27.0113990
H	7.6634214	1.5939834	31.5983730
H	6.8113748	1.6144601	24.5511836
C	8.0899486	4.9745298	28.0808221
H	4.0409429	2.9026132	31.3467561
H	6.5612131	6.5031126	28.4861537
H	3.5971563	3.5009452	25.4943678
C	7.1142810	3.8056029	28.1407205
C	6.8800024	0.8333693	31.3977278
C	7.5591385	6.1936482	28.8569115
H	8.2487509	7.0574514	28.7568199
C	6.7970303	3.1833732	29.3618500
C	5.9457565	0.9828930	24.8425473
H	9.4831998	4.2774729	29.6344225
C	6.4937373	3.3225242	26.9775558
C	9.4947165	4.5710844	28.5637538
H	9.8892340	3.7120491	27.9842598
H	6.7263373	3.8093207	26.0165322
C	4.9707282	2.4787592	31.7740924
H	6.6498255	0.3284242	32.3588378
H	7.3125862	0.0801216	30.7081643
C	5.8976315	2.1061155	29.4400282
C	4.3344836	2.9471214	24.8826681
C	5.5805123	2.2503310	26.9987427
H	5.4683484	0.6117928	23.9118722
H	6.3439852	0.1080118	25.3951493
C	5.6129271	1.4732572	30.8011058
C	5.2934337	1.6282334	28.2443770
C	4.9410280	1.7863877	25.6901828
H	5.6598731	3.3181847	32.0041702
H	5.1110680	3.6558856	24.5267675
H	4.7157429	1.9840003	32.7343097
H	7.4602213	5.9681366	29.9395677
H	3.8147878	2.5540228	23.9842833
H	10.2069598	5.4155366	28.4574745
H	4.8818194	0.6533919	30.6471834
H	4.1039876	1.1071604	25.9529378
H	7.2675234	3.5482922	30.2892635

(S)-TRIP

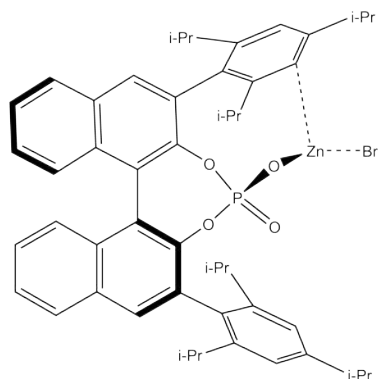


Energy (Hartree) = -2577.42980613

C	-0.0043875	0.8912558	29.2473999
C	0.7949085	-0.1931295	29.6167541
C	0.3400753	-1.0269239	30.7044798
C	1.1382927	-2.0628222	31.2761055
C	-0.9684370	-0.7866748	31.2665653
C	-1.4445924	-1.6339327	32.31115576
C	-1.7369234	0.3263781	30.8185001
H	-2.7154894	0.5150781	31.2849844
C	-1.2561695	1.2110330	29.8613963
C	4.3401277	0.4740676	28.2931262
C	4.7002393	-0.7880578	27.8367162
H	5.7194029	-0.9464020	27.4523676
C	3.7782586	-1.8725550	27.8139334
C	4.1371493	-3.1361083	27.2559725
C	2.4467136	-1.6855546	28.3380006
C	1.5170613	-2.7622149	28.2171004
C	2.0965913	-0.4148759	28.9264511
C	3.0241006	0.6311982	28.8253330
O	0.4103738	1.7058688	28.2012632
O	2.6940526	1.8949358	29.3168133
P	1.6182758	2.7948418	28.4621590
O	1.1483801	3.7362046	29.6963190
H	0.3784693	4.2887215	29.4396337
O	2.0184098	3.4443103	27.1873067
C	-0.6560802	-2.6551463	32.8186886
C	0.6525205	-2.8564974	32.3059685
H	-2.4494774	-1.4464120	32.7217591
H	-1.0337909	-3.2968035	33.6292004
H	2.1558934	-2.2256405	30.8957431
H	1.2910930	-3.6454944	32.7316638
C	1.8925052	-3.9728529	27.6520196
C	3.2173651	-4.1704471	27.1802721
H	0.4856873	-2.6200937	28.5683926
H	1.1539134	-4.7841396	27.5635113
H	3.5056923	-5.1375038	26.7409344
H	5.1603772	-3.2668604	26.8701580
C	-1.9233246	3.5632402	30.4947028
C	-1.9127452	2.5138548	29.5261180
C	-2.4243946	4.8247223	30.1133894
C	-2.4250489	2.7492005	28.2191913
C	-2.9244421	4.0238771	27.9004462
C	-2.9236204	5.0822621	28.8252370
H	-2.4317780	5.6426502	30.8516204
C	-2.4881047	1.6459709	27.1655893
H	-3.3203979	4.1966910	26.8872392
C	-1.8164118	2.0542638	25.8431604
H	-1.7953440	1.1960598	25.1406224
H	-0.7736285	2.3870122	26.0103895
H	-2.3665206	2.8758763	25.3385866

C	-3.9452006	1.1943211	26.9492769
H	-1.9346633	0.7703220	27.5606103
H	-3.9937279	0.3594148	26.2199889
H	-4.5692290	2.0234712	26.5545677
H	-4.4060390	0.8504292	27.8974415
C	-3.4389100	6.4645247	28.4459536
C	-2.5774708	7.1015476	27.3402708
H	-1.5113352	7.1569137	27.6393238
H	-2.9242899	8.1302219	27.1108798
H	-2.6298745	6.5131675	26.4005474
C	-4.9259238	6.4310744	28.0504407
H	-3.3473733	7.1022349	29.3528908
H	-5.0865468	5.8211651	27.1370446
H	-5.3007322	7.4533812	27.8374302
H	-5.5488731	5.9960631	28.8575617
C	-1.4479928	3.3611084	31.9354177
C	-0.5569406	4.4969291	32.4672806
H	-0.2046309	4.2518624	33.4899614
H	-1.1001103	5.4621672	32.5369733
H	0.3386103	4.6426187	31.8333537
C	-2.6596674	3.1496990	32.8658159
H	-0.8369817	2.4364866	31.9592237
H	-3.2995558	2.3107162	32.5274873
H	-3.2973188	4.0581107	32.8946160
H	-2.3285089	2.9331178	33.9024939
H	8.1499809	5.2913314	27.0318894
H	7.6422853	1.6034451	31.6089910
H	6.8011205	1.6102555	24.5651087
C	8.0653444	4.9923651	28.1000576
H	4.0102948	2.8858980	31.3403019
H	6.5289375	6.5113215	28.5092123
H	3.6059091	3.5397732	25.4821055
C	7.0942800	3.8193719	28.1530067
C	6.8650586	0.8383941	31.4016883
C	7.5279831	6.2061115	28.8797024
H	8.2131398	7.0740951	28.7851667
C	6.7789796	3.1897224	29.3701447
C	5.9257271	0.9901905	24.8516138
H	9.4598638	4.2940788	29.6518267
C	6.4749862	3.3416879	26.9875784
C	9.4711420	4.5929733	28.5827250
H	9.8692760	3.7374553	28.0009226
H	6.7044161	3.8357067	26.0296952
C	4.9407268	2.4682312	31.7718001
H	6.6344375	0.3287195	32.3601948
H	7.3076184	0.0912099	30.7121358
C	5.8830094	2.1098029	29.4422545
C	4.3372439	2.9720886	24.8764332
C	5.5650635	2.2672702	27.0019934
H	5.4501293	0.6235809	23.9182941
H	6.3106777	0.1112869	25.4069810
C	5.5967635	1.4706194	30.8000456
C	5.2808081	1.6373018	28.2439499
C	4.9260786	1.8079445	25.6916047
H	5.6211941	3.3131953	32.0071280
H	5.1240592	3.6671108	24.5158717
H	4.6845981	1.9700343	32.7299478
H	7.4273966	5.9758662	29.9610906
H	3.8135744	2.5804713	23.9798656
H	10.1810093	5.4400649	28.4816495
H	4.8728604	0.6454986	30.6397374
H	4.0793271	1.1400905	25.9528139
H	7.2473104	3.5514499	30.2998864

zinc salt of (*S*)-TRIP, most stable conformation according to ΔG data; COSMO

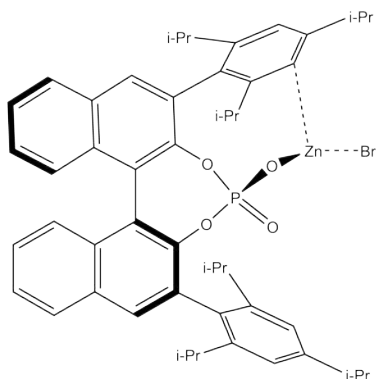


Energy (Hartree) = -6929.285931673

Zn	2.6823475	1.6364635	1.0645451
Br	4.5524310	0.4581576	1.6949215
C	-1.3197290	3.1518337	-0.1519526
C	-2.6662854	2.9156708	0.1392954
C	-3.3621613	3.8819416	0.9572658
C	-4.6847163	3.6706446	1.4514902
C	-2.6878599	5.1060711	1.3256236
C	-3.3866487	6.0866052	2.0923710
C	-1.3161420	5.2883155	0.9826696
H	-0.8040343	6.2057005	1.3123639
C	-0.6051948	4.3074929	0.3042174
C	-3.2903548	-0.8281929	-0.4428181
C	-4.5413358	-0.8045712	-1.0473374
H	-5.0423992	-1.7563645	-1.2815257
C	-5.1775603	0.4155628	-1.4138235
C	-6.4176091	0.4182019	-2.1209840
C	-4.5437246	1.6721007	-1.0936458
C	-5.1571612	2.8735397	-1.5624139
C	-3.3043805	1.6633756	-0.3534616
C	-2.6870944	0.4257705	-0.1120839
O	-0.6323809	2.2576986	-0.9442206
O	-1.4638637	0.3798948	0.5379380
P	-0.0925199	0.8184501	-0.2906407
O	0.8610488	1.1558444	0.9007764
O	0.3631594	-0.0589532	-1.4100397
C	-4.6859583	5.8633831	2.5227914
C	-5.3296747	4.6356530	2.2134708
H	-2.8636465	7.0204529	2.3526254
H	-5.2113696	6.6249937	3.1188273
H	-5.1938223	2.7232029	1.2283423
H	-6.3478866	4.4436859	2.5849737
C	-6.3540764	2.8417102	-2.2653582
C	-7.0014845	1.6062075	-2.5348667
H	-4.6632483	3.8366728	-1.3725322
H	-6.8008563	3.7823812	-2.6221820
H	-7.9542943	1.5935375	-3.0858073
H	-6.8943530	-0.5487007	-2.3467270
C	1.7023973	4.1320300	1.2927234
C	0.8790210	4.2956733	0.1418317
C	3.0897475	3.8673823	1.1044654
C	1.4620655	4.2557803	-1.1585823
C	2.8381474	3.9910959	-1.2967927
C	3.6787278	3.7874361	-0.1907945
H	3.7605556	3.8458907	1.9808572
C	0.6432377	4.5357594	-2.4127062
H	3.2700139	3.9506845	-2.3072099
C	0.8467781	3.4780526	-3.5106662
H	1.8697234	3.5168117	-3.9398150

H	0.1382103	3.6585702	-4.3440749
H	0.6674292	2.4573518	-3.1207380
C	0.9558964	5.9574105	-2.9231122
H	-0.4266360	4.5206906	-2.1259337
H	2.0203326	6.0516917	-3.2244389
H	0.7546026	6.7215791	-2.1451797
H	0.3310334	6.1942366	-3.8083515
C	5.1783298	3.5862345	-0.3373243
C	5.5457657	2.5968416	-1.4525623
H	6.6404819	2.4240901	-1.4625800
H	5.2622389	2.9752718	-2.4563318
H	5.0515576	1.6168600	-1.2955765
C	5.8670705	4.9519015	-0.5324879
H	5.5359769	3.1544606	0.6226216
H	6.9681023	4.8259510	-0.5732967
H	5.6307405	5.6493954	0.2962470
H	5.5420520	5.4286038	-1.4808457
C	1.1768749	4.2110955	2.7245185
C	1.5586945	2.9851391	3.5739071
H	1.1647742	3.0934829	4.6044971
H	2.6574953	2.8490439	3.6688431
H	1.1104684	2.0603237	3.1546608
C	1.6378560	5.5260278	3.3827433
H	0.0716789	4.2294515	2.6726996
H	1.1994671	5.6243999	4.3964727
H	1.3292101	6.4089150	2.7871615
H	2.7425364	5.5608587	3.4870175
H	-0.2434036	-6.3070731	-0.2465603
H	-3.7476694	-3.4682511	3.5521306
H	-3.2485553	-2.9145411	-4.4800269
C	-0.5521545	-5.8765703	0.7314458
H	-2.3293624	-0.6844182	4.1658538
H	1.2652160	-6.6059050	1.7252521
H	-0.8404891	-2.0753553	-4.3993153
C	-1.2617770	-4.5623854	0.4295096
C	-4.1319817	-2.5306768	3.0985211
C	0.7238878	-5.6506618	1.5628570
H	0.4825484	-5.2286213	2.5610074
C	-1.7955856	-3.7687231	1.4609495
C	-3.1608066	-3.2660428	-3.4308215
H	-2.3954128	-7.0759692	0.7956242
C	-1.3908541	-4.0971452	-0.8887033
C	-1.4909795	-6.8904195	1.4096787
H	-0.9765684	-7.8608790	1.5690103
H	-0.9651105	-4.7036396	-1.7045840
C	-1.9069060	-1.3144121	3.3554093
H	-4.5737607	-1.9207209	3.9138703
H	-4.9448046	-2.8067533	2.3962881
C	-2.4491129	-2.5510151	1.2051942
C	-0.7462323	-2.4747788	-3.3679437
C	-2.0297502	-2.8814844	-1.2016482
H	-4.1638112	-3.1987829	-2.9626495
H	-2.8773724	-4.3394907	-3.4561815
C	-3.0140895	-1.7533880	2.3794573
C	-2.5787235	-2.1097248	-0.1411212
C	-2.1130840	-2.4385068	-2.6623173
H	-1.1303619	-0.7259853	2.8285219
H	-0.0152741	-1.8512370	-2.8190440
H	-1.4165633	-2.1880783	3.8337868
H	1.4130951	-4.9439710	1.0582071
H	-0.3495417	-3.5080818	-3.4527300
H	-1.8280730	-6.5250283	2.4024939
H	-3.4757222	-0.8311041	1.9717660
H	-2.4468437	-1.3808575	-2.6686335
H	-1.7008889	-4.1094840	2.5048601

zinc salt of (*S*)-TRIP, most stable conformation according to ΔG data

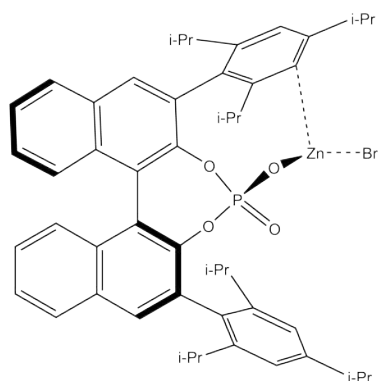


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Zn	2.6689608	1.6000274	1.0766583
Br	4.5493076	0.4970414	1.7777877
C	-1.3288944	3.1547601	-0.1460188
C	-2.6758640	2.9226388	0.1483977
C	-3.3685757	3.8947004	0.9617681
C	-4.6906711	3.6880488	1.4585643
C	-2.6927467	5.1203213	1.3220130
C	-3.3903318	6.1056908	2.0828058
C	-1.3213506	5.2982472	0.9763784
H	-0.8073994	6.2171205	1.2996286
C	-0.6120588	4.3122934	0.3037236
C	-3.2947668	-0.8225906	-0.4339050
C	-4.5457763	-0.8002882	-1.0376372
H	-5.0421677	-1.7537493	-1.2748139
C	-5.1863427	0.4185031	-1.4000222
C	-6.4268742	0.4196986	-2.1052745
C	-4.5554255	1.6760312	-1.0785918
C	-5.1724902	2.8759938	-1.5456021
C	-3.3155438	1.6691590	-0.3393305
C	-2.6962262	0.4323446	-0.0982968
O	-0.6436018	2.2571525	-0.9323327
O	-1.4756816	0.3873265	0.5551190
P	-0.0993016	0.8225001	-0.2667233
O	0.8361250	1.1862710	0.9352737
O	0.3823233	-0.0551247	-1.3721616
C	-4.6890030	5.8867948	2.5156430
C	-5.3338477	4.6582281	2.2145710
H	-2.8662967	7.0407887	2.3366463
H	-5.2129909	6.6528215	3.1071655
H	-5.1997361	2.7395808	1.2402008
H	-6.3519633	4.4695238	2.5878298
C	-6.3703796	2.8421971	-2.2459715
C	-7.0148784	1.6060846	-2.5161271
H	-4.6801145	3.8396952	-1.3552875
H	-6.8198891	3.7823564	-2.6005765
H	-7.9684464	1.5914353	-3.0655821
H	-6.9006724	-0.5482900	-2.3324532
C	1.6971167	4.1402360	1.2919563
C	0.8721348	4.2942922	0.1408190
C	3.0806856	3.8638326	1.1051408
C	1.4531240	4.2329022	-1.1598653
C	2.8265337	3.9561560	-1.2954267
C	3.6673135	3.7602723	-0.1879329
H	3.7504671	3.8352354	1.9817573
C	0.6353618	4.5023928	-2.4174495
H	3.2560852	3.8974725	-2.3059428
C	0.8335972	3.4321791	-3.5040932
H	1.8547175	3.4649997	-3.9385204

H	0.1228661	3.6040482	-4.3374251
H	0.6538162	2.4158729	-3.1033774
C	0.9522224	5.9175770	-2.9424758
H	-0.4342693	4.4936327	-2.1298011
H	2.0171880	6.0067151	-3.2436092
H	0.7527592	6.6908917	-2.1732372
H	0.3298268	6.1480808	-3.8311159
C	5.1655510	3.5449910	-0.3349756
C	5.5228411	2.5295604	-1.4298849
H	6.6166483	2.3516108	-1.4431295
H	5.2346508	2.8848838	-2.4408023
H	5.0277869	1.5548626	-1.2463512
C	5.8654863	4.9001326	-0.5592104
H	5.5220443	3.1268277	0.6314803
H	6.9655901	4.7661785	-0.6003016
H	5.6368794	5.6170716	0.2549690
H	5.5424486	5.3616842	-1.5157236
C	1.1737949	4.2391352	2.7237534
C	1.5270525	3.0104938	3.5816714
H	1.1427763	3.1384352	4.6137728
H	2.6222649	2.8435989	3.6703675
H	1.0533794	2.0954952	3.1703901
C	1.6610538	5.5482153	3.3741805
H	0.0692757	4.2810320	2.6708214
H	1.2246391	5.6641633	4.3870121
H	1.3722681	6.4337747	2.7725128
H	2.7660640	5.5625536	3.4803988
H	-0.2032742	-6.2750927	-0.2720214
H	-3.7538694	-3.5013025	3.5355918
H	-3.2182682	-2.8557523	-4.4876217
C	-0.5167151	-5.8543689	0.7089355
H	-2.3586390	-0.7083538	4.1767554
H	1.3110786	-6.5675251	1.6975313
H	-0.8101685	-2.0132278	-4.3875388
C	-1.2406564	-4.5462740	0.4150931
C	-4.1429402	-2.5626610	3.0884989
C	0.7572441	-5.6185441	1.5405455
H	0.5117478	-5.2048542	2.5410465
C	-1.7887497	-3.7685318	1.4504105
C	-3.1360792	-3.2158958	-3.4409463
H	-2.3459712	-7.0746907	0.7660858
C	-1.3649251	-4.0692125	-0.8987525
C	-1.4430029	-6.8838130	1.3802870
H	-0.9182250	-7.8497388	1.5332664
H	-0.9258734	-4.6618884	-1.7174924
C	-1.9287616	-1.3300445	3.3638051
H	-4.5930385	-1.9638098	3.9075236
H	-4.9503698	-2.8399182	2.3808257
C	-2.4515514	-2.5547842	1.2024889
C	-0.7204670	-2.4298041	-3.3626675
C	-2.0126974	-2.8570760	-1.2044368
H	-4.1411829	-3.1505714	-2.9772284
H	-2.8562485	-4.2899836	-3.4738394
C	-3.0282983	-1.7712107	2.3803622
C	-2.5762811	-2.1020471	-0.1398985
C	-2.0891425	-2.3985472	-2.6606704
H	-1.1536210	-0.7337299	2.8441396
H	0.0130662	-1.8196528	-2.8025047
H	-1.4336221	-2.2028139	3.8386953
H	1.4364063	-4.8994276	1.0404420
H	-0.3289912	-3.4635667	-3.4646114
H	-1.7843335	-6.5296858	2.3756101
H	-3.4958296	-0.8497057	1.9772876
H	-2.4206779	-1.3400722	-2.6571298
H	-1.6965853	-4.1178975	2.4916829

zinc salt of (*S*)-TRIP, second most stable conformation according to ΔG data; COSMO

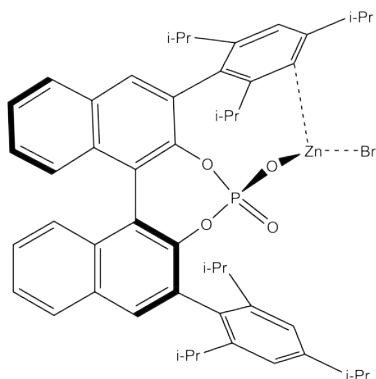


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C	1.3749530	1.8699386	1.1379671
C	2.7784042	1.8852408	1.1714604
C	3.4437400	3.1655784	1.2156188
C	4.8558528	3.3100735	1.0592725
C	2.6526694	4.3608104	1.3849566
C	3.3067557	5.6275932	1.4577450
C	1.2335177	4.2599702	1.4459619
H	0.6417022	5.1763717	1.5935144
C	0.5753656	3.0469741	1.2830279
C	3.8731757	-1.6237347	0.0764882
C	4.9151183	-1.8916573	0.9542469
H	5.4531713	-2.8501001	0.8880076
C	5.2636361	-0.9783798	1.9920480
C	6.2829047	-1.3003750	2.9382002
C	4.5275457	0.2571001	2.1361678
C	4.8002610	1.0702493	3.2775374
C	3.5315129	0.6005642	1.1476954
C	3.2318207	-0.3447879	0.1626441
O	0.7004947	0.6640000	1.0294343
O	2.2985841	-0.0407510	-0.8049862
P	0.6706493	-0.1146442	-0.4378097
O	-0.0883331	0.5229833	-1.5550031
O	0.3447162	-1.5717771	0.0227632
C	4.6843018	5.7286058	1.3323999
C	5.4604132	4.5586945	1.1152326
H	2.6896565	6.5288839	1.5995241
H	5.1752588	6.7124224	1.3831758
H	5.4691053	2.4162272	0.8789417
H	6.5501489	4.6421244	0.9834782
C	5.7839596	0.7182466	4.1920833
C	6.5472090	-0.4664377	4.0143979
H	4.2135482	1.9855310	3.4342641
H	5.9693497	1.3619251	5.0655177
H	7.3314126	-0.7295407	4.7404679
H	6.8445233	-2.2386758	2.8062235
C	-1.6381974	3.4374749	0.1275020
C	-0.9179386	2.9514436	1.2553588
C	-3.0423476	3.3598870	0.1397550
C	-1.6131209	2.3722153	2.3506885
C	-3.0188554	2.3138606	2.3072303
C	-3.7554564	2.8038836	1.2167059
H	-3.5985076	3.7387918	-0.7323968
C	-0.8860384	1.8284416	3.5792446
H	-3.5650694	1.8695774	3.1558820
C	-1.1386295	0.3216409	3.7707661
H	-2.2090854	0.1117066	3.9769514
H	-0.5517566	-0.0654632	4.6297999
H	-0.8419290	-0.2438667	2.8657430

C	-1.2433108	2.6310325	4.8438665
H	0.2027266	1.9594602	3.4133237
H	-2.3214919	2.5397621	5.0922188
H	-1.0195210	3.7092961	4.7119696
H	-0.6662063	2.2642152	5.7181426
C	-5.2767337	2.7186359	1.1960937
C	-5.9265313	4.1115944	1.1134928
H	-7.0327805	4.0350917	1.1587759
H	-5.6664050	4.6210151	0.1619155
H	-5.5910879	4.7631370	1.9456155
C	-5.7743409	1.7999703	0.0651213
H	-5.5864096	2.2605404	2.1613872
H	-6.8790521	1.6969735	0.0955481
H	-5.3299957	0.7873449	0.1440288
H	-5.5029214	2.2077619	-0.9311887
C	-0.9371017	4.0420118	-1.0891974
C	-1.4141303	3.4204353	-2.4133583
H	-0.8277152	3.8340439	-3.2601864
H	-2.4824892	3.6435742	-2.6163681
H	-1.2715825	2.3233045	-2.3945640
C	-1.0869297	5.5751011	-1.1056846
H	0.1434596	3.8087905	-0.9989110
H	-0.5427076	6.0156444	-1.9669542
H	-0.6920960	6.0381551	-0.1786891
H	-2.1545696	5.8678727	-1.1941962
H	0.2115079	-5.7683592	-2.8494104
H	4.9771863	-2.5530149	-4.4271818
C	3.5236522	-5.6217979	2.4529471
C	0.9149925	-5.2057650	-3.5008449
H	3.8556614	0.4818640	-4.1841182
H	-0.5371898	-5.1721463	-5.1275270
H	1.2536603	-4.5481651	2.8429635
C	1.7004349	-4.2753376	-2.5906179
C	5.2844977	-1.8820859	-3.5976952
C	0.0758396	-4.4554664	-4.5453613
H	0.7085896	-3.8993754	-5.2674268
C	2.4398608	-3.1899310	-3.0874174
C	3.4405618	-5.3841856	1.3730644
H	2.4481753	-6.7872404	-3.3968800
C	1.7816059	-4.5393413	-1.1924977
C	1.8731579	-6.2202052	-4.1564986
H	1.3035306	-6.9471297	-4.7704250
H	1.3187757	-5.4666805	-0.8125829
C	3.2406169	-0.3775505	-3.8488684
H	5.9241319	-1.0839193	-4.0266954
H	5.9008073	-2.4753167	-2.8921010
C	3.2298243	-2.3729700	-2.2561427
C	1.1835701	-4.2679629	1.7726276
C	2.5652938	-3.7380223	-0.3127221
H	4.4652873	-5.2572788	0.9688151
H	2.9863652	-6.2619506	0.8675425
C	4.0579275	-1.2648965	-2.8948728
C	3.2696068	-2.6241692	-0.8531925
C	2.5906925	-4.1152952	1.1670815
H	2.3362318	0.0199406	-3.3489122
H	0.6291930	-3.3073680	1.7281501
H	2.9265572	-0.9273368	-4.7606183
H	-0.6160339	-3.7369740	-4.0609621
H	0.5823766	-5.0605599	1.2775092
H	2.6004817	-5.7079386	-4.8205132
H	4.4401799	-0.6188869	-2.0802158
H	3.0826552	-3.2878943	1.7128630
H	2.4081822	-2.9741855	-4.1652265
Zn	-0.0230537	-3.2149499	-0.8352734
Br	-1.9712351	-4.3842971	-1.1823137

zinc salt of (*S*)-TRIP, second most stable conformation according to ΔG data

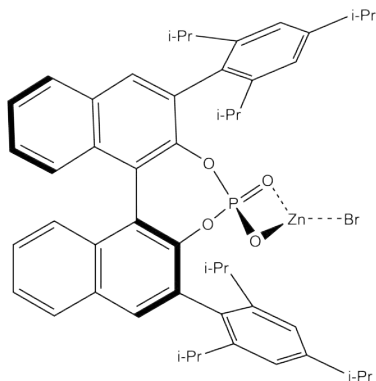


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C	1.3815776	1.8741394	1.1404990
C	2.7850246	1.8889346	1.1766641
C	3.4505930	3.1688847	1.2230106
C	4.8628996	3.3132961	1.0711057
C	2.6593339	4.3641801	1.3898465
C	3.3139866	5.6299711	1.4641130
C	1.2402001	4.2633945	1.4475841
H	0.6470433	5.1790758	1.5939393
C	0.5816601	3.0510926	1.2841971
C	3.8693311	-1.6218841	0.0790748
C	4.9096876	-1.8944884	0.9571597
H	5.4432689	-2.8556037	0.8906305
C	5.2625467	-0.9831780	1.9949184
C	6.2810056	-1.3079136	2.9403311
C	4.5311682	0.2550406	2.1391506
C	4.8078588	1.0670374	3.2801617
C	3.5362735	0.6032325	1.1515039
C	3.2333515	-0.3396974	0.1646175
O	0.7068633	0.6693161	1.0306967
O	2.3041768	-0.0324554	-0.8028006
P	0.6732330	-0.1066557	-0.4380498
O	-0.0876039	0.5177160	-1.5585408
O	0.3625695	-1.5681777	0.0291104
C	4.6914480	5.7309659	1.3435961
C	5.4675648	4.5613002	1.1294789
H	2.6964500	6.5313678	1.6030954
H	5.1821791	6.7147565	1.3957446
H	5.4756902	2.4188136	0.8928266
H	6.5577516	4.6441568	1.0015002
C	5.7910256	0.7120047	4.1933666
C	6.5495489	-0.4750526	4.0156100
H	4.2243299	1.9844655	3.4354092
H	5.9796765	1.3556009	5.0660914
H	7.3336938	-0.7408074	4.7407043
H	6.8393000	-2.2482202	2.8080595
C	-1.6326902	3.4196914	0.1229990
C	-0.9114273	2.9523071	1.2575301
C	-3.0358862	3.3336604	0.1356738
C	-1.6034247	2.3828861	2.3594559
C	-3.0081692	2.3161508	2.3157827
C	-3.7462261	2.7872989	1.2187030
H	-3.5930169	3.6956713	-0.7427824
C	-0.8730133	1.8541656	3.5925259
H	-3.5523021	1.8781076	3.1689551
C	-1.1145198	0.3470430	3.7948835
H	-2.1830834	0.1308301	4.0039457
H	-0.5239197	-0.0307982	4.6555023
H	-0.8168927	-0.2224997	2.8929010

C	-1.2355694	2.6638754	4.8508126
H	0.2149118	1.9917255	3.4256176
H	-2.3132238	2.5686480	5.0995163
H	-1.0191864	3.7424208	4.7107022
H	-0.6573675	2.3077776	5.7288073
C	-5.2664666	2.6874764	1.1956263
C	-5.9304520	4.0712928	1.0827629
H	-7.0360825	3.9855243	1.1266991
H	-5.6731614	4.5640224	0.1218196
H	-5.6030614	4.7436631	1.9011326
C	-5.7509062	1.7396968	0.0832484
H	-5.5746433	2.2464948	2.1695723
H	-6.8545865	1.6252331	0.1111036
H	-5.2952498	0.7344134	0.1845616
H	-5.4790826	2.1281097	-0.9204865
C	-0.9324585	4.0123933	-1.0999204
C	-1.4200984	3.3911268	-2.4201026
H	-0.8289972	3.7926745	-3.2693090
H	-2.4850780	3.6294059	-2.6238198
H	-1.2932135	2.2922959	-2.3979749
C	-1.0692016	5.5466375	-1.1209128
H	0.1464743	3.7696446	-1.0136680
H	-0.5277384	5.9800164	-1.9874874
H	-0.6648046	6.0106323	-0.1986587
H	-2.1349234	5.8479729	-1.2024291
H	0.1878787	-5.7392200	-2.8619055
H	4.9707660	-2.5372484	-4.4276331
H	3.4867983	-5.6278841	2.4480336
C	0.9035924	-5.1873495	-3.5093734
H	3.8512650	0.5008252	-4.1712842
H	-0.5323751	-5.1542849	-5.1507651
H	1.2313195	-4.5332500	2.8391793
C	1.6875553	-4.2585308	-2.5953709
C	5.2781999	-1.8685860	-3.5963246
C	0.0784398	-4.4382975	-4.5655439
H	0.7196316	-3.8878953	-5.2846357
C	2.4315905	-3.1744915	-3.0884143
C	3.4039719	-5.3878751	1.3685671
H	2.4243255	-6.7797469	-3.3829371
C	1.7654219	-4.5241757	-1.1986762
C	1.8597359	-6.2127837	-4.1503956
H	1.2921983	-6.9398112	-4.7661807
H	1.2857922	-5.4424748	-0.8183541
C	3.2358379	-0.3596045	-3.8394897
H	5.9189306	-1.0707274	-4.0242478
H	5.8948934	-2.4647129	-2.8935982
C	3.2230188	-2.3618330	-2.2549095
C	1.1628070	-4.2410699	1.7718510
C	2.5503885	-3.7294788	-0.3168016
H	4.4296402	-5.2754969	0.9623161
H	2.9387524	-6.2607494	0.8644578
C	4.0527814	-1.2528519	-2.8907450
C	3.2617943	-2.6178947	-0.8529149
C	2.5706424	-4.1080983	1.1630770
H	2.3326041	0.0375533	-3.3374658
H	0.6262586	-3.2708173	1.7349375
H	2.9210227	-0.9035764	-4.7546680
H	-0.6162024	-3.7163914	-4.0909058
H	0.5446988	-5.0166853	1.2704268
H	2.5980780	-5.7105679	-4.8099164
H	4.4358693	-0.6107210	-2.0735188
H	3.0748936	-3.2874583	1.7080512
H	2.4011024	-2.9548455	-4.1654348
Zn	-0.0635057	-3.1703353	-0.8649767
Br	-1.9719755	-4.3833953	-1.2246579

zinc salt of (*S*)-TRIP, high energy conformation; COSMO

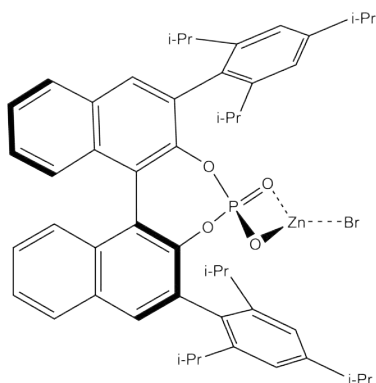


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C	-0.0089901	0.7961219	29.2841903
C	0.7514910	-0.3324283	29.6052936
C	0.2156364	-1.2341520	30.5987037
C	0.9632267	-2.3234301	31.1390050
C	-1.1197168	-1.0070284	31.1012179
C	-1.6690343	-1.9161480	32.0551186
C	-1.8477885	0.1464075	30.6873570
H	-2.8528696	0.3164226	31.1021122
C	-1.2969618	1.0893890	29.8285080
C	4.3192045	0.4187713	28.3750704
C	4.6952454	-0.8089119	27.8444346
H	5.7036665	-0.9270832	27.4198367
C	3.7867920	-1.9050473	27.7728700
C	4.1645118	-3.1286103	27.1416759
C	2.4450251	-1.7633493	28.2896116
C	1.5241802	-2.8330536	28.0771790
C	2.0807650	-0.5372951	28.9613436
C	3.0157160	0.5021240	28.9539213
O	0.4866723	1.7102941	28.3486627
O	2.6920251	1.7153853	29.5698634
P	1.6720237	2.7316115	28.8060257
O	1.2951882	3.8474892	29.8177555
O	2.1963942	3.4294241	27.5218734
C	-0.9266915	-2.9858640	32.5324178
C	0.4065249	-3.1773599	32.0816377
H	-2.6928994	-1.7383155	32.4198839
H	-1.3604863	-3.6748058	33.2730661
H	1.9992532	-2.4793471	30.8081842
H	1.0070338	-4.0061694	32.4866289
C	1.9181395	-4.0024853	27.4408189
C	3.2534903	-4.1622414	26.9840164
H	0.4849231	-2.7214145	28.4156801
H	1.1863859	-4.8097484	27.2845609
H	3.5567269	-5.0975033	26.4893398
H	5.1942403	-3.2275796	26.7638071
C	-1.9646549	3.4176391	30.5321358
C	-1.9208847	2.4150481	29.5213710
C	-2.4301755	4.7006785	30.1854533
C	-2.3535013	2.7160719	28.1993334
C	-2.8063776	4.0142313	27.9096162
C	-2.8396935	5.0287852	28.8835070
H	-2.4539114	5.4874590	30.9562873
C	-2.3640111	1.6631788	27.0929234
H	-3.1329697	4.2442661	26.8829640
C	-1.5949803	2.1190751	25.8404540
H	-2.0946157	2.9755935	25.3415744
H	-1.5376051	1.2955530	25.0990911
H	-0.5617149	2.4244995	26.0976174

C	-3.8083584	1.2498582	26.7515932
H	-1.8541149	0.7580137	27.4817143
H	-4.3879237	2.1098209	26.3549017
H	-4.3408012	0.8712946	27.6477508
H	-3.8187466	0.4509910	25.9812356
C	-3.2528346	6.4513551	28.5294230
C	-2.1974594	7.1132820	27.6227246
H	-2.4612347	8.1701594	27.4103379
H	-2.1203142	6.5836360	26.6497362
H	-1.1915384	7.1003358	28.0900422
C	-4.6552978	6.5181363	27.9010033
H	-3.2831251	7.0244833	29.4822098
H	-4.9523885	7.5707613	27.7145712
H	-5.4167765	6.0569119	28.5619665
H	-4.6892308	5.9879813	26.9262260
C	-1.5234846	3.1547681	31.9722753
C	-0.6062587	4.2540971	32.5357990
H	-0.2295616	3.9581987	33.5366643
H	-1.1409220	5.2184650	32.6630462
H	0.2604228	4.4175288	31.8674399
C	-2.7485643	2.9393710	32.8825991
H	-0.9348751	2.2147755	31.9754048
H	-2.4329549	2.7012908	33.9196910
H	-3.3914667	2.1117670	32.5207376
H	-3.3768306	3.8542349	32.9200354
H	7.1940883	5.8130192	26.9870553
H	7.6147735	1.9370754	31.4540964
H	5.5856153	0.5512814	24.0145963
C	7.0961281	5.5620476	28.0661718
H	4.7059458	1.9816062	32.8351942
H	6.5944588	7.6350170	28.6002802
H	3.6077917	2.1855489	23.9623331
C	6.4655809	4.1776643	28.1414562
C	6.8999307	1.0982929	31.3191089
C	6.1702818	6.6148262	28.7053440
H	6.0324704	6.4178472	29.7895842
C	6.3014450	3.5159666	29.3719230
C	5.9602163	1.0354697	24.9404176
H	9.1746082	4.8564682	28.2117962
C	5.9810542	3.5431651	26.9868934
C	8.5042020	5.6029216	28.6838460
H	8.9602928	6.6061614	28.5555012
H	6.1057838	4.0518686	26.0176096
C	4.8708497	2.5293249	31.8844665
H	6.8077844	0.5724699	32.2921629
H	7.3442722	0.3934479	30.5872223
C	5.6505594	2.2747226	29.4709874
C	4.0508952	2.7036196	24.8377799
C	5.3178167	2.3016023	27.0268396
H	6.4798643	0.2647193	25.5447287
H	6.7181504	1.7915858	24.6456508
C	5.5277877	1.6094598	30.8402709
C	5.1463125	1.6635090	28.2886936
C	4.8056374	1.6943727	25.7204872
H	3.8908102	2.9011315	31.5263150
H	3.2367825	3.1877750	25.4099610
H	5.5093370	3.4068517	32.1176004
H	5.1653239	6.6138493	28.2358585
H	4.7218027	3.4939562	24.4411097
H	8.4761084	5.3899337	29.7729589
H	4.8749414	0.7198464	30.7272204
H	4.0818360	0.8965508	25.9839018
Zn	1.8710034	5.2319457	28.4285332
Br	2.0391482	7.4570024	28.0886658
H	6.6826299	3.9886129	30.2911622

zinc salt of (*S*)-TRIP, high energy conformation



Energy (Hartree) = -6929.26922604

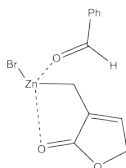
C	-0.0088886	0.7985675	29.2881247
C	0.7522789	-0.3304345	29.6058952
C	0.2188434	-1.2320683	30.6006900
C	0.9671303	-2.3221300	31.1377900
C	-1.1144830	-1.0043678	31.1079436
C	-1.6602253	-1.9136796	32.0629953
C	-1.8434276	0.1490214	30.6961893
H	-2.8471467	0.3203957	31.1136649
C	-1.2957089	1.0915989	29.8354088
C	4.3175568	0.4191805	28.3661726
C	4.6913696	-0.8085142	27.8347970
H	5.6990815	-0.9261371	27.4083921
C	3.7825144	-1.9042059	27.7653688
C	4.1575226	-3.1281313	27.1343490
C	2.4424403	-1.7621497	28.2860381
C	1.5214952	-2.8322119	28.0775606
C	2.0795965	-0.5356778	28.9577253
C	3.0146755	0.5035571	28.9463381
O	0.4824972	1.7134944	28.3524947
O	2.6942212	1.7176081	29.5602325
P	1.6711387	2.7340527	28.8016252
O	1.3072207	3.8516968	29.8166328
O	2.1828980	3.4306883	27.5113732
C	-0.9177398	-2.9842119	32.5366941
C	0.4131109	-3.1763074	32.0811474
H	-2.6824419	-1.7348114	32.4318063
H	-1.3497716	-3.6732784	33.2781734
H	2.0015826	-2.4778579	30.8023282
H	1.0145052	-4.0058463	32.4831760
C	1.9135479	-4.0019730	27.4415693
C	3.2467931	-4.1619020	26.9806003
H	0.4838296	-2.7195574	28.4202710
H	1.1813324	-4.8093865	27.2886631
H	3.5487880	-5.0973585	26.4856578
H	5.1860537	-3.2271066	26.7532835
C	-1.9598660	3.4234141	30.5309552
C	-1.9202394	2.4161332	29.5251205
C	-2.4221457	4.7057376	30.1784285
C	-2.3544723	2.7115118	28.2025072
C	-2.8042559	4.0091424	27.9075441
C	-2.8330336	5.0286179	28.8760096
H	-2.4423470	5.4961583	30.9454966
C	-2.3700184	1.6530705	27.1014284
H	-3.1327274	4.2346542	26.8805238
C	-1.6027170	2.0996344	25.8446888
H	-2.1003038	2.9550642	25.3419693
H	-1.5502780	1.2725751	25.1070324
H	-0.5674677	2.4022792	26.0962144

C	-3.8162458	1.2414388	26.7666934
H	-1.8612342	0.7488383	27.4939666
H	-4.3955133	2.1005127	26.3680122
H	-4.3471439	0.8693929	27.6662503
H	-3.8317740	0.4389375	26.0002634
C	-3.2444601	6.4499762	28.5152558
C	-2.1922083	7.1056838	27.6007261
H	-2.4562429	8.1608746	27.3809383
H	-2.1180054	6.5697410	26.6310319
H	-1.1846321	7.0976172	28.0641718
C	-4.6498876	6.5152746	27.8935655
H	-3.2698965	7.0284581	29.4650811
H	-4.9476215	7.5669116	27.7030177
H	-5.4084650	6.0570637	28.5595812
H	-4.6894242	5.9806218	26.9215685
C	-1.5186617	3.1655016	31.9719144
C	-0.5994012	4.2647032	32.5319236
H	-0.2234215	3.9719531	33.5338366
H	-1.1315841	5.2307271	32.6564742
H	0.2684001	4.4249399	31.8644801
C	-2.7446724	2.9557117	32.8821319
H	-0.9318712	2.2243476	31.9786568
H	-2.4310773	2.7210335	33.9205278
H	-3.3894482	2.1285872	32.5227257
H	-3.3719564	3.8712256	32.9153819
H	7.1833255	5.8243832	27.0051300
H	7.6147546	1.9234035	31.4481649
H	5.5947446	0.5684778	24.0092588
C	7.0877167	5.5665063	28.0829463
H	4.7063794	1.9560273	32.8334045
H	6.5875964	7.6359033	28.6339022
H	3.6130125	2.1996792	23.9563938
C	6.4589206	4.1809503	28.1503032
C	6.9004557	1.0848552	31.3099167
C	6.1631613	6.6150915	28.7304328
H	6.0256819	6.4103754	29.8132179
C	6.2964257	3.5122061	29.3768389
C	5.9648723	1.0505501	24.9378878
H	9.1661355	4.8589789	28.2198325
C	5.9757258	3.5515286	26.9928501
C	8.4974558	5.6035145	28.6968278
H	8.9541976	6.6070241	28.5736024
H	6.0992221	4.0653679	26.0262340
C	4.8689291	2.5089128	31.8853616
H	6.8110503	0.5537676	32.2803152
H	7.3453565	0.3852671	30.5736364
C	5.6483295	2.2694734	29.4696685
C	4.0528712	2.7154961	24.8346339
C	5.3156921	2.3083480	27.0259054
H	6.4847107	0.2794213	25.5414164
H	6.7229874	1.8082388	24.6482587
C	5.5271955	1.5967059	30.8354652
C	5.1452898	1.6637020	28.2842258
C	4.8069422	1.7051963	25.7164055
H	3.8873975	2.8803247	31.5315469
H	3.2357746	3.1969909	25.4045030
H	5.5051069	3.3867035	32.1236571
H	5.1580795	6.6202387	28.2616285
H	4.7229018	3.5081547	24.4413035
H	8.4725917	5.3844214	29.7847117
H	4.8756482	0.7067122	30.7176207
H	4.0836727	0.9054075	25.9755038
Zn	1.8707377	5.2325289	28.4210371
Br	2.0394061	7.4504238	28.0792249
H	6.6773043	3.9803213	30.2984710

4 Uncatalyzed Background Reaction

4.1 Educt Complexes 16

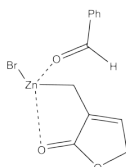
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Energy (Hartree) = -5040.681416145

C	-4.3107479	-0.2200071	-1.2730258
C	-3.2430085	0.6562699	-1.0396990
C	-2.2264541	0.3013295	-0.1238205
C	-2.2857957	-0.9384326	0.5569275
C	-3.3530286	-1.8088816	0.3209050
C	-4.3643499	-1.4495901	-0.5931211
H	-5.1040922	0.0524327	-1.9850442
H	-3.1861123	1.6234020	-1.5642995
C	-1.1183713	1.2306982	0.1057777
H	-1.4818962	-1.1912264	1.2647288
H	-3.4061470	-2.7738067	0.8474319
H	-5.2038259	-2.1381865	-0.7760164
O	-0.1857015	1.0026870	0.8912029
H	-1.1409609	2.1970469	-0.4623520
H	4.2778725	-2.0884782	-1.1851044
Br	0.3587469	4.4226137	0.6889054
H	3.9648162	2.0827706	1.2652310
Zn	1.4935582	2.3902419	0.9388385
C	3.6356965	-1.0599555	0.6381801
C	3.3565108	-1.7465098	-0.6630875
H	4.1449974	-1.5521744	1.4785194
C	3.1822255	0.2213172	0.5808091
C	3.1345203	1.3790867	1.5014321
C	2.5470077	0.3683297	-0.7570460
O	2.6939606	-0.7636775	-1.4847505
O	1.9091278	1.3414488	-1.1626719
H	2.6783099	-2.6244795	-0.5728691
H	3.2332417	1.0859310	2.5640185

ed_{unc.} = 16₁

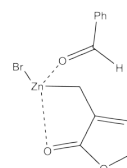


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C	-4.3691152	-0.1719499	-1.2136937
C	-3.3043565	0.7050919	-0.9700760
C	-2.2424686	0.3091144	-0.1269397
C	-2.2536533	-0.9728902	0.4709826
C	-3.3175129	-1.8446406	0.2253495
C	-4.3742840	-1.4441022	-0.6162590
H	-5.1979342	0.1331218	-1.8699127
H	-3.2845681	1.7057875	-1.4306902
C	-1.1342932	1.2395430	0.1161409
H	-1.4127193	-1.2538030	1.1229766

H	-3.3325716	-2.8431309	0.6880365
H	-5.2111396	-2.1336436	-0.8074622
O	-0.1690169	0.9720347	0.8445395
H	-1.1879488	2.2433047	-0.3829860
H	4.2976093	-2.1377222	-1.1053888
Br	0.3483885	4.4047645	0.6129770
H	3.9682829	2.1111298	1.2080994
Zn	1.5016019	2.4023080	0.8763982
C	3.6503516	-1.0544083	0.6861560
C	3.3741835	-1.7783653	-0.5972934
H	4.1582931	-1.5192688	1.5426348
C	3.1976989	0.2240795	0.5890373
C	3.1448026	1.4089120	1.4710163
C	2.5633554	0.3311624	-0.7558613
O	2.7160422	-0.8241119	-1.4493670
O	1.9247739	1.2888305	-1.1874880
H	2.6961836	-2.6547251	-0.4833741
H	3.2501150	1.1537771	2.5424475

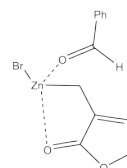
16₂; COSMO



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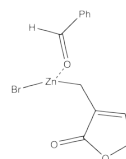
C	-4.5840775	1.2301712	1.0885064
C	-3.4463380	1.3635231	0.2822137
C	-2.6322049	0.2381817	0.0185481
C	-2.9654008	-1.0227970	0.5690172
C	-4.1012865	-1.1505347	1.3728090
C	-4.9096111	-0.0251002	1.6320369
H	-5.2201055	2.1036840	1.2959294
H	-3.1773126	2.3402188	-0.1508070
C	-1.4465375	0.4000888	-0.8252420
H	-2.3157643	-1.8836124	0.3501668
H	-4.3659779	-2.1279178	1.8038520
H	-5.8036702	-0.1302221	2.2660252
O	-0.6786472	-0.5306121	-1.1138880
H	-1.2482247	1.4270388	-1.2288274
H	5.1872420	0.0152320	1.9059005
Br	0.3988539	1.5532842	-3.6666585
H	1.9795673	-2.1262602	-1.0014282
Zn	1.1636821	-0.0455514	-2.1284988
C	4.6855982	-0.6891367	-0.1054626
C	4.9285386	0.3990031	0.8939657
H	5.4494718	-1.4287905	-0.3836817
C	3.4088453	-0.6048128	-0.5661801
C	2.5739719	-1.3514968	-1.5379173
C	2.8161010	0.5873579	0.0985276
O	3.6886406	1.1310913	0.9775278
O	1.7099048	1.0800428	-0.1322009
H	5.7254639	1.1152778	0.5932980
H	3.1793772	-1.8671510	-2.3075318

16₂



Energy (Hartree) = -5040.670706369

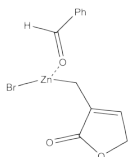
C	-4.6094239	1.2181169	1.0454013
C	-3.4763954	1.3513051	0.2325506
C	-2.6331735	0.2402461	0.0085982
C	-2.9324311	-1.0066671	0.6059015
C	-4.0631832	-1.1350583	1.4166838
C	-4.9008997	-0.0235556	1.6359216
H	-5.2682764	2.0815576	1.2215319
H	-3.2331730	2.3178071	-0.2372325
C	-1.4496446	0.3991267	-0.8441698
H	-2.2577283	-1.8547900	0.4150438
H	-4.3008942	-2.1024845	1.8845087
H	-5.7910155	-0.1286181	2.2754588
O	-0.6652600	-0.5243544	-1.0997276
H	-1.2710869	1.4144934	-1.2872314
H	5.2114881	-0.0438619	1.8998895
Br	0.3833362	1.6084727	-3.6275023
H	1.9425790	-2.0873615	-1.0228499
Zn	1.1820600	0.0133375	-2.1313768
C	4.6891363	-0.6947202	-0.1262012
C	4.9331241	0.3673040	0.9032270
H	5.4543090	-1.4201769	-0.4359738
C	3.4062258	-0.6087322	-0.5679681
C	2.5644650	-1.3281972	-1.5501343
C	2.8109087	0.5619020	0.1376947
O	3.6910074	1.0832822	1.0262544
O	1.7037280	1.0540009	-0.0730355
H	5.7199811	1.1008377	0.6150258
H	3.1603369	-1.8530121	-2.3202884



Energy (Hartree) = -5040.670286015

C	0.9513539	0.5843262	-5.0197904
C	-0.1584642	0.6265256	-4.1693660
C	0.0288207	0.5724420	-2.7677093
C	1.3324486	0.4633465	-2.2342727
C	2.4396526	0.4368172	-3.0895368
C	2.2492002	0.4970995	-4.4809800
H	0.8050114	0.6133911	-6.1100775
H	-1.1778129	0.6655835	-4.5902525
C	-1.1068085	0.6843900	-1.8416864
H	1.4687636	0.4455937	-1.1420477
H	3.4560054	0.3757334	-2.6730891
H	3.1202869	0.4697092	-5.1540083
O	-2.2518387	1.0377992	-2.1524394
H	-0.8996873	0.4157073	-0.7747525
H	1.9026735	3.6411066	-4.6389605
Br	-3.9824028	1.1166635	-5.2577940
H	-2.7880491	4.9472258	-3.6316487
Zn	-2.9432019	2.3882188	-3.6338962
C	-0.0202345	4.6192792	-4.2728298
C	1.4185690	4.3679650	-3.9451578
H	-0.3559425	5.0545174	-5.2245883
C	-0.8020192	4.2110829	-3.2361885
C	-2.2647645	4.1692968	-3.0423479
C	0.1257357	3.6893813	-2.1833786
O	1.4197975	3.8024748	-2.6311576
O	-0.1378263	3.2035652	-1.0983962
H	2.0436660	5.2902492	-3.9400686
H	-2.5155834	4.2741837	-1.9673554

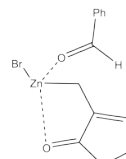
16₃; COSMO



Energy (Hartree) = -5040.6807109

C	0.9661327	0.6950790	-5.0052700
C	-0.1464098	0.7077842	-4.1580257
C	0.0317666	0.5683911	-2.7606248
C	1.3310840	0.4031474	-2.2290998
C	2.4423471	0.4075974	-3.0798861
C	2.2598719	0.5539754	-4.4662841
H	0.8275486	0.7910703	-6.0926075
H	-1.1619593	0.7850234	-4.5816998
C	-1.1000367	0.6432240	-1.8307372
H	1.4614030	0.3070356	-1.1400376
H	3.4552313	0.3000193	-2.6643371
H	3.1335429	0.5516254	-5.1363457
O	-2.2455713	1.0216149	-2.1172913
H	-0.8929745	0.3219141	-0.7790231
H	1.9182402	3.5969750	-4.6302863
Br	-4.0815460	1.0452224	-5.1236398
H	-2.7783924	4.9201450	-3.7308525
Zn	-2.9747288	2.3720347	-3.5646960
C	-0.0056801	4.5856629	-4.3066406
C	1.4278095	4.3390463	-3.9586042
H	-0.3281356	5.0007379	-5.2718950
C	-0.8004180	4.2036469	-3.2694558
C	-2.2656604	4.1752568	-3.0914882
C	0.1127369	3.7059098	-2.1955999
O	1.4110761	3.8008140	-2.6303604
O	-0.1633142	3.2547559	-1.0967277
H	2.0538782	5.2599259	-3.9644483
H	-2.5304924	4.3460393	-2.0278122

16₄; COSMO



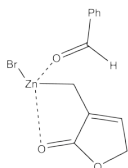
Energy (Hartree) = -5040.67800658

C	0.1991757	-0.6602381	-5.8775010
C	-0.0581888	-0.0299012	-4.6563013
C	0.9470257	0.0057670	-3.6589074
C	2.1995070	-0.6081857	-3.8999276
C	2.4535532	-1.2312752	-5.1273840
C	1.4532319	-1.2549901	-6.1159941
H	-0.5845344	-0.6961637	-6.6490125
H	-1.0508970	0.4048703	-4.4565278
C	0.7364304	0.6689619	-2.3676434
H	2.9734093	-0.5854945	-3.1157115
H	3.4293039	-1.7031381	-5.3168726
H	1.6494012	-1.7487618	-7.0803484
O	-0.2401408	1.3538291	-2.0417846
H	1.5642327	0.5331031	-1.6208965
H	1.8309512	5.2637503	-0.2645853
Br	-3.5842944	0.9993775	-3.3089997
H	-0.0134614	3.8447818	-4.5770356
Zn	-1.8052225	2.4892513	-3.0330053
C	0.9483335	5.3826233	-2.2754960
C	0.9609892	5.6928493	-0.8100295
H	1.7312783	5.7243529	-2.9669144

16₃

C	-0.1652929	4.6607818	-2.5747465
C	-0.7571948	4.0424239	-3.7816267
C	-0.8658991	4.4426438	-1.2803804
O	-0.2326053	5.0832457	-0.2745576
O	-1.8566499	3.7298267	-1.1002296
H	0.9344060	6.7837555	-0.5927314
H	-1.5446511	4.7065371	-4.2042227

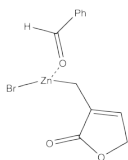
16₄



Energy (Hartree) = -5040.668302984

C	0.1457748	-0.8646882	-5.8232441
C	-0.0611477	-0.1241166	-4.6553790
C	0.9966494	0.0257075	-3.7260680
C	2.2490805	-0.5822508	-3.9790836
C	2.4510985	-1.3159674	-5.1534507
C	1.3983460	-1.4552382	-6.0756129
H	-0.6792456	-0.9887305	-6.5407370
H	-1.0510336	0.3134589	-4.4418093
C	0.8336671	0.8051104	-2.4924458
H	3.0644972	-0.4683409	-3.2461376
H	3.4266454	-1.7841861	-5.3530847
H	1.5538648	-2.0361386	-6.9980169
O	-0.1459844	1.4841260	-2.1750379
H	1.7107982	0.7675796	-1.7881195
H	1.7793880	5.2022184	-0.1556412
Br	-3.5213380	1.0700292	-3.5307308
H	-0.0076650	4.0447124	-4.5789216
Zn	-1.8030388	2.5783420	-3.1273438
C	0.9322389	5.4328792	-2.1747361
C	0.9191531	5.6625760	-0.6926146
H	1.7250675	5.8106069	-2.8353841
C	-0.1783189	4.7335168	-2.5307060
C	-0.7544143	4.1818341	-3.7739726
C	-0.9015784	4.4448644	-1.2595068
O	-0.2818921	5.0324745	-0.2103267
O	-1.8917645	3.7249691	-1.1367634
H	0.8949417	6.7411201	-0.4170716
H	-1.5515930	4.8581158	-4.1574277

16₅; COSMO

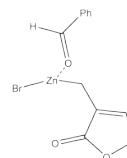


Energy (Hartree) = -5040.679400098

C	-4.4379384	-0.5546414	-0.7099969
C	-3.5082885	0.4921417	-0.7221717
C	-2.1939332	0.2731318	-0.2461447
C	-1.8186815	-0.9963557	0.2632915
C	-2.7569851	-2.0322459	0.2798041
C	-4.0604154	-1.8143667	-0.2104546
H	-5.4594089	-0.3923845	-1.0853160
H	-3.7888069	1.4862386	-1.1056848
C	-1.2319158	1.3719426	-0.2768109

H	-0.8013347	-1.1370890	0.6635767
H	-2.4785361	-3.0184427	0.6808811
H	-4.7929379	-2.6363926	-0.1959689
O	-0.0320520	1.2227385	0.0037937
H	-1.6110381	2.3888666	-0.5615511
H	2.9581830	-1.5946939	-1.8497366
Br	0.3012525	4.6663309	-0.1946501
H	2.7660360	1.6067659	2.2737287
Zn	1.4005839	2.7147956	0.4542130
C	3.7699994	-0.0609705	-0.5151065
C	3.3715149	-1.4700682	-0.8222629
H	4.5404753	0.4833558	-1.0794036
C	3.0318589	0.4061343	0.5284076
C	2.9630587	1.7234688	1.1875086
C	2.1269788	-0.7105675	0.9451018
O	2.3489770	-1.7938259	0.1268695
O	1.3015123	-0.7424520	1.8393606
H	4.2061512	-2.2000276	-0.7138270
H	3.8856907	2.3185131	1.0422492

16₅

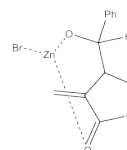


Energy (Hartree) = -5040.668125526

C	-4.4585288	-0.5368715	-0.6598792
C	-3.5216799	0.5022069	-0.6961069
C	-2.1960176	0.2727123	-0.2586674
C	-1.8161546	-0.9990317	0.2408400
C	-2.7629778	-2.0266379	0.2828161
C	-4.0767929	-1.7995310	-0.1718142
H	-5.4888300	-0.3664529	-1.0063811
H	-3.8051304	1.4993801	-1.0697759
C	-1.2264752	1.3652027	-0.3139159
H	-0.7908900	-1.1465184	0.6191439
H	-2.4808982	-3.0141017	0.6781561
H	-4.8152212	-2.6157435	-0.1372309
O	-0.0174050	1.2036954	-0.0897477
H	-1.6072835	2.3922675	-0.5621593
H	3.0683840	-1.5774421	-1.8681890
Br	0.2921128	4.6347032	-0.2449806
H	2.6771235	1.5747102	2.2746892
Zn	1.3987408	2.7130964	0.4155513
C	3.8135146	-0.0545120	-0.4821152
C	3.4307096	-1.4624463	-0.8198170
H	4.6086573	0.4970939	-1.0035042
C	3.0273481	0.3997684	0.5301728
C	2.9254473	1.7087677	1.2010120
C	2.1032477	-0.7226598	0.8936760
O	2.3673161	-1.7976019	0.0736567
O	1.2363283	-0.7590296	1.7441308
H	4.2621893	-2.1917713	-0.6805144
H	3.8531657	2.3066469	1.1106536

4.2 Product Complexes 17

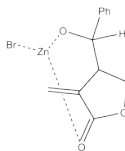
$p_{unc.} = 17_1$; COSMO



Energy (Hartree) = -5040.677055639

C	-1.8519734	12.5797814	84.8459298
C	-0.1689019	8.7216099	85.9347178
C	-1.6982871	11.5687920	83.8796660
C	-0.8830872	11.1061097	86.5231661
C	-0.7421456	10.0846460	85.5649200
C	-1.4397442	12.3472038	86.1673663
C	-1.1460389	10.3307697	84.2371638
O	0.6965430	8.2818959	84.9585031
H	-2.2843843	13.5523942	84.5646923
H	-0.5371482	10.9370633	87.5561036
H	-2.0070187	11.7509796	82.8384540
H	-1.5415136	13.1385785	86.9260212
H	-0.9994749	9.5412524	83.4839829
Br	3.1207399	5.0908195	84.7162082
Zn	1.4573971	6.6037171	85.0480153
H	-2.0578317	9.0369395	87.8149777
C	-1.4112358	7.7022436	86.1507193
C	-2.1427035	7.9880356	87.4734563
C	-0.9145667	6.3262450	86.3817459
C	-0.4949787	5.3850195	85.4847283
C	-0.8332780	6.1221709	87.8699732
O	-1.5083666	7.1471460	88.4666133
O	-0.2894698	5.2317364	88.4860372
H	-3.2173682	7.7183162	87.4169903
H	0.3143174	8.8067552	86.9432003
H	-2.0577899	7.7960840	85.2575103
H	-0.1239137	4.4128987	85.8488558
H	-0.7213095	5.4877378	84.4096764

$P_{unc.} = 17_1$

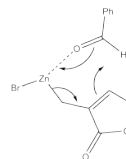


Energy (Hartree) = -5040.664085634

C	-1.8488065	12.5746678	84.8421069
C	-0.1711064	8.7182976	85.9366962
C	-1.6826672	11.5673917	83.8749706
C	-0.8918789	11.1002127	86.5235660
C	-0.7405490	10.0815750	85.5645243
C	-1.4478530	12.3403977	86.1660055
C	-1.1305553	10.3304174	84.2337910
O	0.6910092	8.2714131	84.9640068
H	-2.2805929	13.5469513	84.5592936
H	-0.5512128	10.9306099	87.5582541
H	-1.9799325	11.7525764	82.8310726
H	-1.5568078	13.1302891	86.9250268
H	-0.9683967	9.5440736	83.4807478
Br	3.1301288	5.1337196	84.6757153
Zn	1.4496671	6.5958235	85.0475688
H	-2.0599003	9.0397562	87.8173405
C	-1.4199100	7.7012338	86.1560865
C	-2.1424906	7.9876071	87.4843152
C	-0.9252061	6.3258034	86.3842587
C	-0.5043947	5.3854264	85.4859144
C	-0.8289252	6.1238424	87.8744413
O	-1.5008541	7.1548219	88.4732763
O	-0.2778075	5.2363741	88.4823380
H	-3.2184591	7.7177911	87.4334506
H	0.3100773	8.8033787	86.9466956
H	-2.0671035	7.8039835	85.2641235
H	-0.1284586	4.4155700	85.8514486
H	-0.7405465	5.4829362	84.4123589

4.3 Transition States for Product Formation

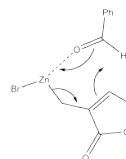
$TS_{unc.} = TS_1$; COSMO



Energy (Hartree) = -5040.667677945

C	-3.9123478	-0.9831607	-0.0128733
C	0.2301636	-0.2383125	0.9157487
C	-3.5073759	0.2841525	0.4483208
C	-1.6159718	-1.7704807	0.1432198
C	-1.2019934	-0.4974764	0.5901214
C	-2.9659813	-2.0107009	-0.1583320
C	-2.1622191	0.5258429	0.7512320
O	0.4947138	0.6788624	1.7897986
H	-4.9710117	-1.1715412	-0.2484685
H	-0.8805689	-2.5868584	0.0589778
H	-4.2508932	1.0858290	0.5769767
H	-3.2815302	-3.0086992	-0.4989542
H	-1.8306560	1.5059390	1.1265051
Br	3.3419832	2.1531319	3.9024635
Zn	2.1721024	1.5955439	2.0197548
H	0.4610995	-1.6489703	-1.5540794
H	1.8602312	3.0206697	-0.0650953
C	0.8687768	0.4502071	-0.9682523
C	1.0994794	-0.7797851	-1.8142268
H	0.0018139	1.1005080	-1.1529538
C	2.1429482	0.9599787	-0.6481141
C	2.5282232	2.1442778	0.0105465
C	3.1338382	-0.1353892	-0.9428985
O	2.4741812	-1.1455656	-1.5895439
O	4.3177184	-0.1765849	-0.6853934
H	0.9562276	-0.5698706	-2.8970674
H	0.8856258	-1.1422795	0.8745130
H	3.6116930	2.3607015	0.0280273

$TS_{unc.} = TS_1$



Energy (Hartree) = -5040.655950981
number of imaginary frequencies: 1

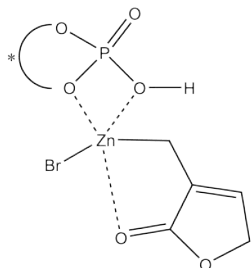
C	-3.9131672	-0.9770090	-0.0110805
C	0.2340508	-0.2403647	0.9055620
C	-3.5039716	0.2871030	0.4530902
C	-1.6192245	-1.7693169	0.1372436
C	-1.2004540	-0.4991457	0.5859969
C	-2.9700120	-2.0058409	-0.1616226
C	-2.1579936	0.5246856	0.7535688
O	0.4999072	0.6741068	1.7819605
H	-4.9727297	-1.1621585	-0.2446907
H	-0.8862233	-2.5878410	0.0514688
H	-4.2453119	1.0898861	0.5866936
H	-3.2888752	-3.0022933	-0.5034282
H	-1.8223349	1.5008547	1.1349825

Br	3.3283027	2.1548864	3.8972261
Zn	2.1731287	1.5940398	2.0210800
H	0.4704343	-1.6574058	-1.5472116
H	1.8514565	3.0213064	-0.0686061
C	0.8671812	0.4434078	-0.9625753
C	1.1070326	-0.7868009	-1.8087172
H	-0.0015548	1.0900982	-1.1527539
C	2.1403538	0.9609556	-0.6473008
C	2.5216473	2.1465697	0.0089553
C	3.1402756	-0.1300705	-0.9417157
O	2.4799755	-1.1459589	-1.5874280
O	4.3207622	-0.1606264	-0.6828916
H	0.9582622	-0.5788963	-2.8920769
H	0.8847404	-1.1491636	0.8677590
H	3.6046120	2.3649615	0.0264648

5 Preactivation of Catalyst

5.1 Educt Complexes and Intermediates

C_{ed}

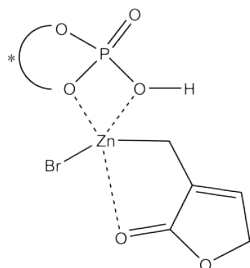


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C	0.6305378	-0.0456053	29.6199214
C	0.2480502	-0.8646554	30.7449093
C	1.1472341	-1.7607576	31.3947648
C	-1.0899223	-0.7408052	31.2710634
C	-1.4912044	-1.5707087	32.3600854
C	-1.9642131	0.2565451	30.7528776
H	-2.9633901	0.3670094	31.1992100
C	-1.5654073	1.1300858	29.7496857
C	4.1623758	0.9715244	28.5200851
C	4.6826604	-0.2593964	28.1334880
H	5.7446869	-0.3218694	27.8507803
C	3.8834343	-1.4342874	28.0701364
C	4.4131551	-2.6681335	27.5868128
C	2.5076158	-1.3755019	28.4973864
C	1.7093813	-2.5524343	28.3698571
C	1.9811074	-0.1308842	28.9996913
C	2.7908248	1.0114455	28.9093068
O	0.0646796	1.6945753	28.0658463
O	2.2659870	2.2590302	29.2630450
P	1.1164075	2.9324259	28.2770445
O	0.4424434	3.9140635	29.3843047
H	-0.5499552	3.8432075	29.4032903
O	1.5578585	3.5290476	26.9921797
C	-0.6028914	-2.4604307	32.9430776
C	0.7317077	-2.5394136	32.4652537
H	-2.5182873	-1.4714086	32.7450065
H	-0.9217469	-3.0875531	33.7894131
H	2.1884402	-1.8180663	31.0509761
H	1.4481847	-3.2161992	32.9551159
C	2.2497494	-3.7326414	27.8799533
C	3.6160629	-3.7984525	27.4964971
H	0.6489969	-2.5118661	28.6552672
H	1.6115740	-4.6241344	27.7827646
H	4.0346211	-4.7427064	27.1163183
H	5.4687063	-2.6996923	27.2742158
C	-2.4689001	3.4450825	30.2270574
C	-2.3528957	2.3334828	29.3313489
C	-3.1193895	4.6106541	29.7667762
C	-2.9008234	2.4176867	28.0195477
C	-3.5484166	3.6006171	27.6259284
C	-3.6619353	4.7146645	28.4763441
H	-3.2051280	5.4737811	30.4453310
C	-2.8408478	1.2441369	27.0453403
H	-3.9706604	3.6564401	26.6100905
C	-2.2171413	1.6333343	25.6939366
H	-2.1075389	0.7382058	25.0481020
H	-1.2140712	2.0819142	25.8312753
H	-2.8494818	2.3598543	25.1420693
C	-4.2381680	0.6193141	26.8706864
H	-2.1931648	0.4655911	27.4964763
H	-4.1920738	-0.2646848	26.2016869
H	-4.9506655	1.3438408	26.4234238
H	-4.6584703	0.2930210	27.8435259
C	-4.3308128	6.0004880	28.0090358
C	-3.5267564	6.6653465	26.8764837
H	-2.4793636	6.8579929	27.1841609
H	-3.9837810	7.6323847	26.5814194
H	-3.4959728	6.0195689	25.9741155
C	-5.7962558	5.7708308	27.5998616
H	-4.3292214	6.6969830	28.8762379
H	-5.8703122	5.0960606	26.7215656
H	-6.2822646	6.7288981	27.3229428
H	-6.3795957	5.3138183	28.4242504
C	-1.9553040	3.3993185	31.6690074
C	-1.2759010	4.6976490	32.1342539
H	-0.7987477	4.5450353	33.1214387
H	-1.9942014	5.5372349	32.2395715
H	-0.4743642	5.0278644	31.4446327
C	-3.0998213	3.0340453	32.6349564
H	-1.1904127	2.5980563	31.7345801
H	-3.5951294	2.0833712	32.3562853
H	-3.8792618	3.8248199	32.6389918
H	-2.7121125	2.9280568	33.6686104
H	8.0836103	5.7474552	27.5353064
H	7.1678332	0.8607887	31.3767497
H	6.6199702	2.1733203	24.9433443
C	7.9636911	5.4194957	28.5913219
H	4.8762770	3.7789426	32.2015740
H	6.5356232	7.0293701	29.0248369
H	3.5301651	4.2903910	25.8071976
C	6.9183176	4.3104366	28.5907275
C	6.0869813	0.6179352	31.3043263
C	7.5038082	6.6426705	29.4032322
H	8.2493800	7.4627624	29.3463224
C	6.5468422	3.6550722	29.7805246
C	5.6956463	1.6075016	25.1853179
H	9.2851414	4.5771664	30.1352931
C	6.2973865	3.9122609	27.3981036
C	9.3322267	4.9095151	29.0771365
H	9.6776840	4.0476652	28.4718030
H	6.5597212	4.4370525	26.4656146
C	5.3787601	2.8007042	32.3476873
H	5.7863182	0.1004542	32.2385104
H	5.9539228	-0.0918856	30.4651446
C	5.6160316	2.6018608	29.7946016
C	4.2362538	3.6826433	25.2113082
C	5.3572610	2.8638591	27.3532050
H	5.2249569	1.3004427	24.2284671
H	5.9990954	0.6883148	25.7248711
C	5.2578103	1.9020933	31.1067326
C	5.0425423	2.1844849	28.5583322
C	4.7275433	2.4694129	26.0179863
H	6.4370447	3.0060069	32.6128048
H	5.0750596	4.3257085	24.8719182
H	4.9051801	2.3060690	33.2187453
H	7.3733676	6.3827865	30.4748122
H	3.6986777	3.3401342	24.3036261
H	10.1002766	5.7079119	29.0116829
H	4.1898955	1.5996509	31.0395013
H	3.8324050	1.8542143	26.2453824
H	7.0011980	3.9734719	30.7307139
C	4.4449525	7.2224443	31.6900225
C	3.4776145	6.2801878	31.5388968
C	2.6395137	6.3501200	32.7693994
O	3.0607774	7.3574402	33.5747776
C	4.2282290	7.9517224	32.9815245
O	1.7269129	5.5868119	33.0724584
C	3.1359217	5.2582241	30.5268770
H	3.9966729	4.9518168	29.9025938

H	5.2623406	7.4532518	30.9945094
H	5.0698912	7.8442102	33.7028320
H	4.0469999	9.0416105	32.8432993
Zn	2.2011255	3.7833009	31.4969219
H	2.3388146	5.6413500	29.8516957
Br	1.5289209	1.9038601	32.6600798

D_{ed}



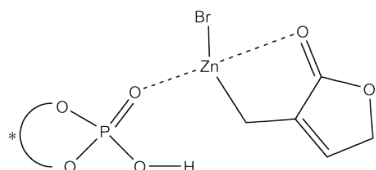
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C	0.3293977	-0.9992813	30.6358884
C	1.1883014	-1.9799969	31.2140897
C	-0.9756870	-0.8064902	31.2206019
C	-1.3919376	-1.6510443	32.2926136
C	-1.7972401	0.2689045	30.7777435
H	-2.7684067	0.4289141	31.2686173
C	-1.3768753	1.1542874	29.7939356
C	4.2754859	0.6575676	28.3281175
C	4.6948114	-0.5889905	27.8748504
H	5.7387268	-0.7115865	27.5477402
C	3.8145165	-1.7036242	27.7989972
C	4.2397195	-2.9499907	27.2491528
C	2.4626588	-1.5692795	28.2820966
C	1.5810504	-2.6836082	28.1420027
C	2.0422240	-0.3133143	28.8517722
C	2.9253850	0.7742279	28.7729903
O	0.2229834	1.6757696	28.0677234
O	2.5024307	2.0389862	29.1954465
P	1.3653178	2.8295902	28.2852144
O	0.8043305	3.8049526	29.4590191
H	-0.1892713	3.8045111	29.5120877
O	1.7966944	3.4499172	27.0081941
C	-0.5459160	-2.6218816	32.8047599
C	0.7608660	-2.7715351	32.2703351
H	-2.3942447	-1.4980312	32.7226266
H	-0.8749699	-3.2597245	33.6390930
H	2.2093039	-2.0935289	30.8265203
H	1.4469544	-3.5144438	32.7047501
C	2.0203839	-3.8770111	27.5873176
C	3.3638484	-4.0194293	27.1480485
H	0.5372153	-2.5832609	28.4705228
H	1.3191383	-4.7188475	27.4821906
H	3.7020589	-4.9737836	26.7165828
H	5.2783782	-3.0400674	26.8942424
C	-2.0975612	3.5033735	30.3994624
C	-2.0943903	2.4251656	29.4565913
C	-2.6857523	4.7277662	30.0142545
C	-2.6878706	2.6009346	28.1740023
C	-3.2695175	3.8396302	27.8560483
C	-3.2728274	4.9216289	28.7540461
H	-2.6847426	5.5652620	30.7292783
C	-2.7461325	1.4686303	27.1520455
H	-3.7281890	3.9662670	26.8625751
C	-2.1497811	1.8731135	25.7927856

H	-2.1263583	1.0012656	25.1074238
H	-1.1139268	2.2476430	25.9066644
H	-2.7518345	2.6631770	25.2972870
C	-4.1885389	0.9462978	27.0105257
H	-2.1361410	0.6301238	27.5443951
H	-4.2287763	0.0908147	26.3050784
H	-4.8669097	1.7351058	26.6229096
H	-4.5920010	0.6070218	27.9860499
C	-3.8744456	6.2664898	28.3685706
C	-3.0828939	6.9228319	27.2224199
H	-2.0114845	7.0345498	27.4838695
H	-3.4879830	7.9285732	26.9869563
H	-3.1386087	6.3137099	26.2960894
C	-5.3700032	6.1493955	28.0257697
H	-3.7847342	6.9258755	29.2598423
H	-5.5310251	5.5164290	27.1282029
H	-5.8034902	7.1473924	27.8092066
H	-5.9423489	5.6985855	28.8612000
C	-1.5294214	3.3633181	31.8146324
C	-0.7450311	4.5933308	32.3002363
H	-0.2395665	4.3683036	33.2590704
H	-1.4000093	5.4732531	32.4696037
H	0.0477256	4.8989372	31.5894086
C	-2.6551720	3.0350027	32.8152646
H	-0.8188658	2.5110224	31.8153528
H	-3.2253504	2.1319444	32.5220396
H	-3.3777705	3.8751961	32.8845437
H	-2.2329558	2.8603916	33.8258235
H	8.4623053	5.2079321	27.3677826
H	7.3787729	0.2312097	31.0481670
H	6.6711765	1.8340087	24.7046250
C	8.3657048	4.8415374	28.4134992
H	5.3206432	3.2541746	32.0853381
H	7.0683574	6.5196953	28.9804235
H	3.7683663	4.1189223	25.7679089
C	7.2495180	3.8037171	28.4137015
C	6.2820456	0.0624251	31.0122144
C	8.0244763	6.0545543	29.2961169
H	8.8198218	6.8263300	29.2380995
C	6.8816202	3.1253348	29.5916572
C	5.7194654	1.3229941	24.9619100
H	9.6915826	3.8449557	29.8586113
C	6.5585806	3.4953599	27.2329932
C	9.7162955	4.2218160	28.8146901
H	9.9770398	3.3678978	28.1579350
H	6.8193283	4.0395974	26.3113003
C	5.7622299	2.2400565	32.1704649
H	5.9849773	-0.4735377	31.9370840
H	6.0686285	-0.6010808	30.1520805
C	5.8845980	2.1345489	29.6033454
C	4.4080855	3.4887300	25.1224333
C	5.5499315	2.5128280	27.1864551
H	5.1933804	1.0871675	24.0137440
H	5.9781379	0.3644384	25.4541660
C	5.5326904	1.4047804	30.9008391
C	5.2371714	1.8066241	28.3766257
C	4.8448496	2.2145861	25.8639184
H	6.8415778	2.3644602	32.3983641
H	5.2758265	4.0865342	24.7732247
H	5.2918702	1.7402863	33.0403690
H	7.9250709	5.7562369	30.3609675
H	3.8146509	3.2189076	24.2251179
H	10.5328356	4.9705324	28.7488758
H	4.4452189	1.1749045	30.8668167
H	3.9188343	1.6522963	26.1043543
H	7.3924181	3.3741975	30.5339457
C	5.1201193	6.7162384	31.7541047
C	4.0787545	5.8568903	31.6012206
C	3.3018700	5.9216992	32.8716559
O	3.8328895	6.8503575	33.7064122
C	5.0151614	7.3887018	33.0895920

O	2.3480683	5.2122519	33.1782536
C	3.6182111	4.9182568	30.5561088
H	4.4255715	4.5855889	29.8763821
H	5.9219811	6.9234688	31.0335251
H	5.8767481	7.1810243	33.7639689
H	4.9110908	8.4948076	33.0153473
Zn	2.6233905	3.4624995	31.4948091
H	2.8219434	5.3926125	29.9402322
Br	1.8713455	1.5827299	32.6062054

$E_{ed} = G1_{ed}$; COSMO



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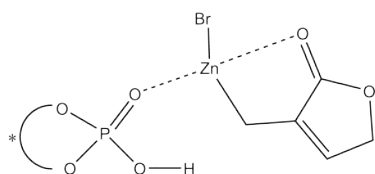
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C	0.9664285	-1.8657846	31.5135400
C	-1.2536257	-0.7977003	31.3954463
C	-1.7067398	-1.7155739	32.3901195
C	-2.1156767	0.2227789	30.8933992
H	-3.1506705	0.2659213	31.2635915
C	-1.6729598	1.1739823	29.9840201
C	4.0624550	1.0537267	28.7078439
C	4.5306446	-0.1448829	28.1804630
H	5.5635927	-0.1968277	27.8037807
C	3.7068565	-1.3027213	28.0917206
C	4.1810741	-2.4982204	27.4721384
C	2.3599668	-1.2607086	28.6089608
C	1.5282727	-2.4056827	28.4187059
C	1.8974834	-0.0583664	29.2598181
C	2.7383082	1.0615787	29.2365902
O	0.1059476	1.9596998	28.5545226
O	2.3040030	2.2572215	29.8132060
P	1.1201264	3.1162327	29.0832822
O	0.4923023	3.8737428	30.3133581
H	0.4213506	4.9021828	30.1464766
O	1.5740694	3.9545291	27.9079638
C	-0.8529554	-2.6686415	32.9259178
C	0.4980008	-2.7320878	32.4924336
H	-2.7498239	-1.6418868	32.7358781
H	-1.2155453	-3.3658161	33.6965443
H	2.0159928	-1.9203541	31.1921628
H	1.1814469	-3.4705707	32.9386697
C	2.0135680	-3.5464957	27.7943826
C	3.3551239	-3.6028224	27.3300658
H	0.4849787	-2.3745792	28.7616804
H	1.3495340	-4.4127699	27.6525828
H	3.7299324	-4.5163379	26.8439259
H	5.2150893	-2.5189603	27.0935859
C	-2.6364893	3.5008758	30.2889158
C	-2.4465188	2.3496328	29.4723838
C	-3.0736843	4.6877774	29.6731037
C	-2.7939296	2.3842045	28.0923964
C	-3.2198240	3.5983059	27.5275623
C	-3.3197992	4.7745121	28.2914411
H	-3.1864665	5.5979465	30.2824277
C	-2.7439001	1.1066410	27.2555357
H	-3.4391301	3.6344491	26.4521819
C	-2.5153230	1.3350043	25.7569501
H	-2.3683138	0.3634331	25.2426752

H	-1.6233618	1.9667028	25.5743558
H	-3.3851473	1.8276204	25.2738561
C	-4.0194625	0.2763464	27.5069496
H	-1.8886680	0.5005437	27.6218897
H	-3.9853386	-0.6809826	26.9462496
H	-4.9200071	0.8355809	27.1769914
H	-4.1447714	0.0404731	28.5832496
C	-3.5731921	6.1369886	27.6577541
C	-2.2179718	6.8065844	27.3403613
H	-1.5651883	6.8544132	28.2353027
H	-2.3604916	7.8376838	26.9541949
H	-1.6789920	6.2259287	26.5602989
C	-4.4687814	6.0976054	26.4123764
H	-4.0810464	6.7612009	28.4269534
H	-3.9679724	5.5786313	25.5687170
H	-4.6990493	7.1263775	26.0681780
H	-5.4279900	5.5783785	26.6124533
C	-2.3900724	3.4649297	31.7967448
C	-1.9073295	4.7946973	32.3983359
H	-1.6215059	4.6468525	33.4595953
H	-2.7032329	5.5681035	32.3845292
H	-1.0292317	5.2040524	31.8645398
C	-3.6665444	2.9996753	32.5289652
H	-1.5957906	2.7111294	31.9810712
H	-4.0311517	2.0242036	32.1523560
H	-4.4856681	3.7348954	32.3831779
H	-3.4849357	2.9016568	33.6196155
H	8.0633795	5.7539010	27.6440393
H	7.3585011	2.0171631	32.1658003
H	6.0300055	2.3622372	24.9696562
C	8.0317307	5.3571049	28.6826484
H	3.7344280	3.2886544	31.7884404
H	6.8264827	7.0741924	29.3532516
H	3.5329308	4.8300649	26.4021198
C	6.9178987	4.3166759	28.7229905
C	6.6013878	1.2539230	31.8893902
C	7.7622805	6.5450870	29.6234050
H	8.5895035	7.2825928	29.5732703
C	6.6196420	3.6097800	29.9029995
C	5.0716737	1.8984160	25.2847766
H	9.4424499	4.3139617	30.0102911
C	6.1572179	4.0264107	27.5779500
C	9.4006879	4.7157068	28.9762324
H	9.6090878	3.8772464	28.2816603
H	6.3500223	4.6023129	26.6588291
C	4.6536211	2.8630346	32.2378270
H	6.3358898	0.7020269	32.8144136
H	7.0818441	0.5403883	31.1895174
C	5.6489586	2.5906221	29.9399170
C	3.9105819	4.1173139	25.6396864
C	5.1651969	3.0254575	27.5649523
H	4.4505285	1.7474153	24.3780094
H	5.3017041	0.9014940	25.7088350
C	5.3494094	1.8918743	31.2637139
C	4.9516835	2.2622470	28.7450276
C	4.3392388	2.7950885	26.3001231
H	5.3247817	3.7045136	32.5116614
H	4.7495384	4.6170784	25.1126120
H	4.3686100	2.3422954	33.1753696
H	7.6735879	6.2147490	30.6795602
H	3.1118556	3.9353895	24.8918615
H	10.2162487	5.4609990	28.8731537
H	4.6368813	1.0677001	31.0554336
H	3.4099977	2.2719270	26.6081362
H	7.1707789	3.8475615	30.8271422
C	3.8571967	6.8317390	28.5265152
C	2.5189779	6.9227237	28.2648927
C	1.8419204	6.4670004	29.4963171
O	2.7391696	6.1359910	30.4473813
C	4.0653975	6.3094613	29.9084859
O	0.6240482	6.3058763	29.6798541

C	1.7404847	7.1605333	27.0427771
H	2.3375227	7.6155077	26.2294013
H	4.6824278	7.0323491	27.8302826
H	4.5733913	5.3183123	29.9235532
H	4.6287646	6.9872636	30.5862071
Zn	1.0430515	5.3623163	26.4699239
H	0.8402432	7.7780494	27.2389950
Br	-0.0708101	4.2513527	24.7526105

H	-3.3396630	1.8330288	25.2553870
C	-3.9954308	0.2792633	27.4814755
H	-1.8657592	0.5042906	27.6162856
H	-3.9572383	-0.6766666	26.9186754
H	-4.8931800	0.8392389	27.1458191
H	-4.1304236	0.0408397	28.5559718
C	-3.5738451	6.1362022	27.6488326
C	-2.2227468	6.8301436	27.3691168
H	-1.5898801	6.8789029	28.2782018
H	-2.3729652	7.8628076	26.9901131
H	-1.6603339	6.2664988	26.5932043
C	-4.4361633	6.0909975	26.3805933
H	-4.1115493	6.7464387	28.4092451
H	-3.9027654	5.5897043	25.5464299
H	-4.6772228	7.1179637	26.0385936
H	-5.3900430	5.5520817	26.5510784
C	-2.4145511	3.4614835	31.7916200
C	-1.9362301	4.7899672	32.3993552
H	-1.6603251	4.6411716	33.4630711
H	-2.7311460	5.5642517	32.3798492
H	-1.0530305	5.1996983	31.8747855
C	-3.6989572	2.9972954	32.5102001
H	-1.6223679	2.7074232	31.9834885
H	-4.0620154	2.0236105	32.1276453
H	-4.5157384	3.7332751	32.3565087
H	-3.5298697	2.8970943	33.6026837
H	8.0452076	5.7620050	27.6192268
H	7.3887705	2.0235106	32.1528733
H	5.9901889	2.3436070	24.9670389
C	8.0296866	5.3585602	28.6558755
H	3.7521449	3.2695115	31.7932293
H	6.8318374	7.0681594	29.3581370
H	3.5243429	4.8401693	26.4068773
C	6.9171216	4.3171540	28.7064628
C	6.6353393	1.2563778	31.8772230
C	7.7744634	6.5409465	29.6074481
H	8.5981053	7.2817002	29.5477269
C	6.6331914	3.6071279	29.8877054
C	5.0294149	1.8910856	25.2909099
H	9.4612335	4.3066184	29.9534333
C	6.1442164	4.0287050	27.5695934
C	9.4034295	4.7164783	28.9234861
H	9.6006697	3.8825826	28.2206295
H	6.3265468	4.6059423	26.6491831
C	4.6782520	2.8524645	32.2359672
H	6.3786199	0.7006534	32.8023448
H	7.1186304	0.5482493	31.1740867
C	5.6636064	2.5876328	29.9331227
C	3.8873699	4.1197467	25.6447848
C	5.1526322	3.0275498	27.5646710
H	4.3999659	1.7435149	24.3895249
H	5.2518617	0.8930018	25.7158948
C	5.3763078	1.8865710	31.2583717
C	4.9529999	2.2621877	28.7456227
C	4.3133652	2.7983939	26.3083762
H	5.3439250	3.6998579	32.5051668
H	4.7235629	4.6081468	25.1023996
H	4.4038624	2.3309081	33.1761345
H	7.7058053	6.2048004	30.6632154
H	3.0764462	3.9399068	24.9098133
H	10.2179471	5.4618760	28.8134671
H	4.6680740	1.0580600	31.0525734
H	3.3829079	2.2839883	26.6269810
H	7.1948718	3.8423401	30.8061449
C	3.8500934	6.8254072	28.5456398
C	2.5112617	6.9253168	28.2917078
C	1.8376503	6.4611501	29.5239680
O	2.7403632	6.1182418	30.4674302
C	4.0623714	6.2845280	29.9206576
O	0.6219844	6.3025127	29.7110488
C	1.7257048	7.1728764	27.0779761

$$\mathbf{E}_{ed} = \mathbf{G}\mathbf{1}_{ed}$$

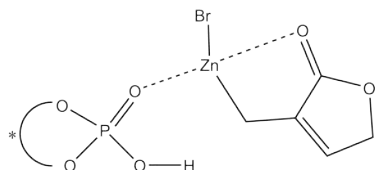


Energy (Hartree) = -7273.236046042

C	-0.3281429	1.0316672	29.5111092
C	0.5520943	0.0244355	29.9055852
C	0.1044562	-0.8891175	30.9292199
C	0.9600672	-1.8625893	31.5251734
C	-1.2585029	-0.7937474	31.3976457
C	-1.7148278	-1.7105628	32.3911418
C	-2.1180812	0.2257031	30.8900142
H	-3.1547015	0.2704626	31.2553996
C	-1.6726358	1.1759902	29.9812196
C	4.0636958	1.0536285	28.7161992
C	4.5321920	-0.1462531	28.1927482
H	5.5650347	-0.1967479	27.8153806
C	3.7096938	-1.3048462	28.1081006
C	4.1833780	-2.5022700	27.4929479
C	2.3628637	-1.2605825	28.6246415
C	1.5312795	-2.4058412	28.4369084
C	1.9000240	-0.0568400	29.2726769
C	2.7403233	1.0637949	29.2474614
O	0.1140046	1.9620641	28.5628671
O	2.3097000	2.2594325	29.8232697
P	1.1208193	3.1206147	29.1005975
O	0.4866420	3.8640154	30.3355544
H	0.4173695	4.8925810	30.1794226
O	1.5758235	3.9707091	27.9343462
C	-0.8642117	-2.6636063	32.9307155
C	0.4876516	-2.7281389	32.5022356
H	-2.7590769	-1.6357555	32.7331156
H	-1.2302876	-3.3598633	33.7004549
H	2.0103926	-1.9172625	31.2065466
H	1.1690408	-3.4669161	32.9510358
C	2.0166594	-3.5485386	27.8171369
C	3.3579360	-3.6069657	27.3540653
H	0.4880360	-2.3722039	28.7793487
H	1.3522485	-4.4148307	27.6776162
H	3.7329357	-4.5219182	26.8709057
H	5.2173832	-2.5241164	27.1143776
C	-2.6460636	3.4991192	30.2814477
C	-2.4444826	2.3501930	29.4646184
C	-3.0820142	4.6848941	29.6636971
C	-2.7779603	2.3863406	28.0814017
C	-3.2020253	3.5999805	27.5148482
C	-3.3154065	4.7735454	28.2801822
H	-3.2050244	5.5930588	30.2739483
C	-2.7180032	1.1103195	27.2428071
H	-3.4094219	3.6374608	26.4373835
C	-2.4745981	1.3406444	25.7470319
H	-2.3227012	0.3698993	25.2327270
H	-1.5809781	1.9719856	25.5725369

H	2.3159294	7.6329778	26.2626301
H	4.6726974	7.0239676	27.8459068
H	4.5611916	5.2885764	29.9200296
H	4.6391869	6.9475148	30.6025462
Zn	1.0146729	5.3780519	26.4983383
H	0.8268030	7.7885748	27.2849125
Br	-0.0840461	4.2890839	24.7714129

$F_{ed} = G2_{ed}$; COSMO



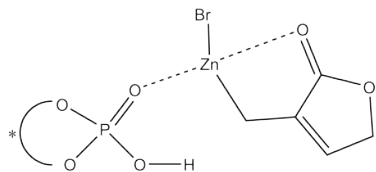
Energy (Hartree) = -7273.226983067

C	0.1529679	1.4662544	29.2425909
C	0.8351036	0.2528158	29.3967901
C	0.2867487	-0.7329331	30.2972542
C	0.9926528	-1.9171459	30.6696139
C	-1.0128070	-0.5038338	30.8762963
C	-1.5752321	-1.4831720	31.7494879
C	-1.7038788	0.7006018	30.5728236
H	-2.7171412	0.8482563	30.9766222
C	-1.1404101	1.7083186	29.7948792
C	4.4658914	0.6616538	28.2288632
C	4.6472368	-0.5151893	27.5088541
H	5.6395175	-0.7331247	27.0857422
C	3.5805648	-1.4254763	27.2611798
C	3.7703019	-2.5807713	26.4440261
C	2.2754223	-1.1659765	27.8199938
C	1.2057078	-2.0499229	27.4870082
C	2.1031318	-0.0096680	28.6650026
C	3.1724506	0.8759039	28.7896625
O	0.7106921	2.4777446	28.4450033
O	2.9816752	2.0356716	29.5588029
P	2.0934770	3.2239459	28.8989867
O	1.8191126	4.1517185	30.1652812
H	1.9571285	5.1199078	29.8732964
O	2.6849557	3.9476001	27.7081332
C	-0.8725816	-2.6340615	32.0716190
C	0.4275493	-2.8418094	31.5368798
H	-2.5746998	-1.2981472	32.1733697
H	-1.3119295	-3.3798807	32.7513389
H	2.0028855	-2.0887120	30.2733131
H	0.9956262	-3.7419913	31.8168514
C	1.4199451	-3.1550351	26.6745132
C	2.7143600	-3.4332667	26.1588290
H	0.1976411	-1.8428053	27.8727043
H	0.5778867	-3.8180770	26.4238639
H	2.8727021	-4.3167800	25.5218984
H	4.7729943	-2.7730994	26.0312212
C	-2.1534733	3.8903648	30.5639092
C	-1.9588893	2.9368387	29.5295684
C	-3.1416181	4.8805645	30.3938397
C	-2.6867932	3.0440122	28.3119295
C	-3.6542054	4.0594871	28.1887964
C	-3.9249895	4.9674134	29.2308649
H	-3.3240977	5.6022373	31.2071078
C	-2.4526439	2.0805260	27.1497936
H	-4.2391613	4.1213745	27.2567331
C	-1.7510856	2.7903186	25.9760244
H	-1.5145212	2.0688571	25.1672201
H	-0.8010909	3.2598353	26.2995635
H	-2.3971388	3.5795132	25.5359469

C	-3.7451685	1.3785738	26.6996463
H	-1.7646659	1.2876397	27.5076992
H	-3.5259964	0.6314602	25.9094408
H	-4.4800689	2.0966264	26.2798596
H	-4.2327388	0.8520145	27.5450587
C	-5.0429213	5.9982620	29.1173746
C	-4.7541137	7.0586749	28.0402314
H	-3.8179832	7.6112271	28.2577340
H	-5.5772448	7.8005383	27.9869532
H	-4.6561830	6.5975485	27.0348880
C	-6.4076531	5.3251904	28.8834925
H	-5.0924712	6.5243348	30.0958778
H	-6.4386627	4.8027252	27.9045359
H	-7.2225018	6.0781148	28.8847441
H	-6.6280179	4.5768243	29.6711189
C	-1.3364750	3.8520834	31.8543275
C	-0.7034047	5.2176255	32.1730233
H	-0.0170703	5.1332723	33.0398531
H	-1.4673892	5.9811815	32.4277337
H	-0.1176135	5.5925835	31.3120165
C	-2.1715481	3.3418616	33.0430881
H	-0.5028808	3.1373327	31.6945574
H	-2.5692713	2.3245516	32.8564667
H	-3.0360908	4.0104214	33.2383758
H	-1.5572259	3.3029492	33.9662139
H	8.7763681	5.1934202	27.9147945
H	7.6983359	0.7895126	31.7334039
H	7.3906856	2.0777823	24.8342318
C	8.7080026	4.6467489	28.8804605
H	4.3378162	2.6800508	31.6865262
H	7.4060007	6.1696514	29.7672937
H	4.2121541	4.0122113	25.8017001
C	7.6043596	3.6101643	28.7167779
C	6.8134525	0.2017856	31.4109065
C	8.3794189	5.6802506	29.9712927
H	9.1623047	6.4657374	30.0128402
C	7.1301950	2.8688293	29.8130058
C	6.4742806	1.4662917	24.9715634
H	10.0546532	3.4010888	30.0907194
C	7.0347274	3.3575130	27.4590191
C	10.0675024	3.9694244	29.1364825
H	10.3238066	3.2574397	28.3257823
H	7.3862636	3.9455372	26.5970427
C	5.1687582	2.0405023	32.0434709
H	6.4800697	-0.4075449	32.2767085
H	7.1446038	-0.4897852	30.6096762
C	6.1120216	1.9092094	29.6831630
C	4.9859631	3.5075229	25.1944402
C	6.0127435	2.4095951	27.2677223
H	6.0498632	1.2632127	23.9662878
H	6.7861766	0.4984194	25.4146294
C	5.6797097	1.1215772	30.9193962
C	5.5505432	1.6748992	28.3965458
C	5.4514213	2.2010271	25.8600916
H	5.9732206	2.7026657	32.4258622
H	5.8183652	4.2260886	25.0521666
H	4.7981040	1.4397845	32.8999274
H	8.3297317	5.2109497	30.9764765
H	4.5546549	3.2915760	24.1950018
H	10.8800017	4.7227032	29.2041356
H	4.8380029	0.4603928	30.6284946
H	4.5571243	1.5511116	25.9464338
H	7.5684128	3.0439356	30.8086680
C	-0.7469547	6.6561009	28.3005034
C	0.6055237	6.7122388	28.1616818
C	0.8740092	6.5010190	26.7179901
O	-0.2715147	6.3867333	26.0227087
C	-1.3704606	6.4548738	26.9561178
O	1.9890299	6.3914357	26.1927106
C	1.7761077	6.8447548	29.0561592
H	1.5042942	6.7878937	30.1303056

H	-1.3359915	6.7321388	29.2240088
H	-1.9432718	5.5059044	26.8813374
H	-2.0434367	7.2841798	26.6494930
Zn	3.2995947	5.9757462	27.9054388
H	2.2352562	7.8538898	28.9425812
Br	5.4843583	6.6332408	27.4745961

$$\mathbf{F}_{ed} = \mathbf{G2}_{ed}$$



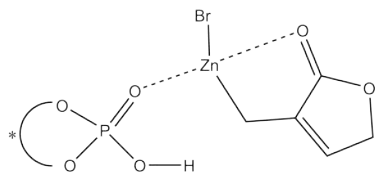
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C	0.1450308	1.4746641	29.2625515
C	0.8330613	0.2640916	29.4125089
C	0.2936613	-0.7244945	30.3150184
C	1.0066090	-1.9062897	30.6805973
C	-1.0032543	-0.5020276	30.9024128
C	-1.5544461	-1.4847695	31.7781254
C	-1.7023859	0.6984396	30.6017373
H	-2.7151512	0.8415224	31.0085847
C	-1.1482008	1.7077368	29.8199181
C	4.4529939	0.6948004	28.2201238
C	4.6311414	-0.4753198	27.4885659
H	5.6212696	-0.6841355	27.0560378
C	3.5674193	-1.3894302	27.2442633
C	3.7543582	-2.5380762	26.4179054
C	2.2673671	-1.1422359	27.8197494
C	1.2004169	-2.0322583	27.4949289
C	2.0972098	0.0090851	28.6715583
C	3.1626629	0.9002785	28.7916497
O	0.6909692	2.4888567	28.4645951
O	2.9698914	2.0557249	29.5653557
P	2.0761338	3.2425066	28.9085201
O	1.8053806	4.1741602	30.1716904
H	1.9276891	5.1439679	29.8609187
O	2.6554457	3.9636715	27.7112704
C	-0.8450860	-2.6326911	32.0941041
C	0.4514464	-2.8344086	31.5499070
H	-2.5516677	-1.3045519	32.2093616
H	-1.2766562	-3.3808431	32.7761613
H	2.0142082	-2.0718455	30.2753378
H	1.0250628	-3.7327622	31.8241715
C	1.4126064	-3.1311931	26.6742272
C	2.7018247	-3.3965799	26.1406729
H	0.1962972	-1.8340983	27.8951593
H	0.5724604	-3.7993497	26.4309557
H	2.8588890	-4.2750033	25.4965092
H	4.7532466	-2.7202769	25.9915413
C	-2.1686762	3.8940493	30.5698172
C	-1.9727409	2.9297921	29.5461623
C	-3.1518757	4.8860994	30.3842842
C	-2.6957368	3.0255333	28.3248439
C	-3.6543296	4.0465854	28.1844269
C	-3.9249754	4.9676474	29.2143067
H	-3.3364029	5.6158311	31.1899005
C	-2.4702856	2.0389503	27.1801984
H	-4.2341906	4.1011734	27.2486842
C	-1.7729448	2.7177822	25.9863208
H	-1.5432760	1.9765776	25.1936697
H	-0.8189494	3.1907442	26.2922761
H	-2.4187114	3.4975779	25.5290784
C	-3.7687338	1.3322041	26.7552155

H	-1.7833406	1.2512276	27.5507523
H	-3.5596338	0.5676275	25.9791613
H	-4.5053518	2.0432243	26.3264994
H	-4.2516940	0.8258236	27.6152557
C	-5.0346711	6.0050919	29.0815982
C	-4.7424861	7.0382659	27.9793424
H	-3.7991288	7.5855425	28.1778527
H	-5.5580821	7.7872559	27.9125616
H	-4.6548117	6.5536814	26.9841677
C	-6.4057289	5.3376668	28.8701399
H	-5.0759571	6.5541348	30.0480069
H	-6.4444348	4.7900744	27.9054035
H	-7.2157875	6.0955489	28.8553046
H	-6.6279111	4.6105514	29.6765700
C	-1.3565409	3.8657979	31.8634867
C	-0.7255720	5.2335913	32.1754343
H	-0.0391178	5.1548125	33.0424994
H	-1.4897583	5.9981652	32.4267268
H	-0.1392246	5.6037347	31.3129632
C	-2.1953734	3.3620425	33.0521583
H	-0.5213021	3.1514745	31.7110415
H	-2.5882867	2.3418480	32.8720276
H	-3.0636159	4.0282700	33.2384853
H	-1.5859269	3.3321276	33.9787272
H	8.7659042	5.2227125	27.9605572
H	7.6886361	0.7646162	31.7229189
H	7.3639644	2.1351275	24.8260085
C	8.7426790	4.6228262	28.8964262
H	4.3406726	2.6807291	31.6912449
H	7.5102114	6.1003399	29.9441390
C	4.2147632	4.0945064	25.8431816
H	7.6206995	3.6066382	28.7309913
C	6.7988145	0.1870400	31.3962411
C	8.4911077	5.5974721	30.0584645
H	9.2805580	6.3765329	30.0905103
C	7.1405639	2.8595061	29.8195575
C	6.4397626	1.5348032	24.9588644
H	10.1314044	3.2902428	29.9554665
C	7.0423992	3.3765068	27.4731058
C	10.1035201	3.9147435	29.0373992
H	10.3043949	3.2480547	28.1744474
H	7.3957658	3.9731236	26.6178444
C	5.1675125	2.0333551	32.0429258
H	6.4618101	-0.4268597	32.2574323
H	7.1252869	-0.4999190	30.5893749
C	6.1103536	1.9142449	29.6824010
C	4.9832442	3.5928926	25.2273645
C	6.0075614	2.4454883	27.2740564
H	6.0066298	1.3551665	23.9529030
H	6.7423745	0.5553804	25.3824995
C	5.6724420	1.1194491	30.9121300
C	5.5417921	1.7018724	28.3954340
C	5.4336243	2.2681796	25.8672066
H	5.9756682	2.6888153	32.4287054
H	5.8231023	4.3049384	25.0975621
H	4.7939814	1.4297217	32.8961072
H	8.5043040	5.0779780	31.0397852
H	4.5473515	3.4028595	24.2248303
H	10.9309856	4.6515651	29.1050524
H	4.8258606	0.4665401	30.6163617
H	4.5301982	1.6299892	25.9487065
H	7.5824439	3.0193460	30.8158115
C	-0.7610556	6.5997438	28.2327574
C	0.5924776	6.6980583	28.1350282
C	0.9105909	6.5109312	26.6961733
O	-0.2115791	6.3787786	25.9652061
C	-1.3369774	6.3989486	26.8660535
O	2.0429214	6.4328475	26.2073823
C	1.7326462	6.8411805	29.0615233
H	1.4293746	6.8091256	30.1278828
H	-1.3794240	6.6392754	29.1390830

H	-1.8775478	5.4341357	26.7608211
H	-2.0285369	7.2106698	26.5515301
Zn	3.3044830	5.9814342	27.9323504
H	2.2114344	7.8399282	28.9383525
Br	5.5154500	6.6193282	27.7367682

$G_{ed} = G3_{ed}$; COSMO



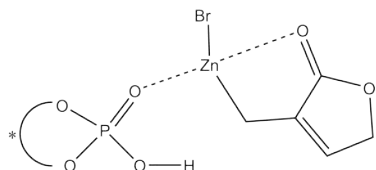
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C	0.6381863	-0.1911430	29.6994456
C	0.0382158	-1.0135891	30.7230554
C	0.7663900	-2.0057777	31.4458992
C	-1.3502075	-0.8042234	31.0591245
C	-1.9627981	-1.6402588	32.0409918
C	-2.0736258	0.2617763	30.4501779
H	-3.1263877	0.4127732	30.7313406
C	-1.4726719	1.1482867	29.5639979
C	4.2447016	0.5362112	28.5860373
C	4.6911582	-0.7307442	28.2345336
H	5.7222773	-0.8602653	27.8725859
C	3.8239684	-1.8608110	28.2579446
C	4.2728029	-3.1372759	27.8028869
C	2.4489703	-1.6987988	28.6692540
C	1.5675693	-2.8117744	28.5171292
C	2.0177539	-0.4191067	29.1839017
C	2.9253146	0.6442176	29.1207197
O	0.4531025	1.7111045	28.2327346
O	2.5573660	1.8917464	29.6278168
P	1.5203344	2.8242340	28.7651406
O	0.8955573	3.7176481	29.8868575
H	0.7593661	4.7568605	29.6301440
O	2.1135994	3.5162044	27.5490648
C	-1.2341674	-2.6187774	32.7005511
C	0.1461754	-2.7881612	32.4107725
H	-3.0258858	-1.4780721	32.2785305
H	-1.7173979	-3.2514043	33.4606248
H	1.8368792	-2.1419605	31.2386722
H	0.7315381	-3.5420821	32.9589310
C	2.0299223	-4.0342964	28.0492358
C	3.3975973	-4.2085049	27.7075996
H	0.5046393	-2.6931231	28.7671571
H	1.3271837	-4.8739655	27.9368639
H	3.7540958	-5.1855498	27.3475577
H	5.3276543	-3.2473334	27.5060975
C	-2.3882223	3.4691500	29.9677043
C	-2.1241759	2.3985881	29.0616769
C	-2.8686337	4.6840777	29.4472365
C	-2.3761115	2.5670857	27.6714258
C	-2.8579795	3.8044238	27.2089491
C	-3.0924394	4.8854045	28.0753613
H	-3.0520766	5.5247371	30.1346541
C	-2.1804996	1.4309774	26.6686577
H	-3.0398489	3.9294249	26.1304279
C	-1.2870208	1.8325940	25.4819175
H	-1.0937166	0.9559641	24.8296690
H	-0.3120358	2.2245729	25.8315411
H	-1.7654853	2.6110888	24.8518031
C	-3.5443018	0.8939067	26.1930611
H	-1.6739559	0.5960136	27.1943756

H	-3.4114979	0.0359381	25.5014675
H	-4.1169768	1.6776607	25.6540822
H	-4.1635193	0.5548022	27.0484030
C	-3.4888808	6.2623594	27.5588399
C	-2.2323023	7.0248356	27.0905254
H	-1.4728304	7.0853423	27.8949634
H	-2.4902776	8.0557682	26.7691496
H	-1.7605518	6.5063925	26.2291766
C	-4.5624405	6.2216242	26.4608056
H	-3.9129135	6.8183571	28.4245173
H	-4.1819303	5.7454737	25.5330061
H	-4.8807519	7.2491793	26.1900380
H	-5.4597731	5.6574693	26.7872529
C	-2.1770310	3.3444811	31.4775820
C	-1.5128288	4.5774761	32.1146576
H	-1.2813680	4.3741261	33.1803560
H	-2.1756714	5.4671085	32.0910486
H	-0.5699633	4.8420177	31.6015826
C	-3.5126376	3.0379262	32.1852464
H	-1.4957540	2.4865789	31.6499785
H	-3.9999115	2.1285095	31.7806506
H	-4.2255930	3.8788787	32.0534494
H	-3.3589527	2.8891052	33.2744432
H	6.9975796	5.7055909	26.3879331
H	7.9038919	2.4110570	31.2427172
H	6.0765292	1.3036222	24.6765997
C	7.2291248	5.4581738	27.4462365
H	4.0911201	2.9700357	31.4803163
H	5.7534468	6.9299143	28.1079687
H	2.9174631	3.3141214	25.3219285
C	6.4290744	4.2047360	27.7819222
C	7.2690491	1.5024773	31.1813565
C	6.8164677	6.6752955	28.2899890
H	7.4289328	7.5593538	28.0183387
C	6.4768424	3.6067336	29.0536188
C	5.2537257	0.7158785	25.1347253
H	9.0363319	4.9472718	28.5939967
C	5.6520099	3.5722929	26.7831066
C	8.7399343	5.1801677	27.5496597
H	9.0376999	4.3208272	26.9154816
H	5.6258681	4.0204331	25.7789333
C	5.1430552	2.7803594	31.7691516
H	7.2768692	1.0241233	32.1822164
H	7.7467627	0.8055136	30.4631592
C	5.7782590	2.4190696	29.3463668
C	3.6041191	2.5959064	24.8379916
C	4.9693349	2.3561391	27.0151380
H	4.7396554	0.1589272	24.3246913
H	5.7105738	-0.0236110	25.8197351
C	5.8292413	1.8435031	30.7581674
C	5.0319787	1.7839424	28.3194832
C	4.2614912	1.6525514	25.8568195
H	5.6630221	3.7591205	31.8324334
H	4.3529063	3.1757331	24.2601187
H	5.1482924	2.3300427	32.7830762
H	6.9550076	6.4910706	29.3761243
H	3.0207799	2.0004923	24.1067658
H	9.3228326	6.0666257	27.2252783
H	5.2567043	0.8925295	30.7466929
H	3.4570522	1.0249190	26.2945895
H	7.0680978	4.0854510	29.8502141
C	3.3118550	8.2069908	29.3991786
C	2.8644692	6.9210313	29.5318169
C	1.3922016	7.0026618	29.3548212
O	1.0040934	8.2695519	29.1287468
C	2.1701304	9.1156186	29.1025953
O	0.5295966	6.1077323	29.3810372
C	3.5775462	5.6422436	29.6553287
H	3.0447293	4.9218234	30.3032706
H	4.3546701	8.5469103	29.4503443
H	2.0220046	9.9325423	29.8426963

H	2.2311303	9.5769013	28.0910934
Zn	3.6142805	4.9609429	27.7294118
H	4.6122310	5.7693678	30.0199796
Br	3.5882972	6.4129386	25.8556526

$$\mathbf{G}_{ed} = \mathbf{G}\mathbf{3}_{ed}$$



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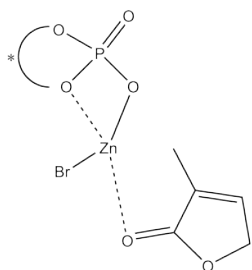
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C	0.6421305	-0.1963699	29.7011954
C	0.0383902	-1.0213479	30.7202826
C	0.7622518	-2.0189996	31.4394380
C	-1.3495233	-0.8090967	31.0556855
C	-1.9649046	-1.6474275	32.0331780
C	-2.0684586	0.2610768	30.4495015
H	-3.1210519	0.4155496	30.7293953
C	-1.4646840	1.1494749	29.5673437
C	4.2488200	0.5296636	28.5889973
C	4.6923606	-0.7363289	28.2312083
H	5.7222110	-0.8637484	27.8647628
C	3.8247485	-1.8657737	28.2520864
C	4.2703670	-3.1409862	27.7918759
C	2.4508753	-1.7034281	28.6664529
C	1.5681740	-2.8147643	28.5117361
C	2.0218005	-0.4252858	29.1866123
C	2.9308077	0.6372335	29.1277267
O	0.4649559	1.7124787	28.2427795
O	2.5665974	1.8820659	29.6406113
P	1.5324039	2.8225256	28.7828442
O	0.9072167	3.7083074	29.9107301
H	0.7585941	4.7414613	29.6540946
O	2.1276482	3.5206452	27.5722608
C	-1.2407720	-2.6311455	32.6888644
C	0.1386625	-2.8038099	32.3995491
H	-3.0275880	-1.4823820	32.2705473
H	-1.7270042	-3.2653461	33.4456274
H	1.8322776	-2.1571505	31.2315597
H	0.7210920	-3.5622112	32.9445522
C	2.0281506	-4.0359943	28.0394204
C	3.3943711	-4.2107104	27.6946572
H	0.5062000	-2.6946349	28.7646268
H	1.3240722	-4.8743004	27.9257456
H	3.7492574	-5.1867539	27.3304888
H	5.3244349	-3.2511520	27.4922691
C	-2.3831857	3.4676924	29.9785544
C	-2.1137471	2.4020563	29.0685097
C	-2.8646868	4.6834330	29.4620648
C	-2.3605263	2.5768022	27.6782911
C	-2.8442391	3.8147971	27.2206330
C	-3.0858031	4.8905501	28.0909877
H	-3.0524180	5.5203794	30.1527431
C	-2.1598771	1.4460860	26.6704597
H	-3.0233607	3.9440358	26.1422543
C	-1.2652088	1.8553075	25.4873425
H	-1.0664777	0.9820594	24.8322618
H	-0.2928071	2.2513459	25.8391277
H	-1.7449778	2.6335360	24.8580494
C	-3.5215285	0.9074849	26.1908700
H	-1.6520164	0.6099744	27.1931091
H	-3.3864766	0.0537343	25.4945459

H	-4.0965538	1.6922758	25.6562251
H	-4.1407218	0.5627153	27.0437263
C	-3.4896009	6.2674267	27.5801864
C	-2.2369184	7.0456889	27.1284730
H	-1.4874421	7.1141016	27.9411858
H	-2.5028060	8.0744395	26.8068052
H	-1.7490675	6.5358480	26.2711091
C	-4.5537078	6.2241995	26.4732735
H	-3.9269787	6.8129180	28.4460719
H	-4.1598639	5.7626709	25.5437621
H	-4.8825170	7.2500944	26.2091592
H	-5.4464575	5.6454905	26.7859663
C	-2.1785159	3.3365574	31.4888744
C	-1.5086640	4.5627096	32.1328890
H	-1.2880575	4.3566986	33.2003433
H	-2.1622126	5.4589383	32.1045036
H	-0.5588801	4.8185465	31.6288532
C	-3.5190275	3.0362084	32.1895555
H	-1.5030062	2.4742605	31.6616049
H	-4.0112927	2.1323755	31.7785397
H	-4.2264461	3.8816030	32.0577199
H	-3.3721459	2.8817275	33.2788893
H	6.9894020	5.7078074	26.3990055
H	7.8936376	2.4118973	31.2590830
H	6.0747318	1.3107447	24.6688627
C	7.2326192	5.4514383	27.4525047
H	4.0776498	2.9670322	31.4802703
H	5.7735549	6.9297838	28.1282193
H	2.9101890	3.3094331	25.3429717
C	6.4309078	4.1989252	27.7880647
C	7.2587028	1.5034887	31.1969848
C	6.8347651	6.6658476	28.3066780
H	7.4531178	7.5466993	28.0379719
C	6.4726792	3.6040528	29.0613266
C	5.2547698	0.7191492	25.1269282
H	9.0490140	4.9209111	28.5770990
C	5.6608543	3.5628915	26.7873695
C	8.7427798	5.1641975	27.5379750
H	9.0289858	4.3073737	26.8953422
H	5.6314338	4.0141473	25.7848031
C	5.1290232	2.7810824	31.7728138
H	7.2637907	1.0272542	32.1988739
H	7.7404044	0.8060094	30.4821810
C	5.7758920	2.4155737	29.3531120
C	3.5977499	2.5971717	24.8516843
C	4.9770514	2.3482863	27.0187168
H	4.7386285	0.1665002	24.3153429
H	5.7163062	-0.0243868	25.8044774
C	5.8208259	1.8432954	30.7666485
C	5.0362603	1.7773269	28.3236153
C	4.2647919	1.6491396	25.8601820
H	5.6459553	3.7614615	31.8355679
H	4.3394014	3.1852970	24.2732774
H	5.1316744	2.3345666	32.7884327
H	6.9770442	6.4743412	29.3911656
H	3.0128098	2.0048767	24.1192225
H	9.3288453	6.0488089	27.2141978
H	5.2490253	0.8918040	30.7541992
H	3.4647938	1.0165135	26.2989239
H	7.0585158	4.0859197	29.8601040
C	3.2778566	8.2210159	29.3286724
C	2.8424615	6.9370099	29.5104455
C	1.3676289	6.9984611	29.3345097
O	0.9682937	8.2540861	29.0626796
C	2.1266896	9.1042526	28.9906612
O	0.5159664	6.0974348	29.3955914
C	3.5648757	5.6688780	29.6651622
H	3.0348048	4.9526369	30.3194275
H	4.3190529	8.5680128	29.3559855
H	1.9724824	9.9592985	29.6858500
H	2.1840482	9.5088311	27.9543354

Zn	3.6074073	4.9842136	27.7363042
H	4.5983953	5.8089620	30.0281413
Br	3.6435406	6.4242037	25.8693113

5.2 Product Complexes

D_{prod}

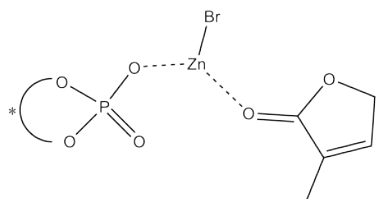


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C	0.3873992	-0.9913722	90.5807179
C	1.2279251	-2.0356530	91.0686941
C	-0.8999290	-0.8049242	91.2031216
C	-1.3153032	-1.7035239	92.2303455
C	-1.7108960	0.3007403	90.8227727
H	-2.6878657	0.4336164	91.3114620
C	-1.2892710	1.2441845	89.8930398
C	4.3545709	0.6171847	88.3173213
C	4.6903983	-0.6009273	87.7372501
H	5.7172569	-0.7548733	87.3708738
C	3.7391096	-1.6490697	87.5856941
C	4.0737652	-2.8638625	86.9159004
C	2.4086723	-1.4816671	88.1187027
C	1.4604454	-2.5286550	87.9134225
C	2.0763263	-0.2587329	88.8062828
C	3.0218550	0.7736045	88.8027887
O	0.3498953	1.8870629	88.2420933
O	2.6854544	2.0114703	89.3418916
P	1.5057960	3.0167982	88.5623885
O	1.1537652	3.8358601	89.8421052
O	1.9460625	3.6631290	87.2930061
C	-0.4857293	-2.7270316	92.6606060
C	0.8021377	-2.8813156	92.0828369
H	-2.3041206	-1.5521719	92.6911096
H	-0.8137440	-3.4069178	93.4615800
H	2.2344134	-2.1559325	90.6457491
H	1.4742471	-3.6722505	92.4492288
C	1.8135430	-3.6916180	87.2440991
C	3.1335564	-3.8689824	86.7502163
H	0.4344791	-2.3983343	88.2850845
H	1.0620195	-4.4809851	87.0904103
H	3.4033759	-4.7988094	86.2266912
H	5.0955804	-2.9820274	86.5222026
C	-2.1907770	3.4941810	90.5962216
C	-2.0855366	2.4781660	89.6040708
C	-2.9712530	4.6314165	90.3165075
C	-2.7329920	2.6394925	88.3485860
C	-3.4936945	3.7992335	88.1205084
C	-3.6328827	4.8067062	89.0908769
H	-3.0590908	5.4214919	91.0799641
C	-2.6497397	1.5811821	87.2504864
H	-3.9969221	3.9171881	87.1472250
C	-2.0262044	2.1424730	85.9599775
H	-1.9137620	1.3400849	85.2015980
H	-1.0246119	2.5712663	86.1575488
H	-2.6608061	2.9355227	85.5117016
C	-4.0263056	0.9423916	86.9894330
H	-1.9837852	0.7711960	87.6111402
H	-3.9489929	0.1371998	86.2295241
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H	-4.4476254	0.5021299	87.9159600
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C	-3.8552310	6.8940369	87.6749933
H	-2.8007075	7.1620967	87.8867379
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H	-4.4211558	6.6758555	89.7419525
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H	-6.3776541	5.1425572	89.3828523
C	-1.4736164	3.3954982	91.9416275
C	-0.7038315	4.6793433	92.3061710
H	-0.0343551	4.4877908	93.1715920
H	-1.3853657	5.5048727	92.5999191
H	-0.0922485	5.0295351	91.4520448
C	-2.4341953	3.0041649	93.0789058
H	-0.7236392	2.5821547	91.8570410
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H	-3.2090830	3.7852746	93.2297231
H	-1.8787620	2.8804730	94.0314249
H	8.6646476	5.1588124	87.9460089
H	7.3531718	-0.0131853	91.1743466
H	7.0795376	2.1924060	84.8724873
C	8.4969600	4.7098738	88.9498743
H	5.1129171	2.8784711	92.2804727
H	7.1584230	6.3454541	89.5585863
H	3.8710426	4.0264356	86.0172660
C	7.3900917	3.6742949	88.7907996
C	6.2656277	-0.1968478	91.0477675
C	8.0874236	5.8477773	89.9021045
H	8.8860968	6.6152518	89.9712989
C	6.9241292	2.9349776	89.8953985
C	6.1732072	1.5708979	85.0318770
H	9.7220030	3.5993713	90.4002280
C	6.8025554	3.4301889	87.5414302
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H	7.1437342	4.0168382	86.6726705
C	5.6123859	1.8901421	92.3226626
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H	6.1263678	-0.7885235	90.1215258
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C	4.6548972	3.5863999	85.3714074
C	5.7864159	2.4689940	87.3615361
H	5.7118087	1.3866382	84.0397819
H	6.5071550	0.5953034	85.4398324
C	5.4944717	1.1365962	90.9902942
C	5.3653111	1.7089014	88.4829070
C	5.1772186	2.2711284	85.9749399
H	6.6697516	2.0496984	92.6206558
H	5.4674558	4.3281400	85.2215086
H	5.1209656	1.3110761	93.1289681
H	7.8996682	5.4672236	90.9281744
H	4.1996020	3.3937562	84.3781691
H	10.6345934	4.8106599	89.4474700
H	4.4201051	0.8844682	90.8654736
H	4.2984507	1.6047222	86.0925631
H	7.3635451	3.1208067	90.8868838
C	4.5749601	7.3994304	90.5730895
C	4.1487073	6.1295826	90.3495612
C	3.6398020	5.6364960	91.6522265
O	3.7633479	6.5940872	92.5959328
C	4.3532798	7.7593758	92.0035995

O	3.1808903	4.5330521	91.9636443
C	4.1398673	5.3121080	89.1095064
H	4.8406881	5.7082239	88.3527244
H	5.0232815	8.0811077	89.8369586
H	5.2930714	7.9944587	92.5513927
H	3.6581778	8.6168507	92.1448615
Zn	2.0499291	2.9458890	91.3437661
H	3.1284545	5.2799592	88.6557677
Br	1.8016086	1.3780631	92.9937532
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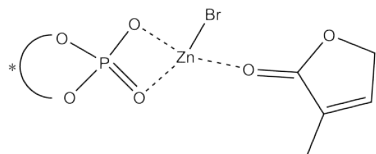
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C	0.8441365	-1.9226845	91.3818643
C	-1.3346219	-0.8352165	91.0275216
C	-1.8664401	-1.6367895	92.0813004
C	-2.1037117	0.2161367	90.4488143
H	-3.1038660	0.4297863	90.8580958
C	-1.5745964	1.0490052	89.4720303
C	4.1378745	0.8209641	88.6649904
C	4.7436224	-0.4102750	88.4444435
H	5.8279421	-0.4493145	88.2606036
C	3.9971792	-1.6221720	88.4066972
C	4.6176017	-2.8637476	88.0749323
C	2.5804823	-1.5923085	88.6779189
C	1.8401706	-2.8044553	88.5341318
C	1.9627012	-0.3416472	89.0427924
C	2.7378807	0.8277694	88.9581444
O	0.1294641	1.3882877	87.8116985
O	2.1463700	2.0629777	89.1930178
P	1.2317428	2.6350529	87.9154792
O	0.5038318	3.8651883	88.5373027
O	1.9512761	2.7646772	86.6104708
C	-1.0711188	-2.5490517	92.7576030
C	0.3008492	-2.6738594	92.4153183
H	-2.9224194	-1.4984745	92.3625781
H	-1.4935028	-3.1575531	93.5716765
H	1.9096658	-2.0268180	91.1380425
H	0.9436258	-3.3688293	92.9770449
C	2.4701021	-3.9919896	88.1894099
C	3.8734033	-4.0290586	87.9730608
H	0.7522396	-2.7855197	88.6887165
H	1.8750264	-4.9110273	88.0759485
H	4.3634106	-4.9781239	87.7073447
H	5.7019286	-2.8730532	87.8817610
C	-2.0363864	3.4030749	90.1760101
C	-2.1352517	2.3999680	89.1599367
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C	-2.5818725	2.7494990	87.8621329
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C	-2.0505832	2.0707425	85.4552465

H	-2.1808410	1.2562141	84.7140109
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H	-4.4001737	0.6162302	85.8046487
H	-4.7815399	2.3289067	86.1642714
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C	-3.4427311	6.5147917	88.3993218
C	-3.7310844	6.8896547	86.9417965
H	-2.8471117	6.7481956	86.2876941
H	-4.0328478	7.9539200	86.8778223
H	-4.5657615	6.2873093	86.5253852
C	-4.7017374	6.7157209	89.2687315
H	-2.6522206	7.1987524	88.7825365
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H	0.2635580	3.6960857	92.7919004
H	-0.4278837	5.0655989	91.8619931
H	0.5448460	3.8219657	91.0173206
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H	-1.1349565	2.0750624	91.5989572
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H	-2.8804303	4.3714468	92.7019369
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H	7.6913168	5.8462444	87.4596726
H	6.5739614	2.7304444	92.3388071
H	7.1400298	1.7335731	85.3690132
C	7.4733688	5.6446346	88.5315243
H	2.9794624	3.5520169	91.2066540
H	5.8964159	7.1791337	88.5814321
H	3.7602489	3.5372747	85.2959194
C	6.5377565	4.4406839	88.5682847
C	5.9245156	1.8632897	92.0959060
C	6.8327643	6.9158799	89.1139284
H	7.5224209	7.7811637	89.0323825
C	6.0372035	3.9321353	89.7808103
C	6.2511252	1.0945186	85.5560772
H	8.6637402	5.1247625	90.3063535
C	6.1822112	3.7736757	87.3851008
C	8.8113844	5.3287483	89.2249787
H	9.2914263	4.4343023	88.7802227
H	6.5547583	4.1694241	86.4267914
C	3.8238036	3.2900053	91.8735717
H	5.5546907	1.4441064	93.0546008
H	6.5597286	1.0965416	91.6082531
C	5.2349033	2.7771810	89.8310235
C	4.6250127	2.9387050	84.9554831
C	5.3799890	2.6157412	87.3764867
H	6.0010514	0.5765833	84.6071255
H	6.5469351	0.3240125	86.2951952
C	4.7502351	2.2701640	91.1883803
C	4.9215483	2.0987945	88.6205780
C	5.0587749	1.9413198	86.0430415
H	4.3706395	4.2211130	92.1362002
H	5.4502117	3.6181453	84.6551299
H	3.4049270	2.8744380	92.8135382
H	6.5928140	6.7911717	90.1915201
H	4.3111193	2.3875244	84.0456799
H	9.5174915	6.1804833	89.1370857
H	4.1485357	1.3562592	91.0110767
H	4.1961307	1.2671031	86.2167591
H	6.3014704	4.4337756	90.7268376
C	3.1396621	6.3894060	89.9867510
C	2.3619804	6.3309894	88.8756968
C	0.9810613	6.6255307	89.3283266
O	0.9728420	6.9115142	90.6487506
C	2.3025611	6.7477369	91.1670292

O	-0.0810408	6.6426447	88.6905692
C	2.7296440	6.0530106	87.4581328
H	3.8262069	6.0931388	87.3195365
H	4.2189590	6.1947105	90.0363888
H	2.2722527	5.9474649	91.9394285
H	2.6115889	7.6936181	91.6640057
Zn	-0.6081482	5.0479999	87.4441553
H	2.2390603	6.7735700	86.7732196
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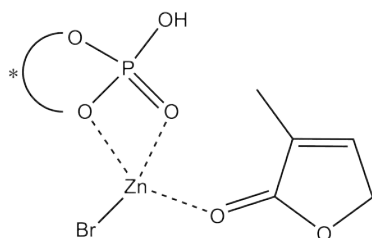
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C	1.0439268	-2.1370614	91.0692943
C	-0.9723327	-0.7243919	91.1345884
C	-1.4983853	-1.5846765	92.1445018
C	-1.6723997	0.4493961	90.7335156
H	-2.6410175	0.6791661	91.2039783
C	-1.1378839	1.3398455	89.8107047
C	4.4211968	0.3334156	88.2514512
C	4.7103802	-0.9219642	87.7329597
H	5.7268722	-1.1321824	87.3678841
C	3.7212039	-1.9442546	87.6394398
C	4.0119430	-3.1967376	87.0206305
C	2.3947036	-1.7080511	88.1583032
C	1.4060347	-2.7205903	87.9745895
C	2.1131691	-0.4506786	88.8081055
C	3.1046909	0.5349120	88.7709274
O	0.5583517	1.8368109	88.1998891
O	2.8347197	1.7896072	89.3170506
P	1.8781132	2.7848652	88.4272185
O	1.6632102	4.0825762	89.2273918
O	2.4065179	3.1225252	87.0132005
C	-0.7778435	-2.6783724	92.5984722
C	0.5113141	-2.9431841	92.0656363
H	-2.4867363	-1.3495991	92.5701175
H	-1.1934074	-3.3296872	93.3823654
H	2.0470209	-2.3495447	90.6752644
H	1.0980143	-3.7916944	92.4495430
C	1.7174939	-3.9208426	87.3510134
C	3.0343263	-4.1702177	86.8819535
H	0.3813064	-2.5356064	88.3258602
H	0.9348217	-4.6826909	87.2145781
H	3.2720410	-5.1285486	86.3956356
H	5.0306875	-3.3684845	86.6388950
C	-1.7442910	3.6965791	90.4745500
C	-1.7725569	2.6587027	89.4980646
C	-2.3497627	4.9270418	90.1656777
C	-2.3643745	2.8937224	88.2301180
C	-2.9636134	4.1423771	87.9768038
C	-2.9811725	5.1710783	88.9314265
H	-2.3305754	5.7316255	90.9198081
C	-2.3932963	1.8306805	87.1347584
H	-3.4332439	4.3022847	86.9955588
C	-1.6952459	2.3160141	85.8511812
H	-1.6575636	1.5018261	85.0983971
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H	-2.2356224	3.1686904	85.3892374
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H	-1.8297309	0.9500170	87.5035891
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H	-4.4654801	2.1824468	86.4724679
H	-4.3121219	0.9671609	87.7786649
C	-3.6874655	6.5043780	88.6964627
C	-4.0333122	6.7764728	87.2270556
H	-3.1541325	6.6558503	86.5623541
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C	-4.9500056	6.6107670	89.5752014
H	-2.9809372	7.2989935	89.0311851
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H	-5.4356237	7.6023115	89.4607514
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H	-1.6766897	3.2629564	93.9435124
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H	7.6859448	1.0431261	91.7338532
H	7.0718665	1.4481084	84.8643457
C	8.0267079	4.9254770	88.7227350
H	4.0475810	2.3034549	91.5185685
H	6.3467105	6.2494245	89.2223504
H	4.2847090	3.9202763	85.5428089
C	7.1471090	3.6898737	88.5839215
C	6.9292909	0.2957454	91.4157678
C	7.3514472	5.9870837	89.6107132
H	7.9622143	6.9130399	89.6541267
C	6.8383440	2.8870199	89.6946116
C	6.0846840	0.9687742	85.0332535
H	9.4042359	4.1489340	90.2527467
C	6.5852031	3.3405304	87.3455891
C	9.4372441	4.5769480	89.2287947
H	9.9311766	3.8330530	88.5714677
H	6.8124431	3.9722088	86.4735579
C	4.9639701	1.8354439	91.9280238
H	6.6848366	-0.3292525	92.2998347
H	7.4035574	-0.3555719	90.6538191
C	5.9754806	1.7819434	89.5994642
C	4.8495982	3.1656137	84.9646528
C	5.7219536	2.2397803	87.1895865
H	5.6542764	0.7153621	84.0419506
H	6.2647710	0.0209519	85.5765185
C	5.6649412	0.9757881	90.8599933
C	5.4115917	1.4552110	88.3355898
C	5.1489992	1.9164897	85.8101336
H	5.6272348	2.6461603	92.2959061
H	5.7771259	3.6468674	84.5902644
H	4.6781637	1.2159982	92.8035669
H	7.2285348	5.6178794	90.6507810
H	4.2446513	2.8890238	84.0776496
H	10.0780906	5.4821571	89.2689773
H	4.9622408	0.1645137	90.5792907
H	4.1830857	1.3954893	85.9734593
H	7.2665001	3.1411788	90.6777017
C	-0.7281667	8.7834137	87.8261761
C	0.0007941	7.6775691	88.1185895
C	0.0947319	6.9002193	86.8595544
O	-0.5871509	7.5239340	85.8746193
C	-1.1208383	8.7552489	86.3862409
O	0.6778907	5.8350931	86.6347911
C	0.6251341	7.2106847	89.3853940

H	0.3111820	7.8280497	90.2470232
H	-1.0042434	9.5929889	88.5160794
H	-2.2208554	8.7575250	86.2277831
H	-0.6880162	9.5925688	85.7946551
Zn	2.4140031	5.1146000	87.4828050
H	1.7334325	7.2563730	89.3037603
Br	3.9981906	6.7825200	87.3562547
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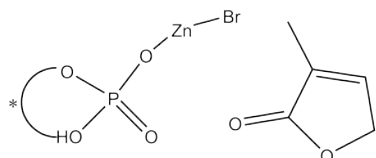
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C	-0.9746951	-0.5541096	91.0278430
C	-1.5549809	-1.5411886	91.8794850
C	-1.6658266	0.6494854	90.7113794
H	-2.6874797	0.7954251	91.0951655
C	-1.0806721	1.6530517	89.9474998
C	4.5004826	0.7047116	88.3048830
C	4.6606235	-0.4408828	87.5341095
H	5.6246073	-0.6157213	87.0330002
C	3.6036655	-1.3711880	87.3289458
C	3.7644764	-2.4871129	86.4548859
C	2.3306612	-1.1556044	87.9710692
C	1.2556589	-2.0372056	87.6512654
C	2.1872270	-0.0337235	88.8662337
C	3.2501521	0.8676014	88.9784763
O	0.8289298	2.4507504	88.7233519
O	3.1119203	1.9564874	89.8310278
P	2.2340208	3.2612802	89.3395058
O	1.9983030	4.1745234	90.4941527
O	2.7181889	3.7750408	87.9490484
C	-0.8646593	-2.6991886	92.2022641
C	0.4428291	-2.9100606	91.6886406
H	-2.5624206	-1.3579563	92.2851687
H	-1.3218560	-3.4498943	92.8647258
H	2.0442354	-2.1460293	90.4598244
H	0.9985393	-3.8190158	91.9651800
C	1.4392792	-3.1028073	86.7819612
C	2.7068295	-3.3423200	86.1885442
H	0.2641548	-1.8543771	88.0870924
H	0.5907058	-3.7618447	86.5428950
H	2.8409831	-4.1935273	85.5038133
H	4.7447241	-2.6421404	85.9773149
C	-2.0244686	3.9079618	90.5942491
C	-1.8211788	2.9088898	89.6078186
C	-2.7992562	5.0379922	90.2602556
C	-2.3481425	3.0763081	88.2923795
C	-3.1008037	4.2292053	88.0116905
C	-3.3518845	5.2166723	88.9842392
H	-2.9716054	5.8132340	91.0248417
C	-2.1558165	2.0024578	87.2204371
H	-3.5159258	4.3570018	87.0007304
C	-2.1479665	2.5465260	85.7848750

H	-1.8277753	1.7525749	85.0819669
H	-1.4384883	3.3899436	85.6694037
H	-3.1523879	2.8934927	85.4637120
C	-3.2085271	0.8869051	87.3739994
H	-1.1618879	1.5353060	87.3853223
H	-3.0374268	0.0836106	86.6281886
H	-4.2304258	1.2914908	87.2176303
H	-3.1744216	0.4295935	88.3824147
C	-4.1960198	6.4430682	88.6579227
C	-3.5654363	7.2946674	87.5414626
H	-2.5367196	7.6098581	87.8079547
H	-4.1680971	8.2063526	87.3483208
H	-3.5021843	6.7277351	86.5888379
C	-5.6453439	6.0558874	88.3125291
H	-4.2256795	7.0675728	89.5780251
H	-5.6868613	5.4367570	87.3921001
H	-6.2676348	6.9579730	88.1377824
H	-6.1094517	5.4693603	89.1304480
C	-1.4350069	3.7910742	91.9984042
C	-0.6003477	5.0237917	92.3870372
H	-0.1737990	4.8888974	93.4023396
H	-1.2110218	5.9509186	92.4082186
H	0.2454262	5.1575623	91.6855938
C	-2.5366584	3.5021783	93.0349162
H	-0.7408590	2.9260376	91.9944014
H	-3.1027456	2.5818479	92.7853417
H	-3.2665964	4.3372990	93.0881559
H	-2.0998621	3.3712541	94.0464191
H	8.8113905	5.2089461	87.6246531
H	8.0880687	0.8115763	91.4851811
H	6.8393035	2.1963104	84.6201736
C	8.7359343	4.7448834	88.6330567
H	4.6779032	2.5958534	91.7894729
H	7.4114446	6.3342624	89.3791192
H	4.1570267	4.3871543	86.1808927
C	7.6333079	3.6963293	88.5537578
C	7.1939047	0.2072526	91.2246709
C	8.3815292	5.8613092	89.6321068
H	9.1616599	6.6508192	89.6395969
C	7.2985067	2.9056457	89.6667375
C	5.9105068	1.6500901	84.8892214
H	10.0999907	3.6429768	89.9615420
C	6.9061255	3.5008889	87.3689737
C	10.1025305	4.1155287	88.9570309
H	10.3700352	3.3317862	88.2200957
H	7.1478385	4.1254706	86.4935672
C	5.5597761	1.9803006	92.0529136
H	6.9580350	-0.4349076	92.0986067
H	7.4717126	-0.4523870	90.3776336
C	6.2819111	1.9362094	89.6182451
C	4.6431616	3.7806862	85.3921937
C	5.8737309	2.5500112	87.2660577
H	5.3086012	1.5173905	83.9665944
H	6.2079869	0.6447874	85.2471312
C	5.9938084	1.1026510	90.8652215
C	5.5706403	1.7465975	88.4018709
C	5.1067974	2.4219086	85.9510374
H	6.3748024	2.6616635	92.3754280
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H	3.9196649	3.6232607	84.5642306
H	10.9042978	4.8829225	88.9523750
H	5.1475265	0.4252997	90.6312221
H	4.1920549	1.8292836	86.1584664
H	7.8494743	3.0459157	90.6108263
C	0.1902782	7.8868314	86.6834418
C	0.3134856	6.6009361	87.1023438
C	0.6412251	5.8090264	85.8923373
O	0.7106917	6.6137522	84.8104975
C	0.4352308	7.9622048	85.2139495

O	0.8140079	4.5936669	85.7569901
C	0.1761967	6.0018663	88.4544381
H	-0.3838257	6.6627404	89.1402325
H	-0.0564748	8.7593108	87.3043452
H	-0.4432032	8.3289135	84.6373797
H	1.3068219	8.5971951	84.9393079
Zn	1.5883435	2.9011999	86.6030055
H	1.1678423	5.7993312	88.9078035
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H	-0.3540745	5.0302811	88.4048701

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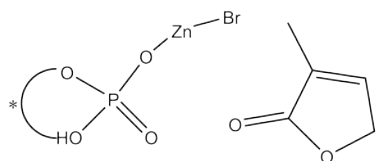
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C	3.7088408	3.5425350	1.1816517
C	1.4951000	4.5688085	1.5507557
C	2.1284551	5.8478507	1.5302813
C	0.0720324	4.4668886	1.6488228
H	-0.5152760	5.3940943	1.7216079
C	-0.5660481	3.2358118	1.5912127
C	2.7302432	-1.5005644	0.4786962
C	3.8055468	-1.7011156	1.3320482
H	4.3827002	-2.6362035	1.2613324
C	4.1628838	-0.7410045	2.3198107
C	5.2136550	-1.0003934	3.2502727
C	3.4241580	0.4960848	2.4047747
C	3.7346072	1.3816173	3.4828466
C	2.3808716	0.7750776	1.4407466
C	2.0215976	-0.2587458	0.5525760
O	-0.3513439	0.8528195	1.4947834
O	1.0134705	-0.1250297	-0.3903364
P	-0.5517313	0.3131707	-0.0759687
O	-0.9573129	1.3523222	-1.0747598
H	-3.0520572	-2.1661662	-1.5275806
O	-1.4891530	-0.9061688	0.2070409
C	3.4975125	5.9673358	1.3394205
C	4.2886929	4.8040290	1.1474155
H	1.5019278	6.7456294	1.6515944
H	3.9687183	6.9617485	1.3195206
H	4.3295579	2.6488824	1.0273919
H	5.3699761	4.9019100	0.9661225
C	4.7489602	1.0923035	4.3856386
C	5.5109718	-0.0996510	4.2616062
H	3.1487592	2.3020014	3.6083373
H	4.9578620	1.7919270	5.2094499
H	6.3189574	-0.3142121	4.9775103
H	5.7735512	-1.9443150	3.1576107
C	-2.6823039	3.2908244	0.1893464
C	-2.0277669	2.9468401	1.4133174
C	-3.9296629	2.7078116	-0.1110265
C	-2.6763409	2.0730682	2.3266863
C	-3.9142207	1.4591875	1.9601027
C	-4.5678367	1.7889989	0.7307724
H	-4.4178269	2.9653501	-1.0620485
C	-2.1252307	1.8356048	3.7289108
H	-4.4950323	0.9450880	2.7444320
C	-2.0808205	0.3562316	4.1396900
H	-1.6155194	0.2466218	5.1399297

H	-1.4591812	-0.2349204	3.4338144
H	-3.0890913	-0.1028142	4.2030389
C	-2.9345691	2.6772424	4.7376441
H	-1.0850835	2.2190992	3.7443420
H	-2.5039324	2.5787165	5.7548243
H	-3.9917977	2.3422041	4.7825911
H	-2.9295028	3.7509660	4.4626393
C	-5.9060608	1.1897214	0.3184987
C	-5.6991075	0.0381943	-0.6889876
H	-5.0713602	0.3299045	-1.5535768
H	-6.6764255	-0.3182818	-1.0736476
H	-5.2218824	-0.8349527	-0.1904683
C	-6.7822666	0.7508149	1.4991191
H	-6.4369651	2.0024074	-0.2244992
H	-6.3471559	-0.1249021	2.0242546
H	-7.7827844	0.4444496	1.1342184
H	-6.9238462	1.5681124	2.2353767
C	-2.0780089	4.2837725	-0.7936485
C	-2.3684691	3.9726513	-2.2698367
H	-1.7822131	4.6611607	-2.9119648
H	-3.4363146	4.1272679	-2.5299397
H	-2.0884777	2.9337016	-2.5256342
C	-2.5510203	5.7090333	-0.4323382
H	-0.9785171	4.2395604	-0.6594115
H	-2.3314910	5.9723697	0.6217922
H	-3.6479757	5.8042200	-0.5744113
H	-2.0569521	6.4569112	-1.0857511
H	0.2088398	-6.0351939	-3.0412521
H	4.9027680	-2.5279283	-3.9347986
H	1.5433641	-5.3741539	1.7998588
C	0.9827771	-5.4028006	-3.5293995
H	2.5372157	0.1203654	-2.4569843
H	-0.5306415	-4.0512153	-4.3859015
H	-1.4242605	-3.3945058	0.4501241
C	1.4634550	-4.4079736	-2.4792168
C	5.1849904	-2.1334267	-2.9364443
C	0.3136258	-4.6881772	-4.7183588
H	-0.0776004	-5.4229364	-5.4521463
C	2.4835931	-3.4824081	-2.7644311
H	1.4957179	-4.3198218	2.1443928
C	2.9161280	-5.7642219	-4.5167909
C	0.8823102	-4.3754012	-1.1993167
C	2.1148239	-6.3330444	-4.0000257
H	2.5789805	-6.48673277	-3.1465563
H	0.0852668	-5.0985146	-0.9673874
C	3.3602260	-0.3637775	-3.0181269
H	5.9744487	-1.3714083	-3.0997378
H	5.6274976	-2.9685862	-2.3564746
C	2.9220387	-2.5387630	-1.8158132
C	-0.8132249	-3.9505231	1.1851173
C	1.2804483	-3.4504390	-0.2154122
H	1.0522437	-4.3121406	3.1616594
H	2.5339302	-3.9420299	2.2225456
C	3.9861572	-1.5120802	-2.2019479
C	2.3116319	-2.5246745	-0.5326604
C	0.6456296	-3.4740567	1.1747259
H	2.9450241	-0.7418470	-3.9767567
H	-0.8972660	-5.0362429	0.9697401
H	4.1182713	0.4099962	-3.2594396
H	1.0358414	-4.0344843	-5.2514615
H	-1.2645126	-3.7814961	2.1833090
H	1.7313188	-7.0905318	-4.7144508
H	4.3733955	-1.0686594	-1.2615411
H	0.6495005	-2.4283163	1.5513444
H	2.9479062	-3.4866691	-3.7631202
C	-0.4489192	-1.1211262	-3.2587308
C	-1.7671181	-1.3156475	-3.0206766
C	-2.4837245	-0.0825177	-3.4545199
O	-1.5679592	0.7875187	-3.9938453
C	-0.2542856	0.2351397	-3.8577163
O	-3.6687615	0.1906732	-3.3818090

C	-2.4912558	-2.4777028	-2.4319316
H	-1.7908137	-3.2820253	-2.1396583
H	0.3771090	-1.8096171	-3.0296887
H	0.3329992	0.8997252	-3.1865933
H	0.2389968	0.2123883	-4.8549908
Zn	-3.0394336	-0.5168643	1.2984776
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Br	-4.2369464	-2.2908595	2.2094908

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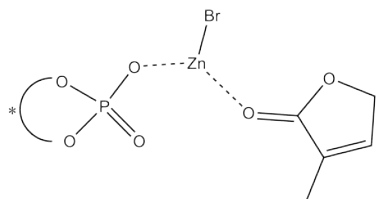
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C	3.7110599	3.5426737	1.1912546
C	1.4948475	4.5663118	1.5490177
C	2.1269459	5.8454330	1.5284408
C	0.0718743	4.4621002	1.6416168
H	-0.5174375	5.3884918	1.7080289
C	-0.5649975	3.2305979	1.5849405
C	2.7331081	-1.5027519	0.4824249
C	3.8068717	-1.7043588	1.3371148
H	4.3812933	-2.6411876	1.2666968
C	4.1653440	-0.7445985	2.3245557
C	5.2153009	-1.0039151	3.2551410
C	3.4278547	0.4931518	2.4091143
C	3.7393718	1.3785419	3.4866216
C	2.3856552	0.7734297	1.4445165
C	2.0272176	-0.2593006	0.5546297
O	-0.3460662	0.8479975	1.4931414
O	1.0235018	-0.1237565	-0.3912335
P	-0.5430759	0.3133257	-0.0814198
O	-0.9449930	1.3569285	-1.0755269
H	-3.0429509	-2.1475693	-1.5341340
O	-1.4777780	-0.9092494	0.1959966
C	3.4961189	5.9666812	1.3435136
C	4.2892461	4.8044378	1.1575236
H	1.4985777	6.7426045	1.6447772
H	3.9658103	6.9617490	1.3235624
H	4.3325620	2.6488769	1.0419075
H	5.3711911	4.9031792	0.9810167
C	4.7536725	1.0890191	4.3887146
C	5.5139971	-0.1033428	4.2654668
H	3.1543768	2.2996034	3.6104197
H	4.9636893	1.7892377	5.2116589
H	6.3218660	-0.3185591	4.9811902
H	5.7738964	-1.9486477	3.1631527
C	-2.6772787	3.2699459	0.1750323
C	-2.0261320	2.9380403	1.4046112
C	-3.9191399	2.6767385	-0.1266882
C	-2.6742701	2.0683655	2.3217401
C	-3.9095865	1.4505500	1.9572427
C	-4.5598767	1.7664960	0.7235658
H	-4.3997770	2.9176168	-1.0858316
C	-2.1247390	1.8420627	3.7270260
H	-4.4868064	0.9316997	2.7404918
C	-2.0655475	0.3654667	4.1460293
H	-1.6063216	0.2667327	5.1503291
H	-1.4339393	-0.2216853	3.4466716
H	-3.0677348	-0.1074183	4.2030064

C	-2.9434926	2.6810244	4.7300945
H	-1.0884048	2.2361973	3.7419231
H	-2.5152868	2.5931256	5.7493767
H	-3.9977413	2.3367856	4.7756120
H	-2.9492283	3.7532562	4.4495053
C	-5.9018406	1.1680871	0.3194280
C	-5.7082072	0.0030134	-0.6748646
H	-5.0825140	0.2782000	-1.5463953
H	-6.6904989	-0.3487945	-1.0511566
H	-5.2395501	-0.8684764	-0.1657966
C	-6.7777270	0.7493589	1.5079826
H	-6.4288493	1.9786252	-0.2311499
H	-6.3483431	-0.1253342	2.0395260
H	-7.7820835	0.4470889	1.1503140
H	-6.9111435	1.5750871	2.2365063
C	-2.0745031	4.2635111	-0.8085669
C	-2.3697356	3.9597127	-2.2847458
H	-1.7863764	4.6516403	-2.9256304
H	-3.4381924	4.1149925	-2.5418081
H	-2.0902873	2.9235693	-2.5505564
C	-2.5448959	5.6881511	-0.4410868
H	-0.9746669	4.2157936	-0.6778163
H	-2.3274889	5.9474058	0.6145410
H	-3.6414702	5.7863049	-0.5836865
H	-2.0499561	6.4387358	-1.0907086
H	0.1908511	-6.0193512	-3.0436797
H	4.9078238	-2.5342645	-3.9254348
H	1.5432125	-5.3675355	1.8042156
C	0.9748108	-5.3964761	-3.5283789
H	2.5354758	0.1181713	-2.4638253
H	-0.5180045	-4.0353006	-4.4062150
H	-1.4280449	-3.4021363	0.4432464
C	1.4561491	-4.4018355	-2.4783394
C	5.1860088	-2.1359556	-2.9274872
C	0.3222598	-4.6832082	-4.7270279
H	-0.0701968	-5.4180789	-5.4599728
C	2.4778946	-3.4784570	-2.7628891
C	1.4898637	-4.3136966	2.1489109
H	2.9146597	-5.7810948	-4.4933530
C	0.8764486	-4.3695276	-1.1982482
C	2.1025106	-6.3398691	-3.9828036
H	2.5535444	-6.8731014	-3.1219723
H	0.0772431	-5.0901653	-0.9664761
C	3.3610315	-0.3665003	-3.0206188
H	5.9766616	-1.3753819	-3.0915342
H	5.6260741	-2.9695726	-2.3438144
C	2.9197000	-2.5380412	-1.8131888
C	-0.8175484	-3.9497458	1.1849028
H	1.2776240	-3.4479745	-0.2128613
C	1.0422050	-4.3084804	3.1642159
H	2.5260502	-3.9320263	2.2323295
C	3.9846589	-1.5122627	-2.1993317
C	2.3116885	-2.5253260	-0.5292645
C	0.6405491	-3.4707818	1.1762970
H	2.9494673	-0.7471966	-3.9797913
H	-0.8990206	-5.0373382	0.9782550
H	4.1187227	0.4076102	-3.2619454
H	1.0547478	-4.0403653	-5.2591634
H	-1.2744459	-3.7751785	2.1794297
H	1.7205108	-7.0977815	-4.6975389
H	4.3688344	-1.0659902	-1.2589734
H	0.6422723	-2.4244011	1.5512993
H	2.9420349	-3.4828228	-3.7617114
C	-0.4575699	-1.0913026	-3.2913457
C	-1.7714355	-1.2809883	-3.0294434
C	-2.4890281	-0.0306416	-3.4179365
O	-1.5780184	0.8381806	-3.9700999
C	-0.2681148	0.2761920	-3.8692919
O	-3.6652335	0.2543129	-3.2967412
C	-2.4915846	-2.4488800	-2.4474197
H	-1.7908357	-3.2592015	-2.1726819

H	0.3686758	-1.7884786	-3.0900882
H	0.3368537	0.9246579	-3.1974076
H	0.2075690	0.2681524	-4.8758370
Zn	-3.0318143	-0.5392368	1.2841654
H	-3.2453066	-2.8407597	-3.1618004
Br	-4.2310871	-2.2780299	2.2392608

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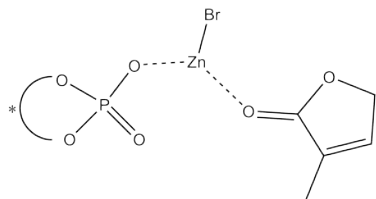
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C	0.3401256	1.6758018	0.9169699
C	1.7299007	1.6732350	1.1191062
C	2.4006184	2.9317119	1.3321008
C	3.8236696	3.0513019	1.3600182
C	1.6133677	4.1296244	1.4866684
C	2.2707395	5.3773448	1.7062309
C	0.1949678	4.0370597	1.4257267
H	-0.4059843	4.9385365	1.6225361
C	-0.4569500	2.8435182	1.1326181
C	3.0641797	-1.7149471	-0.0781939
C	3.9203481	-2.0576030	0.9626996
H	4.4958531	-2.9943732	0.8999452
C	4.0404433	-1.2567153	2.1351278
C	4.8649366	-1.6653956	3.2265639
C	3.2820979	-0.0325187	2.2437270
C	3.3396360	0.6901980	3.4736295
C	2.4789107	0.3873500	1.1216841
C	2.3726127	-0.4671726	0.0234453
O	-0.3124266	0.4991720	0.5848953
O	1.5928309	-0.0671736	-1.0464667
P	-0.0561030	-0.1758304	-0.9290436
O	-0.6697639	0.5715940	-2.0754656
H	-2.4565078	-0.7892181	-2.5936399
O	-0.4220325	-1.6599100	-0.6584888
C	3.6548741	5.4552236	1.7463230
C	4.4344873	4.2818205	1.5592242
H	1.6542988	6.2814112	1.8324973
H	4.1512657	6.4239610	1.9097095
H	4.4391884	2.1540258	1.2053924
H	5.5331988	4.3493483	1.5657226
C	4.1378323	0.2558302	4.5235091
C	4.9205325	-0.9230728	4.3969838
H	2.7342063	1.6000384	3.5885500
H	4.1603241	0.8284632	5.4634136
H	5.5563810	-1.2527747	5.2327959
H	5.4472258	-2.5949365	3.1252381
C	-2.7290801	3.2017773	0.0603420
C	-1.9561843	2.8096215	1.1827965
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C	-2.5901030	2.5145382	2.4243200
C	-3.9850895	2.6757419	2.5278188
C	-4.7685417	3.1222960	1.4451409
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C	-1.7856219	2.0009981	3.6185406
H	-4.4727851	2.4685429	3.4934636
C	-1.8309777	0.4602005	3.6828959
H	-1.1609123	0.0816443	4.4824291
H	-1.5122315	0.0043926	2.7246975
H	-2.8576084	0.1028196	3.9135214

C	-2.2062490	2.6284812	4.9563312
H	-0.7277038	2.2859744	3.4443730
H	-1.5165022	2.3084598	5.7637815
H	-3.2272102	2.3168692	5.2609623
H	-2.1896813	3.7362521	4.9090717
C	-6.2656528	3.3685664	3.3685664
C	-7.0435959	2.0769258	1.9099564
H	-6.9239920	1.3272929	1.1016755
H	-8.1284647	2.2843773	2.0143012
H	-6.7006319	1.6152597	2.8599446
C	-6.5486285	4.4533188	2.6558066
H	-6.6308170	3.7503102	0.6216986
H	-6.2275351	4.1258320	3.6667379
H	-7.6334543	4.6807634	2.7069873
H	-6.0095579	5.3929371	2.4204683
C	-2.0726950	3.5099773	-1.2827108
C	-2.8360329	2.9044208	-2.4705048
H	-2.2639921	3.0605192	-3.4071464
H	-3.8352733	3.3679595	-2.6103821
H	-2.9567395	1.8125435	-2.3399955
C	-1.8741290	5.0270632	-1.4609538
H	-1.0732157	3.0293774	-1.2762054
H	-1.2541269	5.4555876	-0.6483891
H	-2.8491447	5.5590640	-1.4581382
H	-1.3696310	5.2449086	-2.4249476
H	1.1195561	-5.9260233	-4.2899308
H	5.3935334	-1.8023885	-4.2348746
C	2.3564082	-6.4753538	0.0269252
C	1.9038616	-5.2182944	-4.6363981
H	2.1780672	0.1969278	-3.5148117
H	0.4509800	-3.8859713	-5.5953046
H	-0.3321601	-3.7105600	0.5419665
C	2.1959542	-4.2909124	-3.4647799
C	5.3776956	-1.2380648	-3.2788302
C	1.3473016	-4.4800694	-5.8634144
H	1.0587349	-5.2041368	-6.6527414
C	2.8630003	-3.0674985	-3.6354339
C	2.5720334	-5.6298349	0.7128621
H	3.9793195	-5.3761477	-5.3378808
C	1.8456064	-4.6637407	-2.1553289
C	3.1572680	-6.0400878	-4.9959333
H	3.5303081	-6.6123839	-4.1223630
H	1.3284666	-5.6262427	-2.0099444
C	3.2095991	-0.0271297	-3.8492138
H	5.9509665	-0.3002193	-3.4320424
H	5.9106601	-1.8470984	-2.5203987
C	3.1694540	-2.2200557	-2.5553433
C	0.2342510	-4.6656035	0.4788547
C	2.1333598	-3.8596019	-1.0355069
H	2.3477240	-5.9657544	1.7463643
H	3.6586905	-5.4189926	0.6479896
C	3.9352595	-0.9281325	-2.8343410
C	2.8014880	-2.6160552	-1.2397515
C	1.7423534	-4.3839024	0.3491036
H	3.1559797	-0.4999898	-4.8521957
H	-0.1519042	-5.3120560	-0.3401519
H	3.7505793	0.9345063	-3.9669842
H	2.0983545	-3.7941974	-6.3083091
H	-0.0051450	-5.1939189	1.4245349
H	2.9393600	-6.7595868	-5.8125973
H	4.0075948	-0.3620941	-1.8842677
H	1.9778033	-3.5984139	1.0930453
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C	-4.4999277	-0.1341271	-0.2621028
C	-3.8195415	-1.0774205	-0.9631735
C	-3.3991680	-2.0930667	0.0229235
O	-3.8196583	-1.7599551	1.2542097
C	-4.5199467	-0.5048837	1.1779123
O	-2.7646461	-3.1488288	-0.1535158
C	-3.4897524	-1.1622678	-2.4153713
H	-4.1693167	-0.5290669	-3.0156508

H	-4.9572120	0.7836573	-0.6541460
H	-3.9866206	0.2384749	1.8107333
H	-5.5387235	-0.6418289	1.5989126
Zn	-1.1715996	-3.2163360	-1.4601596
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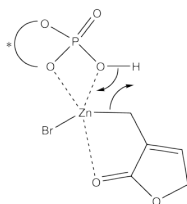
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C	3.8198361	3.0507898	1.3750778
C	1.6078353	4.1229463	1.5086498
C	2.2626121	5.3709735	1.7309197
C	0.1902091	4.0268685	1.4466376
H	-0.4140255	4.9263778	1.6426535
C	-0.4591572	2.8326575	1.1511813
C	3.0655837	-1.7119539	-0.0803484
C	3.9294757	-2.0547839	0.9538227
H	4.5061057	-2.9902896	0.8835898
C	4.0560405	-1.2578492	2.1278321
C	4.8890193	-1.6668222	3.2119922
C	3.2948747	-0.0365886	2.2455711
C	3.3592164	0.6823102	3.4770593
C	2.4832608	0.3846607	1.1302878
C	2.3726020	-0.4653953	0.0288468
O	-0.3115983	0.4875678	0.6090809
O	1.5861296	-0.0630784	-1.0344529
P	-0.0603984	-0.1898625	-0.9073158
O	-0.7004148	0.5436393	-2.0464843
H	-2.4474790	-0.7868623	-2.6106467
O	-0.4016704	-1.6801151	-0.6265802
C	3.6459727	5.4522554	1.7695120
C	4.4276099	4.2817128	1.5774708
H	1.6439955	6.2731543	1.8598873
H	4.1400909	6.4217263	1.9350007
H	4.4363306	2.1550491	1.2166388
H	5.5261136	4.3516479	1.5823517
C	4.1664305	0.2475122	4.5192417
C	4.9512079	-0.9282582	4.3837963
H	2.7523205	1.5903013	3.5977546
H	4.1945173	0.8179060	5.4602975
H	5.5942047	-1.2586434	5.2137707
H	5.4730274	-2.5944636	3.1035176
C	-2.7223084	3.1890985	0.0617747
C	-1.9586290	2.8017163	1.1922664
C	-4.1154165	3.3508279	0.2125320
C	-2.6017421	2.5181434	2.4316306
C	-3.9966954	2.6845856	2.5246919
C	-4.7711928	3.1255739	1.4337322
H	-4.7106234	3.6878633	-0.6518642
C	-1.8054186	2.0110004	3.6339803
H	-4.4910533	2.4868969	3.4889019
C	-1.8372647	0.4699246	3.6981576
H	-1.1716629	0.0970295	4.5038993
H	-1.5052990	0.0153081	2.7441062
H	-2.8625303	0.1027202	3.9193908
C	-2.2439523	2.6344498	4.9676659
H	-0.7485620	2.3055371	3.4692929
H	-1.5567073	2.3244372	5.7809797
H	-3.2625675	2.3096666	5.2666125
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H	-6.9274881	1.3340033	1.0883273
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C	-6.5564594	4.4706777	2.6222320
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H	-6.0117734	5.4061170	2.3845163
C	-2.0559466	3.4878382	-1.2785267
C	-2.8184726	2.8895990	-2.4702585
H	-2.2355826	3.0328945	-3.4017976
H	-3.8096083	3.3672720	-2.6216524
H	-2.9532760	1.7996735	-2.3389447
C	-1.8402164	5.0024375	-1.4571042
H	-1.0621231	2.9960694	-1.2676320
H	-1.2165801	5.4245988	-0.6442967
H	-2.8087292	5.5461334	-1.4569357
H	-1.3309780	5.2134504	-2.4198995
H	1.0973512	-5.9206719	-4.2825963
H	5.3622157	-1.7901077	-4.2526753
H	2.4112560	-6.4639110	0.0329418
C	1.8794693	-5.2125723	-4.6332526
H	2.1466031	0.2041013	-3.5082211
H	0.4179820	-3.8830856	-5.5814683
H	-0.3352863	-3.7589853	0.5494796
C	2.1773358	-4.2855420	-3.4629552
C	5.3512263	-1.2255814	-3.2967753
C	1.3135196	-4.4749310	-5.8560897
H	1.0207604	-5.1989310	-6.6438141
C	2.8384564	-3.0600193	-3.6368148
C	2.6139835	-5.6131325	0.7162557
H	3.9513380	-5.3674647	-5.3460812
C	1.8380010	-4.6607436	-2.1512985
C	3.1318907	-6.0323227	-5.0000966
H	3.5116896	-6.6036649	-4.1289857
H	1.3240432	-5.6246108	-2.0041040
C	3.1757674	-0.0185029	-3.8501733
H	5.9217258	-0.2868485	-3.4545076
H	5.8909999	-1.8338486	-2.5427875
C	3.1514580	-2.2131798	-2.5584618
C	0.2559604	-4.6990850	0.4958229
C	2.1317086	-3.8573897	-1.0328278
H	2.4047612	-5.9526378	1.7518475
H	3.6957862	-5.3821254	0.6422617
C	3.9113661	-0.9188957	-2.8421501
C	2.7956713	-2.6120898	-1.2407953
C	1.7566067	-4.3851752	0.3550855
H	3.1152807	-0.4898259	-4.8534545
H	-0.1225141	-5.3597732	-0.3144958
H	3.7137256	0.9443066	-3.9713190
H	2.0600954	-3.7878535	-6.3066076
H	0.0364452	-5.2222253	1.4493039
H	2.9111849	-6.7521331	-5.8156704
H	3.9892962	-0.3536577	-1.8920668
H	1.9807578	-3.5924447	1.0950725
H	3.1249305	-2.7452515	-4.6521095
C	-4.4780064	-0.1282779	-0.2834269
C	-3.8074544	-1.0792879	-0.9822620
C	-3.3852537	-2.0931777	0.0087668
O	-3.8027192	-1.7501364	1.2404126
C	-4.4889330	-0.4900419	1.1600392
O	-2.7536137	-3.1472778	-0.1665197
C	-3.4774870	-1.1715101	-2.4337472
H	-4.1611081	-0.5475130	-3.0391767

H	-4.9255482	0.7941442	-0.6755868
H	-3.9425898	0.2539356	1.7811190
H	-5.5054969	-0.6096092	1.5925466
Zn	-1.1476203	-3.2110963	-1.4764280
H	-3.5324154	-2.2180675	-2.7968616
Br	-1.5877881	-4.5316130	-3.2929570

5.3 Transition States

D_{TS} ; woelfling data



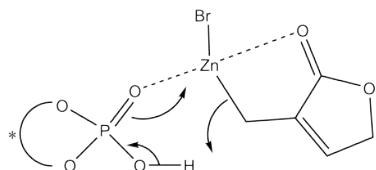
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C	3.378679	2.993110	1.720205
C	1.193542	4.082353	2.015239
C	1.863080	5.341900	2.045416
C	-0.227168	4.011297	2.047124
H	-0.803402	4.944849	2.129604
C	-0.905546	2.806221	1.922183
C	2.592710	-1.741421	0.527421
C	3.649653	-1.991230	1.395147
H	4.311459	-2.848708	1.200647
C	3.882629	-1.185764	2.545918
C	4.905902	-1.516146	3.483818
C	3.068188	-0.016231	2.773922
C	3.295337	0.746160	3.958691
C	2.030853	0.313898	1.826957
C	1.768357	-0.612019	0.809563
O	-0.819852	0.411078	1.913762
O	0.656535	-0.422139	-0.012823
P	-0.852853	-0.633449	0.675820
O	-1.732679	0.074900	-0.483600
H	-1.531997	-0.418973	-1.352732
O	-1.225442	-2.010010	1.095057
C	3.240186	5.421155	1.914056
C	3.998386	4.234723	1.733131
H	1.256846	6.255271	2.151986
H	3.743600	6.399969	1.927431
H	3.979842	2.088984	1.557775
H	5.087890	4.299934	1.590950
C	4.288964	0.389001	4.858857
C	5.109764	-0.744884	4.617516
H	2.659076	1.619238	4.158930
H	4.435973	0.986591	5.771150
H	5.896363	-1.016350	5.337594
H	5.522644	-2.408430	3.294125
C	-3.002205	3.172109	0.573933
C	-2.391851	2.724229	1.779682
C	-4.399327	3.056628	0.446451
C	-3.183788	2.159194	2.815879
C	-4.573192	2.064094	2.632162
C	-5.203657	2.504612	1.455400
H	-4.882155	3.396288	-0.484219
C	-2.573209	1.680496	4.131578
H	-5.184185	1.624549	3.436782

C	-2.884257	0.199986	4.414103
H	-2.369700	-0.135305	5.338317
H	-2.545063	-0.447071	3.582211
H	-3.971333	0.031408	4.561345
C	-3.008627	2.585205	5.298959
H	-1.471682	1.774797	4.046921
H	-2.524644	2.266894	6.245609
H	-4.107285	2.545109	5.452804
H	-2.735537	3.643503	5.111144
C	-6.709549	2.368633	1.271309
C	-7.139305	0.890516	1.245724
H	-6.596804	0.328599	0.459294
H	-8.228179	0.794698	1.052871
H	-6.926357	0.394001	2.215604
C	-7.489349	3.163339	2.333281
H	-6.954031	2.806109	0.277860
H	-7.300653	2.765458	3.352348
H	-8.582324	3.105400	2.150445
H	-7.194389	4.231831	2.332445
C	-2.190611	3.762934	-0.578254
C	-2.582110	3.190425	-1.951301
H	-1.850351	3.505165	-2.722346
H	-3.583527	3.538020	-2.281229
H	-2.603777	2.082003	-1.930184
C	-2.278680	5.301047	-0.589750
H	-1.127375	3.491690	-0.417044
H	-1.946778	5.738590	0.372754
H	-3.322449	5.638693	-0.762961
H	-1.641868	5.725003	-1.393215
H	1.521048	-6.157261	-3.792896
H	5.476783	-1.481925	-2.500193
H	2.273405	-6.301403	0.755267
C	1.986851	-5.213767	-4.153011
H	2.148305	-0.164072	-3.833718
H	0.057472	-4.428873	-4.841776
H	-0.902074	-4.185519	0.306952
C	2.090171	-4.286924	-2.948259
C	4.937984	-0.806307	-1.803261
C	1.069592	-4.634747	-5.244536
H	0.966710	-5.340569	-6.094791
C	2.654755	-3.002266	-3.065490
C	2.192585	-5.404344	1.404562
H	3.893816	-4.666582	-5.105525
C	1.626915	-4.687808	-1.687460
C	3.375846	-5.567146	-4.714191
H	4.022914	-6.010278	-3.930887
H	1.162160	-5.681699	-1.587653
C	3.216272	-0.148709	-3.528910
H	5.384765	0.205667	-1.887525
H	5.114798	-1.170597	-0.772284
C	2.794765	-2.142764	-1.961796
C	-0.203466	-4.943131	0.706876
C	1.740109	-3.867259	-0.546669
H	1.835804	-5.738111	2.400513
H	3.212729	-4.988924	1.528505
C	3.434686	-0.765872	-2.138980
C	2.357271	-2.596933	-0.681972
C	1.222262	-4.373761	0.797531
H	3.792904	-0.673298	-4.318708
H	-0.251520	-5.856421	0.078261
H	3.530364	0.912854	-3.524635
H	1.471149	-3.680572	-5.645667
H	-0.563577	-5.218840	1.718747
H	3.294921	-6.294735	-5.548090
H	2.955302	-0.075959	-1.411592
H	1.174232	-3.501986	1.481699
H	3.002339	-2.658747	-4.051437
C	-1.526382	-1.775238	-5.202106
C	-1.030588	-0.985506	-4.214737
C	-0.938170	0.379847	-4.797072
O	-1.325605	0.383572	-6.085847

C	-1.702344	-0.956750	-6.444998
O	-0.567949	1.398937	-4.211832
C	-0.584752	-1.167317	-2.809968
H	0.386608	-1.710179	-2.772321
H	-1.748772	-2.850569	-5.156541
H	-1.035596	-1.294558	-7.270099
H	-2.742059	-0.929708	-6.837390
Zn	0.120298	0.710400	-2.217871
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Br	1.425669	2.515258	-1.618582

G1_{TS}; COSMO



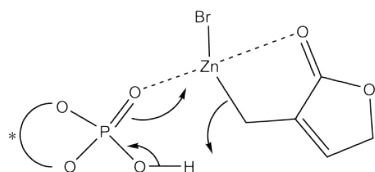
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C	3.7291513	3.2435920	1.2090576
C	1.5812755	4.4301300	1.4465436
C	2.2848708	5.6606716	1.2776018
C	0.1570576	4.4083118	1.5244368
H	-0.3942964	5.3578861	1.4415370
C	-0.5523749	3.2168309	1.6165987
C	2.6126186	-1.5714100	0.5491645
C	3.7183514	-1.8123794	1.3568232
H	4.3243127	-2.7145320	1.1808895
C	4.0958338	-0.9196035	2.4008839
C	5.1813357	-1.2203849	3.2774525
C	3.3753141	0.3193985	2.5709509
C	3.7493498	1.1801342	3.6464209
C	2.2816105	0.6250673	1.6815203
C	1.8758009	-0.3713893	0.7828808
O	-0.4867137	0.8420995	2.0080743
O	0.7168320	-0.1858990	0.0120277
P	-0.7065739	-0.2486388	0.8308378
O	-1.8276699	0.1311026	-0.1652150
H	-2.4618490	-0.8908315	-0.4071872
O	-0.9556462	-1.5967288	1.5382847
C	3.6579462	5.6790200	1.0824888
C	4.3799273	4.4573261	1.0301622
H	1.7085941	6.5991080	1.2864672
H	4.1857011	6.6355170	0.9484682
H	4.3022886	2.3079441	1.1565000
H	5.4641886	4.4702964	0.8410854
C	4.7990264	0.8500297	4.4926261
C	5.5306174	-0.3530854	4.3018699
H	3.1839474	2.1084373	3.8094848
H	5.0625113	1.5239630	5.3219316
H	6.3652351	-0.5998549	4.9755253
H	5.7302474	-2.1636737	3.1303714
C	-2.5322577	3.2667546	0.0718937
C	-2.0239608	3.0781522	1.3913810
C	-3.8712446	2.9207699	-0.1833102
C	-2.8734227	2.5859118	2.4191764
C	-4.2048328	2.2604071	2.1070196
C	-4.7187873	2.3939244	0.8053698
H	-4.2617346	3.0254712	-1.2087765
C	-2.3851826	2.4355200	3.8583024
H	-4.8541289	1.8730779	2.9061921
C	-2.6947078	1.0519372	4.4556908
H	-2.2380006	0.9533703	5.4619031

H	-2.2950859	0.2384611	3.8183552
H	-3.7858149	0.8878083	4.5743396
C	-2.9529731	3.5668657	4.7373850
H	-1.2816693	2.5543617	3.8534375
H	-2.5662078	3.4946231	5.7752999
H	-4.0611305	3.5162830	4.7833666
H	-2.6792295	4.5636521	4.3356683
C	-6.1106986	1.9033295	0.4253477
C	-6.0153323	0.4653097	-0.1281082
H	-5.3346068	0.4159965	-1.0017808
H	-7.0132924	0.0950365	-0.4434521
H	-5.6281280	-0.2264698	0.6513822
C	-7.1408087	1.9952167	1.5590375
H	-6.4629691	2.5528288	-0.4069648
H	-6.9103682	1.2858134	2.3813245
H	-8.1518732	1.7365142	1.1842696
H	-7.1849154	3.0149257	1.9929276
C	-1.6802365	3.7807894	-1.0909140
C	-1.5444076	2.7464430	-2.2237446
H	-0.9036719	3.1471819	-3.0365619
H	-2.5248923	2.4774899	-2.6660478
H	-1.0908925	1.8072834	-1.8528413
C	-2.2177045	5.1252645	-1.6152767
H	-0.6580628	3.9701205	-0.7089967
H	-2.2729397	5.8825490	-0.8062554
H	-3.2367366	5.0164707	-2.0419344
H	-1.5610650	5.5239044	-2.4163330
H	1.2054119	-6.0450505	-3.6238781
H	4.7298403	-1.3495717	-3.8996793
H	2.0027121	-6.0129422	1.0435754
C	1.7113921	-5.1372218	-4.0195679
H	1.7183744	0.4364443	-2.2931291
H	-0.2007067	-4.2841629	-4.6965999
H	-1.0435946	-3.9750802	0.0770626
C	1.8955111	-4.1882565	-2.8409747
C	4.8792252	-0.9917892	-2.8597001
C	0.7989802	-4.5365273	-5.1040540
H	0.6544614	-5.2522439	-5.9392991
C	2.5643006	-2.9584986	-2.9882752
C	1.8854315	-5.0803559	1.6343831
H	3.6141188	-4.7192093	-5.0445946
C	1.4030966	-4.5173179	-1.5665666
C	3.0635696	-5.5786807	-4.6080156
H	3.7115081	-6.0340809	-3.8322322
H	0.8665991	-5.4716330	-1.4415972
C	2.6638084	0.2595986	-2.8437790
H	5.4410188	-0.0371634	-2.9194068
H	5.5157517	-1.7331064	-2.3354726
C	2.7871021	-2.0917875	-1.9023784
C	-0.4484739	-4.6116375	0.7722669
C	1.5722610	-3.6705965	-0.4520552
H	1.4513796	-5.3501450	2.6191556
H	2.8966726	-4.6631453	1.8108060
C	3.5437609	-0.7818675	-2.1258930
C	2.2952073	-2.4607533	-0.6174545
C	0.9858915	-4.0701110	0.8990483
H	2.4115380	-0.0737871	-3.8729673
H	-0.4885280	-5.6355143	0.3473540
H	3.1954856	1.2296016	-2.9298230
H	1.2378474	-3.6101980	-5.5311875
H	-0.9513870	-4.6488398	1.7597434
H	2.9159731	-6.3245123	-5.4160176
H	3.7891473	-0.3657740	-1.1277884
H	0.9300660	-3.1519693	1.5169550
H	2.9463491	-2.6712629	-3.9808556
C	-1.1665148	-2.0728181	-2.7922098
C	-2.3496635	-1.6400786	-2.2946988
C	-2.7979425	-0.4892917	-3.1353816
O	-1.8637196	-0.2817377	-4.1194438
C	-0.8006006	-1.2305576	-3.9726907
O	-3.7972497	0.1953389	-3.0263525

C	-3.1265396	-2.0153007	-1.0825343
H	-3.2140195	-3.1283909	-1.0408974
H	-0.5164947	-2.8696417	-2.4025672
H	0.1541872	-0.6831896	-3.8101798
H	-0.6976356	-1.8082322	-4.9179158
Zn	-2.6235251	-2.4965338	0.9589070
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Br	-4.0704849	-3.6027146	2.3468052

G1_{TS}



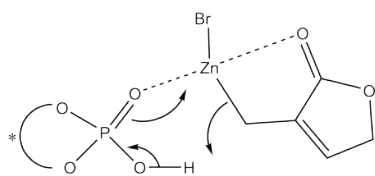
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C	3.7308379	3.2549980	1.2117448
C	1.5788150	4.4328124	1.4510076
C	2.2790172	5.6655837	1.2882987
C	0.1549401	4.4055968	1.5285522
H	-0.4004718	5.3531827	1.4501410
C	-0.5518040	3.2121660	1.6147610
C	2.6214279	-1.5708688	0.5473675
C	3.7277109	-1.8086245	1.3547642
H	4.3333087	-2.7112443	1.1798535
C	4.1053815	-0.9133667	2.3962271
C	5.1910319	-1.2103748	3.2731847
C	3.3829670	0.3245988	2.5640761
C	3.7553757	1.1866950	3.6387776
C	2.2897624	0.6287649	1.6734388
C	1.8850314	-0.3693465	0.7758543
O	-0.4765930	0.8363893	1.9940174
O	0.7309483	-0.1853449	-0.0004084
P	-0.6994145	-0.2442481	0.8080460
O	-1.8099153	0.1537065	-0.1927377
H	-2.4648042	-0.8550955	-0.4281787
O	-0.9645588	-1.5952714	1.5014290
C	3.6518353	5.6898490	1.0956928
C	4.3777256	4.4713536	1.0396681
H	1.6994463	6.6019402	1.3001334
H	4.1762513	6.6488019	0.9667233
H	4.3063915	2.3210002	1.1571202
H	5.4623329	4.4886985	0.8531556
C	4.8054389	0.8598837	4.4850316
C	5.5391120	-0.3415539	4.2959853
H	3.1877532	2.1138947	3.7993862
H	5.0673240	1.5354036	5.3134803
H	6.3740401	-0.5862587	4.9699223
H	5.7409548	-2.1533527	3.1278447
C	-2.5336149	3.2711235	0.0728264
C	-2.0228911	3.0705321	1.3896205
C	-3.8711286	2.9217606	-0.1841807
C	-2.8687769	2.5634150	2.4130829
C	-4.1992272	2.2371834	2.0992194
C	-4.7160125	2.3837937	0.8003522
H	-4.2627554	3.0342594	-1.2082618
C	-2.3797702	2.4014803	3.8508121
H	-4.8466077	1.8408866	2.8954334
C	-2.6836728	1.0116658	4.4362776
H	-2.2291082	0.9065086	5.4427208

H	-2.2786617	0.2044505	3.7947301
H	-3.7739091	0.8402868	4.5517838
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H	-1.2766522	2.5245590	3.8471752
H	-2.5658012	3.4442065	5.7769949
H	-4.0595819	3.4691291	4.7840058
H	-2.6821541	4.5242524	4.3457844
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H	-5.6367357	-0.2336052	0.6183601
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H	-8.1494640	1.7337663	1.1849362
H	-7.1729285	2.9963081	2.0064302
C	-1.6864817	3.8028659	-1.0856116
C	-1.5440753	2.7823741	-2.2300602
H	-0.9088129	3.1975968	-3.0397606
H	-2.5217469	2.5075421	-2.6747383
H	-1.0800591	1.8439708	-1.8704307
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H	-0.6651809	3.9960642	-0.7030677
H	-2.2971655	5.8966029	-0.7770110
H	-3.2526754	5.0375152	-2.0220381
H	-1.5819454	5.5621924	-2.3911881
H	1.1865376	-6.0519858	-3.6079378
H	4.7396484	-1.3753796	-3.9000273
H	2.0379946	-5.9916762	1.0747837
C	1.7005233	-5.1497098	-4.0065767
H	1.7286721	0.4260768	-2.3072577
H	-0.2027390	-4.2826354	-4.6908705
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C	1.8902101	-4.1974661	-2.8314484
C	4.8873118	-1.0124060	-2.8616027
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H	0.6443044	-5.2653034	-5.9278134
C	2.5635894	-2.9713868	-2.9839411
C	1.9041097	-5.0560436	1.6571965
H	3.6092732	-4.7523945	-5.0282819
C	1.3999185	-4.5203769	-1.5550595
C	3.0500599	-5.6052330	-4.5899750
H	3.6925815	-6.0614760	-3.8105355
H	0.8603795	-5.4723211	-1.4256914
C	2.6747416	0.2447632	-2.8550433
H	5.4524411	-0.0601276	-2.9262490
H	5.5210249	-1.7529616	-2.3332528
C	2.7915448	-2.1022248	-1.9014799
C	-0.4363049	-4.6288846	0.7894933
C	1.5743698	-3.6719464	-0.4429836
H	1.4716107	-5.3247291	2.6428955
H	2.9083016	-4.6228207	1.8341900
C	3.5512970	-0.7951895	-2.1311650
C	2.3012440	-2.4652039	-0.6145607
C	0.9906168	-4.0663964	0.9110906
H	2.4232956	-0.0923118	-3.8832378
H	-0.4584283	-5.6604995	0.3816209
H	3.2077049	1.2136421	-2.9448879
H	1.2421799	-3.6273340	-5.5271766
H	-0.9417069	-4.6563900	1.7758731
H	2.8997138	-6.3533192	-5.3953246
H	3.7963656	-0.3746410	-1.1348790
H	0.9205497	-3.1426921	1.5193545
H	2.9454409	-2.6888744	-3.9779831
C	-1.1887009	-2.0699791	-2.8015463
C	-2.3649304	-1.6217095	-2.3026263
C	-2.7971073	-0.4572785	-3.1374373
O	-1.8599334	-0.2631123	-4.1235948
C	-0.8125964	-1.2255665	-3.9791349
O	-3.7816683	0.2427043	-3.0168779

C	-3.1464988	-1.9829520	-1.0900705
H	-3.2211523	-3.0959399	-1.0271911
H	-0.5467230	-2.8739209	-2.4129797
H	0.1507543	-0.6940988	-3.8119802
H	-0.7145303	-1.8018471	-4.9264521
Zn	-2.6891127	-2.4182941	0.9772467
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Br	-4.1176678	-3.5421014	2.3510580

G2_{TS}; COSMO



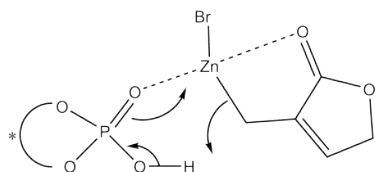
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C	2.5288868	2.9386172	0.6930187
C	3.9235857	3.0591624	0.4099422
C	1.7591948	4.1472115	0.8483824
C	2.4163546	5.4126535	0.7776930
C	0.3551460	4.0540590	1.0500943
H	-0.2219067	4.9784637	1.2054509
C	-0.3207447	2.8370841	1.0351844
C	3.0839880	-1.7874133	-0.3469512
C	4.1797556	-1.9718157	0.4903810
H	4.8025467	-2.8703899	0.3639869
C	4.4960671	-1.0599819	1.5376943
C	5.5718271	-1.3170569	2.4404920
C	3.6998119	0.1310244	1.7130098
C	3.9854723	0.9811939	2.8231899
C	2.6333310	0.3940457	0.7778543
C	2.3354741	-0.5856493	-0.1689993
O	-0.2201840	0.4290786	0.9074373
O	1.2566067	-0.3607890	-1.0356418
P	-0.2372897	-0.5396899	-0.4153442
O	-1.1819809	0.0153316	-1.5355902
H	-2.0577612	-0.6908535	-1.6070138
O	-0.5862747	-1.9492267	0.0536454
C	3.7776141	5.4930160	0.5275445
C	4.5306633	4.3046285	0.3272961
H	1.8151099	6.3256891	0.9113183
H	4.2735800	6.4737261	0.4679364
H	4.5188820	2.1511961	0.2423119
H	5.6052284	4.3711416	0.0984578
C	5.0279128	0.6929660	3.6936928
C	5.8385566	-0.4569559	3.4952036
H	3.3617118	1.8699218	2.9930909
H	5.2240425	1.3589794	4.5477858
H	6.6668270	-0.6704703	4.1878693
H	6.1779297	-2.2241329	2.2900993
C	-2.6457943	3.3017968	0.1731388
C	-1.8083452	2.8530790	1.2291381
C	-3.9967996	3.5867946	0.4555799
C	-2.3566970	2.6017358	2.5172535
C	-3.7149302	2.8953238	2.7446577
C	-4.5456368	3.4263306	1.7386572
H	-4.6434377	3.9729385	-0.3495479
C	-1.5077472	2.0296736	3.6505183
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C	-1.8959522	0.5665187	3.9383798
H	-1.2288970	0.1277231	4.7086277
H	-1.8161282	-0.0563529	3.0257271

H	-2.9363069	0.4924025	4.3205978
C	-1.5593543	2.8928596	4.9222773
H	-0.4531650	2.0253178	3.3067884
H	-0.8700128	2.4902167	5.6924825
H	-2.5756981	2.9117991	5.3680717
H	-1.2639780	3.9404760	4.7102569
C	-5.9828499	3.8445629	2.0310467
C	-6.8821373	2.6518982	2.4003639
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H	-7.9200947	2.9883960	2.6007207
H	-6.5179775	2.1366840	3.3140439
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H	-5.6727462	4.5567721	4.0909471
H	-7.0773644	5.2941773	3.2618778
H	-5.4094428	5.8089101	2.8382490
C	-2.1126958	3.5037011	-1.2444729
C	-2.9797511	2.7823853	-2.2906715
H	-2.5093042	2.8477829	-3.2927872
H	-3.9930026	3.2281916	-2.3700213
H	-3.0882295	1.7106630	-2.0380743
C	-1.9596960	4.9968082	-1.5882729
H	-1.1047340	3.0414994	-1.2858964
H	-1.2729259	5.5098094	-0.8860360
H	-2.9387572	5.5185206	-1.5430709
H	-1.5550597	5.1236311	-2.6136019
H	0.8979956	-6.5423156	-3.7864120
H	4.5359675	-1.9855384	-4.8805870
H	3.0266345	-6.4532303	0.2955799
C	1.4199078	-5.7344518	-4.3442867
H	1.3379150	-0.2422604	-3.6190004
H	-0.4562659	-4.7203420	-4.8478343
H	-0.0794971	-4.2261494	0.7352705
C	1.8541787	-4.7034817	-3.3108326
C	4.6523671	-1.3529528	-3.9758337
C	0.4212784	-5.1599703	-5.3629297
H	0.0606618	-5.9562043	-6.0465564
C	2.3420257	-3.4422997	-3.6938449
C	3.1749426	-5.5138763	0.8684501
H	3.2084824	-5.5899331	-5.6120152
C	1.7950733	-4.9931263	-1.9386516
C	2.6425219	-6.3583215	-5.0437343
H	3.3391184	-6.8134123	-4.3106013
H	1.4006205	-5.9729272	-1.6272483
C	2.2970065	-0.3995177	-4.1501476
H	5.0798043	-0.3802527	-4.2971167
H	5.3884223	-1.8502842	-3.3117931
C	2.7490207	-2.4800388	-2.7540567
C	0.6932684	-4.9972949	0.9105730
C	2.1874288	-4.0700854	-0.9519817
H	3.1456303	-5.7681304	1.9484432
H	4.1918367	-5.1397995	0.6311840
C	3.3039932	-1.1487419	-3.2594156
C	2.6725372	-2.7970402	-1.3684264
C	2.0877197	-4.4786674	0.5190016
H	2.0857911	-0.9574171	-5.0862444
H	0.4027965	-5.9012204	0.3378133
H	2.6979491	0.5938632	-4.4401896
H	0.8861888	-4.3722250	-5.9924369
H	0.6738352	-5.2620625	1.9879671
H	2.3312735	-7.1471214	-5.7600899
H	3.5062189	-0.5044374	-2.3798125
H	2.2754907	-3.5759498	1.1345753
H	2.4084163	-3.1955881	-4.7655013
C	-4.7180912	-0.0013992	0.3278370
C	-4.0624327	-1.0584739	-0.2252120
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O	-4.3931024	-1.5843984	2.0222098
C	-4.9629958	-0.2800407	1.7758204
O	-3.2070004	-3.0820674	0.8088342
C	-3.4800345	-1.3841629	-1.5423685

H	-3.6534003	-0.5912181	-2.2968413
H	-5.0254506	0.9319021	-0.1620217
H	-4.4546573	0.4461982	2.4463037
H	-6.0385256	-0.3093350	2.0529426
Zn	-2.0406643	-2.9624960	-0.9702783
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Br	-1.8550824	-4.9485040	-2.1464437

G2TS



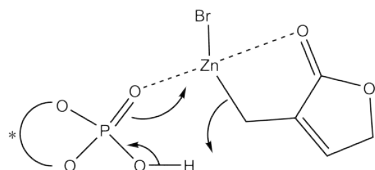
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C	3.9225851	3.0547667	0.4197824
C	1.7578886	4.1446365	0.8482381
C	2.4160362	5.4089177	0.7758851
C	0.3535915	4.0517279	1.0460467
H	-0.2253761	4.9756818	1.1973791
C	-0.3219803	2.8348576	1.0333023
C	3.0840317	-1.7891027	-0.3402230
C	4.1780125	-1.9738940	0.4990974
H	4.7994337	-2.8732748	0.3718337
C	4.4936124	-1.0633591	1.5474733
C	5.5680610	-1.3203257	2.4511522
C	3.6984248	0.1282824	1.7222178
C	3.9851388	0.9788939	2.8314342
C	2.6321992	0.3911843	0.7870294
C	2.3349939	-0.5878918	-0.1605680
O	-0.2242136	0.4279152	0.9128504
O	1.2554698	-0.3626230	-1.0256706
P	-0.2365227	-0.5510732	-0.4041811
O	-1.1821917	0.0045167	-1.5270774
H	-2.0402322	-0.6988422	-1.6018807
O	-0.5827212	-1.9579303	0.0665210
C	3.7776172	5.4882499	0.5301981
C	4.5303094	4.2993357	0.3359885
H	1.8145831	6.3225506	0.9044602
H	4.2739655	6.4686281	0.4693342
H	4.5169652	2.1454331	0.2572800
H	5.6056387	4.3644538	0.1106557
C	5.0271642	0.6907147	3.7017995
C	5.8358737	-0.4600758	3.5048090
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H	5.2242501	1.3577043	4.5548576
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H	6.1726972	-2.2285281	2.3017966
C	-2.6466071	3.2924412	0.1664513
C	-1.8095623	2.8524272	1.2260912
C	-3.9974727	3.5791615	0.4466723
C	-2.3577988	2.6109521	2.5159520
C	-3.7162816	2.9047186	2.7402089
C	-4.5469744	3.4270362	1.7301054
H	-4.6433265	3.9602779	-0.3615408
C	-1.5076160	2.0495290	3.6536365
H	-4.1290964	2.7528718	3.7509447
C	-1.8902347	0.5873518	3.9528280
H	-1.2216080	0.1567133	4.7261492
H	-1.8081262	-0.0433994	3.0460788

H	-2.9298873	0.5113518	4.3366026
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H	-0.4533014	2.0459406	3.3092491
H	-0.8706437	2.5293377	5.6918330
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H	-1.2693369	3.9698665	4.6979085
C	-5.9850550	3.8450210	2.0185919
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H	-6.9213991	1.9026939	1.5818693
H	-7.9218313	2.9879863	2.5933138
H	-6.5179947	2.1464699	3.3142854
C	-6.0426568	4.9472245	3.0919399
H	-6.3871688	4.2761762	1.0754294
H	-5.6776433	4.5760688	4.0722552
H	-7.0832250	5.3037165	3.2370485
H	-5.4158136	5.8164755	2.8094821
C	-2.1128474	3.4823214	-1.2525349
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H	-2.5077051	2.8074492	-3.2950024
H	-3.9920137	3.1991313	-2.3791795
H	-3.0887881	1.6834385	-2.0312319
C	-1.9578617	4.9722279	-1.6082545
H	-1.1055780	3.0184937	-1.2897120
H	-1.2695190	5.4895495	-0.9109599
H	-2.9355027	5.4967693	-1.5666307
H	-1.5534364	5.0908158	-2.6345187
H	0.8641359	-6.5105268	-3.7985697
H	4.5368825	-1.9741243	-4.8710596
H	3.0232942	-6.4653057	0.2651201
C	1.3950388	-5.7065498	-4.3534932
H	1.3444357	-0.2217924	-3.6064246
H	-0.4709959	-4.6720646	-4.8502446
H	-0.0684892	-4.2251472	0.7563670
C	1.8404586	-4.6850199	-3.3157338
C	4.6548216	-1.3448097	-3.9643965
C	0.4012234	-5.1179969	-5.3684545
H	0.0315335	-5.9079187	-6.0544133
C	2.3332551	-3.4244073	-3.6925952
C	3.1798918	-5.5319927	0.8452251
C	3.1857331	-5.5752243	-5.6197349
H	1.7862210	-4.9831112	-1.9454981
C	2.6113970	-6.3398920	-5.0550011
H	3.3038040	-6.8041996	-4.3239062
H	1.3867850	-5.9622657	-1.6389949
C	2.3037534	-0.3803610	-4.1363492
H	5.0872634	-0.3732581	-4.2825196
H	5.3879411	-1.8484786	-3.3022012
C	2.7469400	-2.4695969	-2.7489982
C	0.7008044	-5.0036355	0.9119940
C	2.1868563	-4.0688908	-0.9544811
H	3.1587351	-5.7964901	1.9229178
H	4.1967483	-5.1614949	0.6020067
C	3.3067305	-1.1379953	-3.2484117
C	2.6732137	-2.7946620	-1.3652096
C	2.0946968	-4.4888102	0.5138296
H	2.0905751	-0.9327848	-5.0751071
H	0.3966802	-5.8973863	0.3307856
H	2.7085965	0.6126826	-4.4220623
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H	0.6892353	-5.2818112	1.9860271
H	2.2931095	-7.1225196	-5.7749538
H	3.5112344	-0.4980877	-2.3659423
H	2.2915939	-3.5925801	1.1361014
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C	-4.6978881	-0.0183093	0.3283369
C	-4.0537550	-1.0839839	-0.2219457
C	-3.8315456	-2.0385708	0.8899637
O	-4.3751148	-1.5910844	2.0335083
C	-4.9333890	-0.2855286	1.7811035
O	-3.1989060	-3.1013814	0.8247714
C	-3.4772002	-1.4226940	-1.5357122

H	-3.6513959	-0.6386644	-2.2992171
H	-4.9989150	0.9154393	-0.1644091
H	-4.4143213	0.4420953	2.4420411
H	-6.0074996	-0.3006625	2.0672025
Zn	-2.0261895	-3.0022652	-0.9532957
H	-3.9641753	-2.3325119	-1.9588116
Br	-1.8442531	-4.9597774	-2.1610738

G3_{TS}; woelfling data



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C	2.051766	2.031024	0.965549
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C	4.074546	3.521494	0.860391
C	1.825884	4.501100	1.125044
C	2.433299	5.792509	1.155439
C	0.410395	4.348709	1.188768
H	-0.212822	5.245915	1.324196
C	-0.211207	3.111598	1.043936
C	3.286358	-1.498063	0.000261
C	4.242899	-1.720670	0.984264
H	4.786166	-2.676378	0.990694
C	4.503075	-0.781141	2.021971
C	5.440166	-1.081293	3.055287
C	3.769469	0.462403	2.074086
C	3.962344	1.312881	3.203600
C	2.854030	0.767264	1.000199
C	2.668442	-0.209379	0.019489
O	0.028398	0.734016	0.774676
O	1.763420	0.086227	-1.018742
P	0.227262	-0.137821	-0.586394
O	-0.499802	0.595825	-1.814135
H	-1.417805	0.243138	-1.909620
O	-0.182638	-1.558294	-0.278891
C	3.806285	5.939266	1.029654
C	4.629755	4.793159	0.869808
H	1.784302	6.676070	1.260795
H	4.259093	6.942365	1.039764
H	4.719086	2.641117	0.727878
H	5.716706	4.913844	0.745386
C	4.871487	0.982757	4.199418
C	5.630378	-0.214690	4.119779
H	3.376028	2.238254	3.285577
H	5.000173	1.653593	5.062376
H	6.353241	-0.461596	4.912024
H	5.996942	-2.029649	2.997144
C	-2.469729	3.444390	-0.069225
C	-1.708180	2.966038	1.033501
C	-3.875462	3.347915	-0.016788
C	-2.378339	2.379314	2.147693
C	-3.783054	2.300589	2.139789
C	-4.561166	2.793733	1.075519
H	-4.467959	3.735520	-0.861702
C	-1.607786	1.935092	3.390777
H	-4.287804	1.842988	3.003237
C	-2.139242	0.636271	4.014560
H	-1.462057	0.296867	4.824683
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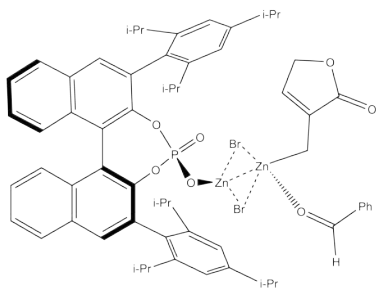
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H	-1.123898	4.001672	3.993143
C	-6.089802	2.758545	1.090724
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H	-7.766524	1.363546	0.875281
H	-6.302883	0.635018	1.623962
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H	-6.423693	3.393205	0.239581
H	-6.396711	2.775735	3.270848
H	-7.790516	3.359294	2.322177
H	-6.347547	4.409285	2.531244
C	-1.828601	4.106000	-1.289286
C	-2.336768	3.522083	-2.618791
H	-1.786549	3.965151	-3.473815
H	-3.414758	3.730396	-2.778138
H	-2.194480	2.424840	-2.658289
C	-2.042077	5.632369	-1.255439
H	-0.736632	3.914753	-1.243825
H	-1.641888	6.082656	-0.325204
H	-3.123441	5.879638	-1.300357
H	-1.544992	6.124988	-2.116676
H	0.872504	-6.408148	-3.052695
H	5.043814	-2.469253	-4.360862
H	2.885258	-5.813430	1.303378
C	1.441507	-5.690625	-3.684494
H	2.084720	-0.133302	-3.590464
H	-0.397184	-4.660544	-4.312756
H	-0.336988	-4.051480	0.595780
C	1.929414	-4.587892	-2.752700
C	5.196338	-1.764886	-3.516411
C	0.477827	-5.170257	-4.764486
H	0.102898	-6.006103	-5.391128
C	2.603894	-3.449294	-3.223597
C	2.858466	-4.797071	1.749243
H	3.233119	-5.800723	-4.954125
C	1.728533	-4.694345	-1.369595
C	2.622819	-6.460203	-4.302369
H	3.290682	-6.864312	-3.515307
H	1.186913	-5.574123	-0.990469
C	3.039216	-0.505348	-4.010364
H	5.805284	-0.916279	-3.890717
H	5.783693	-2.298203	-2.741891
C	3.068305	-2.442714	-2.355926
C	0.428080	-4.552037	1.214524
C	2.158755	-3.717053	-0.454303
H	2.586436	-4.905434	2.819505
H	3.883411	-4.383630	1.698327
C	3.849564	-1.273977	-2.952001
C	2.848006	-2.570788	-0.955461
C	1.816977	-3.924393	1.022114
H	2.802245	-1.143756	-4.886889
H	0.420593	-5.633199	0.963314
H	3.612964	0.367518	-4.384343
H	0.976055	-4.446352	-5.442703
H	0.095316	-4.458010	2.265830
H	2.264773	-7.309364	-4.920894
H	4.081624	-0.564222	-2.131524
H	1.796670	-2.924382	1.503775
H	2.784261	-3.339679	-4.305069
C	-5.194228	-2.536225	-2.007869
C	-4.373799	-1.667231	-1.363893
C	-5.000025	-1.376057	-0.040483
O	-6.189017	-2.032335	0.057100
C	-6.361096	-2.843861	-1.115120
O	-4.515269	-0.703099	0.853679
C	-3.025000	-1.121583	-1.563141
H	-3.069955	-0.011680	-1.439819

H	-5.043719	-2.996424	-2.994212
H	-7.351773	-2.617999	-1.566866
H	-6.372356	-3.909428	-0.788567
Zn	-2.197054	-1.856296	0.154971
H	-2.550445	-1.414925	-2.520563
Br	-2.586054	-3.026530	2.108121

6 Structures of the proposal in the main text of the paper

6.1 Educt Complexes 14

14 α -ma



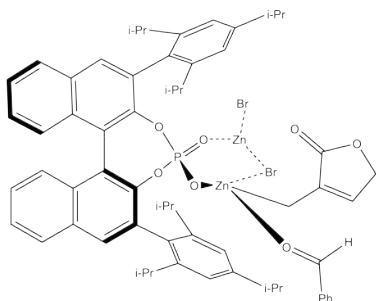
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C	0.2118237	-0.3317098	89.0266963
C	0.9534342	-1.5515135	89.0527293
C	-1.1396659	-0.3466495	89.5336906
C	-1.7061626	-1.5799602	89.9743585
C	-1.8714979	0.8724262	89.6203282
H	-2.9060510	0.8449346	89.9948306
C	-1.3054240	2.0932055	89.2777171
C	4.3931870	1.9900772	87.8753345
C	4.7537007	1.1265264	86.8485897
H	5.7833892	1.1505910	86.4609937
C	3.8173807	0.2321276	86.2527829
C	4.1850998	-0.5852945	85.1422589
C	2.4632620	0.1740313	86.7515587
C	1.5260699	-0.6548050	86.0646238
C	2.1065309	0.9792938	87.8949360
C	3.0610404	1.8771009	88.3832759
O	0.5206687	3.2948778	88.2968515
O	2.7152415	2.7012744	89.4471637
P	1.8077710	4.0206972	89.0495280
O	1.3517034	4.5321698	90.4638122
O	2.4112096	5.0075186	88.0964556
C	-0.9672559	-2.7529354	89.9565722
C	0.3792000	-2.7309131	89.5060493
H	-2.7426335	-1.5767952	90.3472095
H	-1.4148584	-3.6957061	90.3062501
H	1.9992482	-1.5479906	88.7158973
H	0.9761426	-3.6556251	89.5212869
C	1.9123365	-1.4232682	84.9751897
C	3.2562128	-1.4030426	84.5170109
H	0.4812517	-0.6732918	86.4040917
H	1.1681749	-2.0496786	84.4599196
H	3.5534552	-2.0233403	83.6577216
H	5.2244293	-0.5403707	84.7801668
C	-2.0152963	4.0416109	90.7301200
C	-2.0114686	3.4037229	89.4551496
C	-2.6094581	5.3094317	90.8414226
C	-2.6191607	4.0362623	88.3418533
C	-3.2141135	5.3028508	88.5122655
C	-3.2118574	5.9649488	89.7487664
H	-2.5963001	5.8219673	91.8156630
C	-2.6466899	3.3796002	86.9631943
H	-3.6734122	5.7891429	87.6388655
C	-1.8484486	4.1911834	85.9279927
H	-2.2818903	5.2023839	85.7784491
H	-1.8456517	3.6773693	84.9440007

H	-0.7997797	4.3217552	86.2563497
C	-4.0893734	3.1190894	86.4936431
H	-2.1524190	2.3903169	87.0554915
H	-4.6509182	4.0667104	86.3560531
H	-4.6469657	2.5036949	87.2285328
H	-4.0956154	2.5842842	85.5212404
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C	7.8040494	6.1334915	90.2360454
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H	4.1564486	5.9452975	85.0555960
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C	4.7687867	2.0095940	91.9310814
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C	4.6653858	5.8705645	86.0400455
C	5.6413431	4.1887015	87.7036830
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H	7.0927891	4.6226199	85.3370414
C	5.4879383	1.6347617	90.6225358
C	5.3147071	3.0216032	88.4508625
C	5.1234829	4.4210777	86.2839700
H	3.8528022	2.5958360	91.7223591
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H	5.4219935	2.6102904	92.5981651
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H	9.0617486	4.8797066	91.5359439
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H	7.0014900	3.7434382	91.3506069
Zn	1.3981211	6.4014150	90.7071800
Br	-0.0625632	8.0130488	91.7432111
C	3.2196303	10.1804621	84.3708982
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C	3.4037506	9.4725757	85.5739122
C	1.4490451	11.4902787	85.3867918
C	1.6213253	10.7785891	86.5979974

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H	0.6678955	12.2633802	85.3207937
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H	2.0942425	11.7261438	83.3290914
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Br	3.1959255	7.9065379	89.9954709
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H	1.4225215	5.6972315	86.1704095
C	0.0881797	7.3425655	86.7348211
C	-0.2305091	7.2086344	88.1664797
C	-0.4368893	8.4917185	85.9456077
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H	0.3804789	6.5448258	83.7593134
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14β-ma



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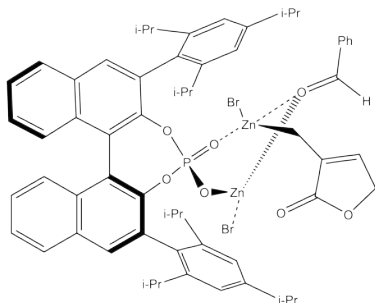
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H	5.9757486	0.3655762	88.1784602
C	4.2761232	-0.8614483	88.7783340
C	4.8615552	-2.0941544	88.3615692
C	2.9651938	-0.8728313	89.3822504
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O	2.5022780	2.7858248	89.8371830
P	1.2024812	3.3038011	88.9610550
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O	1.5343547	3.5653621	87.4865170
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H	0.1988992	-2.1593297	95.2152119
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C	4.1783192	-3.2923370	88.5011069
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H	4.6394702	-4.2349026	88.1692918
H	5.8669031	-2.0720967	87.9123577
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C	-3.0225924	3.4232803	93.5385373
H	-1.0543763	2.9364460	92.8192466
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H	3.0085927	3.6264995	84.7169215
C	6.4235690	5.3937537	88.4763784
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C	6.3537115	4.7433125	89.7206868
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C	5.8111989	4.7747659	87.3777293
C	8.6088749	6.6679723	88.6623905
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H	5.8449258	5.2879410	86.4041199
C	5.7512406	3.8280208	92.4324276
H	6.7592827	1.2743887	92.3567776
H	6.7152965	1.0132818	90.5836089
C	5.6974771	3.5131871	89.8876399
C	3.8176347	4.0396891	85.3504784
C	5.1266627	3.5482534	87.4892473
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H	6.7528119	4.2999446	92.5117781
H	5.3259765	7.8876375	88.9418248
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H	3.4484971	2.2041993	97.2922941
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Br	2.5909221	6.8023726	88.2514768
Zn	1.2760784	6.1659384	90.4330656
H	5.1074723	7.9753535	92.5983962
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C	4.2233451	8.5965158	92.8765798
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P	1.6371681	3.0267048	88.1854510
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H	0.3991084	-2.3983097	88.9138868
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C	-5.2020198	5.1190813	85.3261714
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C	5.9698936	5.8312952	86.1782756
H	5.0038084	3.1823672	91.9047647
H	4.8419833	7.7238824	86.1941406
H	2.6552392	0.3122126	84.1794950
C	5.7499880	4.3945101	86.6320295
C	7.0462889	2.1527672	90.2836620
C	4.7512703	6.6863642	86.5794193
H	4.6461656	6.7438082	87.6843351
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14δ-ma

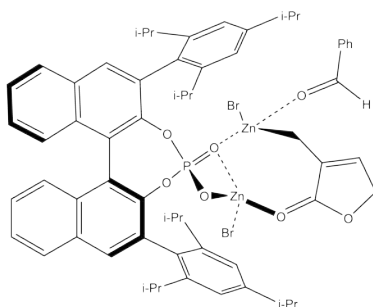


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H	5.5579968	-0.9508561	87.2575920
C	3.6630597	-1.7957780	87.9308328
C	3.9991322	-3.1342933	87.5676521
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C	5.3639993	3.4070539	85.7114257	C	0.6803967	-0.2859589	90.6096087
C	7.2835378	6.4409350	86.6908485	C	1.5151755	-1.3973244	90.9342076
H	7.4294441	7.4615645	86.2807731	C	-0.5301406	-0.0946918	91.3720237
H	5.3054183	3.6825662	84.6489401	C	-0.8722122	-1.0387082	92.3856437
C	4.9724660	3.5123573	90.8461642	C	-1.3666945	1.0229638	91.0895365
H	7.1501279	1.8628954	91.3501540	H	-2.3306619	1.1160626	91.6132968
H	7.4608382	1.3344930	89.6608200	C	-1.0098815	1.9895170	90.1571859
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C	2.9627879	1.0819104	84.9173398	C	4.5791039	-0.0331192	87.2167725
C	4.9783070	2.1136055	86.1064767	H	5.5296390	-0.2529553	86.7081966
H	6.2432864	1.4065642	83.7326439	C	3.5212423	-0.9851166	87.1427551
H	4.7577949	2.2522019	83.1822561	C	3.6459067	-2.1676310	86.3550012
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H	5.0123562	1.4933037	90.1126313	C	-0.0470878	-2.1175858	92.6635536
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H	6.1722386	4.7824970	88.7232895	H	-1.8042724	-0.8855938	92.9519200
Zn	1.5793054	5.9413065	89.2508014	H	-0.3200785	-2.8349538	93.4523637
Br	2.5255563	7.4467010	90.6927456	H	2.4571532	-1.5359236	90.3859075
C	0.5904135	10.2615407	83.7841513	H	1.8276193	-3.1315392	92.1756423
C	1.0906913	7.9868523	87.3427731	C	1.3818191	-2.8248309	86.9403220
C	1.1606134	8.9762847	83.7045792	C	2.6006615	-3.0730896	86.2557589
C	0.3977345	10.0530941	86.1938411	O	0.2813113	-1.5035535	88.2439976
C	0.9667888	8.7587059	86.1186806	H	0.5430847	-3.5299287	86.8365803
C	0.2088766	10.7999949	85.0273965	H	2.7073728	-3.9754725	85.6347551
C	1.3477570	8.2231794	84.8657639	H	4.5875583	-2.3376738	85.8099262
O	1.4721003	6.7919384	87.3872921	C	-1.8716518	4.3774032	90.3487190
H	0.4425896	10.8523647	82.8665515	C	-1.9426106	3.0909340	89.7519100
H	0.0853813	10.4521012	87.1713079	C	-2.7594887	5.3741086	89.9016314
H	1.4602473	8.5508725	82.7349984	C	-2.8968313	2.8189526	88.7312695
H	-0.2414071	11.8022138	85.0805470	C	-3.7639108	3.8507049	88.3282186
H	1.7907323	7.2179899	84.8001549	C	-3.7118995	5.1348744	88.8965274
Br	2.5361308	4.9799131	83.5701187	H	-2.7134156	6.3772069	90.3530520
Zn	1.1684692	4.5862175	85.4425074	C	-2.9605613	1.4592334	88.0347565
H	-1.8562397	8.4097819	83.4903013	H	-4.4993217	3.6430661	87.5355834
H	-1.2215020	3.8094464	85.3558728	C	-2.2188798	1.4918948	86.6851846
C	-1.8459649	6.3016857	84.0820504	H	-2.7156722	2.1877304	85.9766306
C	-2.4140513	7.6823531	84.1251145	H	-2.2044612	0.4867712	86.2160089
H	-1.7798655	5.7017848	83.1638934	H	-1.1659503	1.8185356	86.7889438
C	-1.4226933	5.9363155	85.3265777	C	-4.3973886	0.9376824	87.8705756
C	-0.7910428	4.7116649	85.8347307	H	-2.4273940	0.7317738	88.6800768
C	-1.7031587	7.1009598	86.2171958	H	-4.9870042	1.5553924	87.1614095
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O	-1.4611794	7.2486599	87.4072202	H	-4.3874381	-0.0951877	87.4664718
H	-3.4878200	7.7334349	83.8320053	C	-4.6825210	6.2303439	88.4706972
H	-0.9439769	4.6207991	86.9280418	C	-4.6870699	6.4620594	86.9503896
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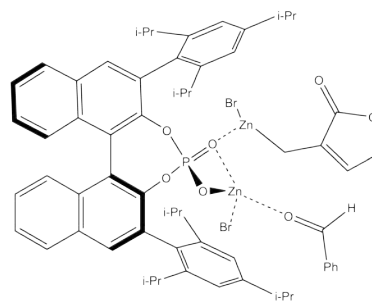
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H	5.1596928	1.9878518	83.6473933
C	8.4600093	5.3914242	88.4357116
H	5.1702237	1.5573231	92.4656924
H	8.5685657	7.3420385	89.4449886
H	3.9263316	4.2066989	84.1764612
C	7.4715291	4.2439881	88.2723338
C	7.2154081	0.6222991	90.7970265
C	7.8858648	6.4694169	89.3750495
H	7.7472297	6.0667880	90.4006122
C	7.1941918	3.3610125	89.3299023
C	5.7642932	2.1026886	84.5705117
H	10.2648692	4.1525429	88.2154916
C	6.7590774	4.0765844	87.0741689
C	9.8469149	4.9173171	88.9008517
H	10.5591219	5.7670575	88.9460311
H	6.9604574	4.7710500	86.2436219
C	5.4292678	2.2383948	91.6285249
H	6.9968185	-0.0695621	91.6369073
H	7.5714446	0.0190966	89.9374046
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C	4.6653164	4.3356979	84.9917545
C	5.7792138	3.0795680	86.9115976
H	5.9776065	1.0886185	84.9613470
H	6.7356110	2.5663948	84.2962115
C	5.9662248	1.4411556	90.4250839
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H	4.0482241	2.4624760	85.8138844
H	7.7357492	3.4761910	90.2826447
Zn	2.2811174	6.2862044	88.5295207
Br	4.0017775	7.7444953	88.0904981
C	1.9525699	10.1181087	82.5221064
C	2.0077208	6.4998103	84.7784098
C	1.5030074	8.9225990	81.9232004
C	2.4609060	8.9244385	84.5760698
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C	2.4292698	10.1198450	83.8441977
C	1.5295206	7.7273252	82.6457661
O	1.5903072	5.4032661	84.3811691
H	1.9304258	11.0572548	81.9477313
H	2.8303570	8.9038049	85.6153238
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H	1.1823843	6.7783185	82.2097148
Br	1.3720820	1.7714094	85.0003277
Zn	0.8256428	3.9187667	85.7475562
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H	-1.7070935	4.4137494	85.6646344
C	-1.3754706	7.1726431	85.1365652
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H	-1.9423416	6.8810885	84.2424035
C	-0.8892736	6.3292873	86.1070252
C	-0.9069719	4.8831602	86.2669299
C	-0.1970849	7.2213160	87.0646748
O	-0.3033981	8.5133011	86.7048364
O	0.4304626	6.9110058	88.0915638
H	-1.9342428	9.2316902	85.6421333
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H	2.4176575	6.6099873	85.8163629



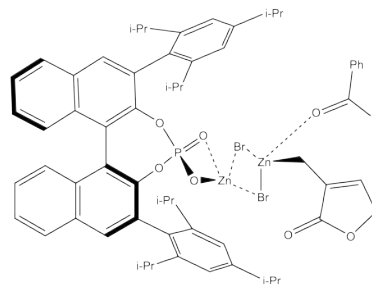
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C	-1.0719812	0.3674814	91.3493082
C	-1.4531694	-0.0132132	92.6709331
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H	-2.8849957	1.5170873	90.9577526
C	-1.5182961	1.6506021	89.2998459
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H	5.2682731	-1.5164311	87.4165750
C	3.3297127	-2.1162502	88.2167344
C	3.5941037	-3.5153323	88.1317227
C	2.0581234	-1.6711114	88.7344694
C	1.0874900	-2.6561506	89.0820129
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C	2.7479868	0.6051714	88.2751080
O	0.0805420	1.6247584	87.5258389
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P	1.3654043	2.5956795	87.2871685
O	1.2342512	4.0849450	87.6185124
O	1.6143805	2.4621828	85.7369342
C	-0.6098436	-0.7729298	93.4664454
C	0.6590410	-1.1722005	92.9694170
H	-2.4300129	0.3237374	93.0519673
H	-0.9139457	-1.0539421	94.4861754
H	2.0395864	-1.1447196	91.3135820
H	1.3406543	-1.7502723	93.6118174
C	1.3690555	-4.0100173	88.9670034
C	2.6373423	-4.4471442	88.5029892
H	0.0957369	-2.3321293	89.4257738
H	0.5976210	-4.7501422	89.2286992
H	2.8512298	-5.5236104	88.4208387
H	4.5714233	-3.8412344	87.7426224
C	-2.5362540	3.9346764	88.9142925
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H	-3.5397723	5.8125622	88.5084810
C	-2.8219279	0.7194960	86.7602908
H	-4.4281485	2.6108356	85.7537507
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H	-3.0989775	1.1643893	84.6048278
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H	-1.4860185	1.5218453	85.2305549
C	-4.0869806	-0.1474286	86.8850297
H	-2.0290063	0.2189626	87.3501077
H	-4.9324132	0.2845410	86.3099491
H	-4.4091019	-0.2377005	87.9423207
H	-3.9003048	-1.1683946	86.4933976
C	-5.1340651	5.2311274	86.3830945
C	-5.4452988	4.8565814	84.9261030
H	-6.0488363	5.6518951	84.4434644

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H	-6.0412001	3.9220865	84.8687678	Zn	0.7849470	1.0412031	84.4118483
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H	-7.1458819	6.0380765	86.7612512	C	0.0204705	5.6011569	82.4142493
H	-6.2267862	5.6422208	88.2531010	H	1.8993690	4.3044371	82.2832449
H	-6.9275884	4.3273750	87.2618813	C	-0.0244741	3.2643387	82.6074453
C	-1.7854271	4.5168447	90.1116607	C	0.2195220	1.8169926	82.6499570
C	-0.9224764	5.7268604	89.7117022	C	-1.4035652	3.8272117	82.7630137
H	-0.3594885	6.1070553	90.5891442	O	-1.3401918	5.2042792	82.6342941
H	-1.5375733	6.5659351	89.3236821	O	-2.4570959	3.2658188	82.9890186
H	-0.1893727	5.4380868	88.9340956	H	0.0846212	6.1389334	81.4408307
C	-2.7465349	4.8591526	91.2642817	H	-0.7040015	1.2654105	82.3802575
H	-1.0896855	3.7367338	90.4815908	H	-2.5059360	4.9475401	85.0405322
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H	7.5440030	4.4509289	84.7824698				
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H	4.6935065	2.9091188	91.4731569				
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H	3.2458168	0.7923317	83.0061486				
C	6.6612320	3.3479053	86.3757572				
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C	6.8665390	5.8590991	86.2649576				
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C	6.4850523	3.0906612	87.7459537				
C	5.3087760	-0.5444318	84.3568353				
H	9.4370160	3.4627547	86.1121548				
C	5.9846998	2.5233973	85.4626255				
C	8.9649268	4.4236222	86.4005381				
H	9.5798672	5.2489790	85.9857767				
H	6.1111817	2.7208169	84.3865593				
C	4.8736858	3.1007855	90.3949456				
H	6.6866761	1.2657467	91.4588748				
H	7.2391289	0.5423475	89.9105925				
C	5.6489697	2.0616122	88.2124361				
C	3.9126128	1.4268382	83.6273562				
C	5.1374572	1.4777522	85.8742855				
H	5.6472760	-1.1741876	85.2023335				
H	6.2144617	-0.1676306	83.8362227				
C	5.4903147	1.8621111	89.7188541				
C	4.9682521	1.2461409	87.2671230				
C	4.4235502	0.6219105	84.8334965				
H	3.9083822	3.3708834	89.9237838				
H	3.3524076	2.3279241	83.9474007				
H	5.5471205	3.9802178	90.3210784				
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H	4.7358545	1.7637909	82.9634579				
H	9.0118669	4.5011910	87.5070204				
H	4.7881254	1.0176394	89.8758836				
H	3.5345172	0.1759430	85.3259717				
H	7.0029448	3.7258506	88.4826069				
Zn	1.4383086	4.5828284	85.5657453				
Br	2.9442869	6.1170177	84.7614712				
C	-1.3526353	9.5352054	86.1554778				
C	-1.5233462	5.3467896	85.3743656				
C	-0.3301289	8.7044246	86.6506408				
C	-2.4754453	7.6135435	85.1882486				
C	-1.4440184	6.7745195	85.6736999				
C	-2.4228096	8.9919382	85.4217888				
C	-0.3688263	7.3285574	86.4075524				
O	-0.5796261	4.5366933	85.4440955				
H	-1.3153799	10.6188662	86.3461679				
H	-3.2962148	7.1716329	84.6027690				
H	0.5008467	9.1334123	87.2296936				
H	-3.2157462	9.6482717	85.0333696				
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Br	1.0210914	-1.0881822	85.3314376				

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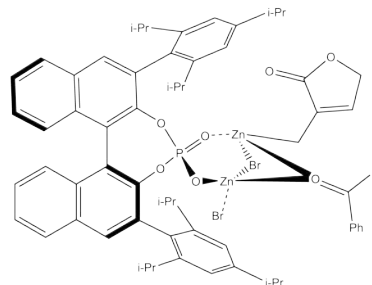


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C	0.3799380	-0.6035051	91.2855115
C	1.1897946	-1.4324618	92.1177502
C	-0.9725575	-0.3208641	91.7057465
C	-1.4687737	-0.9295421	92.8973326
C	-1.7789089	0.5791918	90.9484778
H	-2.8133278	0.7646233	91.2739881
C	-1.2819134	1.2542890	89.8407254
C	4.2110171	0.4378066	88.2313961
C	4.6013261	-0.8785488	88.0220801
H	5.5146312	-1.0821394	87.4420790
C	3.7971940	-1.9745433	88.4492893
C	4.1782427	-3.3183383	88.1566678
C	2.5290374	-1.7235602	89.0959538
C	1.6658752	-2.8367893	89.3287224
C	2.1756964	-0.3635897	89.4369405
C	3.0447683	0.6528395	89.0259650
O	0.5277611	1.6074454	88.3100116
O	2.7760701	1.9698704	89.3867920
P	1.5996446	2.8081658	88.6199486
O	1.0984559	3.8875439	89.6232974
O	1.9886268	3.4892236	87.2980112
C	-0.6634380	-1.7532034	93.6693323
O	0.6815733	-1.9924615	93.2816246
H	-2.5056099	-0.7164810	93.2017898
H	-1.0589431	-2.2088772	94.5898709
H	2.2341808	-1.6171101	91.8289909
H	1.3286698	-2.6223307	93.9109815
C	2.0591640	-4.1303548	89.0140761
C	3.3341177	-4.3801526	88.4421630
H	0.6705945	-2.6632581	89.7585241
H	1.3710093	-4.9681183	89.2043115
H	5.1536432	-3.4922204	87.6755425
C	-2.2899318	3.5752145	89.6439727
C	-2.0356387	2.2947565	89.0691946
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C	-2.4000584	2.0415956	87.7179745

C	-3.0075740	3.0649234	86.9681739	C	0.6532334	11.2275893	80.7901380
C	-3.2624560	4.3338811	87.5069921	C	0.8932699	8.6761375	84.2062263
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C	-3.2627491	2.8630219	85.9181120	C	0.8254052	9.5531757	83.0381197
H	-1.3418292	0.8120923	85.7543714	C	-0.5036993	10.5960887	81.2787322
H	-1.8769259	1.3875788	84.9716644	C	1.9843555	10.2015186	82.5472818
H	-1.1203254	-0.1934589	85.3398269	O	1.9258601	8.5394513	84.9028228
H	-0.3851790	1.3338961	85.9420575	H	0.5880028	11.8827124	79.9078957
C	-3.5104069	-0.0281415	86.7971010	H	-1.3225048	9.2693547	82.7982086
H	-1.5939429	0.0509945	87.7477483	H	2.7950767	11.5328208	81.0399290
H	-4.1491010	0.5483963	86.0955826	H	-1.4727185	10.7594202	80.7837271
H	-4.0807059	-0.1574287	87.7395415	H	2.9410714	10.0322036	83.0637627
H	-3.3443209	-1.0319689	86.3534458	Br	3.2599803	6.8528675	88.2115609
C	-3.9184380	5.4510161	86.7030456	Zn	2.1751686	6.8164801	85.9689345
C	-3.6603086	5.3611624	85.1928732	H	-0.8410156	6.9752876	81.9221451
H	-4.0227066	6.2776032	84.6828074	H	3.5168398	5.7361669	84.0492151
H	-4.2002292	4.5055676	84.7356481	C	1.1801696	6.3497418	82.5096760
H	-2.5846079	5.2325559	84.9641252	C	-0.1913690	6.0704901	81.9775154
C	-5.4281640	5.5178812	87.0075563	H	1.8981177	7.0147133	82.0109877
H	-3.4621942	6.4003621	87.0649243	C	1.4131631	5.5604554	83.6064237
H	-5.9067661	6.3684008	86.4780849	C	2.5484783	5.4603064	84.5068658
H	-5.6187601	5.6361388	88.0933150	C	0.1480876	4.7781813	83.8500343
H	-5.9320816	4.5842932	86.6801337	O	-0.7743951	5.1331079	82.8843649
C	-1.9131290	3.9134339	91.0866580	O	-0.0997340	3.9655808	84.7115176
C	-1.3252128	5.3256742	91.2484424	H	-0.1765285	5.6245853	80.9556049
H	-0.9223690	5.4571811	92.2732513	H	2.6031036	4.4965205	85.0483416
H	-2.0871805	6.1175612	91.0936241	H	-0.0559152	8.1695566	84.5127216
H	-0.4975192	5.4952365	90.5347777	H	3.6391062	-5.4108555	88.2053525
C	-3.1229528	3.7347376	92.0253547	H	1.8120760	0.7985238	84.1314728
H	-1.1240108	3.1988444	91.3980470	H	2.9420358	2.1214768	83.7337547
H	-2.8407037	3.9360861	93.0798545	H	1.9444819	2.2163837	85.2207462
H	-3.5420141	2.7105975	91.9739541				
H	-3.9376977	4.4371564	91.7501163				
H	6.1907211	4.8163080	84.2234577				
H	8.0571740	3.0051939	89.5682789				
H	3.7442073	-0.8712988	83.9393363				
C	6.5842732	4.8993622	85.2613668				
H	5.6164713	3.5754794	91.5279860				
H	6.6346860	7.0904604	85.1600990				
C	5.9475886	3.7679514	86.0604569				
C	7.4202834	2.1707158	89.9298437				
C	6.1973712	6.2896425	85.7921360				
H	6.5602595	6.4465711	86.8289386				
C	6.1772225	3.6222015	87.4400942				
C	4.4177293	-0.1585985	84.4590013				
H	8.3941485	3.7487064	84.7722060				
C	5.1243234	2.8224250	85.4296377				
C	8.1139324	4.7361675	85.1907354				
H	8.5710246	5.5241831	84.5564596				
H	4.9135047	2.9418344	84.3544910				
C	5.4447374	3.6965920	90.4384263				
H	7.6174589	2.0442080	91.0146507				
H	7.7509839	1.2486993	89.4100173				
C	5.6353693	2.5552012	88.1784100				
C	2.5208954	1.5288749	84.5730730				
C	4.5439736	1.7440313	86.1224973				
H	5.1596247	-0.7470726	85.0355279				
H	4.9735766	0.4095375	83.6835381				
C	5.9284674	2.4521000	89.6726786				
C	4.8362362	1.5920183	87.5086056				
C	3.6144061	0.7916026	85.3664961				
H	4.3621289	3.8663157	90.2798926				
H	5.9841456	4.6114559	90.1158078				
H	5.0977976	6.4233893	85.8121322				
H	8.5685614	4.8121359	86.2006217				
H	5.3607713	1.5823937	90.0638703				
H	3.0908320	0.1669234	86.1182130				
H	6.8033119	4.3630061	87.9629501				
Zn	1.3330886	5.2993593	88.1987638				
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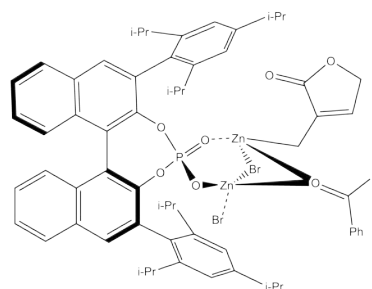


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C	3.3307523	3.3743175	0.8852290
C	4.7348748	3.5497929	0.7017617
C	2.5071425	4.5477306	1.0596943
C	3.1275417	5.8330872	1.0852664
C	1.0974093	4.4029090	1.2129449
H	0.4895046	5.2966235	1.4224204
C	0.4717275	3.1671212	1.0889146
C	3.7718559	-1.5629986	0.2301228
C	4.7488050	-1.7393466	1.2014338
H	5.2421514	-2.7183794	1.2977243
C	5.0809695	-0.7092573	2.1276140
C	6.0306349	-0.9414257	3.1678355
C	4.3895836	0.5580707	2.0683477
C	4.6237326	1.4964035	3.1192806
C	3.4703540	0.7993576	0.9778177
C	3.2096270	-0.2569269	0.1005121
O	0.6490142	0.8208285	0.6829466
O	2.3699371	-0.0324475	-0.9873751
P	0.7498005	0.0470870	-0.7578695
O	0.2273360	0.8995959	-1.9295452

O	0.1108565	-1.3162824	-0.4854813	H	6.3264363	-3.1017351	-2.1882044
C	4.4980086	5.9679166	0.9181394	C	3.5752534	-2.8513149	-1.9462783
C	5.3041729	4.8158835	0.7134413	C	0.4155038	-3.7113057	1.7713603
H	2.4914984	6.7208178	1.2286868	C	2.3083565	-3.6011520	0.0298491
H	4.9615296	6.9661318	0.9321044	H	3.8484701	-4.2442619	2.2445504
H	5.3647901	2.6640243	0.5358676	H	2.5710047	-5.4868680	2.0936142
H	6.3880091	4.9279375	0.5573799	C	4.5431496	-1.8935030	-2.6363172
C	5.5384055	1.2313375	4.1298377	C	3.2264639	-2.6964540	-0.5830756
C	6.2659535	0.0119722	4.1467224	C	1.9113543	-3.4791507	1.5031647
H	4.0641572	2.4409726	3.1332525	H	2.9831895	-0.6165016	-3.5006055
H	5.6948995	1.9728475	4.9282149	H	-0.2226562	-3.0254004	1.1850050
H	6.9961123	-0.1824258	4.9470741	H	3.5871281	-1.8743347	-4.6222035
H	6.5588856	-1.9076771	3.1883579	H	-0.4396326	-5.8838000	-1.9292185
C	-1.9253931	3.5656885	0.3596543	H	0.1084373	-4.7557992	1.5520518
C	-1.0028708	2.9845564	1.2738201	H	1.9007490	-5.3808786	-4.9284720
C	-3.3049563	3.4504138	0.6212023	H	4.8305083	-1.1202616	-1.8938569
C	-1.4853190	2.2407579	2.3907934	H	2.1356660	-2.4396645	1.8207809
C	-2.8734876	2.1460428	2.5946130	H	3.3158671	-4.0386381	-3.7305894
C	-3.8038826	2.7597491	1.7396400	Zn	-0.6097954	0.2096019	-3.5805016
H	-4.0214811	3.9111008	-0.0788991	Br	-1.1558014	1.5789964	-5.3637999
C	-0.5663066	1.5555948	3.4024037	C	-6.3656600	2.1899844	-3.1148521
H	-3.2360756	1.5791497	3.4653982	C	-3.1178051	-0.0786846	-1.5798790
C	-0.7981745	0.0326941	3.4353980	C	-5.3955529	1.6877672	-4.0065648
H	-1.8191629	-0.2215206	3.7876775	C	-5.1982486	1.1878391	-1.2399308
H	-0.0742479	-0.4533248	4.1223104	C	-4.2190893	0.6827398	-2.1312307
H	-0.6770090	-0.4163296	2.4317219	C	-6.2712769	1.9367616	-1.7340194
C	-0.7071113	2.1851759	4.8012562	C	-4.3276622	0.9296292	-3.5236229
H	0.4828873	1.7225041	3.0875819	O	-2.1863917	-0.5763791	-2.2609179
H	-1.7279804	2.0409636	5.2128015	H	-7.2059189	2.7859465	-3.5033439
H	-0.5050817	3.2755056	4.7752150	H	-5.0956448	0.9903694	-0.1632673
H	0.0076268	1.7197525	5.5112523	H	-5.4758450	1.8957966	-5.0838195
C	-5.2988745	2.7370380	2.0384708	H	-7.0341098	2.3304673	-1.0458211
C	-5.7983222	1.3944718	2.5981300	H	-3.5565359	0.5467657	-4.2082131
H	-6.9056954	1.3888436	2.6617296	Br	0.0893930	-2.1248424	-3.8968170
H	-5.4154839	1.2159245	3.6242861	Zn	-1.0107601	-2.4450502	-1.6405174
H	-5.4822167	0.5281884	1.9806289	H	-6.1562179	-1.2805767	-0.8131176
C	-5.6686074	3.8983640	2.9832704	H	-2.5692439	-4.4837504	-1.9599415
H	-5.8218292	2.9263127	1.0742635	C	-4.8463757	-2.9838867	-1.2543356
H	-6.7627623	3.9298697	3.1677618	C	-5.7535545	-2.2120882	-0.3521454
H	-5.3597700	4.8754560	2.5603406	H	-5.1657834	-3.3905109	-2.2241004
H	-5.1596370	3.7799678	3.9627924	C	-3.6243343	-3.1326147	-0.6664432
C	-1.4710105	4.2786204	-0.9131879	C	-2.3914267	-3.7954100	-1.1124570
C	-2.0570329	3.6154306	-2.1705763	C	-3.6828283	-2.3877723	0.6323710
H	-1.6577534	4.0863745	-3.0913190	O	-4.9502214	-1.8532709	0.7805082
H	-3.1640488	3.6889594	-2.2077309	O	-2.8073726	-2.1998069	1.4531453
H	-1.7846165	2.5438504	-2.2123397	H	-6.6273887	-2.8075713	-0.0018197
C	-1.7909774	5.7834523	-0.8712223	H	-1.9111176	-4.3406162	-0.2735755
H	-0.3697369	4.1705825	-0.9813459	H	-3.0880275	-0.2008408	-0.4708163
H	-1.4150125	6.2903378	-1.7838675				
H	-1.3282976	6.2745414	0.0091194				
H	-2.8855407	5.9613857	-0.8145687				
H	1.8074719	-6.9407415	-2.2612998				
H	5.6332995	-3.4033541	-3.8122509				
H	2.5175375	-4.3069704	3.4450364				
C	1.5568028	-6.0354044	-2.8616145				
H	4.5966105	-0.4367705	-4.2704779				
H	-0.3985358	-6.8578914	-3.4297207				
H	0.1914811	-3.5298702	2.8424568				
C	2.1422314	-4.8477992	-2.0962967				
C	5.8365337	-2.6157928	-3.0565316				
C	0.0191349	-5.9570653	-2.9346996				
H	-0.3005436	-5.0675407	-3.5166279				
C	3.0308336	-3.9280235	-2.6747945				
C	2.7634081	-4.4285828	2.3696501				
H	3.2535888	-6.3336080	-4.2356210				
C	1.7916097	-4.6544012	-0.7438561				
C	2.1498614	-6.2326931	-4.2612702				
H	1.7373904	-7.1495524	-4.7284603				
H	1.0985077	-5.3670428	-0.2688942				
C	3.8888937	-1.1653363	-3.8235643				
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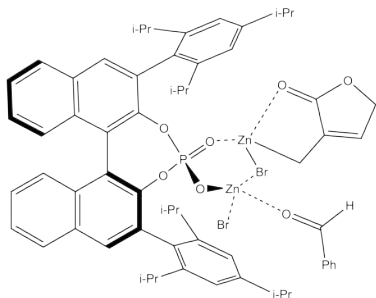


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C	3.3314681	3.3741383	0.8870233
C	4.7355012	3.5499598	0.7053981
C	2.5080874	4.5471873	1.0630532
C	3.1290562	5.8316507	1.0916187
C	1.0985817	4.4015720	1.2149798
H	0.4891973	5.2939919	1.4256478

C	0.4730824	3.1663241	1.0878376	H	0.1901707	-3.5217953	2.8452118
C	3.7713320	-1.5634896	0.2305006	C	2.1409829	-4.8487193	-2.0928190
C	4.7473792	-1.7397614	1.2023806	C	5.8308508	-2.6174903	-3.0604701
H	5.2381611	-2.7200866	1.2988100	C	0.0190089	-5.9591008	-2.9324453
C	5.0805434	-0.7099683	2.1280093	H	-0.2995387	-5.0697723	-3.5151991
C	6.0293895	-0.9414782	3.1684039	C	3.0275542	-3.9283483	-2.6725809
C	4.3901854	0.5576563	2.0675737	C	2.7590126	-4.4341857	2.3712262
C	4.6250135	1.4962547	3.1178314	H	3.2543230	-6.3358792	-4.2291113
C	3.4715568	0.7992633	0.9765680	C	1.7918871	-4.6553264	-0.7404170
C	3.2103206	-0.2569634	0.0991278	C	2.1506445	-6.2362109	-4.2560134
O	0.6499720	0.8216448	0.6775274	H	1.7400277	-7.1539167	-4.7230919
O	2.3726249	-0.0333729	-0.9891468	H	1.1005045	-5.3686764	-0.2639156
P	0.7523861	0.0469435	-0.7633831	C	3.8832362	-1.1627088	-3.8203762
O	0.2283798	0.8970152	-1.9347147	H	6.5530873	-1.9037205	-3.5081250
O	0.1140537	-1.3167589	-0.4889532	H	6.3215328	-3.1063947	-2.1944821
C	4.4992042	5.9668055	0.9265686	C	3.5724813	-2.8517341	-1.9450599
C	5.3049601	4.8154342	0.7206618	C	0.4146770	-3.7033583	1.7744149
H	2.4927563	6.7191012	1.2355184	C	2.3083164	-3.6017547	0.0326196
H	4.9626451	6.9649610	0.9429579	H	3.8448806	-4.2546804	2.2468322
H	5.3643002	2.6636624	0.5388944	H	2.5631205	-5.4912275	2.0933862
H	6.3889774	4.9273271	0.5661660	C	4.5395683	-1.8939999	-2.6363561
C	5.5395152	1.2314389	4.1279986	C	3.2252736	-2.6971389	-0.5815922
C	6.2657349	0.0120411	4.1461370	C	1.9118163	-3.4795047	1.5061092
H	4.0658989	2.4410055	3.1302284	H	2.9817547	-0.6098059	-3.4933556
H	5.6966228	1.9737428	4.9254474	H	-0.2193193	-3.0129423	1.1888427
H	6.9956667	-0.1825317	4.9465800	H	3.5751001	-1.8692638	-4.6186411
H	6.5564286	-1.9083625	3.1898428	H	-0.4409488	-5.8847971	-1.9276105
C	-1.9232667	3.5640126	0.3573323	H	0.1012595	-4.7460413	1.5550617
C	-1.0013832	2.9828310	1.2717367	H	1.9008528	-5.3857705	-4.9244912
C	-3.3026439	3.4472564	0.6180949	H	4.8297910	-1.1224663	-1.8932390
C	-1.4835030	2.2368312	2.3871097	H	2.1415486	-2.4417792	1.8253601
C	-2.8715088	2.1398238	2.5891326	H	3.3112946	-4.0387797	-3.7286476
C	-3.8014747	2.7549744	1.7353092	Zn	-0.5870442	0.2248423	-3.6015828
H	-4.0188986	3.9085918	-0.0820305	Br	-1.1883863	1.5851445	-5.3652333
C	-0.5643348	1.5526924	3.3991510	C	-6.3839435	2.1785872	-3.0979956
H	-3.2336762	1.5692771	3.4575412	C	-3.1074209	-0.0622976	-1.5765628
C	-0.7933466	0.0295383	3.4329765	C	-5.4042487	1.6996325	-3.9908177
H	-1.8140036	-0.2287532	3.7826600	C	-5.2048863	1.1778711	-1.2290113
H	-0.0697039	-0.4544693	4.1214549	C	-4.2186847	0.6935243	-2.1228183
H	-0.6697039	-0.4201397	2.4300627	C	-6.2885510	1.9142054	-1.7196035
C	-0.7069946	2.1835052	4.7971713	C	-4.3272679	0.9508100	-3.5125624
H	0.4847550	1.7217216	3.0851423	O	-2.1893365	-0.5663519	-2.2664992
H	-1.7274340	2.0378026	5.2090560	H	-7.2316298	2.7665374	-3.4829858
H	-0.5079308	3.2742120	4.7704467	H	-5.1010325	0.9720612	-0.1540047
H	0.0080882	1.7203522	5.5081536	H	-5.4804963	1.9194983	-5.0660581
C	-5.2962071	2.7350075	2.0360131	H	-7.0574056	2.2905827	-1.0282433
C	-5.7979278	1.3953961	2.6006473	H	-3.5450903	0.5914107	-4.1979831
H	-6.9053305	1.3915157	2.6660208	Br	0.0839276	-2.1236290	-3.9021075
H	-5.4159843	1.2207274	3.6276681	Zn	-1.0069736	-2.4369559	-1.6519858
H	-5.4828032	0.5245739	1.9892464	H	-6.1678113	-1.3085526	-0.8672150
C	-5.6627139	3.9006083	2.9766054	H	-2.5490464	-4.4997186	-1.9329050
H	-5.8194509	2.9217726	1.0710717	C	-4.8461342	-3.0151589	-1.2589315
H	-6.7563203	3.9358866	3.1639904	C	-5.7589352	-2.2235289	-0.3778128
H	-5.3515077	4.8752619	2.5502626	H	-5.1617548	-3.4539869	-2.2158035
H	-5.1516680	3.7854095	3.9552012	C	-3.6213068	-3.1326853	-0.6711260
C	-1.4678873	4.2779501	-0.9146071	C	-2.3809470	-3.7895169	-1.1017399
C	-2.0499365	3.6142519	-2.1732576	C	-3.6843372	-2.3497412	0.6068009
H	-1.6489355	4.0829005	-3.0941859	O	-4.9603823	-1.8249454	0.7413002
H	-3.1569722	3.6867093	-2.2138704	O	-2.8089850	-2.1242920	1.4150833
H	-1.7752943	2.5433672	-2.2143940	H	-6.6292404	-2.8145305	-0.0093659
C	-1.7899922	5.7821642	-0.8725826	H	-1.8948022	-4.3086073	-0.2497779
H	-0.3663964	4.1714360	-0.9809117	H	-3.0647068	-0.1740641	-0.4664657
H	-1.4136450	6.2903570	-1.7842295				
H	-1.3302853	6.2740007	0.0088018				
H	-2.8846833	5.9594808	-0.8173682				
H	1.8073847	-6.9419416	-2.2556421				
H	5.6255568	-3.4035874	-3.8170034				
H	2.5136926	-4.3136911	3.4467456				
C	1.5564579	-6.0373516	-2.8571533				
H	4.5913270	-0.4363929	-4.2701200				
H	-0.3990383	-6.8599061	-3.4272937				

14 γ -ma



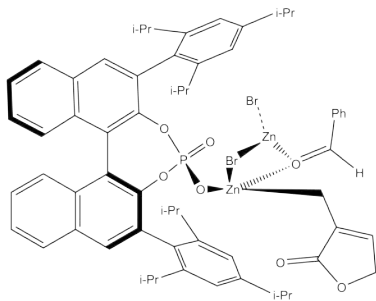
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C	0.4894074	0.2508772	90.7169353
C	1.2683723	-0.5990588	91.5592789
C	-0.7596078	0.7587489	91.2323552
C	-1.2001952	0.3490423	92.5265278
C	-1.5158829	1.6794061	90.4540586
H	-2.4751355	2.0498908	90.8478681
C	-1.0590408	2.1567246	89.2308085
C	4.4150685	0.4330516	87.8174858
C	4.6137181	-0.9411002	87.7838308
H	5.5907294	-1.3356953	87.4671215
C	3.5822125	-1.8610541	88.1336075
C	3.7759640	-3.2690126	88.0063384
C	2.3120970	-1.3669743	88.6105663
C	1.2772208	-2.3113467	88.8815957
C	2.1324338	0.0569273	88.7645412
C	3.1514831	0.8925039	88.3026192
O	0.5690289	2.0807955	87.4836997
O	2.9622589	2.2706234	88.3647243
P	1.9591087	2.9226059	87.2452121
O	1.8130872	4.4034067	87.6195795
O	2.3838536	2.5641268	85.8173766
C	-0.4315443	-0.5008020	93.3064298
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H	-2.1606468	0.7375547	92.9002551
H	-0.7795401	-0.8031046	94.3058684
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H	2.9193485	-5.2443819	88.1921560
H	4.7534829	-3.6333010	87.6529231
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C	9.0839046	5.1935625	87.4143221
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H	4.1051428	0.5389604	85.3204950
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Zn	3.1147127	5.8751601	87.2409827
Br	4.7981266	6.5232768	88.6797394
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C	-1.5875495	7.7727050	85.4952851
C	-0.4398304	8.1255615	86.2399783
C	-2.5197227	8.7597793	85.1487020
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O	1.6391541	7.3427577	87.0798879
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Zn	2.1191319	3.6944679	84.2193974
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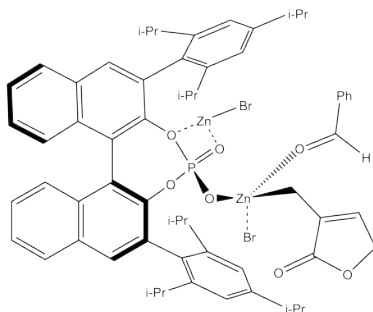
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O	0.1305412	2.6248803	87.1714847
O	2.4754932	2.6414471	88.2902733
P	1.5124245	3.5648472	87.3136931
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H	3.7075849	1.3007836	91.9137372
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C	7.3942505	3.6191294	88.4800875
C	6.1176702	0.2513844	90.9735702
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H	7.8484286	5.1168912	90.8425373
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H	6.1653955	0.9370919	84.7565961
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C	5.0749332	1.0847975	90.2095191
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H	3.4531146	2.5141940	90.6134214
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H	6.1159966	4.7770825	84.7035676
H	9.5474156	3.1561261	90.2746105
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H	4.2400888	2.4132859	85.3830607	O	1.7916713	4.9435500	87.8763660
H	7.1630258	2.7879002	90.4689111	O	1.7388257	3.4327278	85.7272032
Zn	2.1163116	4.9281135	84.5124573	C	-1.0199074	-2.1358200	91.3339197
Br	2.3841726	7.1900665	84.6914338	C	0.2487543	-2.3022113	90.7204915
C	-2.3813281	8.6966770	85.5055677	H	-2.7566547	-0.8562690	91.5197891
C	-1.2660309	4.7758436	84.3128450	H	-1.3811868	-2.8754733	92.0642878
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C	-2.7043874	6.7715628	84.0669408	H	0.8790339	-3.1630582	90.9910706
C	-1.6472229	6.1085580	84.7376895	C	1.1675382	-2.8575530	85.8997681
C	-3.0599520	8.0694717	84.4422736	C	2.4713427	-3.0794915	85.3837051
C	-0.9668216	6.7445799	85.8073618	H	-0.1241205	-1.5602910	87.0405278
O	-0.2017159	4.2347082	84.6925134	H	0.3626853	-3.5761286	85.6839980
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H	-3.2257171	6.2617687	83.2413627	H	4.4913130	-2.3182958	85.2290423
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Br	2.1007073	3.3742283	82.6240007	C	-3.2228882	3.6853612	87.8529745
Zn	0.7346342	2.3103448	84.5534070	C	-3.9365853	4.8963227	87.8325947
H	0.4047473	-0.1932759	79.9624233	C	-3.7417272	5.8965475	88.8015828
H	0.6822956	-0.2931268	84.8321846	H	-2.5933533	6.4571293	90.5439876
C	0.1684040	-0.7061591	82.0811992	C	-3.4455876	2.6625220	86.7427911
C	-0.3830454	-0.4000339	80.7229204	H	-4.6638962	5.0663651	87.0226693
H	0.8174242	-1.5666078	82.2962135	C	-3.2440521	3.2857759	85.3498944
C	-0.2588481	0.2346155	82.9642693	H	-4.0092893	4.0580944	85.1267299
C	0.0129205	0.4692406	84.3929245	H	-3.3039522	2.5136000	84.5563009
C	-1.0846007	1.2053920	82.1818567	H	-2.2490009	3.7712091	85.2827537
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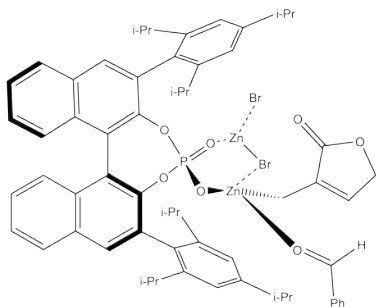


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C	-1.3276963	-0.0486137	90.0904306	H	8.2310762	6.0248549	91.5805778
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C	4.0381664	1.1174080	87.3624527	H	8.4555481	4.2764316	91.3102826
C	4.2884699	-0.0688590	86.6895743	C	6.4992638	2.9141523	89.6494117
H	5.3086016	-0.3047260	86.3516074	C	6.0061666	3.0054302	84.8844687
C	3.2353344	-0.9938239	86.4146637	H	8.4137768	5.8097211	87.7952588
C	3.4810266	-2.1639121	85.6376938	C	5.8989160	4.4146852	87.8613348
C	1.9066372	-0.7671621	86.9387905	C	8.6554591	5.6050296	88.8575851
C	0.8927149	-1.7302603	86.6609626	H	9.2038123	6.4822342	89.2571531
C	1.6436304	0.4467570	87.6776764	H	6.0054921	5.3897553	87.3595068
C	2.6893472	1.3607660	87.7486048	C	4.2756741	0.8774109	90.8990115
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O	2.3992978	2.6297570	88.2400175				
P	1.4410193	3.5982834	87.1990307				

H	6.4558631	-0.8953126	91.0871608	H	0.3597916	5.6339556	0.9273378
H	7.5296242	-0.0445520	89.9295222	C	0.2540750	3.5063585	0.6188537
C	5.6901989	1.8923671	89.0986864	C	3.5658828	-1.1748801	-0.7140733
C	4.4231289	4.9440577	85.2955650	C	4.6326374	-1.4295629	0.1383295
C	5.1974797	3.3791738	87.1896214	H	5.2168345	-2.3541244	0.0115432
H	6.2691661	1.9648290	85.1595171	C	4.9583571	-0.5519812	1.2149992
H	6.9075318	3.6396000	85.0211619	C	5.9962208	-0.8775428	2.1388005
C	5.4316766	0.6242011	89.9073793	C	4.1970981	0.6602845	1.4127935
C	5.0399565	2.1180795	87.8576700	C	4.4699433	1.4476695	2.5709754
C	4.8210499	3.5278102	85.7248638	C	3.1808789	1.0100433	0.4477346
H	3.3521938	1.2054868	90.3820971	C	2.8858932	0.0740721	-0.5450626
H	3.6375318	5.3717293	85.9506763	O	0.3346427	1.1131801	0.3533640
H	4.5426627	1.6734763	91.6243311	O	1.9167093	0.3842351	-1.4883423
H	6.8364090	4.9144785	91.7764614	P	0.3255535	0.4021815	-1.1306348
H	5.2886919	5.6395149	85.2783407	O	-0.2795199	1.3180657	-2.2047295
H	9.3411427	4.7326970	88.8833614	O	-0.2737029	-0.9948647	-0.9510096
H	5.0958246	-0.1592794	89.1982309	C	4.4059144	6.1163638	0.5964357
H	3.9692679	2.8544021	85.5078911	C	5.1601019	4.9320364	0.3852640
H	7.0080561	2.7195542	90.6024026	H	2.4281918	6.9534074	0.8705667
Zn	3.5373960	4.4424557	88.8335364	H	4.9135562	7.0922006	0.6328022
Br	3.8377044	5.0412923	91.0351486	H	5.1308441	2.7873052	0.1718741
C	-2.9372830	6.8779771	80.8557132	H	6.2496865	4.9956169	0.2432452
C	-0.7290243	3.7477571	82.7238259	C	5.4735225	1.0905762	3.4614309
C	-1.6366381	7.1451945	81.3287900	C	6.2565859	-0.0721789	3.2373568
C	-2.7632316	4.5733412	81.5999215	H	3.8676736	2.3473436	2.7588241
C	-1.4582624	4.8405662	82.0760542	H	5.6598885	1.7131078	4.3498431
C	-3.4996518	5.5965295	80.9886376	H	7.0565114	-0.3409679	3.9439361
C	-0.8945468	6.1297447	81.9377403	H	6.5777957	-1.7974225	1.9696883
O	0.4293334	3.8423271	83.1604425	C	-2.0553898	3.6222197	-0.4441683
H	-3.5180223	7.6818665	80.3769124	C	-1.2373886	3.3853354	0.6966736
H	-3.1745465	3.5565151	81.7144272	C	-3.4338623	3.3755001	-0.3390890
H	-1.2087583	8.1532403	81.2180535	C	-1.8209123	2.9543753	1.9156208
H	-4.5149451	5.3976941	80.6137369	C	-3.2061686	2.7007009	1.9599115
H	0.1226771	6.3038780	82.3203224	C	-4.0292222	2.8846150	0.8383295
Br	3.1672541	1.2966699	83.2227660	H	-4.0789556	3.5483877	-1.2147881
Zn	1.1698099	2.1012354	84.2191420	C	-0.9817835	2.7669667	3.1793575
H	-0.0537944	-1.5115584	80.8381369	H	-3.6436391	2.3416781	2.9035580
H	-0.0769698	0.3197022	85.4927750	C	-0.9260204	1.2963812	3.6232380
C	-0.0141486	-1.0668662	82.9790509	H	-1.9262093	0.9314470	3.9335103
C	-0.6980636	-1.5626652	81.7465554	H	-0.2419988	1.1691819	4.4879143
H	0.9118395	-1.4988640	83.3809547	H	-0.5643634	0.6484272	2.7999790
C	-0.6821400	0.0175565	83.4683646	C	-1.4691438	3.6800384	4.3184307
C	-0.4137142	0.8989983	84.6139245	H	0.0554705	3.0764825	2.9387944
C	-1.8303039	0.2535654	82.5405722	H	-2.4989590	3.4179414	4.6396859
O	-1.8220509	-0.6947496	81.5517755	H	-1.4764474	4.7439963	4.0067888
O	-2.6771725	1.1368497	82.5675731	H	-0.8098395	3.5855217	5.2060818
H	-1.0706558	-2.6104238	81.8258166	C	-5.5098608	2.5176447	0.8208777
H	-1.3081130	1.4869507	84.8891439	C	-5.7105236	1.2000684	0.0422112
H	-1.2986522	2.7908819	82.8201211	H	-6.7826317	0.9156261	0.0038140
				H	-5.1393756	0.3725192	0.5119155
				H	-5.3367173	1.2804628	-0.9977657
				C	-6.1602897	2.4506969	2.2082157
				H	-6.0301232	3.3199771	0.2499200
				H	-7.2519805	2.2802013	2.1173518
				H	-6.0055968	3.3875151	2.7806012
				H	-5.7498547	1.6171664	2.8159939
				C	-1.4662279	4.1445938	-1.7537296
				C	-2.2116423	3.6428727	-3.0023833
				H	-1.5810948	3.7386153	-3.9095048
				H	-3.1469083	4.2077790	-3.1975837
				H	-2.5306444	2.5838008	-2.8781388
				C	-1.4088556	5.6847338	-1.7701966
				H	-0.4277794	3.7609954	-1.8146710
				H	-0.9701443	6.0515743	-2.7211561
				H	-0.7947007	6.0818021	-0.9396421
				H	-2.4270053	6.1160343	-1.6724333
				H	-0.2778494	-4.9932812	-3.7483723
				H	4.6568193	-1.8703717	-5.2632283
				H	2.5857621	-5.5003006	1.4534706
				C	0.1909100	-4.1773764	-4.3413554
				H	3.6578471	1.1651911	-4.8610727

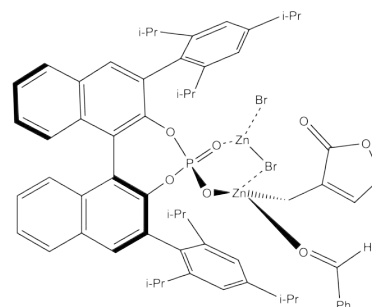
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C	3.1227548	3.5746866	0.5160584
C	4.5353534	3.6934439	0.3475044
C	2.3528831	4.7847293	0.6780432
C	3.0286227	6.0403075	0.7334154
C	0.9328429	4.7095885	0.7583258

H	-1.7296004	-3.6200088	-5.2672556
H	1.1290142	-3.5066721	2.0840476
C	1.2453986	-3.5355943	-3.4498494
C	4.9899555	-1.2604942	-4.3975093
C	-0.9099111	-3.1543529	-4.6819732
H	-0.5128429	-2.3040702	-5.2758172
C	2.0552504	-2.4888063	-3.9270225
C	2.3965173	-5.2352689	0.3924825
H	1.5673097	-5.5515285	-5.3647398
C	1.3922994	-3.9308353	-2.1109416
C	0.7881494	-4.8030023	-5.6127219
H	0.0021021	-5.3081598	-6.2111549
H	0.7719054	-4.7576292	-1.7331196
C	3.0056488	0.3228761	-4.5517653
H	5.6599491	-0.4630429	-4.7813002
H	5.5828145	-1.9204793	-3.7323005
C	2.9148990	-1.7734182	-3.0800943
C	1.1203651	-3.1331489	1.0379548
C	2.2548192	-3.2581873	-1.2223369
H	3.2251057	-5.6503741	-0.2163261
H	1.4574265	-5.7405049	0.0915294
C	3.7818376	-0.6552516	-3.6553825
C	2.9762644	-2.1285763	-1.7022798
C	2.3072273	-3.7066184	0.2405551
H	2.1282995	0.7464645	-4.0268121
H	1.1409433	-2.0256761	1.0551284
H	2.6376600	-0.1596807	-5.4802570
H	-1.3584105	-2.7272320	-3.7619421
H	0.1665054	-3.4417952	0.5660559
H	1.2542530	-4.0331829	-6.2625448
H	4.1883579	-0.0724157	-2.8023070
H	3.2249236	-3.2828982	0.6923961
H	1.9872462	-2.1930370	-4.9856642
Zn	-1.3310411	0.8778953	-3.7764348
Br	-0.7101304	1.1687596	-5.9556831
C	-3.8718858	-1.4216857	5.6217343
C	-2.2709034	-1.5588945	1.6662891
C	-4.6240303	-0.8982356	4.5510410
C	-2.1008805	-2.0558080	4.0868668
C	-2.8504556	-1.5293693	3.0101392
C	-2.6123831	-2.0013890	5.3899308
C	-4.1178529	-0.9505803	3.2495205
O	-2.8118494	-1.0630788	0.6601656
H	-4.2719519	-1.3741283	6.6461938
H	-1.1061447	-2.4886167	3.8921243
H	-5.6078662	-0.4423620	4.7402551
H	-2.0269141	-2.4042367	6.2298446
H	-4.6798784	-0.5374570	2.3994838
Br	-3.2574662	-0.3406384	-2.9410178
Zn	-2.0738064	-1.7785032	-1.1970631
H	-2.5841325	-4.6373926	3.1642055
H	-3.9184875	-3.4267119	-1.5310971
C	-3.4895730	-4.2025917	1.2166271
C	-2.9373378	-5.1471478	2.2371460
H	-4.3720609	-3.5729492	1.3926856
C	-2.7752504	-4.3139694	0.0554772
C	-2.8712473	-3.6357348	-1.2352092
C	-1.7166910	-5.3478299	0.3095429
O	-1.8245114	-5.7884199	1.6069967
O	-0.8797938	-5.7839756	-0.4550585
H	-3.6682919	-5.9267051	2.5535635
H	-2.3583147	-4.2144863	-2.0280455
H	-1.2572572	-2.0237513	1.5835983



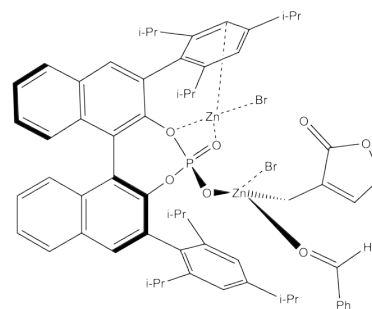
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C	-0.0170879	-0.9042144	90.3924000
C	0.7580239	-1.9976905	90.8835421
C	-1.2903984	-0.6364377	91.0178674
C	-1.7556669	-1.5032236	92.0514081
C	-2.0538825	0.4938278	90.6064488
H	-3.0458739	0.6573847	91.0544649
C	-1.5790375	1.3921799	89.6603809
C	3.9210954	0.5079509	87.7788471
C	4.1898519	-0.7470369	87.2488418
H	5.1597457	-0.9350344	86.7635367
C	3.2177043	-1.7912572	87.2644445
C	3.4763158	-3.0432680	86.6304560
C	1.9298248	-1.5708199	87.8820853
C	0.9414066	-2.5932019	87.7686171
C	1.6906920	-0.3209344	88.5643143
C	2.6718606	0.6661231	88.4627694
O	0.1423751	2.0211560	88.0985732
O	2.4628550	1.8751952	89.1096282
P	1.4129012	2.9795295	88.5217385
O	1.0950458	3.8614883	89.7379372
O	1.8973753	3.6541640	87.2402230
C	-0.9889264	-2.5736055	92.4850531
C	0.2848634	-2.8102834	91.9041683
H	-2.7345853	-1.2935122	92.5105795
H	-1.3569194	-3.2293227	93.2887495
H	1.7504276	-2.1858529	90.4515599
H	0.9068846	-3.6413268	92.2701117
C	1.2201299	-3.7919749	87.1261955
C	2.5027299	-4.0287371	86.5657842
H	-0.0568151	-2.4196985	88.1939601
H	0.4381459	-4.5626874	87.0483704
H	2.7165154	-4.9862959	86.0670439
H	4.4658402	-3.2047980	86.1745205
C	-2.2996054	3.8304121	89.8443113
C	-2.3508803	2.5787253	89.1678192
C	-2.9114297	4.9403822	89.2398661
C	-3.0586146	2.4587078	87.9445263
C	-3.6309576	3.6103257	87.3680999
C	-3.5474026	4.8675573	87.9852723
H	-2.8744650	5.9163938	89.7482840
C	-3.2145415	1.1103811	87.2409134
H	-4.1477779	3.5114400	86.4020506
C	-2.4547761	1.0644886	85.9057672
H	-2.8711197	1.7931378	85.1809276
H	-2.5239116	0.0575500	85.4441667
H	-1.3821651	1.3023649	86.0512947
C	-4.6973092	0.7404593	87.0571226
H	-2.7683824	0.3376085	87.8992923
H	-5.2158679	1.4502867	86.3792390
H	-5.2371878	0.7474614	88.0254974
H	-4.7959296	-0.2724873	86.6148108
C	-4.0629548	6.1509660	87.3399880
C	-2.8746112	7.0384529	86.9121839

14λ-ma

H	-3.2290358	7.9853544	86.4540909	Br	1.0243860	7.0436545	88.2644428
H	-2.2282932	6.5103004	86.1811283	Zn	1.7345863	5.4430631	86.3919414
H	-2.2236334	7.2961877	87.7708335	H	-0.5451466	7.6645008	82.3483593
C	-5.0300499	5.9241774	86.1719696	H	3.3415160	7.2072925	85.3798686
H	-4.6193162	6.7036196	88.1314693	C	1.3913795	7.7552497	83.3731536
H	-5.4321690	6.8916542	85.8092899	C	0.5360790	7.4473438	82.1835739
H	-5.8888504	5.2863208	86.4636367	H	1.4920659	8.7619896	83.8018475
H	-4.5251361	5.4358583	85.3121829	C	1.9850442	6.6121466	83.8147356
C	-1.6149262	3.9712466	91.2029289	C	2.8506286	6.3074950	84.9629849
C	-1.0201666	5.3680073	91.4500211	C	1.5211841	5.5177035	82.9086517
H	-0.2597515	5.3400788	92.2566380	O	0.6804135	6.0403768	81.9580216
H	-1.7870808	6.1109607	91.7530422	O	1.7717609	4.3249218	82.9581856
H	-0.5644169	5.7780386	90.5212106	H	0.8434300	7.9905837	81.2604809
C	-2.5744799	3.6053226	92.3523926	H	3.6154565	5.5520450	84.6912815
H	-0.7733671	3.2492889	91.2154190	H	0.3825058	3.0775487	85.1296712
H	-2.0651085	3.6955106	93.3341489				
H	-2.9481312	2.5676917	92.2595030				
H	-3.4551216	4.2811803	92.3585481				
H	6.0543486	6.1373069	86.1894940				
H	7.4341903	2.1513427	90.4617093				
H	4.8243715	1.4488344	82.9173344				
C	6.1108087	5.8616522	87.2659218				
H	4.7267413	2.0548826	92.2101500				
H	5.3073666	7.8130573	87.8933838				
H	2.5493085	1.0605181	83.9884463				
C	5.7305080	4.3909642	87.3684567				
C	6.7412662	1.2853869	90.4119881				
C	5.0905291	6.7326208	88.0236859				
H	5.0940121	6.5185504	89.1130094				
C	5.7185487	3.7360275	88.6112841				
C	5.0688255	2.1213279	83.7643049				
H	8.2821960	5.5219222	87.1837180				
C	5.3383688	3.6592802	86.2347013				
C	7.5470610	6.1331971	87.7449135				
H	7.8124255	7.2023060	87.6116200				
H	5.3915895	4.1525334	85.2527294				
C	4.7544482	2.6276805	91.2606636				
H	6.7968804	0.7498455	91.3825681				
H	7.1129800	0.6049178	89.6192416				
C	5.2423971	2.4229472	88.7523270				
C	2.8519512	1.6718287	84.8642825				
C	4.8481480	2.3420291	86.3148028				
H	6.1719937	2.1554168	83.8697212				
H	4.7130646	3.1320699	83.4763988				
C	5.2999515	1.7503117	90.1226528				
C	4.7515287	1.7395305	87.6043160				
C	4.3817428	1.6202289	85.0443281				
H	3.7279676	2.9808226	91.0457879				
H	2.3115551	1.2915710	85.7521778				
H	5.3845468	3.5226796	91.4406106				
H	4.0593957	6.5515023	87.6589506				
H	2.5273064	2.7120867	84.6706133				
H	7.6642104	5.8954644	88.8227946				
H	4.6719278	0.8363589	90.0775247				
H	4.6611888	0.5532918	85.1605067				
H	6.0645547	4.2736440	89.5076697				
Zn	1.6851338	5.6674296	90.1465808				
Br	3.0264303	6.2483841	91.9049756				
C	-3.0434934	3.3814806	81.6976391				
C	-0.2841507	3.9429518	84.8970364				
C	-3.1020346	4.5639907	82.4605732				
C	-1.1903188	2.5796592	83.0429344				
C	-1.2518828	3.7586485	83.8173539				
C	-2.0843076	2.3938905	81.9827240				
C	-2.2018051	4.7591766	83.5115683				
O	-0.1662477	5.0039596	85.5353075				
H	-3.7506886	3.2321705	80.8670449				
H	-0.4276094	1.8210053	83.2773304				
H	-3.8529761	5.3337701	82.2266715				
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14 μ -ma

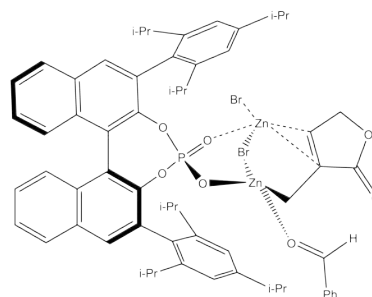


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C	0.7690532	-1.6285665	88.9674499
C	-1.0815800	-0.3156120	89.9149312
C	-1.4615013	-1.4628191	90.6729489
C	-1.7736988	0.9198167	90.0561407
H	-2.6474848	0.9704304	90.7239381
C	-1.3665264	2.0721047	89.3976132
C	3.8604561	1.4081287	86.6934981
C	3.9552540	0.4177515	85.7287540
H	4.8966014	0.2638297	85.1809028
C	2.8402169	-0.4304572	85.4385459
C	2.9306782	-1.4315784	84.4252146
C	1.6061070	-0.3057763	86.1853392
C	0.5107036	-1.1512113	85.8403863
C	1.5251773	0.6704424	87.2454141
C	2.6168600	1.5190064	87.3902491
O	0.0922483	3.1487257	87.8591995
O	2.5132972	2.5460300	88.3201513
P	1.5440146	3.8971659	87.9167323
O	1.9293373	4.7071789	89.1766564
O	1.8341767	4.4191680	86.5223612
C	-0.7490058	-2.6482751	90.5821647
C	0.3863982	-2.7209773	89.7337367
H	-2.3273985	-1.3793700	91.3482443
H	-1.0480690	-3.5233942	91.1786722
H	1.6612968	-1.7039065	88.3316424
H	0.9759243	-3.6493444	89.6867640
C	0.6338225	-2.1086125	84.8444571
C	1.8573096	-2.2620678	84.1407386
H	-0.4411095	-1.0295387	86.3760670
H	-0.2277789	-2.7432921	84.5891624
H	1.9456191	-3.0285226	83.3559220
H	3.8753022	-1.5295301	83.8676382
C	-1.7561647	4.2951420	90.5482739
C	-2.1181145	3.3596714	89.5453123

C	-2.5322758	5.4605065	90.6855817	H	5.1578494	-0.0128162	88.2190295
C	-3.2057689	3.6233442	88.6709982	H	3.7023428	3.4609699	85.0545666
C	-3.9519283	4.7981065	88.8585792	H	6.0526593	2.9403526	90.4330571
C	-3.6354361	5.7297169	89.8609106	Zn	3.4108121	3.6560953	90.0431734
H	-2.2586038	6.2011079	91.4523783	Br	3.4762634	3.3059393	92.3322534
C	-3.5784916	2.6603283	87.5443241	C	-1.3061046	-0.6034911	82.0054373
H	-4.7924214	5.0081942	88.1794304	C	0.1658576	2.6078725	84.3980256
C	-3.8488294	3.3856592	86.2159810	C	-2.1985850	0.1137868	82.8283034
H	-4.7463079	4.0352336	86.2717393	C	0.5462650	0.7530210	82.7964610
H	-4.0421904	2.6482878	85.4081812	C	-0.3468467	1.4809096	83.6126465
H	-2.9847283	4.0134134	85.9246617	C	0.0609554	-0.2814048	81.9859453
C	-4.7648142	1.7675974	87.9532817	C	-1.7248109	1.1603324	83.6234444
H	-2.7066939	1.9937093	87.3732952	O	-0.5564244	3.4201599	84.9908213
H	-5.6663359	2.3815861	88.1602749	H	-1.6844272	-1.4216072	81.3727964
H	-4.5382948	1.1884153	88.8712352	H	1.6142648	1.0189291	82.7892224
H	-5.0205184	1.0470643	87.1478691	H	-3.2679585	-0.1466941	82.8383328
C	-4.4247750	7.0238434	90.0097950	H	0.7531468	-0.8430879	81.3415101
C	-4.2471508	7.9273078	88.7755096	H	-2.3961429	1.7511955	84.2642763
H	-4.7571751	8.9024669	88.9214984	Br	-0.8980496	6.4116914	87.1229148
H	-4.6776379	7.4534137	87.8686709	Zn	0.3173860	5.3890975	85.3822214
H	-3.1758148	8.1145690	88.5635975	H	-0.7010340	2.7494505	80.8782631
C	-5.9113236	6.7632121	90.3089912	H	0.2919559	6.9279498	83.3664279
H	-3.9962836	7.5619159	90.8843018	C	-0.3576580	4.7729571	81.6433986
H	-6.4564298	7.7166635	90.4690970	C	-0.0347895	3.6332267	80.7330485
H	-6.0385126	6.1363158	91.2147181	H	-1.3222148	5.2994678	81.6324362
H	-6.4056173	6.2372220	89.4653389	C	0.7051492	5.0372628	82.4600500
C	-0.5598935	4.0558318	91.4677405	C	0.8933748	6.0130466	83.5377913
C	0.1923475	5.3484682	91.8207690	C	1.7571201	4.0325520	82.1021972
H	1.1371908	5.1039753	92.3456890	O	1.3004797	3.2445757	81.0691815
H	-0.4016813	5.9982743	92.4964472	O	2.8512399	3.8388376	82.6030738
H	0.4433094	5.9218593	90.9077103	H	-0.0689912	3.8994964	79.6513965
C	-0.9714366	3.2931766	92.7412127	H	1.9614542	6.2909495	83.6373243
H	0.1548927	3.4054688	90.9172147	H	1.2805085	2.7240032	84.4242200
H	-0.0840163	3.0891499	93.3753969				
H	-1.4508703	2.3227754	92.5021981				
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H	6.7662176	6.3250114	89.1869272				
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H	5.3742559	3.3726772	83.2760650				
C	6.0983595	5.6905485	89.8114708				
H	4.3536212	-0.7502599	90.4384045				
H	5.1262305	7.4897405	90.6154961				
H	4.1761632	5.5123315	83.8605981				
C	5.7360294	4.4960187	88.9317884				
C	6.7825763	0.2954159	89.5910244				
C	4.8437298	6.5322885	90.1330786				
H	4.1834150	6.0002948	90.8543417				
C	5.6936163	3.1585871	89.4166263				
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H	7.7577547	4.7175820	90.8841806				
C	5.4486070	4.7043472	87.5670073				
C	6.8507081	5.3192597	91.0948162				
H	7.1681510	6.2364051	91.6294766				
H	5.5283265	5.7262463	87.1702675				
C	4.3111195	0.3237240	90.1655467				
H	6.8444957	-0.7801693	89.8535905				
H	7.5504114	0.5067843	88.8199388				
C	5.3198790	2.0776019	88.5717551				
C	4.5195164	5.4304907	84.9084517				
C	5.0163192	3.6752458	86.7128809				
H	5.8665381	2.2160858	84.5563811				
H	6.7074726	3.7876399	84.4198583				
C	5.3667892	0.6403804	89.0911110				
C	4.8721173	2.3640417	87.2558127				
C	4.6798563	3.9478334	85.2550829				
H	3.2797737	0.5305714	89.8159817				
H	3.7613647	5.9138128	85.5549111				
H	4.4753337	0.9123329	91.0907078				
H	4.2455374	6.7616730	89.2293352				
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H	6.2018846	4.7452664	91.7889746				

14*ν*-2-ma

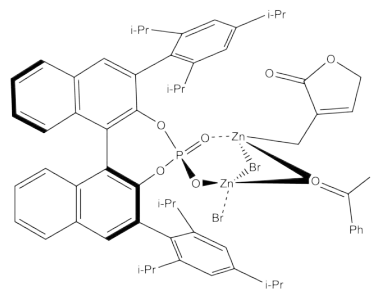


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C	-0.3436652	0.6996270	92.0636916
C	-0.0103262	0.3464575	93.4056860
C	-1.4927925	1.4941453	91.7837328
H	-2.1359862	1.8088512	92.6193436
C	-1.7876412	1.9268665	90.4972746
C	2.5487215	0.8077649	86.6260191
C	2.9978050	-0.5057316	86.5612473
H	3.8312079	-0.7558176	85.8862712
C	2.3926157	-1.5431909	87.3281388
C	2.7855696	-2.9059781	87.1718990
C	1.3661223	-1.2127067	88.2882723
C	0.7496212	-2.2768285	89.0119595
C	0.9839034	0.1685845	88.4649646
C	1.4884820	1.0967005	87.5426490
O	-1.3233331	1.7892778	88.1509016
O	1.0809132	2.4165568	87.5773017
P	-0.4622952	2.9402341	87.3761445

O	-0.4435112	4.2839657	88.1264746	H	5.7223076	2.6907516	89.4520066
O	-1.0087567	2.9001621	85.9472348	H	5.9394559	1.8010575	87.9069807
C	1.1570302	-0.3425360	93.6956013	C	3.8516662	2.9688210	86.5107074
C	2.0471510	-0.6900286	92.6460420	C	0.8728755	1.4917435	83.2030852
H	-0.6949205	0.6524104	94.2124660	C	3.0206075	1.9657917	84.4198784
H	1.4042166	-0.6023058	94.7361721	H	3.9913174	-0.0873274	82.7863919
H	2.4473982	-0.6503263	90.5305894	H	3.2262696	1.0976665	81.6832970
H	2.9919829	-1.2049832	92.8776816	C	4.0776465	2.9655849	88.0229632
C	1.1420623	-3.5945704	88.8220309	C	3.1567153	1.9236423	85.8339633
C	2.1775453	-3.9142112	87.9044461	C	2.2282618	0.9159774	83.6440724
H	-0.0586384	-2.0417117	89.7189135	H	2.4590746	4.3846135	88.4608496
H	0.6413186	-4.3981503	89.3833004	H	0.2808521	1.8288176	84.0758128
H	2.4855919	-4.9618283	87.7667446	H	4.0845582	5.1406700	88.3620065
H	3.5764444	-3.1430406	86.4429660	H	3.2604313	6.6971140	84.0565713
C	-2.7532527	4.2589756	90.6250125	H	0.9958145	2.3641889	82.5289682
C	-2.8767772	2.9080387	90.1887357	H	6.7975569	5.2886376	84.5900129
C	-3.7718338	5.1723799	90.2902252	H	3.5256482	2.1068438	88.4542216
C	-4.0026621	2.5152243	89.4110798	H	2.0115426	0.0761669	84.3335192
C	-4.9819994	3.4728960	89.0958241	H	4.9276163	4.8292690	86.2879836
C	-4.8903617	4.8086737	89.5234945	Zn	-1.4298646	4.2193998	84.4961998
H	-3.6863141	6.2177497	90.6282654	Br	-2.1963099	3.2747884	82.5095033
C	-4.2062561	1.0767565	88.9394671	C	5.4362223	9.8562422	86.6425194
H	-5.8521740	3.1592101	88.4972298	C	1.5592231	8.1297352	86.9356728
C	-4.3844621	0.9821319	87.4135967	C	5.1968185	8.8560130	87.6068063
H	-5.3185251	1.4793555	87.0775976	C	3.1214137	9.7550645	85.9231486
H	-4.4467717	-0.0788747	87.0958330	C	2.8771649	8.7487867	86.8866215
H	-3.5322615	1.4474259	86.8809709	C	4.4024442	10.3064486	85.8027221
C	-5.3796119	0.4196322	89.6910333	C	3.9220624	8.3001262	87.7311284
H	-3.2959627	0.5007114	89.2009551	O	1.2804687	7.1934336	87.7149032
H	-6.3375123	0.9385725	89.4772277	H	6.4449175	10.2861965	86.5431044
H	-5.2215371	0.4482812	90.7882602	H	2.3016994	10.0836270	85.2644619
H	-5.4967906	-0.6412390	89.3872259	H	6.0161194	8.5094610	88.2544207
C	-5.9692217	5.8268888	89.1746662	H	4.6013084	11.0837780	85.0501869
C	-6.1229641	6.0052808	87.6533786	H	3.7063820	7.5061561	88.4616594
H	-6.8805749	6.7819894	87.4210024	Br	0.6670012	5.5202115	84.8882784
H	-6.4539322	5.0633617	87.1676908	Zn	-0.3105963	6.0021753	87.1713533
H	-5.1660784	6.3092479	87.1842245	H	-3.0628168	5.8445581	82.7333802
C	-7.3128811	5.4700095	89.8358831	H	-2.7736146	6.0772462	87.8600718
H	-5.6373343	6.8027680	89.5931847	C	-3.1403396	5.7534313	84.9576187
H	-8.0772159	6.2469854	89.6270940	C	-3.3719257	6.4347932	83.6204675
H	-7.2080501	5.3747395	90.9353055	H	-3.8184400	4.9627070	85.3213028
H	-7.7035993	4.5043911	89.4522418	C	-2.5327851	6.6911399	85.7937946
C	-1.5613105	4.7541907	91.4459208	C	-2.2160410	6.7513287	87.1855170
C	-0.9672646	6.0719829	90.9190124	C	-2.0550595	7.8145802	84.8976619
H	-0.0467688	6.3303478	91.4814003	O	-2.5798739	7.6374210	83.6600562
H	-1.6683454	6.9250572	91.0295152	O	-1.3285681	8.7451354	85.1930304
H	-0.6981355	5.9818435	89.8505402	H	-4.4401637	6.7215679	83.4893353
C	-1.9394817	4.8939537	92.9333961	H	-2.0953467	7.7866704	87.5560707
H	-0.7624627	3.9896232	91.3671719	H	0.7867426	8.5058083	86.2162078
H	-1.0627450	5.2068130	93.5377349				
H	-2.3216935	3.9425173	93.3533956				
H	-2.7350627	5.6565508	93.0682500				
H	4.5027659	5.1438943	82.5214380				
H	6.1944268	3.5711636	87.9631005				
H	2.4384452	-0.4772846	81.9719804				
C	4.8510043	5.2582743	83.5716079				
H	3.6359089	4.1724301	89.7980958				
H	4.7721059	7.4469107	83.4400972				
H	0.2681674	0.7355985	82.6621923				
C	4.2518281	4.1011177	84.3623433				
C	5.5654138	2.7440621	88.3544473				
C	4.3663746	6.6302112	84.0725834				
H	4.6982210	6.8260470	85.1139028				
C	4.3864801	4.0278235	85.7595499				
C	3.0177351	0.3330592	82.4601951				
H	6.7417474	4.2084987	83.1646235				
C	3.5692330	3.0582850	83.7188056				
C	6.3893443	5.1810650	83.5628848				
H	6.8264469	5.9892179	82.9398613				
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C	3.5307553	4.2376515	88.6952739				

14*ν*-ma; COSMO

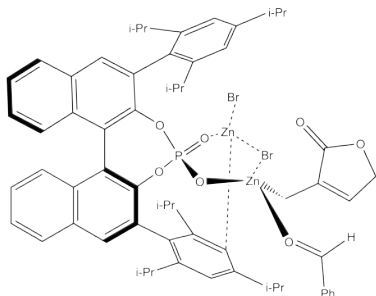


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C	0.9777961	-1.6708260	91.7118197
C	-1.2500953	-0.6293385	91.8169976
C	-1.4753426	-1.3148532	93.0487980
C	-2.1862841	0.3294270	91.3327643

H	-3.0902577	0.5341939	91.9262494	H	6.4716376	6.9899373	84.9317743
C	-1.9333414	1.0771228	90.1903838	H	1.4638164	0.3741288	83.2596488
C	3.2911944	0.4673087	87.6628415	C	5.0436995	3.8386314	85.5504721
C	3.7530256	-0.8284627	87.4574033	C	6.2247729	2.4229088	89.5644849
H	4.6754088	-0.9816657	86.8768040	C	6.1282751	6.1693312	85.5923127
C	3.0206449	-1.9693119	87.8909780	H	6.9672634	5.9131989	86.2734092
C	3.4576147	-3.2899611	87.5689535	C	5.1382065	3.7395728	86.9477636
C	1.7765612	-1.7883606	88.5994578	C	4.1025057	-0.1868711	83.9104159
C	0.9853434	-2.9449799	88.8733309	H	6.5575522	3.5929917	83.2530691
C	1.3724536	-0.4517298	88.9697477	C	4.3408116	2.8221888	84.8740904
C	2.1238860	0.6233250	88.4735196	C	6.8699827	4.4255346	83.9152035
O	-0.6369119	1.3846594	88.1940716	H	7.3000864	5.2259257	83.2780099
O	1.7566530	1.9244210	88.8078997	H	4.2433812	2.8880167	83.7771429
P	0.4621554	2.6044672	88.0589842	C	4.1571659	3.8810043	89.8611833
O	0.1108331	3.8237073	88.9298767	H	6.3390557	2.3418872	90.6654304
O	0.6661153	2.8106136	86.5568134	H	6.6316267	1.4980659	89.1070588
C	-0.5058935	-2.1453874	93.5903549	C	4.5730887	2.6677954	87.6670614
C	0.7380733	-2.3047513	92.9235886	C	1.9870295	1.2030044	83.7799333
H	-2.4295130	-1.1507342	93.5737579	C	3.7758764	1.7188929	85.5370527
H	-0.6882676	-2.6619214	94.5449686	H	4.8691396	-0.6401160	84.5709401
H	1.9491917	-1.7978941	91.2152314	H	4.6360862	0.4476780	83.1716363
H	1.5230943	-2.9315630	93.3734774	C	4.7466058	2.6306097	89.1836668
C	1.4264128	-4.2147892	88.5259646	C	3.9025628	1.6376724	86.9577448
C	2.6823265	-4.3948536	87.8867357	C	3.0752421	0.6403937	84.7072015
H	0.0068610	-2.8236724	89.3578589	H	3.0868518	4.0063916	89.6060602
H	0.7931687	-5.0885903	88.7429962	H	1.2394536	1.7830068	84.3527058
H	3.0262406	-5.4073770	87.6259702	H	4.6939523	4.8032719	89.5556983
H	4.4162764	-3.4110000	87.0404186	H	5.2930483	6.5653621	86.2025994
C	-2.4696857	3.4862033	90.6133618	H	2.4125970	1.8602896	82.9938493
C	-2.6967166	2.3140039	89.8336551	H	7.6765449	4.0436245	84.5761219
C	-3.0710998	4.6996105	90.1961766	H	4.1887158	1.7524877	89.5671447
C	-3.5351831	2.3716186	88.6898722	H	2.5649962	-0.0476473	85.4092062
C	-4.1630217	3.5872966	88.3502742	H	5.6708381	4.5215300	87.5079742
C	-3.9501331	4.7668335	89.0801005	Zn	-1.2331176	5.2791706	88.7093030
H	-2.9458843	5.5971119	90.8222657	Br	-0.8405956	7.4283870	89.5914608
C	-3.7813535	1.1446862	87.8196907	C	2.6513601	4.2114177	79.0965419
H	-4.8195609	3.6125274	87.4696037	C	1.8123025	4.8136691	83.2244031
C	-3.3935829	1.3959759	86.3511894	C	1.5762019	3.5134820	79.6849423
H	-4.0448945	2.1613033	85.8804304	C	3.1375237	5.3021489	81.2093069
H	-3.4984617	0.4615096	85.7626188	C	2.0633136	4.5971702	81.8048494
H	-2.3457453	1.7436272	86.2681209	C	3.4281306	5.1068172	79.8533947
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H	-5.9523211	1.4309535	87.5842018	H	2.8829196	4.0549546	78.0314853
H	-5.4967677	0.4417925	89.0076990	H	3.7155788	6.0135021	81.8215218
H	-5.3997746	-0.2576331	87.3566758	H	0.9758229	2.8182785	79.0790210
C	-4.6458731	6.0872861	88.7703562	H	4.2588518	5.6528157	79.3820768
C	-5.2578825	6.1640778	87.3678180	H	0.4460652	3.1731580	81.5229145
H	-5.6529825	7.1826088	87.1818367	Br	-1.6695051	5.2688327	86.2770583
H	-6.1063613	5.4574299	87.2518033	Zn	0.8159704	4.7102100	85.8916852
H	-4.5094519	5.9398758	86.5821203	H	0.1648026	9.8097407	84.8550069
C	-5.7059328	6.3885724	89.8504209	H	1.8730744	6.1194940	87.7001788
H	-3.8599104	6.8739595	88.8472271	C	0.9628691	8.4467520	86.3708413
H	-6.1683751	7.3809910	89.6737675	C	1.1004212	9.5863214	85.4169269
H	-5.2692472	6.3935739	90.8690441	H	0.2664703	8.4396368	87.2223914
H	-6.5121427	5.6255393	89.8302859	C	1.8197876	7.4463655	86.0185865
C	-1.6633054	3.4664446	91.9108183	C	2.0589324	6.1149040	86.6068382
C	-0.6584368	4.6184335	92.0597347	C	2.5418097	7.9247597	84.8029183
H	-0.0972096	4.4988866	93.0086471	O	2.1072747	9.1803946	84.4765446
H	-1.1455638	5.6139969	92.0889392	O	3.3930158	7.3559410	84.1286235
H	0.0743758	4.6224286	91.2300382	H	1.4283203	10.5342338	85.9010500
C	-2.6347668	3.4295459	93.1093852	H	3.0947845	5.7663754	86.4215202
H	-1.0776521	2.5267165	91.9242665	H	2.5388413	5.4801980	83.7512481
H	-2.0723150	3.3350538	94.0607562				
H	-3.3439677	2.5802822	93.0432401				
H	-3.2344017	4.3625301	93.1596481				
H	4.9181915	5.3357091	84.0440234				
H	6.8537787	3.2716434	89.2231514				
H	3.6018565	-1.0063199	83.3538320				
C	5.6920343	4.9655991	84.7511087				
H	4.2390795	3.7999317	90.9648460				

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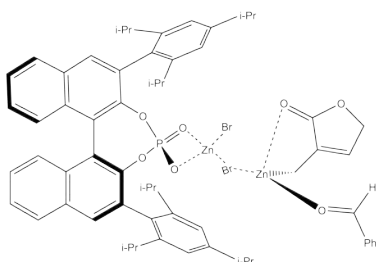
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C	0.9817350	-1.6649784	91.7194741
C	-1.2453068	-0.6236199	91.8300647
C	-1.4643044	-1.3043054	93.0651293
C	-2.1829215	0.3331428	91.3455166
H	-3.0835668	0.5429529	91.9424766
C	-1.9361106	1.0758540	90.1987625
C	3.2812159	0.4636833	87.6593530
C	3.7449187	-0.8319116	87.4584230
H	4.6670858	-0.9838053	86.8771431
C	3.0162115	-1.9728109	87.8969722
C	3.4550200	-3.2936283	87.5802756
C	1.7734265	-1.7917641	88.6072665
C	0.9861280	-2.9490868	88.8881336
C	1.3667374	-0.4547707	88.9727500
C	2.1141679	0.6204894	88.4705581
O	-0.6497036	1.3731060	88.1953658
O	1.7438653	1.9212552	88.7984586
P	0.4465833	2.5941678	88.0469065
O	0.0944795	3.8192764	88.9085976
O	0.6488301	2.7881421	86.5430377
C	-0.4931456	-2.1326820	93.6055840
C	0.7472925	-2.2944623	92.9340921
H	-2.4160607	-1.1378309	93.5937704
H	-0.6715466	-2.6454145	94.5629393
H	1.9504240	-1.7934335	91.2182366
H	1.5343973	-2.9195833	93.3825622
C	1.4297093	-4.2190081	88.5461701
C	2.6839669	-4.3988249	87.9049177
H	0.0089520	-2.8268828	89.3748600
H	0.7992614	-5.0932675	88.7691608
H	3.0301073	-5.4115237	87.6480330
H	4.4126755	-3.4144203	87.0498640
C	-2.4734960	3.4849987	90.6195591
C	-2.7008290	2.3116167	89.8417729
C	-3.0772688	4.6958168	90.2027745
C	-3.5390738	2.3674354	88.6978288
C	-4.1653806	3.5828359	88.3565819
C	-3.9530243	4.7631004	89.0858217
H	-2.9415226	5.5975831	90.8201551
C	-3.7873912	1.1384311	87.8305140
H	-4.8195822	3.6080622	87.4742174
C	-3.4054299	1.3847039	86.3599040
H	-4.0558938	2.1505374	85.8889197
H	-3.5149512	0.4493086	85.7736852
H	-2.3572345	1.7288221	86.2703169
C	-5.2437013	0.6570386	87.9707170
H	-3.1357060	0.3260433	88.2126505
H	-5.9597186	1.4224928	87.6049364
H	-5.4973585	0.4370536	89.0275149
H	-5.4083735	-0.2660199	87.3777941
C	-4.6446882	6.0850623	88.7718199
C	-5.2579722	6.1588340	87.3697604
H	-5.6500539	7.1777915	87.1797425

H	-6.1095827	5.4552544	87.2567771
H	-4.5110570	5.9302644	86.5840688
C	-5.7020263	6.3958559	89.8514098
H	-3.8548086	6.8683856	88.8438893
H	-6.1607948	7.3895847	89.6723933
H	-5.2644319	6.4030545	90.8695084
H	-6.5119905	5.6366770	89.8366098
C	-1.6588185	3.4706504	91.9124044
C	-0.6420547	4.6148832	92.0414005
H	-0.0764131	4.5028085	92.9886541
H	-1.1173075	5.6163529	92.0586656
H	0.0861815	4.6011162	91.2080691
C	-2.6210401	3.4535975	93.1184577
H	-1.0814956	2.5258766	91.9315413
H	-2.0534720	3.3647320	94.0673628
H	-3.3375915	2.6093800	93.0663164
H	-3.2140111	4.3910137	93.1643027
H	4.9167884	5.3177540	84.0251439
H	6.8380307	3.2724336	89.2179218
H	3.6079454	-1.0205037	83.3523926
C	5.6853074	4.9560409	84.7422896
H	4.2189953	3.8047050	90.9550091
H	6.4456811	6.9884894	84.9177886
H	1.4663464	0.3544735	83.2506597
C	5.0355868	3.8304186	85.5422559
C	6.2082085	2.4250529	89.5607290
C	6.1063828	6.1676506	85.5798308
H	6.9438056	5.9222105	86.2667647
C	5.1262643	3.7348573	86.9397192
C	4.1043493	-0.1979514	83.9081384
H	6.5737277	3.5771887	83.2633661
C	4.3356973	2.8117157	84.8668368
C	6.8744452	4.4164908	83.9222913
H	7.3079180	5.2143718	83.2842532
H	4.2412510	2.8751362	83.7693956
C	4.1389569	3.8827072	89.8511049
H	6.3216906	2.3471221	90.6619348
H	6.6161353	1.4995686	89.1059893
C	4.5603223	2.6648611	87.6602795
C	1.9853301	1.1856778	83.7714628
C	3.7701087	1.7095924	85.5307961
H	4.8719789	-0.6467652	84.5703836
H	4.6381122	0.4360065	83.1691375
C	4.7306627	2.6315629	89.1773468
C	3.8923531	1.6325446	86.9518901
C	3.0735775	0.6278938	84.7015728
H	3.0688844	4.0065982	89.5950718
H	1.2332633	1.7622601	84.3416132
H	4.6743227	4.8054581	89.5448792
H	5.2643283	6.5597751	86.1829004
H	2.4104196	1.8438488	82.9856709
H	7.6756766	4.0425877	84.5938608
H	4.1725327	1.7540727	89.5618584
H	2.5635535	-0.0602522	85.4036308
H	5.6565894	4.5189787	87.4989301
Zn	-1.2249607	5.2944969	88.6720799
Br	-0.8761458	7.4304228	89.5767552
C	2.6934632	4.2862113	79.0892900
C	1.8083090	4.8070267	83.2197865
C	1.6392421	3.5452447	79.6614317
C	3.1306268	5.3644477	81.2195932
C	2.0772175	4.6159352	81.7976683
C	3.4343860	5.1968624	79.8626912
C	1.3251143	3.7100192	81.0125931
O	0.8490191	4.2848214	83.8219266
H	2.9366290	4.1516722	78.0237511
H	3.6768267	6.0878582	81.8472622
H	1.0664776	2.8380698	79.0426207
H	4.2482538	5.7774656	79.4032923
H	0.5102494	3.1458824	81.4906548
Br	-1.6903279	5.2455596	86.2489495

Zn	0.7875789	4.6879056	85.8724650
H	0.1869610	9.8206023	84.8872015
H	1.8689500	6.0823964	87.6794126
C	0.9781624	8.4295749	86.3820848
C	1.1250784	9.5764559	85.4372972
H	0.2899182	8.4219795	87.2405787
C	1.8184197	7.4226414	86.0106697
C	2.0453505	6.0829021	86.5844343
C	2.5361862	7.9047320	84.7923637
O	2.1153599	9.1690842	84.4835570
O	3.3713910	7.3291449	84.1048140
H	1.4703203	10.5150596	85.9287217
H	3.0769227	5.7260732	86.3911802
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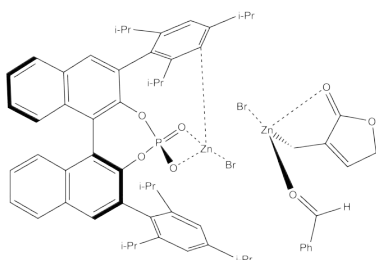
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C	4.7114906	4.1856082	0.1153876
C	2.5122594	5.0522523	0.8064485
C	2.9925208	6.3718342	0.5510850
C	1.1580794	4.8238998	1.1833312
H	0.4865691	5.6881189	1.2990623
C	0.6475895	3.5418778	1.3480292
C	4.1019428	-0.9458105	0.0355605
C	5.3583692	-0.9793379	0.6290918
H	5.9594661	-1.8990794	0.5593338
C	5.8551224	0.1077465	1.4051176
C	7.1094856	0.0151315	2.0796126
C	5.0455048	1.2911086	1.5820798
C	5.5021165	2.2874994	2.4965151
C	3.8005906	1.3966629	0.8583844
C	3.3805005	0.2870005	0.1164305
O	1.0576072	1.1826691	1.4987743
O	2.1945546	0.3709227	-0.5990526
P	0.7682766	0.2119908	0.2027467
O	-0.3436058	0.6917131	-0.7499831
O	0.4613612	-1.2099425	0.7086427
C	4.2832729	6.5866825	0.0932881
C	5.1411795	5.4798322	-0.1424981
H	2.3056075	7.2185603	0.7075019
H	4.6377248	7.6094529	-0.1063446
H	5.3820739	3.3380371	-0.0815782
H	6.1540612	5.6475585	-0.5394069
C	6.7190489	2.1575457	3.1517071
C	7.5414961	1.0216678	2.9296443
H	4.8722931	3.1672111	2.6866073
H	7.0446661	2.9400768	3.8540782
H	8.5085376	0.9328739	3.4477950
H	7.7207482	-0.8881097	1.9255012
C	-1.7317480	3.5070849	0.5025166
C	-0.8111046	3.2780074	1.5651620
C	-3.0973465	3.2524380	0.7317294
C	-1.2747377	2.7686366	2.8098889
C	-2.6502161	2.5388226	2.9830924

C	-3.5831793	2.7811375	1.9607127
H	-3.8108811	3.4211717	-0.0906560
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H	-3.0031260	2.1562997	3.9541958
C	-0.4037072	1.0105161	4.4200439
H	-1.3987707	0.7609387	4.8443924
H	0.3528843	0.8023558	5.2046270
H	-0.2131992	0.3295176	3.5680815
C	-0.5870859	3.4468928	5.1484363
H	0.7052356	2.6699108	3.6271406
H	-1.6086973	3.3177238	5.5636194
H	-0.4867891	4.5041562	4.8291945
H	0.1343628	3.2659196	5.9721112
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C	-5.3953892	1.1043992	2.5661018
H	-6.4909555	0.9524989	2.6618969
H	-4.9329837	0.8278854	3.5362061
H	-5.0138897	0.3943070	1.8067779
C	-5.6410860	3.5497731	3.2149072
H	-5.5764725	2.7614440	1.2120509
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H	-5.4417201	4.5989396	2.9172326
H	-5.1798695	3.3937596	4.2123490
C	-1.2989529	4.0304927	-0.8677686
C	-1.8888071	3.2258159	-2.0389425
H	-1.4685240	3.5940554	-2.9976381
H	-2.9913976	3.3222622	-2.1093965
H	-1.6392514	2.1532558	-1.9421222
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H	-0.1968645	3.9263555	-0.9299820
H	-1.2811860	5.9220411	-1.9832823
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H	-2.7360546	5.6890533	-0.9608143
H	1.5884995	-6.4864133	-1.5775992
H	4.1733298	-2.6267803	-4.4329683
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C	1.0318943	-5.5669495	-1.8752205
H	2.6533580	0.1952092	-4.3678705
H	-0.8978686	-6.4768275	-1.3531664
H	2.2820875	-3.1726968	3.8122097
C	1.9028571	-4.3846686	-1.4485856
C	4.5684861	-1.7758355	-3.8390986
C	-0.3043762	-5.5733958	-1.1019339
H	-0.9092031	-4.6821620	-1.3677418
C	2.2946945	-3.3550020	-2.3192016
C	4.4356687	-4.1388098	2.2813860
H	1.7138815	-5.6811311	-3.9682140
C	2.3139754	-4.2881539	-0.1075328
C	0.7718409	-5.6479663	-3.3842716
H	0.1885905	-6.5596293	-3.6270147
H	2.0229023	-5.0870534	0.5932938
C	2.3051534	-0.6199596	-3.7002045
H	4.9261583	-1.0038060	-4.5520393
H	5.4418677	-2.1464877	-3.2648037
C	3.0528265	-2.2507738	-1.8830824
C	2.0609609	-3.3513647	2.7393357
C	3.0379274	-3.1937851	0.3906595
H	5.3738987	-3.9520335	1.7202389
H	4.1243955	-5.1826039	2.0651233
C	3.4862990	-1.2013041	-2.9046439
C	3.4219660	-2.1601562	-0.5152389
C	3.3295694	-3.1412371	1.8915915
H	1.5296497	-0.2069391	-3.0272871
H	1.2609693	-2.6567080	2.4178393
H	1.8206809	-1.3870451	-4.3391577
H	-0.1498983	-5.5606256	-0.0048555
H	1.6725742	-4.3881771	2.6545785
H	0.1783112	-4.7772086	-3.7325205
H	3.9537691	-0.3635739	-2.3474760
H	3.7015656	-2.1245148	2.1276632
H	1.9953208	-3.3953715	-3.3757027

Zn	-1.1736023	-1.2369432	-0.6475252	H	-2.2652464	-1.2696512	93.0452089
Br	-1.3101242	-2.1584130	-2.7890097	H	-0.4492938	-2.6327161	94.0896644
H	-6.9812659	3.1127334	-2.6040076	H	2.2593408	-1.5056127	90.8972176
Br	-2.8803880	-1.6246014	1.0886922	H	1.8296828	-2.7024369	93.0245377
H	-7.2722416	-1.4475640	-1.0234772	C	1.8650122	-3.8883798	88.1197229
Zn	-4.8495172	-1.5955451	-0.3331843	C	3.1751682	-4.0325885	87.5929169
C	-7.1436650	1.7377426	-0.9040575	H	0.3487995	-2.5448887	88.8475147
C	-6.3924943	2.7246511	-1.7435213	H	1.2270358	-4.7758405	88.2495273
C	-6.4977615	0.5413808	-0.9279042	H	3.5577990	-5.0314710	87.3339739
C	-6.6983707	-0.7987254	-0.3233646	H	4.9594519	-2.9954596	86.9357768
C	-5.2766169	0.7584971	-1.7503338	C	-2.7351255	3.3601583	89.9233720
O	-5.2494789	2.0084430	-2.2528536	C	-2.6740318	2.1435785	89.1819970
O	-4.3650001	-0.0574281	-1.9274453	C	-3.1652323	4.5355956	89.2535763
H	-6.0110312	3.6013331	-1.1730410	C	-3.1491883	2.1106480	87.8385110
H	-7.2554905	-0.7576276	0.6309714	C	-3.5964993	3.2947461	87.2210827
H	-8.0751597	1.9827764	-0.3752812	C	-3.5968461	4.5256051	87.8989009
C	-3.3287590	-6.9674776	-3.2264647	H	-3.2734004	5.4724330	89.8235938
C	-3.7172463	-5.7961497	-2.5696972	C	-3.2014124	0.8038322	87.0549219
C	-3.7495220	-4.5723396	-3.2760756	H	-3.9320986	3.2592461	86.1732131
C	-3.3895100	-4.5348127	-4.6422651	C	-2.5229985	0.9040524	85.6790279
C	-2.9976184	-5.7087440	-5.2939851	H	-3.0681356	1.5720322	84.9841685
C	-2.9666065	-6.9239295	-4.5858509	H	-2.4498201	-0.0996709	85.2135739
H	-3.2958981	-7.9213771	-2.6788226	H	-1.4913852	1.2921041	85.8115571
H	-3.9885067	-5.7971067	-1.5037446	C	-4.6627376	0.3306498	86.9248709
C	-4.1345935	-3.3330512	-2.5978201	H	-2.6594955	0.0358694	87.6437790
H	-3.3947197	-3.5719263	-5.1769295	H	-5.2672550	1.0581130	86.3443619
H	-2.7054214	-5.6805524	-6.3542450	H	-5.1391840	0.2089016	87.9186489
H	-2.6510102	-7.8462347	-5.0975561	H	-4.7083615	-0.6440583	86.3975411
O	-4.4774506	-3.3071054	-1.3961350	C	-4.1379277	5.7979857	87.2650661
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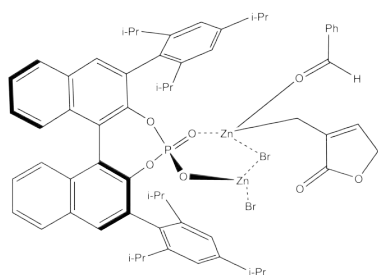


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C	0.2357683	-0.7124062	90.7081282	H	3.5897229	0.8810245	82.6941848
C	1.2610482	-1.4646613	91.3534792	C	5.8682640	4.3730922	86.2415391
C	-1.0529204	-0.6183074	91.3567870	C	6.1048598	2.5122317	90.1911581
C	-1.2746613	-1.3383136	92.5685711	C	6.2687690	6.8908020	86.4815527
C	-2.0661388	0.2365769	90.8250667	H	6.5668103	6.8755777	87.5502863
H	-3.0237908	0.3133647	91.3609453	C	5.5719541	4.1649976	87.5981412
C	-1.8369566	1.0117317	89.6979931	C	5.7695119	0.3757967	84.2969772
C	3.7078155	0.8383532	87.5555037	H	8.4669182	4.4097380	85.3303476
C	4.2210233	-0.4416432	87.3925983	C	5.4801980	3.3772926	85.3298133
H	5.2299094	-0.5620594	86.9725178	C	8.1727028	5.3212183	85.8881850
C	3.4641942	-1.6052916	87.6929084	H	8.7633897	6.1750773	85.4953837
C	3.9550522	-2.9071795	87.3787376	H	5.7319881	3.5136787	84.2647834
C	2.1607760	-1.4595705	88.2853685	C	4.0419846	4.0003003	90.2609863
C	1.3722943	-2.6363111	88.4599085	H	5.9992284	2.3004913	91.2755493
C	1.6834122	-0.1401455	88.6414872	H	6.5788641	1.6311883	89.7127781
C	2.4177318	0.9641693	88.1719278	C	4.8915103	3.0210057	88.0500189
O	-0.3670369	1.5858644	87.8875274	C	3.8334529	1.7130893	83.3861415
O	2.0155144	2.2856905	88.3672273				
P	0.5290443	2.9260025	88.2123595				
O	0.1594383	3.6067957	89.5572849				
O	0.2574366	3.9358380	87.0807602				
C	-0.2644671	-2.0886981	93.1509766				
C	1.0180225	-2.1342759	92.5451503				

C	4.7927528	2.2119854	85.7210217	H	4.8102058	-2.1771116	0.7814700
H	6.2637291	-0.0581051	85.1894056	C	4.7493382	-0.2235688	1.7488467
H	6.5112570	1.0416720	83.8072209	C	5.7598689	-0.5368608	2.7067254
C	4.7330994	2.8202382	89.5579824	C	4.1082373	1.0703132	1.7976912
C	4.4707008	2.0440515	87.1022280	C	4.4646926	1.9580416	2.8571898
C	4.4872263	1.1524817	84.6590009	C	3.1132945	1.3939415	0.8014752
H	3.0307985	4.1821110	89.8493167	C	2.7322677	0.3820353	-0.0845886
H	2.8882047	2.2349220	83.6236401	O	0.2987130	1.6307365	0.7729381
H	4.6278963	4.9383516	90.1684550	O	1.7770275	0.6607063	-1.0556829
H	5.1749945	7.0673965	86.4438078	P	0.2063390	0.8158035	-0.6479110
H	4.5001379	2.4125392	82.8386503	O	-0.4021505	1.6502877	-1.7936406
H	8.4572604	5.1686919	86.9503695	O	-0.4888255	-0.5143921	-0.3385572
H	4.1023091	1.9246644	89.7227760	C	4.5589266	6.4527041	0.5463225
H	3.7578717	0.4358068	85.0866940	C	5.2585357	5.2284899	0.3786726
H	5.8946309	4.9110738	88.3402904	H	2.6303005	7.3859882	0.8560563
Zn	-0.9054884	5.0704389	88.5775493	H	5.1044568	7.4075563	0.5021034
Br	-0.8371572	7.3721778	88.5310616	H	5.1350723	3.0754145	0.3026960
C	2.3982933	7.6845428	84.5579601	H	6.3430992	5.2395482	0.1915282
C	0.2987672	3.9697326	84.5755127	C	5.4387400	1.6141791	3.7843943
C	3.1073109	6.4860391	84.3448663	C	6.1066958	0.3641037	3.7015897
C	0.3278873	6.4385059	84.7618158	H	3.9505459	2.9250091	2.9414647
C	1.0359594	5.2340869	84.5533086	H	5.6901588	2.3161486	4.5940269
C	1.0090672	7.6616024	84.7686725	H	6.8837426	0.1059401	4.4370289
C	2.4339649	5.2618292	84.3482315	H	6.2482769	-1.5223225	2.6489320
O	0.8162613	2.8674060	84.3207084	C	-2.0529079	4.1507045	-0.0048101
H	2.9384090	8.6440032	84.5695981	C	-1.1742344	3.9319444	1.0920194
H	-0.7595556	6.4049174	84.9245392	C	-3.4268917	3.9092834	0.1789451
H	4.1958606	6.5094668	84.1893936	C	-1.6893076	3.5009638	2.3453722
H	0.4579486	8.5951003	84.9547206	C	-3.0692884	3.2610967	2.4680762
H	2.9775854	4.3163808	84.2146384	C	-3.9563158	3.4415765	1.3936731
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Zn	-0.1344287	1.0999322	83.7348728	C	-0.7844838	3.2865101	3.5585872
H	-0.5491167	6.0600287	82.0733819	H	-3.4612124	2.9089608	3.4357635
H	-0.9058654	1.1590485	81.3022510	C	-0.7482396	1.8116944	3.9976005
C	-0.7752222	4.0030233	81.3550767	H	-1.7454653	1.4671008	4.3417458
C	-1.3066731	5.3735431	81.6282521	H	-0.0360776	1.6695979	4.8367847
H	0.0651500	3.8080999	80.6742271	H	-0.4347920	1.1572603	3.1610302
C	-1.4808568	3.0793315	82.0682288	C	-1.1789642	4.2138979	4.7223744
C	-1.3427817	1.6226675	82.2095998	H	0.2473946	3.5654235	3.2620078
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O	-2.3627355	5.1885482	82.5786375	H	-1.1683853	5.2778910	4.4106345
O	-3.3272856	3.4424894	83.6492518	H	-0.4760588	4.0965377	5.5730462
H	-1.7229940	5.8777731	80.7260762	C	-5.4468061	3.1592733	1.5376485
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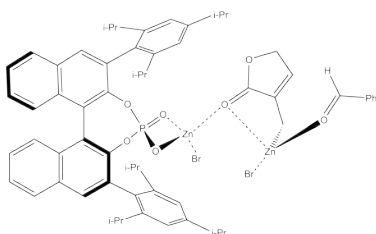
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C	3.1775074	3.9680074	0.6715476	C	4.9145806	-1.3302826	-3.7089123
C	4.5850331	4.0166235	0.4418217				
C	2.4600800	5.2151693	0.7976845				
C	3.1869766	6.4419700	0.7468758				
C	1.0432032	5.2049637	0.9595724				
H	0.5187512	6.1606492	1.1101293				
C	0.3128998	4.0246595	0.9242874				
C	3.2915348	-0.9321115	-0.1016415				
C	4.3291507	-1.1870675	0.7867661				

C	0.5680024	-4.5367333	-5.0081251
H	1.5159393	-4.3982418	-5.5688208
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C	2.6307628	-4.3708323	1.5970244
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C	1.3305692	-3.9686386	-1.2895657
C	1.6786202	-6.2622649	-3.5232258
H	1.1944387	-7.0783707	-4.0991504
H	0.7319476	-4.7869466	-0.8558213
C	2.7994796	0.0358499	-4.0976844
H	5.5295829	-0.5195380	-4.1517423
H	5.5334513	-1.8606534	-2.9568563
C	2.8195314	-1.8679700	-2.4082325
C	0.2984576	-3.3822157	1.5147413
C	1.9325288	-3.0352277	-0.4275424
H	3.6993582	-4.2320968	1.3362968
H	2.3058640	-5.3345450	1.1514215
C	3.6311434	-0.7598216	-3.0758682
C	2.6953772	-1.9732228	-0.9970152
C	1.7626276	-3.2062278	1.0828428
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H	2.3097122	-2.7446765	-4.3128834
Zn	-1.8648582	0.7382312	-2.7267988
Br	-1.5666427	-0.2908472	-4.7668420
H	-3.2447593	-5.4418526	2.4317892
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H	-3.5368987	-0.2127982	2.6514024
Zn	-2.2810878	-0.8224481	0.5518614
C	-2.9062749	-3.4559847	3.2874232
C	-3.7953349	-4.6072404	2.9271781
C	-3.3089581	-2.3468106	2.6131035
C	-2.7603631	-0.9872983	2.4856065
C	-4.4899473	-2.7494921	1.7856064
O	-4.7543967	-4.0848263	2.0026872
O	-5.1338545	-2.0743954	1.0071335
H	-4.3338271	-5.0435674	3.7999732
H	-1.9003087	-0.8038402	3.1551252
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C	-3.2057128	-6.4697366	-2.2782512
C	-2.9569336	-5.2732883	-1.6022527
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C	-2.9521532	-5.3251927	-4.4260195
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H	-3.4145036	-7.3909104	-1.7136351
H	-2.9790022	-5.2109974	-0.5036812
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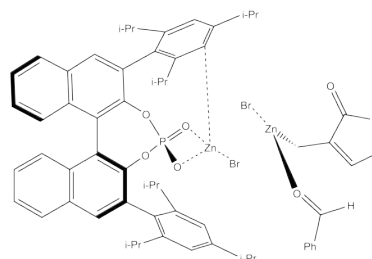
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O	0.0949994	2.4731053	87.7034459
O	2.3570135	2.6147872	88.8902963
P	1.4344049	3.4453182	87.8197919
O	1.2325447	4.8660065	88.3496471
O	2.0757907	3.4731507	86.4122677
C	-1.1649240	-0.9130819	93.0548971
C	0.1524922	-1.2251364	92.6248051
H	-2.9608852	0.2241618	92.6425256
H	-1.5579889	-1.3531778	93.9839380
H	1.6846395	-0.9252225	91.1360624
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H	-0.0335166	-1.8344628	88.9717796
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C	-2.6757460	4.3852759	88.6522192
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H	-3.6714436	6.2407837	88.1337712
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C	-2.3709726	0.7205386	85.9206615
H	-2.7575778	1.1945469	84.9927682
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H	-2.9322000	0.3982936	87.9681001
H	-5.1630367	0.6064845	85.8393136
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H	-6.2594507	6.0186810	84.3197422
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C	-1.7781999	5.0398106	89.6981135
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H	-0.8383140	6.4171942	88.2778565
C	-2.4818346	5.0739851	91.0685959
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14ζ-2-ma



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H	4.8267502	-0.1770910	83.5755990
C	6.7908897	5.6776731	85.7703565
H	4.6214811	3.9039016	91.5847131
H	7.7707735	7.5416139	86.3263687
H	2.9031324	1.4422914	83.1343491
C	6.0753861	4.4620002	86.3543810
C	6.6782095	2.4826074	90.2865121
C	7.3256203	6.6552916	86.8215349
H	8.1195787	6.1911224	87.4448165
C	5.9927156	4.2037290	87.7319485
C	5.2680056	0.5496569	84.2894135
H	7.5385700	4.6083004	83.9865713
C	5.4582595	3.5386228	85.4870013
C	7.9156614	5.2499752	84.8068900
H	8.3880797	6.1394660	84.3417561
H	5.4832771	3.7419663	84.4055241
C	4.7378308	4.1183108	90.5022712
H	6.6514159	2.2961662	91.3803923
H	7.0449396	1.5622825	89.7883603
C	5.3152368	3.0816548	88.2495308
C	3.3945727	2.1799348	83.8027683
C	4.7923951	2.3903635	85.9451226
H	5.8223574	-0.0209013	85.0614720
H	6.0118316	1.1610622	83.7369467
C	5.2857921	2.8841045	89.7636517
C	4.7128363	2.1584792	87.3545936
C	4.1785034	1.4483861	84.9074356
H	3.7501690	4.4190734	90.1018267
H	2.6154744	2.8245240	84.2489345
H	5.4212561	4.9878269	90.4104355
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H	4.6043849	2.0369703	89.9831367
H	3.4535513	0.7932001	85.4315001
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Zn	2.4830844	5.4779614	86.5627835
Br	3.6133745	7.4460393	86.9069225
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C	-1.0028573	8.8739854	86.6272381
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O	1.1201555	7.4862217	82.5495391
H	-3.1681308	8.7304748	86.7424277
H	1.1414324	8.8721714	86.2298516
H	-3.4404216	8.0211164	84.3559076
H	-0.8891437	9.1750636	87.6788822
H	-1.3896556	7.7210504	82.9011680
Br	4.5297343	6.1425533	82.3797495
Zn	2.2846965	5.6248192	82.3166473
H	-2.4767880	5.2374496	85.1921663
H	0.1609057	4.4728571	81.1617424
C	-1.4098925	4.1400847	83.6058093
C	-1.6895916	4.4709765	85.0322559
H	-2.1573645	3.6898471	82.9379137
C	-0.1154734	4.4535025	83.3000471
C	0.7472378	4.3539844	82.0937020
C	0.4302269	5.0210683	84.5423347
O	-0.4562530	5.0271349	85.5336455
O	1.5724113	5.5114904	84.6845828
H	-1.9533870	3.5939482	85.6616605
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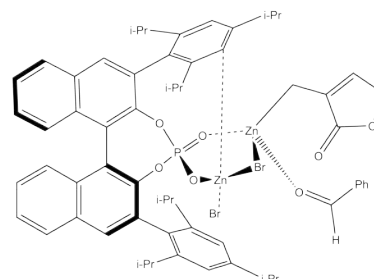
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C	-1.0119995	-0.5276833	91.1054345
C	-1.2512881	-1.3966439	92.2116151
C	-1.9992593	0.4237994	90.7042463
H	-2.9501784	0.4595399	91.2562901
C	-1.7499125	1.3361537	89.6897653
C	3.7664221	1.2473092	87.4516044
C	4.2247017	-0.0204560	87.1190922
H	5.2221928	-0.1240211	86.6686644
C	3.4259831	-1.1826335	87.2825448
C	3.8586781	-2.4507677	86.7936621
C	2.1385071	-1.0627651	87.9133190
C	1.3039176	-2.2201568	87.9473438
C	1.7202811	0.2177345	88.4451204
C	2.4917069	1.3452158	88.1042137
O	-0.2659510	2.1042163	87.9654887
O	2.1509419	2.6500446	88.4643984
P	0.6805249	3.3446347	88.4836498
O	0.3710118	3.8097481	89.9289804
O	0.4151766	4.5355240	87.5391479
C	-0.2638093	-2.2510387	92.6782556
C	1.0133061	-2.2563895	92.0595654
H	-2.2364744	-1.3605029	92.7027892
H	-0.4620982	-2.9101110	93.5370553
H	2.2660311	-1.4526352	90.4984085
H	1.8079233	-2.9099711	92.4504300
C	1.7393565	-3.4356917	87.4385338
C	3.0355124	-3.5626189	86.8741896
H	0.2894993	-2.1401073	88.3602024
H	1.0659646	-4.3059614	87.4631795
H	3.3724374	-4.5336362	86.4807444
H	4.8525648	-2.5198463	86.3243612
C	-2.5524920	3.6640726	90.2467522
C	-2.5413425	2.5615814	89.3422788
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C	-3.0112486	2.7394886	88.0080875
C	-3.3939690	4.0187288	87.5618749
C	-3.3347348	5.1426128	88.4023012
H	-2.9926250	5.7930055	90.4435677
C	-3.1227547	1.5597511	87.0485985
H	-3.7208335	4.1461968	86.5183276
C	-2.4422295	1.8224432	85.6955774
H	-2.9528657	2.6079150	85.1053174
H	-2.4180547	0.8928682	85.0918160
H	-1.3939102	2.1402732	85.8747740
C	-4.6042142	1.1753529	86.8645724
H	-2.6152495	0.6929771	87.5190919
H	-5.1758045	2.0038770	86.3972150
H	-5.0844254	0.9363356	87.8349519
H	-4.6948116	0.2876971	86.2057089
C	-3.7753030	6.5214367	87.9353322
C	-3.0339831	6.9714316	86.6675642
H	-3.3366055	8.0011934	86.3886119
H	-3.2385047	6.3124098	85.7992505

14ζ-ma

H	-1.9410605	6.9880113	86.8525997	H	-0.0933964	7.2616410	82.6551395
C	-5.3034841	6.5571844	87.7450532	H	-0.7330303	2.4905383	81.4188351
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H	-5.6356173	7.5794676	87.4715600	C	-0.8892662	6.6677594	82.1478969
H	-5.8370589	6.2572998	88.6696214	H	0.3874362	5.1219015	81.0421862
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C	-2.2217964	3.5046364	91.7269351	C	-1.1510597	2.8879355	82.3655753
C	-1.5411444	4.7178987	92.3768266	C	-2.1704691	5.1051521	83.2280054
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H	-2.1878591	5.6191679	92.3910127	O	-3.0203424	4.6754015	83.9889512
H	-0.5903391	4.9752647	91.8703585	H	-1.2716427	7.2805453	81.2995352
C	-3.5146078	3.1431850	92.4901998	H	-2.1626627	2.4606371	82.5208598
H	-1.5177154	2.6526979	91.8122100	H	-0.6135143	4.9412325	85.2002074
H	-3.2916102	2.9263367	93.5549909				
H	-4.0216399	2.2586656	92.0560892				
H	-4.2377712	3.9847609	92.4576971				
H	6.7587425	6.3250664	85.2543012				
H	7.0115697	3.2413834	90.2650608				
H	5.3303027	0.3917287	83.2757042				
C	7.1215487	5.9094448	86.2226173				
H	4.1628524	3.7142905	91.5592041				
H	7.6893170	7.9136126	86.8869568				
H	3.4946349	2.0288667	82.6622602				
C	6.2035683	4.7399535	86.5665177				
C	6.2558952	2.4281747	90.2693733				
C	7.1068155	7.0450041	87.2552685				
H	7.5676475	6.7302863	88.2145111				
C	5.8818608	4.3942805	87.8879092				
C	5.6640709	1.0795399	84.0798627				
H	8.5888164	4.6179864	85.2060358				
C	5.7096316	3.9156999	85.5398680				
C	8.5594803	5.4033727	85.9874216				
H	9.2294915	6.2304759	85.6727054				
H	5.9607601	4.1682905	84.4962942				
C	4.2998258	4.0388715	90.5072228				
H	6.1234821	2.0967854	91.3202677				
H	6.6742696	1.5797300	89.6907538				
C	5.0970640	3.2683746	88.2000631				
C	3.8657503	2.7253789	83.4423770				
C	4.9137401	2.7818447	85.7887129				
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H	6.4603111	1.7316632	83.6623580				
C	4.9152473	2.9022955	89.6737568				
C	4.5917053	2.4590913	87.1435899				
C	4.4804827	1.9201491	84.5997654				
H	3.3072036	4.3355160	90.1177665				
H	3.0068864	3.3302339	83.7874037				
H	4.9490539	4.9390092	90.5230840				
H	6.0768771	7.3897825	87.4798645				
H	4.6023620	3.4003748	82.9576949				
H	8.9717584	4.9627206	86.9191241				
H	4.2228609	2.0398683	89.7325658				
H	3.6897912	1.2256817	84.9479219				
H	6.2687374	5.0070862	88.7155213				
Zn	-0.6372543	5.4711662	89.1941348				
Br	-0.4464861	7.7366838	89.5546976				
C	2.7375426	8.3935844	85.7669075				
C	0.4902519	4.8348976	85.0747313				
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C	0.6111075	7.2854393	85.4022191				
C	1.2819709	6.0473814	85.2853365				
C	1.3397424	8.4576852	85.6392169				
C	2.6873326	5.9869538	85.4176441				
O	0.9791219	3.7385374	84.7437373				
H	3.3115659	9.3113515	85.9683030				
H	-0.4848468	7.3176567	85.3063692				
H	4.4997080	7.1106562	85.7750119				
H	0.8160969	9.4195815	85.7422468				
H	3.1977913	5.0144411	85.3684496				
Br	0.9523319	0.1794444	84.6431618				
Zn	-0.0026823	2.1307638	83.8366562				

14 γ -int1-mi

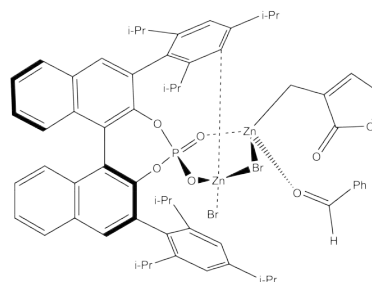


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C	2.7478854	4.3942788	2.0400832
C	3.5123961	5.5855278	2.2232407
C	1.3259101	4.4170097	2.0989495
H	0.8197150	5.3706566	2.3123422
C	0.5581834	3.2906591	1.8258200
C	3.3578937	-1.5301339	0.1356831
C	4.4175638	-1.9583942	0.9245060
H	4.8477588	-2.9573701	0.7544820
C	4.9019320	-1.1782244	2.0138524
C	5.9306412	-1.6732309	2.8702023
C	4.2863429	0.0942243	2.3107600
C	4.6778576	0.7654653	3.5081337
C	3.2840190	0.6137239	1.4091313
C	2.8602433	-0.2088611	0.3600373
O	0.4750591	0.9161766	1.4465217
O	1.9110695	0.2694099	-0.5351092
P	0.3317725	0.2838117	-0.0659975
O	-0.3683486	1.2345122	-1.0373979
O	-0.2076901	-1.1377886	0.1571938
C	4.8899120	5.5803397	2.0686513
C	5.5544398	4.3784424	1.7071872
H	2.9797936	6.5172044	2.4709249
H	5.4666493	6.5077260	2.2052392
H	5.3686720	2.2792798	1.2533018
H	6.6437078	4.3821473	1.5491808
C	5.6673648	0.2464240	4.3314964
C	6.3159633	-0.9729882	4.0027914
H	4.1796257	1.7052162	3.7819662
H	5.9464342	0.7838269	5.2506447
H	7.1064154	-1.3696825	4.6578608
H	6.3993715	-2.6386862	2.6224936
C	-1.4952268	4.0577641	0.5770189
C	-0.9297615	3.3548573	1.6798568
C	-2.8974262	4.0929720	0.4429092
C	-1.7775427	2.6983683	2.6140642

C	-3.1693568	2.7630003	2.4293129	H	1.8791077	-2.8667269	-4.1224195
C	-3.7569862	3.4669350	1.3606884	Zn	-1.0055699	-2.4323410	-1.1158975
H	-3.3289611	4.6470104	-0.4035698	Br	-2.5964638	-4.0634315	-0.5877494
C	-1.2221493	1.9992673	3.8535325	H	-3.1344722	-3.1646048	3.4674578
H	-3.8287316	2.2658259	3.1603383	H	-5.3121434	-2.6850565	4.6180965
C	-1.6574630	0.5287649	3.9448801	C	-3.8075214	-2.3873060	3.0758993
H	-2.7572947	0.4273045	4.0521572	C	-5.0310265	-2.1174949	3.7172738
H	-1.1931908	0.0376576	4.8250128	C	-3.4444604	-1.6666879	1.9357272
H	-1.3496313	-0.0290465	3.0401038	C	-5.9026402	-1.1327141	3.2153996
C	-1.5922545	2.7829036	5.1272485	H	-2.4941684	-1.8548090	1.4194391
H	-0.1158360	2.0107359	3.7797908	H	-6.8607895	-0.9348469	3.7187428
H	-2.6914950	2.8082470	5.2806224	C	-4.3141677	-0.6738779	1.4272370
H	-1.2379875	3.8322253	5.0715871	C	-5.5483304	-0.4142968	2.0680805
H	-1.1382532	2.3129867	6.0242939	H	-5.1339181	-1.4882012	-5.1500974
C	-5.2745084	3.6156673	1.3014982	H	-3.4729077	0.5655593	-5.7991492
C	-5.7239527	4.7016635	2.3017732	C	-5.4166973	-0.4123543	-5.0781976
H	-6.8304832	4.7811193	2.3313472	C	-4.2295761	0.4946285	-5.0057211
H	-5.3174000	5.6914512	2.0060830	H	-6.2245461	0.3473608	1.6481245
H	-5.3640140	4.4862778	3.3279249	C	-3.9557266	0.0959225	0.2409273
C	-5.8391880	3.8930834	-0.0968860	O	-2.9085296	-0.1099966	-0.4016653
H	-5.7023704	2.6501491	1.6559080	H	-6.1015814	-0.1909702	-5.9287354
H	-6.9469462	3.9226881	-0.0620705	Br	-1.3281284	-1.2194956	-3.2193688
H	-5.5558445	3.1114323	-0.8293990	C	-4.2311620	1.1522975	-3.8141839
H	-5.5034656	4.8781998	-0.4829716	O	-6.1289254	-0.2118747	-3.8527158
C	-0.6418633	4.8244656	-0.4354363	H	-2.6308843	2.5904317	-3.9207717
C	-0.9767905	4.4905025	-1.8973002	Zn	-2.0814949	0.9401068	-2.0211693
H	-0.3005135	5.0438208	-2.5806618	C	-3.2622085	2.0608726	-3.1810727
H	-2.0159636	4.7691900	-2.1674938	C	-5.4500036	0.6923311	-3.0798074
H	-0.8477901	3.4097994	-2.0918816	H	-3.7679027	2.8006864	-2.5284597
C	-0.7467634	6.3421270	-0.1858535	O	-5.8489672	1.0146222	-1.9720768
H	0.4145972	4.5302140	-0.2772329	H	-4.6724481	0.8767668	-0.1055079
H	-0.0799292	6.9024208	-0.8735926				
H	-0.4700007	6.6098748	0.8536476				
H	-1.7839983	6.7011503	-0.3525778				
H	-0.8784283	-4.9562858	-2.9277851				
H	4.2884227	-2.4129192	-4.4793043				
H	2.6008333	-5.2845980	2.5788591				
C	0.1330805	-4.9326839	-3.3952298				
H	3.3816133	0.6344769	-4.0840223				
H	-0.7286974	-5.1244708	-5.3855440				
H	0.4206242	-4.0864442	2.9489306				
C	0.9764177	-4.0102108	-2.5215187				
C	4.6748119	-1.8087018	-3.6319663				
C	-0.0259757	-4.4602452	-4.8439129				
H	0.9388093	-4.4884452	-5.3932062				
C	1.8393427	-3.0297571	-3.0365321				
C	2.5325797	-5.0641902	1.4936439				
H	0.7657785	-6.7496560	-2.3080539				
C	0.9376084	-4.1738529	-1.1133559				
C	0.6969592	-6.3678583	-3.3461080				
H	0.0490964	-7.0613972	-3.9202024				
H	0.2926810	-4.9614615	-0.6938590				
C	2.7213335	-0.1727009	-3.7056988				
H	5.3492552	-1.0342898	-4.0520989				
H	5.2797154	-2.4798628	-2.9892078				
C	2.6381077	-2.2222928	-2.2037580				
C	0.3397640	-3.8436842	1.8695010				
C	1.7616126	-3.4279637	-0.2407513				
H	3.5633723	-5.0038359	1.0896608				
H	2.0335947	-5.9259071	1.0029309				
C	3.5262548	-1.1572428	-2.8388344				
C	2.6114580	-2.4284527	-0.7994509				
C	1.7451395	-3.7600919	1.2516890				
H	1.9021043	0.2934185	-3.1254016				
H	-0.1872837	-2.8753800	1.7749329				
H	2.2710490	-0.6742737	-4.5872338				
H	-0.4255382	-3.4282691	-4.8961141				
H	-0.2946248	-4.6227584	1.4002253				
H	1.7148667	-6.4045944	-3.7880673				
H	3.9880254	-0.5745560	-2.0155446				
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14 γ -int2-mi; COSMO

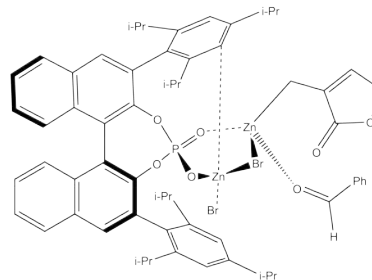


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C	2.5096011	4.3424496	1.3669868
C	3.1377311	5.6205111	1.4711202
C	1.0954904	4.2086676	1.4418839
H	0.4866743	5.1086145	1.6166915
C	0.4545803	2.9903012	1.2391217
C	3.8447809	-1.5886034	-0.0831469
C	4.9199667	-1.8228026	0.7640511
H	5.4794669	-2.7668563	0.6805950
C	5.2635023	-0.9110084	1.8035566
C	6.3117460	-1.2111898	2.7249776
C	4.4876529	0.2941211	1.9811508
C	4.7502643	1.0976368	3.1318206
C	3.4652525	0.6167687	1.0119648
C	3.1797229	-0.3287773	0.0233908
O	0.6296548	0.6074483	0.9503856
O	2.2127523	-0.0368295	-0.9338179
P	0.6262021	-0.1545170	-0.5067108
O	-0.1394560	0.6317833	-1.5751951
O	0.2271428	-1.6030703	-0.1819816

C	4.5089281	5.7548299	1.3154173	C	3.3894716	-2.5648559	-2.3866085
C	5.3034819	4.6105510	1.0352005	C	1.0042460	-4.1739484	1.6751095
H	2.5054872	6.5025650	1.6590004	C	2.4884220	-3.6770048	-0.3792376
H	4.9809328	6.7463686	1.3895129	H	4.4302869	-4.7733943	1.2021708
H	5.3518209	2.4782976	0.7223897	H	3.0962235	-5.9625177	1.1181510
H	6.3871407	4.7230276	0.8780721	C	4.1927237	-1.4562340	-3.0572692
C	5.7627702	0.7666501	4.0223299	C	3.2637144	-2.6389455	-0.9758386
C	6.5657767	-0.3856450	3.8098829	C	2.4110543	-3.8747623	1.1345207
H	4.1336749	1.9875284	3.3168390	H	2.4377742	-0.2211989	-3.5198121
H	5.9399435	1.4014064	4.9039334	H	0.3038761	-3.3468167	1.4501104
H	7.3722774	-0.6317735	4.5172425	H	2.9795237	-1.2458734	-4.8863452
H	6.9025422	-2.1272023	2.5673963	H	0.6644041	-4.3531448	-5.1221707
C	-1.7130214	3.5525646	0.0820167	H	0.5741310	-5.1095675	1.2639764
C	-1.0386659	2.9198569	1.1653458	H	3.0981000	-6.9248468	-3.6636689
C	-3.1202031	3.5840348	0.0811938	H	4.5420605	-0.7697050	-2.2588411
C	-1.7937020	2.2926265	2.1927376	H	2.7442967	-2.9317115	1.6107880
C	-3.1991975	2.3662527	2.1483399	H	2.8800466	-3.4763485	-4.2809915
C	-3.8954636	3.0224394	1.1139812	Zn	-0.1842706	-3.1383466	-1.3751142
H	-3.6268537	4.0687989	-0.7632113	Br	-1.6947416	-4.8853094	-0.9020566
C	-1.1331997	1.5878495	3.3770510	H	-3.6369022	-4.1051146	2.7518232
H	-3.7619493	1.9039481	2.9717658	H	-5.5078002	-3.0267959	4.0290351
C	-1.4949954	0.0919840	3.4237749	C	-4.0182788	-3.1196922	2.4444061
H	-2.5838013	-0.0624633	3.5764695	C	-5.0704771	-2.5131424	3.1588252
H	-0.9659799	-0.4111034	4.2596078	C	-3.4555613	-2.4720594	1.3412961
H	-1.2061932	-0.4162591	2.4833135	C	-5.5686075	-1.2562875	2.7684276
C	-1.4608367	2.2929145	4.7062000	H	-2.6375350	-2.9342585	0.7683136
H	-0.0349072	1.6550714	3.2414018	H	-6.3942895	-0.7896625	3.3264635
H	-2.5460978	2.2475286	4.9357033	C	-3.9438221	-1.2016869	0.9532132
H	-1.1686166	3.3623285	4.6768055	C	-5.0029700	-0.5981190	1.6703184
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C	-5.4265139	3.1146165	1.0978530	H	-5.0989312	-1.5711716	-2.9952517
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H	-5.6761932	3.8823597	3.1395460	H	-5.3746907	0.3886438	1.3575506
H	-5.8267068	2.1040634	3.0339678	C	-3.3442557	-0.4872355	-0.1699304
C	-5.9472201	4.3430447	0.3316623	O	-2.4967838	-0.9954998	-0.9250646
H	-5.7979936	2.2290607	0.5266741	H	-7.4257463	-0.2167788	-2.4982666
H	-7.0530435	4.3903469	0.3979797	Br	-0.5112932	-2.1091634	-3.5866686
H	-5.6882754	4.2954278	-0.7433385	C	-4.4708503	0.5416389	-3.1134748
H	-5.5374766	5.2834271	0.7566343	O	-6.2724652	1.4015912	-1.8899284
C	-0.9693486	4.2348343	-1.0680706	H	-3.1475371	-0.0800784	-4.6859990
C	-1.4089960	3.7134547	-2.4460149	Zn	-1.6926154	-0.0378802	-2.6393779
H	-0.8180504	4.2018988	-3.2481878	C	-3.1812301	0.6134657	-3.8216730
H	-2.4826002	3.8985984	-2.6486049	C	-5.1312094	1.7696326	-2.5702271
H	-1.2413529	2.6227586	-2.5192771	H	-2.9807244	1.6463563	-4.1658723
C	-1.1203732	5.7664638	-0.9911817	O	-4.7951359	2.9359548	-2.6654951
H	0.1080245	3.9972319	-0.9618758	H	-3.6612435	0.5773334	-0.3130521
H	-0.5340862	6.2591771	-1.7942736				
H	-0.7721104	6.1678643	-0.0180290				
H	-2.1816653	6.0675899	-1.1149355				
H	0.2907963	-5.7774674	-3.0597203				
H	5.1755185	-2.7226185	-4.5680142				
H	3.4231421	-5.0921342	2.6529203				
C	1.3169835	-5.6545030	-3.4765725				
H	3.9172471	0.2130738	-4.4425255				
H	0.6050304	-6.1075400	-5.4836143				
H	1.0478861	-4.2882118	2.7773827				
C	1.9770760	-4.5636011	-2.6428825				
C	5.4462738	-2.0259997	-3.7471385				
C	1.1857661	-5.3183568	-4.9657189				
H	2.1769463	-5.2619092	-5.4629368				
C	2.7643894	-3.5402922	-3.1900551				
C	3.3993566	-4.9852858	1.5490130				
H	2.1143261	-7.2784827	-2.2075470				
C	1.8311405	-4.5980344	-1.2298683				
C	2.0595186	-6.9923026	-3.2769636				
H	1.5430054	-7.8087590	-3.8217780				
H	1.2706316	-5.4322282	-0.7800279				
C	3.3296626	-0.6327031	-4.0302518				
H	6.0528310	-1.2084317	-4.1880236				
H	6.0852683	-2.5809178	-3.0304486				

14 γ -int2-mi

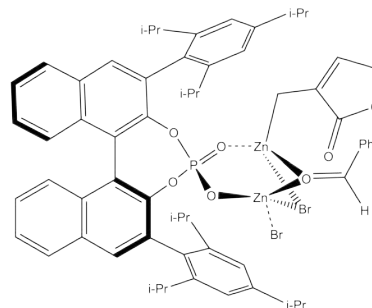


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C	3.3305233	3.1825806	1.1290758
C	4.7334863	3.3668243	0.9391621
C	2.5163266	4.3498728	1.3619379
C	3.1409991	5.6291807	1.4655121
C	1.1033340	4.2108494	1.4403671
H	0.4905335	5.1078315	1.6165665
C	0.4649561	2.9911464	1.2377412

C	3.8643284	-1.5796126	-0.0881750	C	1.9829139	-4.5669381	-2.6217512
C	4.9412749	-1.8093173	0.7577489	C	5.4377073	-2.0237007	-3.7601031
H	5.4996696	-2.7542876	0.6761750	C	1.1737826	-5.3296706	-4.9362536
C	5.2862926	-0.8947317	1.7938982	H	2.1617319	-5.2784403	-5.4406734
C	6.3368474	-1.1898434	2.7136011	C	2.7603642	-3.5413132	-3.1793294
C	4.5083310	0.3090226	1.9703225	C	3.4228520	-4.9834379	1.5641718
C	4.7720734	1.1153563	3.1185124	H	2.1128565	-7.2816988	-2.1765402
C	3.4832139	0.6278171	1.0026980	C	1.8546738	-4.6001083	-1.2081780
C	3.1980869	-0.3198580	0.0157833	C	2.0518065	-6.9994590	-3.2465378
O	0.6474151	0.6104314	0.9429300	H	1.5290774	-7.8168501	-3.7839620
O	2.2309886	-0.0318411	-0.9407515	H	1.2914743	-5.4283962	-0.7511544
P	0.6448306	-0.1504733	-0.5151194	C	3.3159558	-0.6370329	-4.0378638
O	-0.1229426	0.6345283	-1.5825012	H	6.0398965	-1.2077887	-4.2099762
O	0.2469694	-1.5989994	-0.1887697	H	6.0824928	-2.5730795	-3.0444965
C	4.5109045	5.7681877	1.3074834	C	3.3914445	-2.5629416	-2.3850965
C	5.3081311	4.6270096	1.0250840	C	1.0369132	-4.1445583	1.6974794
H	2.5060478	6.5089716	1.6547636	C	2.5148553	-3.6744377	-0.3667799
H	4.9796777	6.7612189	1.3813102	H	4.4545338	-4.7838382	1.2119419
H	5.3616976	2.4949975	0.7102166	H	3.1093396	-5.9597744	1.1388799
H	6.3911130	4.7427820	0.8660551	C	4.1862381	-1.4542702	-3.0663554
C	5.7875093	0.7890974	4.0067355	C	3.2807245	-2.6350778	-0.9729697
C	6.5921737	-0.3615019	3.7953784	C	2.4446362	-3.8648915	1.1485900
H	4.1536811	2.0042055	3.3017948	H	2.4280904	-0.2216830	-3.5239944
H	5.9654627	1.4267024	4.8860592	H	0.3458586	-3.3102669	1.4710108
H	7.4010452	-0.6043289	4.5010940	H	2.9590819	-1.2545313	-4.8879774
H	6.9289153	-2.1052163	2.5569302	H	0.6529721	-4.3645365	-5.0938890
C	-1.7046979	3.5722006	0.0961537	H	0.5914964	-5.0755764	1.2923299
C	-1.0284006	2.9213376	1.1675010	H	3.0883582	-6.9386648	-3.6396517
C	-3.1111039	3.6157947	0.1049215	H	4.5381128	-0.7630700	-2.2730388
C	-1.7828091	2.2835938	2.1889537	H	2.7909999	-2.9236703	1.6189557
C	-3.1879630	2.3668946	2.1523458	H	2.8621025	-3.4779571	-4.2716327
C	-3.8850316	3.0447807	1.1328090	Zn	-0.2047100	-3.1311737	-1.3682746
H	-3.6189084	4.1159442	-0.7293401	Br	-1.6653964	-4.8979395	-0.8583206
C	-1.1228806	1.5565168	3.3600842	H	-3.8742070	-4.1666284	2.6175972
H	-3.7492108	1.8959975	2.9720515	H	-5.7323982	-3.0424044	3.8775653
C	-1.4954833	0.0627408	3.3851184	C	-4.2008021	-3.1544555	2.3350623
H	-2.5846389	-0.0865701	3.5408284	C	-5.2445851	-2.5222891	3.0384420
H	-0.9665533	-0.4581830	4.2099105	C	-3.5741446	-2.4997082	1.2712435
H	-1.2138992	-0.4332975	2.4358941	C	-5.6705724	-1.2312240	2.6764727
C	-1.4401865	2.2437440	4.7008767	H	-2.7617316	-2.9848055	0.7081017
H	-0.0247137	1.6175624	3.2215649	H	-6.4896199	-0.7425782	3.2255109
H	-2.5247956	2.2041108	4.9339613	C	-3.9903695	-1.1959246	0.9126430
H	-1.1403222	3.3111409	4.6861658	H	-5.0415382	-0.5655700	1.6181118
H	-0.9019916	1.7460980	5.5340688	C	-6.4849997	-0.5915297	-0.9671020
C	-5.4153349	3.1500569	1.1251105	H	-5.0685594	-1.6219884	-3.0429063
C	-6.0291382	3.0759420	2.5333613	C	-6.4278804	-0.1170804	-1.9747132
H	-7.1319908	3.1734121	2.4777473	C	-5.2483928	-0.5710568	-2.7754474
H	-5.6464163	3.8949970	3.1775186	H	-5.3549353	0.4475510	1.3272879
H	-5.8125703	2.1200696	3.0519767	C	-3.3293319	-0.4764334	-0.1734590
C	-5.9286219	4.3915697	0.3754855	O	-2.4787059	-0.9983730	-0.9151483
H	-5.7984149	2.2759328	0.5439733	H	-7.4050101	-0.3011953	-2.4783574
H	-7.0329162	4.4528183	0.4538131	Br	-0.5162028	-2.1147181	-3.5854886
H	-5.6824827	4.3458584	-0.7023990	C	-4.4618174	0.0984305	-3.0882965
H	-5.5021644	5.3232328	0.8028242	O	-6.2567826	1.2951064	-1.8096490
C	-0.9659490	4.2541677	-1.0573541	H	-3.1355594	-0.0597680	-4.6821226
C	-1.4080773	3.7208746	-2.4303813	Zn	-1.6776017	-0.0440589	-2.6335978
H	-0.8280813	4.2119226	-3.2388693	C	-3.1786180	0.6106887	-3.8005204
H	-2.4852767	3.8916883	-2.6266928	C	-5.1235010	1.7005369	-2.4874619
H	-1.2251533	2.6323256	-2.4982887	H	-2.9972375	1.6561926	-4.1156214
C	-1.1237350	5.7851673	-0.9886655	O	-4.7913495	2.8683718	-2.5350763
H	0.1128011	4.0221930	-0.9536562	H	-3.6009957	0.6031543	-0.2978184
H	-0.5412286	6.2763531	-1.7953110				
H	-0.7754339	6.1936212	-0.0184043				
H	-2.1860143	6.0823451	-1.1116683				
H	0.2895055	-5.7764471	-3.0230124				
H	5.1648385	-2.7264024	-4.5750054				
H	3.4509875	-5.0869148	2.6683310				
C	1.3137098	-5.6595948	-3.4466230				
H	3.8997015	0.2065462	-4.4599034				
H	0.5878203	-6.1192526	-5.4475403				
H	1.0837178	-4.2542622	2.8001480				

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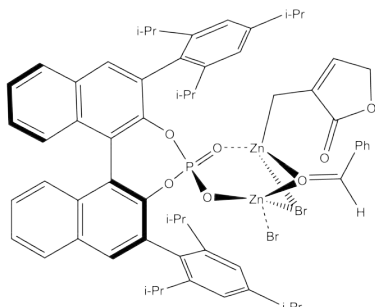


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C	4.5670961	3.4413689	1.1737649
C	2.2446531	4.2484700	1.3459859
C	2.7518822	5.5800979	1.4342194
C	0.8426170	3.9954206	1.3306276
H	0.1494441	4.8435955	1.4374063
C	0.3302000	2.7172347	1.1384593
C	4.2393252	-1.6304894	0.4252978
C	5.2159006	-1.7010202	1.4115410
H	5.8702005	-2.5851715	1.4574508
C	5.3423265	-0.6994801	2.4158926
C	6.2886552	-0.8401140	3.4757371
C	4.4556554	0.4405085	2.4040227
C	4.5098541	1.3417728	3.5104603
C	3.5347252	0.6000622	1.3000942
C	3.4450398	-0.4444697	0.3726133
O	0.7350685	0.3726556	0.8935885
O	2.5802508	-0.3274832	-0.7072600
P	0.9531478	-0.4112300	-0.5253142
O	4.0222200	0.3621004	-1.7343717
O	0.4293711	-1.8265687	-0.2531690
C	4.1154050	5.8293119	1.3876570
C	5.0269484	4.7496016	1.2402806
H	2.0335991	6.4103121	1.5227936
H	4.4922716	6.8617107	1.4479860
H	5.2822258	2.6158135	1.0516468
H	6.1069059	4.9512375	1.1723182
C	5.4270591	1.1651667	4.5378109
C	6.3398868	0.0772901	4.5142476
H	3.8055356	2.1833633	3.5530494
H	5.4412771	1.8730272	5.3806854
H	7.0698102	-0.0464181	5.3287324
H	6.9665124	-1.7081547	3.4608752
C	-1.8509626	2.9419042	-0.1198579
C	-1.1352649	2.4409656	1.0064042
C	-3.2304788	2.6829615	-0.2139945
C	-1.8139953	1.6598440	1.9839751
C	-3.1945043	1.4290869	1.8370154
C	-3.9292020	1.9424076	0.7562454
H	-3.7879040	3.0679962	-1.0840895
C	-1.1141232	1.0849889	3.2153001
H	-3.7107412	0.8279614	2.6000015
C	-1.2451059	-0.4483626	3.2847116
H	-2.3010664	-0.7661689	3.4066043
H	-0.6716563	-0.8459183	4.1483775
H	-0.8514707	-0.9216171	2.3639514
C	-1.6249919	1.7553676	4.5047177
H	-0.0338768	1.3214161	3.1404730
H	-2.7041855	1.5519898	4.6667253
H	-1.4924350	2.8557659	4.4651567
H	-1.0746541	1.3741190	5.3899863
C	-5.4390807	1.7743022	0.6383893
C	-5.9830873	0.5008938	1.3004772
H	-7.0530904	0.3603817	1.0424986
H	-5.9270203	0.5643390	2.4076918
H	-5.4228998	-0.4053353	0.9930490
C	-6.1552141	3.0296285	1.1773605
H	-5.6612599	1.7149897	-0.4501727
H	-7.2539608	2.9509717	1.0393351
H	-5.8072556	3.9481554	0.6628215
H	-5.9548784	3.1560513	2.2621889
C	-1.1737886	3.7393685	-1.2342273
C	-1.4801707	3.1669253	-2.6259580
H	-0.8760302	3.6748146	-3.4045922
H	-2.5478827	3.2848380	-2.9036908
H	-1.2329509	2.0905409	-2.6707610
C	-1.5455807	5.2322751	-1.1607172
H	-0.0781265	3.6550527	-1.0887510
H	-1.0185426	5.8085924	-1.9491660
H	-1.2829848	5.6757146	-0.1790125
H	-2.6367781	5.3763621	-1.3078898
H	3.4178067	-7.1185228	-2.4513217
H	6.2488650	-2.6300670	-3.8222455
H	3.6363304	-5.0574977	3.3943750
C	2.9673876	-6.2442728	-2.9758837
H	4.4769816	-0.0037873	-4.0500367
H	1.1997968	-7.4269884	-3.5282836
H	1.2206483	-4.3974137	2.8495419
C	3.3221180	-5.0191657	-2.1337203
C	6.2802007	-1.8607837	-3.0224162
C	1.4421696	-6.4758939	-3.0106579
H	0.9344926	-5.6513839	-3.5517636
C	3.8992086	-3.8549453	-2.6660390
C	3.8862147	-5.0218366	2.3135281
H	4.6371499	-6.0728933	-4.4018178
C	3.0487043	-5.0352396	-0.7532814
C	3.5375083	-6.2145656	-4.3985083
H	3.3157853	-7.1654350	-4.9237131
H	2.5949417	-5.9394403	-0.3149279
C	3.9983259	-0.9150869	-3.6363059
H	6.7760117	-0.9607564	-3.4417135
H	6.9156292	-2.2540527	-2.2028205
C	4.2094544	-2.7361181	-1.8673344
C	1.4798903	-4.4126787	1.7702397
C	3.3274076	-3.9452281	0.0871939
H	4.9507485	-4.7267223	2.2182922
H	3.7893131	-6.0516355	1.9095583
C	4.8654488	-1.5195920	-2.5174865
C	3.9343116	-2.7849345	-0.4767517
C	2.9589429	-4.0444854	1.5681425
H	2.9976455	-0.6322356	-3.2568832
H	0.8197624	-3.6940905	1.2471516
H	3.8526720	-1.6265415	-4.4752919
H	1.0072307	-6.5222629	-1.9917359
H	1.2529603	-5.4314530	1.3909582
H	3.0865593	-5.3952637	-4.9968885
H	4.9813100	-0.7421718	-1.7345773
H	3.0999721	-3.0423141	2.0194361
H	4.1182694	-3.8024753	-3.7421430
Zn	-0.1691140	-0.4106145	-3.4611022
Br	-0.1174083	0.8460293	-5.4106807
C	-5.8740677	1.5497039	-4.1991984
C	-3.1394912	-0.9838912	-2.1522831
C	-4.5356029	1.5028575	-4.6383432
C	-5.3842391	-0.0667474	-2.4587170
C	-4.0319992	-0.1076529	-2.8869814
C	-6.3005599	0.7624892	-3.1140456
C	-3.6148706	0.6772521	-3.9903653
O	-1.9104714	-1.1423831	-2.3662325
H	-6.5938224	2.2050853	-4.7137190
H	-5.6971799	-0.6864742	-1.6039662
H	-4.2106756	2.1154199	-5.4925233
H	-7.3480520	0.8007941	-2.7802111
H	-2.5722477	0.6387802	-4.3409186
Br	0.4912791	-2.7880658	-3.5655156
Zn	-0.7574548	-2.9319112	-1.3880854
H	-3.1142650	-4.7071690	3.6874692
H	-2.9258820	-4.2617426	-1.3467961
C	-1.9006430	-4.6589650	1.8616647
C	-2.5453979	-4.0041185	3.0388013
H	-1.1569447	-5.4608919	1.9543726
C	-2.3646572	-4.0997994	0.7102297
C	-2.0200264	-4.3233445	-0.7078184
C	-3.3785324	-3.0845177	1.1229134
O	-3.4618892	-3.0474923	2.4861829
O	-4.0815077	-2.3668682	0.4237061
H	-1.8205528	-3.4608569	3.6871333
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H -3.5899160 -1.5746656 -1.3183081

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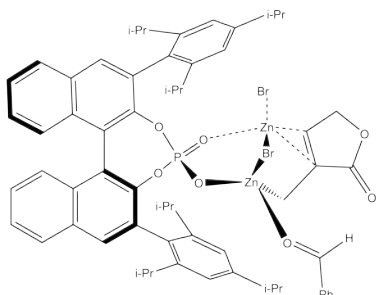
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C	4.5564074	3.4375174	1.1730449
C	2.2330920	4.2414974	1.3397580
C	2.7387130	5.5733470	1.4257133
C	0.8319042	3.9856885	1.3242378
H	0.1360778	4.8318577	1.4292312
C	0.3213631	2.7066195	1.1350785
C	4.2398706	-1.6344478	0.4317712
C	5.2154162	-1.7008904	1.4190269
H	5.8708991	-2.5841873	1.4655189
C	5.3389549	-0.6980843	2.4220490
C	6.2844467	-0.8338249	3.4825983
C	4.4498149	0.4397269	2.4073017
C	4.5018977	1.3434821	3.5114911
C	3.5290687	0.5953702	1.3027309
C	3.4418678	-0.4508683	0.3768580
O	0.7296765	0.3624873	0.8939352
O	2.5780398	-0.3391036	-0.7030889
P	0.9508984	-0.4209408	-0.5253640
O	0.3994183	0.3514048	-1.7335173
O	0.4262561	-1.8370349	-0.2540251
C	4.1013936	5.8244820	1.3812463
C	5.0142000	4.7460614	1.2380412
H	2.0189557	6.4026469	1.5106177
H	4.4765073	6.8575563	1.4398627
H	5.2719181	2.6119752	1.0542371
H	6.0939981	4.9487641	1.1717564
C	5.4191266	1.1714179	4.5389896
C	6.3336795	0.0857205	4.5185860
H	3.7958682	2.1836812	3.5505706
H	5.4317529	1.8816926	5.3797796
H	7.0636527	-0.0347030	5.3334425
H	6.9639247	-1.7006182	3.4699908
C	-1.8640677	2.9208677	-0.1173894
C	-1.1443119	2.4286479	1.0094272
C	-3.2449507	2.6658595	-0.2007432
C	-1.8191817	1.6570281	1.9968940
C	-3.2006609	1.4282143	1.8595924
C	-3.9401292	1.9362595	0.7797536
H	-3.8064328	3.0458063	-1.0704890
C	-1.1122995	1.0907197	3.2281020
H	-3.7143344	0.8340161	2.6297897
C	-1.2384986	-0.4425524	3.3053187
H	-2.2932984	-0.7629666	3.4302237
H	-0.6615611	-0.8338121	4.1696316

H	-0.8446732	-0.9181195	2.3858097
C	-1.6186476	1.7663494	4.5162708
H	-0.0330517	1.3295862	3.1467998
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14ν-2-mi; COSMO



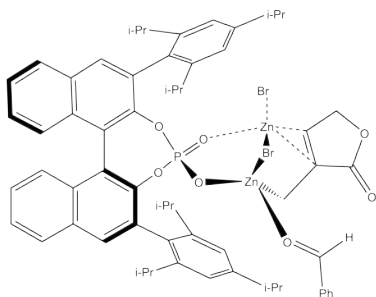
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Zn	0.4661472	5.7501975	87.7152189
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14ν-2-mi



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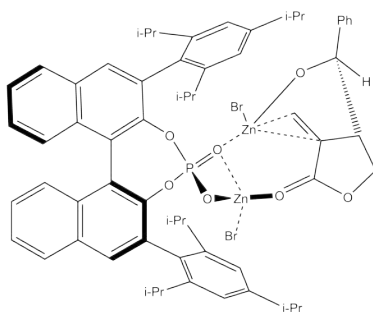
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H	3.8099100	6.4351552	85.7210461	O	2.9854112	2.6255691	89.2686102
H	1.5184217	2.0340791	82.4700368	P	1.8415849	3.6921751	88.8429054
H	6.9098018	4.5382391	84.5288053	O	1.8173198	4.7346997	89.9826759
H	3.8381223	1.3270647	88.9273066	O	2.0250402	4.4406418	87.4880629
H	1.5591173	0.0728486	84.8549573	C	0.0333296	-2.3515498	92.4928441
H	5.1277483	4.2550656	86.9766513	C	1.2443791	-2.4487816	91.7579399
Zn	0.4796635	5.7174268	87.6737895	H	-1.7546058	-1.1845399	92.8519997
Br	1.9905654	7.0445935	88.8343001	H	-0.2172181	-3.1173566	93.2425494
C	-2.1768783	4.5075878	78.5018197	H	2.5134855	-1.5796619	90.2461297
C	-1.8498101	4.6324887	82.7442923	H	1.9350838	-3.2837784	91.9503902
C	-1.7904739	3.3441158	79.1978688	C	1.4447860	-2.7609340	86.7690730
C	-2.3472260	5.7324630	80.5890248	C	2.6509623	-2.9296681	86.0396299
C	-1.9639143	4.5660749	81.2921420	H	0.3318230	-1.5438583	88.1589792
C	-2.4546909	5.6996911	79.1935547	H	0.6318243	-3.4945668	86.6584157
C	-1.6830988	3.3683771	80.5900098	H	2.7748351	-3.7996419	85.3770519
O	-1.5401295	3.6439606	83.4425076	H	4.5913944	-2.0933770	85.5687718
H	-2.2591790	4.4829256	77.4040972	C	-1.8588060	4.2400894	90.6424766
H	-2.5557798	6.6568416	81.1514001	C	-1.9581200	3.0113878	89.9308057
H	-1.5718200	2.4194892	78.6427796	C	-2.7081460	5.2956349	90.2750984
H	-2.7526635	6.6027149	78.6403206	C	-2.9077252	2.8616581	88.8869247
H	-1.3777514	2.4789949	81.1620325	C	-3.7322105	3.9574677	88.5555832
Br	0.8604258	5.4052604	85.2449515	C	-3.6454782	5.1851150	89.2295957
Zn	-1.1776121	3.9508505	85.4495993	H	-2.6382040	6.2509096	90.8176518
H	-0.4095912	8.5300056	87.9695451	C	-3.0733671	1.5485951	88.1208429
H	-2.9796053	4.2107034	87.3355817	H	-4.4617499	3.8350270	87.7413925
C	-1.6301824	6.6813968	87.9756595	C	-2.7136417	1.6885286	86.6315057
C	-1.4391014	8.1642282	87.7663364	H	-3.3475056	2.4479244	86.1263177
H	-1.7018187	6.2233180	88.9757041	H	-2.8648304	0.7253231	86.1023297
C	-2.2054256	6.1506326	86.8304221	H	-1.6508138	1.9693409	86.4928189
C	-2.7080692	4.8467645	86.4734077	C	-4.4874263	0.9707191	88.3137370
C	-2.1823251	7.2521451	85.7960189	H	-2.3634626	0.8152024	88.5538063
O	-1.7404046	8.3973833	86.3796923	H	-5.2642131	1.6335031	87.8782548
O	-2.5131551	7.1912697	84.6257457	H	-4.7257298	0.8389439	89.3888206
H	-2.1451063	8.7629264	88.3861246	H	-4.5769800	-0.0173636	87.8171672
H	-3.5198726	4.9184511	85.7227009	C	-4.4920318	6.4006007	88.8577788
H	-2.0555020	5.6193432	83.2331481	C	-3.6384972	7.4469903	88.1118355
				H	-4.2268108	8.3634467	87.8983297
				H	-3.2835420	7.0342571	87.1438683
				H	-2.7481843	7.7418252	88.7020659
				C	-5.7593235	6.0655766	88.0625105
				H	-4.8110920	6.8645176	89.8185881
				H	-6.3825967	6.9721273	87.9257407
				H	-6.3765676	5.3001839	88.5744435
				H	-5.5163860	5.6825372	87.0490787
				C	-0.8903959	4.3933486	91.8135094
				C	-0.3896252	5.8304392	92.0202830
				H	0.4525889	5.8398882	92.7404515
				H	-1.1811326	6.4899637	92.4336997
				H	-0.0362057	6.2747822	91.0710783
				C	-1.5197683	3.8534475	93.1132771
				H	-0.0007366	3.7697005	91.5851064
				H	-0.8074907	3.9402970	93.9596678

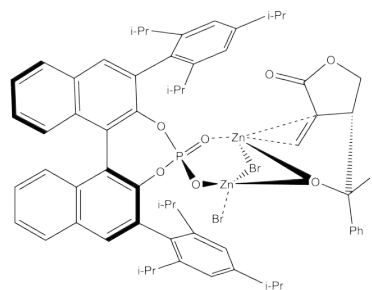
6.2 Product Complexes 15

15c-ma



Energy (Hartree) = -11970.02055173

H	-1.8067864	2.7880796	93.0206434
H	-2.4330897	4.4286376	93.3728197
H	8.3886619	6.1310943	87.7190454
H	8.1342572	1.2272249	90.9122995
H	4.8045621	2.5991333	83.6823885
C	8.2218878	5.6249905	88.6957137
H	5.2647211	1.1085027	92.2876527
H	8.1401837	7.5383499	89.7798722
H	3.6916500	4.8131812	84.4130411
C	7.3034907	4.4404276	88.4235058
C	7.3511363	0.5521394	90.5086146
C	7.5157525	6.6339194	89.6239078
H	7.3205572	6.1794752	90.6181929
C	7.1277840	3.4080366	89.3591614
C	5.4472060	2.6139107	84.5865104
H	10.1004775	4.4846440	88.5888009
C	6.5331930	4.4001747	87.2493143
C	9.5963113	5.2187985	89.2491704
H	10.2559149	6.1053026	89.3466963
H	6.6605804	5.2091095	86.5139453
C	5.4502666	1.9029107	91.5350462
H	7.1964415	-0.2575702	91.2515764
H	7.7494792	0.0959055	89.5798629
C	6.1996515	2.3701887	89.1592379
C	4.4352872	4.8347807	85.2350544
C	5.5886133	3.3885608	86.9998253
H	5.6393541	1.5644121	84.8817166
H	6.4206906	3.0730648	84.3145885
C	6.0352070	1.3038655	90.2417518
C	5.4200113	2.3643371	87.9706202
C	4.7667901	3.4121989	85.7141151
H	4.4928840	2.4233257	91.3360994
H	4.0258256	5.4563851	86.0566376
H	6.1471062	2.6387048	91.9885160
H	6.5391894	6.9529535	89.2063680
H	5.3318132	5.3549910	84.8392005
H	9.5139997	4.7637457	90.2583438
H	5.3076748	0.5539649	89.8688424
H	3.8089974	2.8906077	85.9374126
H	7.7168116	3.4177143	90.2897950
Zn	1.9687372	6.3729572	88.8774996
Br	3.4365867	8.0085550	88.2713794
C	2.4453492	9.1067469	81.2715309
C	1.2266990	6.6105719	84.6095639
C	1.6918913	7.9404230	81.0483960
C	2.4423315	8.6388204	83.6588872
C	1.6711978	7.4806474	83.4417318
C	2.8245840	9.4515900	82.5779876
C	1.3097329	7.1298828	82.1264885
O	1.3040578	5.2770586	84.3078223
H	2.7479176	9.7398771	80.4231900
H	2.7660676	8.8911270	84.6827770
H	1.4084254	7.6571720	80.0226522
H	3.4324276	10.3517423	82.7582708
H	0.7477238	6.1974476	81.9645579
Br	1.0763839	1.6654726	85.2949951
Zn	1.3325278	3.9395714	85.6269586
H	0.2835597	9.1346965	85.1201640
C	-0.2984242	6.9845956	84.9897451
C	-0.4497208	8.4122841	85.5249740
C	-0.6479451	6.1770134	86.1911949
C	-1.0233463	4.8747304	86.3020151
C	-0.2820577	7.0317345	87.3379088
O	-0.1917519	8.3057238	86.9605047
O	-0.0116585	6.6828774	88.5033547
H	-1.4750543	8.8155914	85.3980504
H	-1.3439746	4.3040371	85.4173619
H	-1.1461390	4.4072954	87.2923651
H	1.8463805	6.9088176	85.4994971
H	-0.9132061	6.7791547	84.0936480



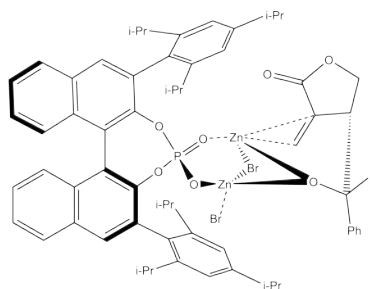
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C	0.0710610	1.7252576	88.9814183
C	0.8211198	0.8323500	89.7569969
C	0.3075433	0.4826386	91.0587879
C	1.0734067	-0.2478186	92.0163012
C	-1.0209040	0.9113236	91.4255612
C	-1.5406271	0.5501758	92.7053375
C	-1.7854264	1.6892088	90.5102364
H	-2.8169896	1.9644445	90.7782723
C	-1.2566417	2.1375028	89.3037132
C	4.2577258	0.5255409	88.0506097
C	4.4619722	-0.8476752	88.1027358
H	5.3885066	-1.2688278	87.6839474
C	3.4756990	-1.7361781	88.6174385
C	3.6710428	-3.1498256	88.5789606
C	2.2305203	-1.2055301	89.1200151
C	1.2055739	-2.1320827	89.4815499
C	2.0651630	0.2289147	89.2013056
C	3.0693271	1.0358734	88.6579693
O	0.5902324	2.1936052	87.7764044
O	2.9432945	2.4209529	88.7465645
P	1.8647650	3.2193223	87.8050579
O	1.5769262	4.5405848	88.5263796
O	2.3055350	3.2808518	86.3238009
C	-0.7763498	-0.1767962	93.6057615
C	0.5459795	-0.5659501	93.2603415
H	-2.5593193	0.8750159	92.9693074
H	-1.1858758	-0.4413065	94.5925562
H	2.1003263	-0.5470511	91.7628577
H	1.1601464	-1.1192594	93.9871190
C	1.4186769	-3.5023225	89.4121610
C	2.6675333	-4.0200333	88.9767424
H	0.2288610	-1.7532179	89.8107332
H	0.6082280	-4.1925233	89.6921782
H	2.8279930	-5.1081646	88.9360215
H	4.6325573	-3.5359556	88.2056067
C	-2.4762105	4.2860691	88.7696373
C	-2.0548587	2.9866554	88.3650548
C	-3.3272525	5.0164002	87.9203772
C	-2.4339837	2.4855622	87.0868116
C	-3.2585227	3.2757493	86.2635974
C	-3.7369974	4.5336886	86.6645309
H	-3.6660468	6.0157179	88.2401647
C	-2.0155326	1.1085694	86.5711355
H	-3.5449977	2.8791327	85.2782196
C	-1.1757884	1.2150279	85.2841247
H	-1.7500412	1.6730449	84.4521564
H	-0.8491901	0.2090347	84.9482876
H	-0.2689120	1.8274211	85.4463584
C	-3.2375655	0.1903152	86.3794860
H	-1.3786921	0.6295148	87.3413009
H	-3.9212665	0.5790036	85.5961362
H	-3.8208639	0.0945448	87.3179921
H	-2.9166989	-0.8254049	86.0683623
C	-4.6941372	5.3536136	85.8055237
C	-4.5130264	5.1350853	84.2966178
H	-5.1089162	5.8718174	83.7211148

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H	-4.8540203	4.1258315	83.9855243	Zn	3.1698598	4.9288948	85.7240879
H	-3.4515083	5.2302372	83.9902950	H	-1.4306411	6.4007266	83.9200895
C	-6.1529324	5.0910060	86.2300935	C	0.7929088	6.4243971	84.0257060
H	-4.4792310	6.4252142	86.0196370	C	-0.5419938	6.1066052	83.3319659
H	-6.8571513	5.7248795	85.6520162	C	1.6356710	5.2836538	83.5818792
H	-6.3034397	5.3014155	87.3080169	C	2.9998956	5.1729688	83.4968915
H	-6.4228593	4.0286822	86.0538458	C	0.6920800	4.1536429	83.2246969
C	-1.9932086	4.9395625	90.0638829	O	-0.5679552	4.6688277	83.1736739
C	-1.2661335	6.2654104	89.7819983	O	0.9522842	2.9949390	82.9968849
H	-0.8082758	6.6703004	90.7067267	H	-0.6058665	6.5745993	82.3286809
H	-1.9463653	7.0420070	89.3757144	H	3.4352348	4.2397396	83.0992294
H	-0.4491953	6.1237154	89.0493726	H	3.6382834	6.0722282	83.5530645
C	-3.1376575	5.1340252	91.0741405	H	1.2134597	7.4112323	83.7550392
H	-1.2489551	4.2594771	90.5244348	H	0.0376786	5.4986475	85.8734987
H	-2.7567065	5.5799113	92.0160133				
H	-3.6320584	4.1734882	91.3252936				
H	-3.9172031	5.8150418	90.6723462				
H	8.2982786	3.5047957	84.3039272				
H	8.3750963	2.4578532	89.6363230				
H	4.3869369	-1.4084948	84.0285255				
C	7.7377909	4.1526738	85.0173523				
H	5.8820631	3.5625021	91.2570522				
H	7.5191721	5.7379686	83.5109040				
H	2.7715168	0.4812522	83.4591246				
C	6.8641571	3.2114104	85.8481713				
C	7.5690699	1.7680876	89.9637156				
C	6.8795316	5.1145203	84.1688284				
H	6.2953314	5.7947474	84.8232363				
C	6.9064835	3.1571980	87.2505476				
C	5.0431977	-0.6892954	84.5610977				
H	9.4315082	4.2691693	86.4203360				
C	5.9662671	2.3465717	85.1898281				
C	8.7682245	4.9381814	85.8361937				
H	9.4084798	5.5483392	85.1678711				
H	5.9382014	2.3493010	84.0882499				
C	5.8428527	3.6308719	90.1502046				
H	7.6210211	1.6940470	91.0697325				
H	7.7906496	0.7670675	89.5404906				
C	6.0764313	2.2934417	87.9937505				
C	3.4654560	1.1944040	83.9481767				
C	5.1249811	1.4577294	85.8810993				
H	5.5558005	-1.2340991	85.3786348				
H	5.8235330	-0.3481121	83.8484620				
C	6.1839037	2.2713784	89.5166365				
C	5.1792044	1.4405984	87.3057451				
C	4.2267234	0.5069405	85.0895166				
H	4.8276818	3.9615818	89.8579140				
H	2.8535273	2.0332150	84.3244766				
H	6.5581988	4.4197226	89.8374584				
H	6.1668926	4.5671218	83.5191938				
H	4.1458067	1.5735950	83.1561410				
H	8.2727184	5.6327485	86.5465452				
H	5.4380558	1.5389634	89.8897162				
H	3.4628864	0.1099273	85.7888854				
H	7.5956857	3.8145040	87.7993701				
Zn	2.2827561	6.4010523	88.1584585				
Br	2.0948731	8.1236016	89.6794065				
C	-1.5841864	9.9218987	86.8911840				
C	0.6275505	6.4155904	85.6197605				
C	-0.1999909	10.0033565	86.6582771				
C	-1.5332678	7.5610947	86.3112740				
C	-0.1512413	7.6409441	86.0630111				
C	-2.2494401	8.6975745	86.7193494				
C	0.5132501	8.8703681	86.2426901				
O	1.8998594	6.3934807	86.1800757				
H	-2.1413616	10.8118734	87.2218611				
H	-2.0428239	6.5895826	86.2268200				
H	0.3305138	10.9549434	86.8145547				
H	-3.3292759	8.6200752	86.9216256				
H	1.6016622	8.9213888	86.0872717				
Br	4.7200965	5.8727802	87.3161118				

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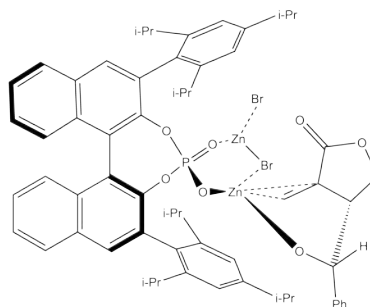


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C	0.8218860	0.8361411	89.7521165
C	0.3084156	0.4881417	91.0542546
C	1.0723092	-0.2457911	92.0102852
C	-1.0176199	0.9218723	91.4230628
C	-1.5360896	0.5623952	92.7032718
C	-1.7801519	1.7019970	90.5084301
H	-2.8104748	1.9818887	90.7762966
C	-1.2518351	2.1477282	89.3010946
C	4.2560621	0.5219146	88.0430222
C	4.4559925	-0.8518185	88.0932722
H	5.3812069	-1.2735852	87.6721560
C	3.4686777	-1.7385089	88.6082456
C	3.6598033	-3.1522033	88.5691007
C	2.2259343	-1.2050358	89.1133723
C	1.1999197	-2.1291794	89.4771113
C	2.0639220	0.2296448	89.1953849
C	3.0692938	1.0348856	88.6515418
O	0.5928664	2.1990426	87.7722988
O	2.9472537	2.4191960	88.7402809
P	1.8706370	3.2214159	87.8007707
O	1.5885096	4.5456599	88.5153068
O	2.3119923	3.2781101	86.3179107
C	-0.7740988	-0.1680315	93.6020043
C	0.5454088	-0.5625841	93.2543796
H	-2.5527318	0.8921293	92.9690036
H	-1.1833031	-0.4308500	94.5893201
H	2.0972505	-0.5488553	91.7539318
H	1.1584000	-1.1189223	93.9797448
C	1.4098687	-3.4994468	89.4075685
C	2.6557927	-4.0199499	88.9690740
H	0.2254577	-1.7470424	89.8088875
H	0.5985487	-4.1875807	89.6899289
H	2.8137851	-5.1083615	88.9277356
H	4.6194332	-3.5404575	88.1931335
C	-2.4660999	4.2975938	88.7619868
C	-2.0506944	2.9952882	88.3616681
C	-3.3228545	5.0235208	87.9150122

C	-2.4374777	2.4879628	87.0884047	H	3.4781972	0.0957589	85.7762496
C	-3.2670830	3.2743031	86.2670871	H	7.5887294	3.8153011	87.8036255
C	-3.7428966	4.5336898	86.6657258	Zn	2.2903684	6.4149666	88.1795746
H	-3.6568071	6.0254493	88.2316158	Br	2.1006668	8.1507503	89.6698277
C	-2.0204897	1.1094521	86.5757768	C	-1.6157108	9.9027125	86.8987791
H	-3.5595938	2.8728913	85.2854443	C	0.6253530	6.4124541	85.6345267
C	-1.1834960	1.2122087	85.2866874	C	-0.2254025	9.9831123	86.7115700
H	-1.7573477	1.6692702	84.4540358	C	-1.5533767	7.5520140	86.2816347
H	-0.8583683	0.2057206	84.9514369	C	-0.1641734	7.6321293	86.0758418
H	-0.2752303	1.8233210	85.4456318	C	-2.2782898	8.6838603	86.6855494
C	-3.2427568	0.1905515	86.3901605	C	0.4971986	8.8558173	86.2977433
H	-1.3821172	0.6326481	87.3460739	O	1.8973769	6.3993809	86.1892451
H	-3.9285761	0.5754951	85.6069333	H	-2.1800599	10.7881184	87.2292592
H	-3.8245450	0.0984153	87.3297795	H	-2.0621046	6.5826163	86.1717570
H	-2.9229253	-0.8262394	86.0818267	H	0.3043163	10.9276640	86.9067832
C	-4.7091774	5.3468892	85.8105083	H	-3.3637406	8.6053778	86.8546417
C	-4.5312950	5.1308182	84.3007477	H	1.5905034	8.9042213	86.1829402
H	-5.1334305	5.8635140	83.7264751	Br	4.7352327	5.8923368	87.3029613
H	-4.8674127	4.1199714	83.9899391	Zn	3.1723339	4.9355170	85.7483183
H	-3.4712476	5.2304388	83.9908723	H	-1.4345741	6.3903496	83.9298316
C	-6.1643503	5.0731764	86.2397405	C	0.7879578	6.4264351	84.0364337
H	-4.5010982	6.4201614	86.0239956	C	-0.5448659	6.1002039	83.3413563
H	-6.8768528	5.7009048	85.6650347	C	1.6379652	5.2936377	83.5891641
H	-6.3122436	5.2805855	87.3184150	C	3.0026415	5.1877439	83.5114345
H	-6.4260751	4.0087596	86.0650161	C	0.7025862	4.1565766	83.2302636
C	-1.9695644	4.9579995	90.0475664	O	-0.5631894	4.6659745	83.1794574
C	-1.2467500	6.2830331	89.7519127	O	0.9717745	3.0020116	83.0013031
H	-0.7730260	6.6913759	90.6666723	H	-0.6117648	6.5727492	82.3391176
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C	-3.1028665	5.1564564	91.0693508	H	1.1997352	7.4194869	83.7741173
H	-1.2196332	4.2806019	90.5029292	H	0.0415575	5.4904526	85.8845457
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H	-3.5942165	4.1973900	91.3316275				
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H	8.3178967	3.4918546	84.3126321				
H	8.3610812	2.4608172	89.6464836				
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H	5.8602047	3.5721366	91.2507504				
H	7.5418431	5.7255918	83.5118416				
H	2.7837639	0.4815004	83.4490682				
C	6.8747790	3.2018794	85.8494978				
C	7.5527691	1.7727544	89.9714596				
C	6.8995981	5.1023382	84.1675381				
H	6.3122040	5.7821040	84.8194478				
C	6.9055229	3.1542687	87.2520194				
C	5.0602448	-0.6945421	84.5457000				
H	9.4383057	4.2607415	86.4337138				
C	5.9839515	2.3330118	85.1881706				
C	8.7788532	4.9287183	85.8443375				
H	9.4237101	5.5376403	85.1793730				
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C	5.8255089	3.6364581	90.1436371				
H	7.5996409	1.7018662	91.0778383				
H	7.7768353	0.7709350	89.5518964				
C	6.0718492	2.2921101	87.9922657				
C	3.4794077	1.1901071	83.9418592				
C	5.1372311	1.4470717	85.8759486				
H	5.5727484	-1.2429754	85.3607956				
H	5.8418116	-0.3495927	83.8364071				
C	6.1701916	2.2753465	89.5158497				
C	5.1810541	1.4352508	87.3007877				
C	4.2418332	0.4975879	85.0795269				
H	4.8111019	3.9656122	89.8479064				
H	2.8684319	2.0275853	84.3226194				
H	6.5409479	4.4255975	89.8322129				
H	6.1899357	4.5536620	83.5154806				
H	4.1589703	1.5720169	83.1502208				
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15λ-ma

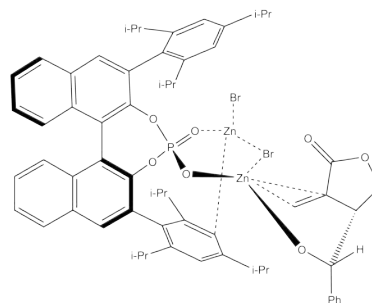


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C	-1.2557151	-0.5856721	90.9610965
C	-1.7287016	-1.4503056	91.9929446
C	-2.0080273	0.5559168	90.5579315
H	-2.9937419	0.7308159	91.0147637
C	-1.5242673	1.4556441	89.6179444
C	3.9614929	0.4841312	87.6943825
C	4.2074007	-0.7785105	87.1728647
H	5.1750503	-0.9857191	86.6905103
C	3.2161603	-1.8039877	87.1987888
C	3.4498307	-3.0657011	86.5744576
C	1.9367822	-1.5551582	87.8227720
C	0.9307117	-2.5620520	87.7241828
C	1.7180175	-0.2937326	88.4934471
C	2.7114351	0.6788663	88.3639828
O	0.1911303	2.0531018	88.0416732
O	2.5411709	1.9143683	88.9806776
P	1.4359606	3.0061832	88.5096964
O	1.1103845	3.7854486	89.7977724

O	1.8448931	3.8439860	87.2859737	H	7.2102187	0.4988673	89.5313369
C	-0.9707339	-2.5270727	92.4265293	C	5.3498233	2.3434699	88.6837452
C	0.3020949	-2.7728019	91.8477707	C	2.8325211	1.9197379	84.8316377
H	-2.7063194	-1.2334204	92.4515266	C	4.8924156	2.3265807	86.2577740
H	-1.3451508	-3.1808799	93.2287951	H	6.1920379	1.9639544	83.8281183
H	1.7733399	-2.1595625	90.3957859	H	4.8957835	3.1395266	83.4361489
H	0.9172919	-3.6087443	92.2140226	C	5.4021300	1.6468583	90.0423009
C	1.1848150	-3.7709320	87.0907414	C	4.8229495	1.6942342	87.5322919
C	2.4595602	-4.0350757	86.5249347	C	4.3448707	1.6665948	84.9874803
H	-0.0629285	-2.3681141	88.1510259	H	3.8306676	2.8687179	90.9787362
H	0.3884699	-4.5277270	87.0233608	H	2.2485813	1.5081290	85.6778879
H	2.6537032	-5.0005644	86.0335400	H	5.4884549	3.3990687	91.3866540
H	4.4336984	-3.2476523	86.1141294	H	3.9353678	6.2623608	87.2368403
C	-2.2570995	3.8711115	89.9548710	H	2.6296276	3.0076221	84.7936065
C	-2.2558429	2.6837869	89.1686809	H	7.2872207	6.1064385	89.0803818
C	-2.8638002	5.0244163	89.4258305	H	4.7678396	0.7376990	89.9793132
C	-2.8701103	2.6775105	87.8890463	H	4.4777923	0.5710489	85.0958979
C	-3.4447715	3.8645388	87.3991738	H	6.2025553	4.1705965	89.4630851
C	-3.4454181	5.0532371	88.1439329	Zn	1.6880932	5.5513212	90.3065932
H	-2.8704744	5.9512537	90.0217238	Br	3.1202210	6.2244953	91.9439863
C	-2.9279801	1.4165394	87.0298616	C	-3.6901324	3.3288027	81.9360148
H	-3.8869262	3.8554937	86.3924322	C	-0.1995989	4.5734475	84.2092287
C	-2.2436895	1.6187868	85.6693394	C	-3.7257230	4.4998100	82.7138779
H	-2.7963164	2.3444323	85.0406323	C	-1.3864008	2.9594716	82.6249421
H	-2.1943007	0.6641030	85.1061276	C	-1.4124470	4.1344991	83.3988244
H	-1.2135719	2.0046930	85.7969435	C	-2.5168314	2.5602841	81.8924615
C	-4.3791106	0.9282544	86.8656824	C	-2.5938488	4.9001172	83.4380698
H	-2.3784637	0.6154365	87.5647605	O	-0.5747367	5.0875395	85.4268590
H	-4.9969780	1.6773470	86.3277296	H	-4.5805451	3.0116395	81.3718584
H	-4.8570872	0.7422046	87.8489376	H	-0.4848298	2.3251370	82.6289316
H	-4.4124514	-0.0149150	86.2817317	H	-4.6469511	5.1014044	82.7628215
C	-3.9813698	6.3670728	87.5841811	H	-2.4851175	1.6327812	81.3003261
C	-2.8150530	7.2220355	87.0443695	H	-2.6224279	5.7993351	84.0713812
H	-3.1848966	8.1833379	86.6299309	Br	0.8516102	7.0305121	88.5087485
H	-2.2651509	6.6746429	86.2497012	Zn	0.8067060	5.4020467	86.6604625
H	-2.0841727	7.4538210	87.8447288	H	0.9419617	4.0584662	81.8347248
C	-5.0730597	6.1917638	86.5199943	C	0.6080512	5.6709434	83.3350681
H	-4.4323947	6.9190566	88.4397312	C	1.3370650	5.0493759	82.1287115
H	-5.4995874	7.1755095	86.2374940	C	1.7314239	6.2422435	84.1155595
H	-5.9009154	5.5492443	86.8822921	C	1.6981222	7.1240394	85.1558458
H	-4.6707480	5.7319711	85.5935334	C	3.0066844	5.6203140	83.6264881
C	-1.6164715	3.9088144	91.3423728	O	2.7157818	4.8743747	82.5222052
C	-0.9579788	5.2598972	91.6737027	O	4.1260016	5.7299724	84.0795161
H	-0.2073045	5.1559096	92.4832203	H	1.3101168	5.7138579	81.2399109
H	-1.6903479	6.0245743	92.0059682	H	2.6410376	7.4327707	85.6364760
H	-0.4789474	5.7004041	90.7700933	H	0.7779051	7.6794167	85.3947713
C	-2.6295651	3.5459561	92.4454602	H	-0.1441968	6.4297782	83.0458210
H	-0.8137953	3.1437300	91.3463773	H	0.4935796	3.6955396	84.2946917
H	-2.1487063	3.5613638	93.4456158				
H	-3.0587638	2.5375496	92.2917851				
H	-3.4712487	4.2695723	92.4574960				
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H	7.5361012	2.0298995	90.3989323				
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C	6.0853760	5.8365593	87.2546052				
H	4.8222002	1.9228231	92.1337867				
H	4.9516139	7.6915560	87.6366324				
H	2.4502863	1.4594660	83.8964708				
C	5.8091438	4.3416985	87.3362767				
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H	4.6805148	6.4047754	88.8564455				
C	5.8366186	3.6550895	88.5618732				
C	5.0960470	2.0847560	83.7128321				
H	8.2499546	5.7263602	87.6169429				
C	5.3891746	3.6409316	86.1935257				
C	7.3614062	6.2771378	87.9861139				
H	7.5433847	7.3615058	87.8387064				
H	5.3887151	4.1700684	85.2306634				
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15*ν*-ma; COSMO

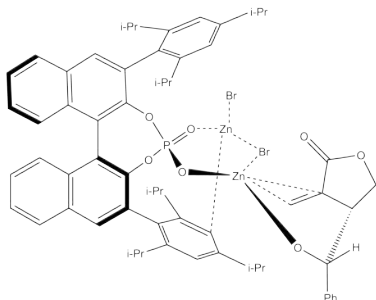


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C	3.0580983	3.3721025	2.1655375
C	4.4833606	3.3123360	2.2312898
C	2.4256387	4.6598759	2.3267679
C	3.2266435	5.8026953	2.6267877
C	1.0231721	4.7842469	2.1150306

H	0.5589760	5.7780438	2.2051450	H	1.5569698	-3.5284241	-6.7282705
C	0.2438955	3.6973613	1.7412221	H	-0.1709644	-4.3770843	0.9560613
C	3.2828913	-1.1135688	0.3365133	C	2.7283456	-3.1396445	-3.4560089
C	4.1795841	-1.5897556	1.2868230	C	5.7656580	-0.0393988	-2.6454910
H	4.7578717	-2.4997272	1.0663418	C	1.7575884	-2.9692352	-5.7906536
C	4.3545773	-0.9522254	2.5479518	H	2.3396118	-2.0636808	-6.0631933
C	5.2035347	-1.5111901	3.5502682	C	3.3911900	-1.9021092	-3.3834238
C	3.6543366	0.2783705	2.8244133	C	2.6346097	-4.8532109	0.7560865
C	3.7973202	0.8644977	4.1179927	H	4.3850770	-5.0157080	-4.6602203
C	2.8149594	0.8492485	1.7995086	C	2.2449768	-3.6952267	-2.2608905
C	2.5874266	0.0951311	0.6417274	C	3.8562544	-4.3479774	-5.3705506
O	0.0418353	1.3075650	1.4934542	H	3.6918487	-4.9092867	-6.3139682
O	1.6843924	0.5680027	-0.3183132	H	1.7012000	-4.6506916	-2.3132220
P	0.0918949	0.5035172	0.0545228	C	3.5559530	1.1767278	-3.0075943
O	-0.6454772	1.2662586	-1.0549870	H	6.3040049	0.9298720	-2.5940464
O	-0.3626787	-0.9345654	0.3617882	H	6.3124638	-0.7707908	-2.0160954
C	4.6059841	5.7000363	2.7226427	C	3.5735082	-1.2195208	-2.1681456
C	5.2366242	4.4463574	2.5028161	C	0.3297214	-4.1407518	-0.0048044
H	2.7261336	6.7745854	2.7605166	C	2.3902957	-3.0514958	-1.0187189
H	5.2141645	6.5893456	2.9474664	H	3.6649003	-4.5298867	1.0053585
H	4.9902677	2.3541188	2.0552212	H	2.7125870	-5.6577037	-0.0052624
H	6.3341032	4.3725077	2.5423065	C	4.3079823	0.1206428	-2.1760842
C	4.6159576	0.2854106	5.0780466	C	3.0747026	-1.8065933	-0.9721312
C	5.3369930	-0.9047201	4.7903754	C	1.7797248	-3.6858123	0.2301357
H	3.2378918	1.7802841	4.3558820	H	2.5186168	1.3037452	-2.6405029
H	4.7021746	0.7496901	6.0723107	H	-0.2463464	-3.3396159	-0.5058478
H	5.9887415	-1.3501448	5.5573377	H	3.5097173	0.8912841	-4.0793678
H	5.7407502	-2.4451908	3.3224308	H	0.7892904	-2.6462703	-5.3622238
C	-1.4395746	4.1340028	-0.0730239	H	0.2719037	-5.0430138	-0.6479089
C	-1.1788455	3.8364471	1.2984494	H	4.5337177	-3.4982268	-5.5998432
C	-2.7900684	4.1471385	-0.5103233	H	4.3486755	0.4940843	-1.1324004
C	-2.2489816	3.6426737	2.2062171	H	1.7466111	-2.9031652	1.0151760
C	-3.5781357	3.7206905	1.7359830	H	3.7754701	-1.4444138	-4.3093845
C	-3.8781492	3.9525781	0.3879108	Zn	-2.5622556	1.8686911	-1.0387180
H	-3.0156082	4.4418617	-1.5478348	Br	-3.6717488	1.7760837	-3.1056426
C	-1.9869972	3.3253857	3.6739413	C	-6.3290365	-6.7862618	1.7195684
H	-4.3995873	3.5623186	2.4491703	C	-3.2164622	-4.3025488	-0.0313649
C	-2.3723581	1.8719432	4.0082737	C	-6.5170812	-5.3992895	1.5734804
H	-3.4607716	1.7020100	3.8738340	C	-4.1052251	-6.5725816	0.7537913
H	-2.1188524	1.6410493	5.0632521	C	-4.2933261	-5.1875519	0.5898726
H	-1.8382006	1.1570680	3.3529732	C	-5.1194102	-7.3705528	1.3126574
C	-2.6831291	4.3299301	4.6087705	C	-5.5049293	-4.6062404	1.0152261
H	-0.8941421	3.4240231	3.8389209	O	-3.0774143	-3.1476575	0.6851931
H	-3.7886475	4.2640935	4.5351812	H	-7.1233238	-7.4087810	2.1598424
H	-2.3893623	5.3735264	4.3753930	H	-3.1473444	-7.0310929	0.4573727
H	-2.4107947	4.1238246	5.6638904	H	-7.4591942	-4.9339282	1.9032258
C	-5.2976325	4.0480349	-0.1517969	H	-4.9577792	-8.4524485	1.4384573
C	-6.3308319	3.2638557	0.6655640	H	-5.6297229	-3.5163561	0.9184891
H	-7.3138246	3.2832910	0.1541322	Br	-3.5551814	0.4020788	0.7077201
H	-6.4798231	3.7016289	1.6747974	Zn	-2.1752839	-1.6210805	0.1138444
H	-6.0299163	2.2041747	0.7894627	H	-3.4799547	-6.2423632	-1.8459272
C	-5.7040291	5.5290320	-0.2975710	H	-3.5609000	-1.1430482	-1.8703011
H	-5.2658967	3.6051630	-1.1732333	C	-3.6400044	-4.0356520	-1.5799222
H	-6.7082063	5.6130585	-0.7608291	C	-3.4254194	-5.3015546	-2.4253846
H	-4.9876712	6.0901888	-0.9308827	H	-4.6878533	-3.6804856	-1.5646791
H	-5.7405091	6.0251852	0.6949421	C	-2.7018018	-3.0862308	-2.2185988
C	-0.3217978	4.5508048	-1.0287044	C	-2.6732372	-1.7210250	-2.1780074
C	-0.5320518	4.1577684	-2.4983524	C	-1.6641277	-3.8964380	-2.9431404
H	0.3560181	4.4601610	-3.0886311	O	-2.0872835	-5.1940572	-2.9682635
H	-1.4085719	4.6650274	-2.9509675	O	-0.6321010	-3.5249584	-3.4591327
H	-0.6579674	3.0662803	-2.6279298	H	-1.4426628	-5.3613938	-3.2698063
C	-0.1226149	6.0788003	-0.9208942	H	-1.8664020	-1.1769919	-2.6974771
H	0.6098233	4.0580412	-0.6808196	H	-2.2697942	-4.8996539	-0.1004513
H	0.7283004	6.3999859	-1.5553089				
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H	-1.0308196	6.6138936	-1.2684207				
H	1.8844606	-4.7365142	-4.5775541				
H	5.8171252	-0.3955218	-3.6955939				
H	2.1839671	-5.2925831	1.6703426				
C	2.5213844	-3.8503314	-4.7868587				
H	4.0681427	2.1595181	-2.9456268				

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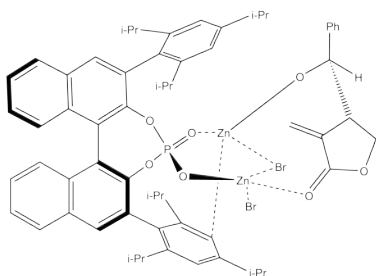
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C	4.4842626	3.3095856	2.2434989
C	2.4285741	4.6595182	2.3330885
C	3.2307751	5.8009521	2.6329633
C	1.0269973	4.7844650	2.1176257
H	0.5628862	5.7787983	2.2036259
C	0.2466805	3.6982803	1.7445699
C	3.2806402	-1.1123449	0.3409577
C	4.1783730	-1.5893978	1.2895892
H	4.7552833	-2.4992925	1.0652949
C	4.3556273	-0.9544168	2.5514212
C	5.2058288	-1.5140801	3.5516365
C	3.6563866	0.2758923	2.8308093
C	3.8025373	0.8602845	4.1245150
C	2.8152028	0.8480735	1.8084080
C	2.5855437	0.0957240	0.6498138
O	0.0413576	1.3091916	1.5046524
O	1.6811796	0.5695963	-0.3070084
P	0.0885722	0.5015233	0.0664268
O	-0.6497653	1.2646997	-1.0413598
O	-0.3647943	-0.9361537	0.3752230
C	4.6092547	5.6969559	2.7320366
C	5.2382028	4.4425423	2.5153212
H	2.7313688	6.7738379	2.7639155
H	5.2179087	6.5858799	2.9568550
H	4.9890487	2.3499326	2.0699275
H	6.3354203	4.3669698	2.5573134
C	4.6231909	0.2804918	5.0818092
C	5.3426215	-0.9092859	4.7916329
H	3.2437091	1.7761263	4.3632368
H	4.7118402	0.7440159	6.0761598
H	5.9957149	-1.3560645	5.5565814
H	5.7415171	-2.4484572	3.3218144
C	-1.4327349	4.1299709	-0.0751420
C	-1.1748555	3.8388702	1.2981498
C	-2.7814058	4.1439018	-0.5143936
C	-2.2468486	3.6492294	2.2044683
C	-3.5743532	3.7244948	1.7304103
C	-3.8712998	3.9516016	0.3808120
H	-3.0045121	4.4245522	-1.5561308
C	-1.9877050	3.3365333	3.6740217
H	-4.3975435	3.5659370	2.4414862
C	-2.3605329	1.8802502	4.0097795
H	-3.4462554	1.6986841	3.8696977
H	-2.1109036	1.6531648	5.0665165
H	-1.8165221	1.1688626	3.3591680
C	-2.6950383	4.3361830	4.6054457
H	-0.8961685	3.4454070	3.8419745
H	-3.7997857	4.2601478	4.5306662
H	-2.4120590	5.3824119	4.3708540
H	-2.4239644	4.1356523	5.6619459
C	-5.2893463	4.0383435	-0.1646771
C	-6.3229781	3.2587227	0.6562481
H	-7.3039071	3.2681100	0.1406575

H	-6.4796698	3.7061844	1.6602242
H	-6.0184160	2.2016367	0.7915874
C	-5.7004852	5.5158825	-0.3278734
H	-5.2520537	3.5832596	-1.1807245
H	-6.7025996	5.5928299	-0.7967555
H	-4.9834528	6.0734307	-0.9634906
H	-5.7431552	6.0236017	0.6585280
C	-0.3112929	4.5336428	-1.0327123
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H	-1.3942407	4.6453082	-2.9583811
H	-0.6586328	3.0432562	-2.6251231
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H	0.6161443	4.0351949	-0.6815366
H	0.7534866	6.3721690	-1.5706669
H	0.1117075	6.3886039	0.1015200
H	-1.0028713	6.6016443	-1.2827471
H	1.8697465	-4.7240786	-4.5769085
H	5.7998715	-0.3802186	-3.6935416
H	2.1938531	-5.3024263	1.6655697
C	2.5069152	-3.8380153	-4.7856923
H	4.0421490	2.1713090	-2.9394785
H	1.5395206	-3.5143656	-6.7248579
H	-0.1654744	-4.3823061	0.9635516
C	2.7167975	-3.1298754	-3.4540698
C	5.7481361	-0.0234072	-2.6438105
C	1.7411187	-2.9561760	-5.7869944
H	2.3215446	-2.0497779	-6.0599689
C	3.3753020	-1.8905732	-3.3805306
C	2.6409236	-4.8577076	0.7521624
H	4.3716133	-5.0023314	-4.6622446
C	2.2408189	-3.6900940	-2.2584810
C	3.8411810	-4.3347524	-5.3712575
H	3.6765414	-4.8950114	-6.3151959
H	1.6993711	-4.6467416	-2.3119734
C	3.5340758	1.1864003	-3.0023055
H	6.2843710	0.9471165	-2.5938420
H	6.2976690	-0.7535510	-2.0156696
C	3.5609028	-1.2107237	-2.1647918
C	0.3333032	-4.1434401	0.0023496
C	2.3893577	-3.0497236	-1.0153405
H	3.6716365	-4.5350427	1.0001691
H	2.7189308	-5.6582124	-0.0131827
C	4.2905863	0.1320333	-2.1728561
C	3.0698638	-1.8028804	-0.9682876
C	1.7839160	-3.6886826	0.2337792
H	2.4959052	1.3080190	-2.6361849
H	-0.2444043	-3.3408736	-0.4943340
H	3.4881250	0.9029523	-4.0744827
H	0.7731291	-2.6344751	-5.3576074
H	0.2734447	-5.0431729	-0.6441348
H	4.5186686	-3.4850448	-5.6002505
H	4.3318676	0.5050972	-1.1290000
H	1.7524458	-2.9092312	1.0220670
H	3.7527078	-1.4286914	-4.3071176
Zn	-2.5722952	1.8429576	-1.0422881
Br	-3.6951345	1.7806603	-3.0913332
C	-6.3217050	-6.7856672	1.7163404
C	-3.2107631	-4.3001315	-0.0319691
C	-6.4982728	-5.3952838	1.5967737
C	-4.1076164	-6.5748296	0.7309221
C	-4.2855817	-5.1861739	0.5909225
C	-5.1220898	-7.3731920	1.2872737
C	-5.4858864	-4.6016021	1.0413652
O	-3.0715685	-3.1454061	0.6783541
H	-7.1164657	-7.4085983	2.1549568
H	-3.1550934	-7.0352297	0.4201857
H	-7.4316531	-4.9273974	1.9469736
H	-4.9682324	-8.4581315	1.3947456
H	-5.5966122	-3.5085091	0.9684835
Br	-3.5498900	0.3957635	0.7275794

Zn	-2.1762565	-1.6188288	0.1008673
H	-3.4862598	-6.2387179	-1.8502657
H	-3.5678075	-1.1352891	-1.8833084
C	-3.6422718	-4.0335039	-1.5836317
C	-3.4244134	-5.2983147	-2.4300194
H	-4.6915650	-3.6828503	-1.5595346
C	-2.7079282	-3.0827468	-2.2238400
C	-2.6799560	-1.7167579	-2.1846272
C	-1.6635562	-3.8932052	-2.9400307
O	-2.0865621	-5.1929486	-2.9654496
O	-0.6283196	-3.5207086	-3.4456399
H	-4.1403861	-5.3575658	-3.2768410
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H	-2.2640382	-4.8969059	-0.1078399

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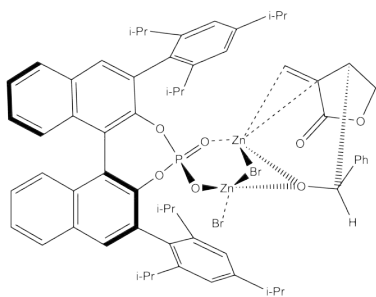
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C	4.2769102	4.4696337	-0.0603581
C	2.1349753	5.3725128	0.7609673
C	2.6511309	6.6864730	0.5526726
C	0.7989869	5.1699806	1.2140072
H	0.1823459	6.0492853	1.4510684
C	0.2459961	3.9006822	1.3305681
C	3.5609842	-0.6617067	-0.1774632
C	4.7978619	-0.7380502	0.4490090
H	5.3859204	-1.6655574	0.3723105
C	5.3037663	0.3319174	1.2408462
C	6.5391739	0.2039916	1.9435987
C	4.5203140	1.5349701	1.3970802
C	4.9805118	2.5173514	2.3257236
C	3.3001146	1.6804214	0.6374953
C	2.8654856	0.5867386	-0.1211810
O	0.5647891	1.5188541	1.2336981
O	1.7149016	0.7091571	-0.8933614
P	0.2392239	0.7171197	-0.1544086
O	-0.7129504	1.5063269	-1.0535350
O	-0.1699824	-0.6970722	0.2856665
C	3.9295470	6.8807007	0.0524644
C	4.7409510	5.7607120	-0.2697625
H	2.0026625	7.5469762	0.7804600
H	4.3105165	7.9000056	-0.1121784
H	4.9093696	3.6098670	-0.3224308
H	5.7435327	5.9166668	-0.6962098
C	6.1765369	2.3532386	3.0102334
C	6.9756467	1.1974404	2.8058932
H	4.3717240	3.4138469	2.5029786
H	6.5048116	3.1257506	3.7222018
H	7.9272519	1.0837932	3.3469410
H	7.1309150	-0.7139888	1.8013329
C	-2.2331081	3.9299126	0.7958047
C	-1.1800381	3.6428650	1.7110661
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C	-2.8089878	2.7427087	3.2868938
C	-3.8669633	3.0188234	2.4045264
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C	-0.3855105	2.7165308	3.9907504
H	-3.0272078	2.2713608	4.2584970
C	-0.3651302	1.2230782	4.3646933
H	-1.2923158	0.9211494	4.8954064
H	0.4872716	1.0031051	5.0403855
H	-0.2626910	0.5904280	3.4613951
C	-0.5193866	3.6126175	5.2360740
H	0.5960648	2.9522102	3.5319143
H	-1.4807746	3.4334518	5.7613456
H	-0.4830330	4.6868138	4.9635688
H	0.3003278	3.4120671	5.9569774
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C	-5.4861114	1.1052314	2.6794937
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H	-4.8559991	0.5997633	3.4414686
H	-5.1952751	0.7042919	1.6869753
C	-5.7670946	3.2014709	4.0913613
H	-5.9470716	3.0786962	1.9494390
H	-6.8359307	2.9650961	4.2722726
H	-5.6459971	4.3026596	4.1294064
H	-5.1876487	2.7708129	4.9345318
C	-1.9786666	4.5386698	-0.5831524
C	-2.9000610	3.9645291	-1.6728100
H	-2.5102065	4.2134869	-2.6796344
H	-3.9310190	4.3708310	-1.6043986
H	-2.9788138	2.8624331	-1.6038642
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H	-0.9375724	4.2820422	-0.8693718
H	-1.9020312	6.4994650	-1.5609059
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H	-0.3802406	-5.0371775	-2.1144979
H	4.4506313	-2.6655683	-4.6357946
H	3.2372961	-3.2317279	3.2076686
C	0.5938180	-5.0797859	-2.6527545
H	3.7012025	0.3841163	-4.5920843
H	-0.4162945	-5.7101750	-4.4736284
C	1.4305076	-3.9526608	-2.0611466
C	4.9351555	-2.0034154	-3.8883239
C	0.3058233	-4.9335503	-4.1508700
H	1.2219782	-5.0604704	-4.7651770
C	2.3130948	-3.1539293	-2.8003479
C	3.2250341	-3.3405886	2.1040085
H	1.4005544	-6.5794911	-1.2497962
C	1.3177517	-3.6960012	-0.6665483
C	1.2344467	-6.4460977	-2.3377045
H	0.5793637	-7.2708325	-2.6852514
H	0.6887714	-4.3710175	-0.0641664
C	3.0490569	-0.2950941	-4.0058365
H	5.6103220	-1.3225115	-4.4453779
H	5.5574165	-2.6394169	-3.2263580
C	3.0309785	-2.0876561	-2.2129661
C	0.7292238	-3.0475788	2.1578516
C	2.0689285	-2.6836852	-0.0210970
H	4.1969403	-2.9814368	1.7179279
H	3.1444752	-4.4219901	1.8674361
C	3.9020488	-1.1915823	-3.0876739
C	2.8984942	-1.8420429	-0.8233446
C	2.0327187	-2.5654096	1.5022369
H	2.3360913	0.3244776	-3.4287521
H	2.4558546	-0.8989310	-4.7229241
H	-0.1304277	-3.9421317	-4.3861633
H	2.2166375	-6.5481183	-2.8450360
H	4.4667126	-0.5228594	-2.4052654
H	2.1580798	-1.4910710	1.7523267
H	2.4137861	-3.3235608	-3.8818632
Zn	-1.2882349	1.1772721	-2.9304312
Br	-0.6154373	2.6635726	-4.5571583

H	-5.0526875	-3.1644770	-3.2244927
Br	-0.4853410	-1.2056419	-3.2851999
Zn	-0.4722525	-2.1734151	-1.0106849
C	-4.0825389	-2.5278191	-1.3167160
C	-5.0522451	-2.3338437	-2.4936564
C	-3.6142380	-1.1150841	-1.1076563
C	-3.1227882	-0.5116620	-0.0030412
C	-3.7786642	-0.4272139	-2.4086945
O	-4.5844376	-1.1449635	-3.2005226
O	-3.2873417	0.6382409	-2.8095586
H	-6.0942495	-2.1406344	-2.1653249
C	-3.9588888	-7.0506358	-0.8406659
C	-3.5321195	-5.7220989	-0.7079484
C	-3.3343335	-4.9160559	-1.8472498
C	-3.5517510	-5.4751478	-3.1214601
C	-3.9790502	-6.8074112	-3.2576503
C	-4.1875477	-7.5969562	-2.1165213
H	-4.1081693	-7.6711308	0.0569430
H	-3.3169269	-5.2928820	0.2826549
C	-2.8610580	-3.4771088	-1.6816282
H	-3.3603183	-4.8653692	-4.0202406
H	-4.1394750	-7.2320061	-4.2608838
H	-4.5184459	-8.6419142	-2.2198068
O	-1.8768476	-3.3938913	-0.7094182
H	-0.1640120	-2.5593420	1.7256174
H	0.7488822	-2.8065117	3.2395347
H	0.6025876	-4.1467997	2.0746503
H	-2.5126718	-3.1312504	-2.6910274
H	-4.5808034	-2.9478611	-0.4213655
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H	-3.0345221	-1.0559981	0.9475895

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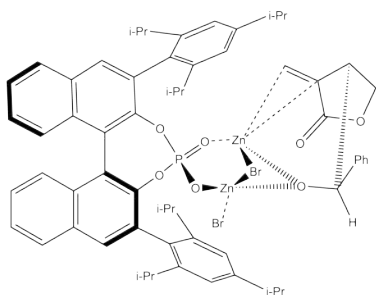
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C	4.6777593	3.2480847	1.3167695
C	2.5749258	4.4666207	1.7172530
C	3.3353824	5.6673926	1.8518047
C	1.1532039	4.4825448	1.7813839
H	0.6416467	5.4351873	1.9853052
C	0.3931959	3.3414526	1.5504894
C	3.3391969	-1.5418410	0.1818776
C	4.3514012	-1.8917656	1.0680867
H	4.8289363	-2.8787186	0.9719715
C	4.7361722	-1.0458146	2.1467151
C	5.7115102	-1.4669018	3.1005582
C	4.0828865	0.2296682	2.3189089
C	4.3864873	0.9878840	3.4902218
C	3.1320771	0.6645389	1.3219859
C	2.7812246	-0.2331503	0.3093040
O	0.3127693	0.9632101	1.1972469
O	1.8655381	0.1748542	-0.6617065
P	0.2710024	0.2524466	-0.2824789
O	-0.3443673	1.2076681	-1.3347159
O	-0.3573229	-1.1281455	-0.0696660

C	4.7155259	5.6549107	1.7175769
C	5.3870744	4.4358384	1.4310957
H	2.7994036	6.6095400	2.0470407
H	5.2902881	6.5884906	1.8152393
H	5.2094290	2.3142376	1.0871438
H	6.4790923	4.4328811	1.2931398
C	5.3251250	0.5410317	4.4106226
C	6.0093530	-0.6873762	4.2081010
H	3.8601213	1.9353718	3.6686368
H	5.5356075	1.1426024	5.3080844
H	6.7582613	-1.0266232	4.9398989
H	6.2095470	-2.4372696	2.9477636
C	-1.7576290	3.9995698	0.4001541
C	-1.1018691	3.3959448	1.5116578
C	-3.1608435	4.1090301	0.4237350
C	-1.8596357	2.8814749	2.5955543
C	-3.2603253	3.0306409	2.5770543
C	-3.9323167	3.6580995	1.5143361
H	-3.6755363	4.5883573	-0.4251427
C	-1.1985446	2.2078735	3.7965802
H	-3.8382831	2.6603728	3.4373886
C	-1.6429626	0.7418302	3.9459255
H	-2.7250717	0.6670586	4.1836668
H	-1.0891382	0.2498771	4.7719486
H	-1.4524589	0.1705579	3.0162829
C	-1.4321866	3.0089638	5.0903808
H	-0.1043014	2.1999419	3.6176384
H	-2.5094976	3.0498635	5.3553585
H	-1.0714981	4.0526723	4.9877654
H	-0.8960469	2.5416316	5.9420766
C	-5.4309665	3.9396187	1.5483300
C	-6.2396892	2.9631620	2.4136498
H	-7.3261570	3.1438762	2.2865232
H	-6.0153853	3.0858846	3.4940033
H	-6.0368907	1.9042884	2.1521545
C	-5.6775412	5.3951434	1.9970828
H	-5.7949162	3.8525016	0.5022696
H	-6.7593999	5.6411273	1.9679574
H	-5.1435677	6.1149919	1.3448991
H	-5.3174878	5.5503919	3.0360181
C	-0.9657218	4.5665041	-0.7789380
C	-1.5373836	4.1773629	-2.1495620
H	-0.8325518	4.4650526	-2.9559963
H	-2.5077596	4.6638181	-2.3643178
H	-1.6920333	3.0822342	-2.2179993
C	-0.8528352	6.1009401	-0.6791927
H	0.0570530	4.1428509	-0.7205268
H	-0.2424885	6.5056787	-1.5129571
H	-0.3842641	6.4207317	0.2720676
H	-1.8568349	6.5716580	-0.7325051
H	-0.1621830	-5.4185481	-3.1967103
H	4.9332784	-2.5140445	-4.2352098
H	2.4393085	-5.1279557	2.7694341
C	0.8841047	-5.3172651	-3.5652868
H	3.8282334	0.4692008	-4.0659459
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H	0.1280650	-4.1269201	2.6650850
C	1.5543724	-4.3172849	-2.6288183
C	5.1736282	-1.8707910	-3.3627729
C	0.8191502	-4.8670245	-5.0291322
H	1.8289841	-4.8100208	-5.4879121
C	2.3919736	-3.2837087	-3.0766848
C	2.5501559	-4.9849803	1.6742835
H	1.5646462	-7.0626923	-2.4004296
C	1.3413531	-4.4346221	-1.2410148
C	1.5559969	-6.7003448	-3.4480497
H	1.0242422	-7.4536434	-4.0658678
H	0.6756652	-5.2327891	-0.8780700
C	3.1622224	-0.3532371	-3.7313068
H	5.8550409	-1.0683101	-3.7145216
H	5.7247670	-2.4936366	-2.6289431

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C	0.2204259	-4.0013730	1.5663255	C	4.3572150	-1.8946927	1.0669459
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H	-0.3926044	-3.1297110	1.2697467	O	0.3152766	0.9495074	1.2073748
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H	0.3418575	-3.8714787	-5.1302905	P	0.2789859	0.2436749	-0.2749288
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Br	-2.3276151	-4.3678372	-1.2604975	H	5.2082661	2.3109867	1.1178325
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C	-4.9157259	-2.1770153	-0.0114407	H	5.5367808	1.1212429	5.3206566
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H	-4.9044073	-2.5349812	-1.0522768	H	6.2126911	-2.4477814	2.9464757
H	-4.8330269	-0.9774533	3.7101892	C	-1.7511122	3.9897113	0.3804552
C	-4.3940158	-0.9073063	0.3040110	C	-1.1058482	3.3875051	1.4989728
C	-4.3656531	-0.4855199	1.6467198	C	-3.1528355	4.1162046	0.3985942
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O	-2.8287201	-0.6370635	-1.5208296	H	-3.8566448	2.6956508	3.4192866
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Br	-0.6409561	-1.4131474	-3.6713543	H	-2.7674166	0.6803089	4.1676845
C	-4.3816865	1.3647829	-2.8161584	H	-1.1375545	0.2461425	4.7591812
O	-5.8429004	2.6457934	-1.5448429	H	-1.4972117	0.1725628	3.0036605
Zn	-1.6680068	0.5141216	-2.6073121	C	-1.4551162	3.0109550	5.0784605
C	-3.5182335	1.1229161	-3.8524688	H	-0.1298821	2.1879702	3.6115716
C	-4.9034040	2.7470125	-2.5209521	H	-2.5327406	3.0640508	5.3399275
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H	-3.2170191	1.9671007	-4.4964837	H	-0.9278216	2.5389458	5.9330068
H	-3.3678779	0.0958514	-4.2264680	C	-5.4260381	3.9945770	1.5215943
H	-3.4417251	0.9216690	-0.2859101	C	-6.2528786	3.0482472	2.4028537
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				H	-6.0242697	3.1820853	3.4810302
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				C	-5.6437841	5.4611500	1.9482886
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				H	-5.2787284	5.6259499	2.9838479
				C	-0.9492932	4.5371775	-0.8013567
				C	-1.5226668	4.1433517	-2.1702642
				H	-0.8097549	4.4105285	-2.9766141
				H	-2.4849963	4.6410993	-2.3953752
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				C	-0.8188985	6.0709611	-0.7160490
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				H	-0.2045367	6.4614491	-1.5535446
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				H	-1.8170524	6.5532542	-0.7725764
				H	-0.1588144	-5.3962908	-3.2200471
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				H	2.4646175	-5.1756155	2.7296769
				C	0.8865582	-5.2901913	-3.5897190
				H	3.8226725	0.5021889	-4.0580018
				H	0.2288113	-5.5506454	-5.6529062
				H	0.1580041	-4.1606118	2.6555004

15 γ -mi



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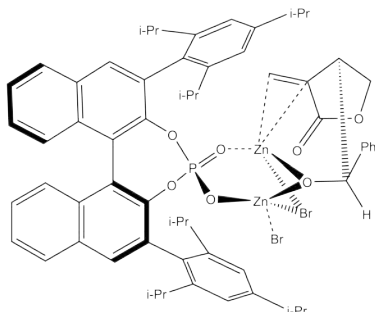
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C	1.1458300	4.4719450	1.7844735
H	0.6297459	5.4235110	1.9820262
C	0.3889329	3.3296036	1.5501869

C	1.5571894	-4.2960041	-2.6475902
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C	0.8176782	-4.8300418	-5.0501078
H	1.8262041	-4.7674736	-5.5110681
C	2.3896387	-3.2558743	-3.0892321
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H	1.5750718	-7.0416017	-2.4388340
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C	1.5623723	-6.6721171	-3.4837095
H	1.0311643	-7.4228385	-4.1049945
H	0.6893690	-5.2302607	-0.9018255
C	3.1570155	-0.3211893	-3.7252594
H	5.8508266	-1.0353822	-3.7178666
H	5.7222653	-2.4675967	-2.6410812
C	2.9928054	-2.3505959	-2.1948798
C	0.2440767	-4.0145149	1.5588866
C	1.9432895	-3.5655359	-0.3220397
H	3.6428095	-4.8760242	1.4084606
H	2.2429519	-5.9499791	1.1264523
C	3.8947541	-1.2466273	-2.7424331
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H	-0.2117004	-4.8984172	1.0691771
H	2.6151670	-6.6207674	-3.8333785
H	4.2184173	-0.6222936	-1.8837536
H	2.0758239	-2.9244016	1.7215077
H	2.5684999	-3.1263968	-4.1666581
Zn	-1.5169867	-2.2186039	-1.2898526
Br	-2.3049448	-4.3938821	-1.2738526
H	-5.6928918	-4.0681913	0.8222552
H	-5.8132648	-3.2276637	3.1852360
C	-5.3601724	-3.0476557	1.0644799
C	-5.4189015	-2.5790298	2.3880120
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H	-4.7790272	-2.6141855	-0.9803969
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H	-6.0755439	1.1833777	-0.0204620
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H	-7.0821660	0.9387040	-1.4909502
Br	-0.6513813	-1.3966098	-3.6805717
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O	-5.8481961	2.6080927	-1.5068539
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C	-3.5292321	1.0865751	-3.8223853
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O	-4.5982382	3.7585704	-3.0067921
H	-3.2353082	1.9357333	-4.4634686
H	-3.3729074	0.0615525	-4.1983355
H	-3.4422753	0.8967131	-0.2521325
H	-5.3228566	-0.5489621	-2.2140498

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C	2.6565664	4.5194364	1.1052824
C	3.2506666	5.8164877	1.0512241
C	1.2613211	4.3556961	1.3412959
H	0.6478468	5.2474119	1.5416838
C	0.6500403	3.1074571	1.2896637
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C	5.1181212	-1.6734947	1.1865523
H	5.6618991	-2.6284534	1.2507930
C	5.4871107	-0.6132058	2.0628694
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C	3.6983167	0.7948558	1.0573858
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O	0.8568418	0.7384381	1.0186684
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P	0.8524500	-0.1192943	-0.3761537
O	0.1508027	0.5775476	-1.5486610
O	0.3424430	-1.5105356	0.0640356
C	4.6020520	5.9712757	0.7802680
C	5.4127924	4.8283701	0.5448122
H	2.6080444	6.6960030	1.2142192
H	5.0454432	6.9775406	0.7329003
H	5.5045195	2.6752770	0.4192626
H	6.4789780	4.9551678	0.3025243
C	6.0371805	1.3809984	3.9872546
C	6.8239398	0.1994765	3.9477134
H	4.4144329	2.4998205	3.1236215
H	6.2323540	2.1426295	4.7576402
H	7.6373732	0.0551670	4.6750085
H	7.1202501	-1.7191479	2.9881985
C	-1.7385492	3.4671401	0.5369513
C	-0.8225663	2.9194538	1.4775315
C	-3.1196916	3.2889342	0.7536846
C	-1.3113465	2.1848062	2.5982462
C	-2.6984821	2.0239871	2.7534702
C	-3.6255178	2.5678752	1.8464709
H	-3.8301224	3.7254955	0.0332979
C	-0.3905970	1.5982900	3.6687204
H	-3.0691281	1.4604588	3.6247762
C	-0.5696387	0.0754968	3.8149933
H	-1.5811736	-0.1823336	4.1933412
H	0.1678413	-0.3353369	4.5353249
H	-0.4190603	-0.4345405	2.8435401
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H	0.6580327	1.7761826	3.3577927
H	-1.6077027	2.1830930	5.4102747
H	-0.4058521	3.4135556	4.9112186
H	0.1289249	1.9321256	5.7739890
C	-5.1258642	2.4010456	2.0566015
C	-5.5413537	0.9225800	2.1568015
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H	-5.0888581	0.4326307	3.0439545
H	-5.2270345	0.3559629	1.2569432
C	-5.6065993	3.1993554	3.2828706
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H	-5.1399843	2.8166377	4.2148360
C	-1.2852727	4.2189337	-0.7134428
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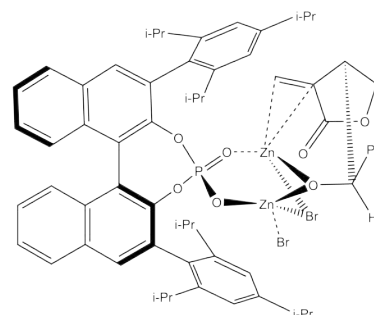
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H	2.0804633	-7.1024926	-1.8248483
H	5.3517111	-3.3325417	-3.9314614
H	3.4725617	-4.5665862	3.6938157
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C	3.9961998	-0.4791469	-4.3176168
H	-0.3257629	-7.1851430	-2.4963288
H	1.1049908	-3.6535435	3.4669840
C	2.2847578	-4.9909247	-1.6969060
C	5.5920196	-2.4958743	-3.2423647
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H	1.5133367	-7.3089718	-4.2297986
H	1.6776537	-5.5958996	0.2917305
C	3.4311108	-1.2524708	-3.7575280
H	6.1717184	-1.7434283	-3.8163626
H	6.2461688	-2.8972768	-2.4416618
C	3.5546022	-2.8824738	-1.8030568
C	1.1665297	-3.7888403	2.3674131
C	2.7655980	-3.7292167	0.3710905
H	4.5994848	-4.5286826	2.2976074
H	3.2512696	-5.7030826	2.3233999
C	4.3121822	-1.8689977	-2.6574513
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C	2.6225451	-3.6413827	1.8923466
H	2.5291474	-0.7764607	-3.3269185
H	0.5286016	-3.0220379	1.8887688
H	3.0937295	-2.0149797	-4.4897323
H	-0.1310637	-6.1994588	-1.0232585
H	0.7509350	-4.7928113	2.1378561
H	1.5064610	-5.5325003	-4.4251939
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H	2.9535109	-2.6307627	2.2043471
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Zn	-1.2118025	-0.0860271	-2.8504881
Br	-1.9122728	0.9812199	-4.7668225
C	-6.2973791	1.6046613	-3.0220255
C	-3.5458117	-1.5518423	-1.8971062
C	-5.4407651	1.7696629	-1.9204083
C	-5.3585833	-0.6043865	-3.4061543
C	-4.5135591	-0.4512713	-2.2902689
C	-6.2509853	0.4166765	-3.7684977
C	-4.5508842	0.7493768	-1.5547028
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Br	-0.2891244	-2.5761675	-3.4015502
Zn	-0.9298638	-2.4223439	-1.0977353
H	-6.0591815	-3.4801411	-0.3675157
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C	-5.3558534	-3.2750642	-1.1998576
C	-3.1788799	-3.5375392	-0.3784996
C	-2.1077874	-3.5399189	0.4719294
C	-3.5866534	-4.7657111	-1.1648200
O	-4.8251374	-4.5371088	-1.6732310
O	-2.9677578	-5.7930564	-1.3256413
H	-5.9127927	-2.8075702	-2.0327281
H	-1.9296602	-2.7016501	1.1666162
H	-1.5416763	-4.4756421	0.6221498
H	-3.4062618	-2.2276116	-2.7800369

H -4.3660512 -1.7785494 0.1207102

$p_{dis.} = 15\gamma\text{-sim-mi}$



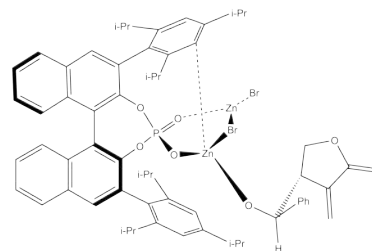
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C	2.8914708	2.0445357	0.9854541
C	3.4850007	3.3574419	0.9131685
C	4.8667923	3.5591555	0.6202759
C	2.6500548	4.5174003	1.1143689
C	3.2407726	5.8157331	1.0667132
C	1.2552186	4.3479676	1.3464650
H	0.6372187	5.2362615	1.5481702
C	0.6476617	3.0984243	1.2880981
C	4.0502223	-1.5617927	0.3140340
C	5.1272207	-1.6688495	1.1851724
H	5.6700050	-2.6243676	1.2500964
C	5.4945099	-0.6085776	2.0617979
C	6.5502431	-0.7741770	3.0076340
C	4.7348914	0.6199368	2.0552464
C	5.0192070	1.5859501	3.0675369
C	3.7039420	0.7967688	1.0555698
C	3.4091602	-0.2880332	0.2246410
O	0.8613092	0.7317807	1.0081596
O	2.4526644	-0.1290238	-0.7744135
P	0.8639774	-0.1240066	-0.3895305
O	0.1590399	0.5665338	-1.5592745
O	0.3601967	-1.5188967	0.0510956
C	4.5917349	5.9757621	0.7995835
C	5.4058534	4.8365517	0.5613021
H	2.5948755	6.6925455	1.2311762
H	5.0320458	6.9835320	0.7570940
H	5.5032208	2.6840442	0.4272525
H	6.4721001	4.9672014	0.3216348
C	6.0393233	1.3850053	3.9873209
C	6.8282453	0.2057013	3.9476159
H	4.4144960	2.5006242	3.1232941
H	6.2325999	2.1468723	4.7578775
H	7.6416795	0.0624246	4.6750277
H	7.1282760	-1.7114839	2.9876475
C	-1.7394010	3.4617682	0.5337715
C	-0.8250058	2.9077368	1.4720017
C	-3.1206328	3.2847962	0.7495099
C	-1.3154800	2.1675565	2.5880922
C	-2.7027353	2.0084897	2.7417201
C	-3.6283990	2.5597313	1.8382135
H	-3.8294703	3.7268569	0.0308928
C	-0.3965061	1.5737133	3.6560593
H	-3.0744877	1.4419049	3.6106510
H	-0.5751685	0.0498886	3.7908207
H	-1.5872576	-0.2116741	4.1653149
H	0.1603675	-0.3668878	4.5096359

H	-0.4215733	-0.4525858	2.8159549
C	-0.5875535	2.2891428	5.0067611
H	0.6525299	1.7537093	3.3480598
H	-1.6156248	2.1468794	5.4007778
H	-0.4144978	3.3800511	4.9106463
H	0.1201668	1.8935966	5.7644903
C	-5.1292145	2.3986814	2.0498833
C	-5.5525781	0.9220115	2.1420610
H	-6.6541093	0.8331797	2.2401961
H	-5.0989763	0.4238702	3.0240932
H	-5.2457104	0.3604522	1.2365788
C	-5.6042605	3.1932497	3.2805767
H	-5.6303565	2.8329704	1.1568698
H	-6.7052730	3.1223724	3.4004142
H	-5.3338314	4.2647691	3.1955021
H	-5.1383015	2.8040366	4.2100006
C	-1.2850994	4.2181655	-0.7134570
C	-1.8376449	3.5824962	-1.9983205
H	-1.4148770	4.0719860	-2.8984875
H	-2.9421570	3.6542792	-2.0711508
H	-1.5714970	2.5112393	-2.0583916
C	-1.6421857	5.7133347	-0.6283629
H	-0.1811564	4.1401352	-0.7695728
H	-1.2685297	6.2567876	-1.5204936
H	-1.2053594	6.1906113	0.2725925
H	-2.7413795	5.8627570	-0.5815108
H	2.0667474	-7.0934982	-1.8281487
H	5.3346967	-3.3419856	-3.9338176
H	3.4921878	-4.5775277	3.6973479
C	1.6179122	-6.2053635	-2.3314383
H	3.9889338	-0.4845790	-4.3255956
H	-0.3582446	-7.1683512	-2.4554429
H	1.1322993	-3.6297401	3.4816920
C	2.2705443	-4.9827166	-1.6862343
C	5.8800867	-2.5037242	-3.2486533
C	0.1029909	-6.2440069	-2.0531246
H	-0.4078716	-5.3839490	-2.5313401
C	2.9481724	-3.9947685	-2.4183138
C	3.5517240	-4.6736993	2.5932942
H	2.9734473	-6.3603653	-4.0627670
C	2.2023887	-4.8206756	-0.2885385
C	1.8888806	-6.3398046	-3.8340865
H	1.4440825	-7.2776877	-4.2227591
H	1.6852192	-5.5902304	0.3077098
C	3.4223594	-1.2528961	-3.7604405
H	6.1610201	-1.7559897	-3.8274125
H	6.2351226	-2.9055961	-2.4491561
C	3.5480301	-2.8794446	-1.8017257
C	1.1890209	-3.7680534	2.3822306
C	2.7779197	-3.7266063	0.3785559
H	4.6123343	-4.5500758	2.2956977
H	3.2525638	-5.7089529	2.3261606
C	4.3044998	-1.8700321	-2.6618580
C	3.4702089	-2.7459770	-0.3927161
C	2.6448239	-3.6392697	1.9007924
H	2.5252176	-0.7690586	-3.3290955
H	0.5586761	-2.9953541	1.9028582
H	3.0775980	-2.0150291	-4.4894150
H	-0.1300161	-6.2112413	-0.9708314
H	0.7610503	-4.7679514	2.1568992
H	1.4346412	-5.4998484	-4.4000710
H	4.6306336	-1.0432151	-1.9977292
H	2.9894522	-2.6333087	2.2127326
H	3.0178305	-4.0839433	-3.5113369
Zn	-1.2029278	-0.0732592	-2.8792689
Br	-1.9439033	0.9924314	-4.7688349
C	-6.2861847	1.5960497	-3.0334610
C	-3.5260376	-1.5494566	-1.9018087
C	-5.4364618	1.7619975	-1.9272931
C	-5.3348636	-0.6061844	-3.4185394
C	-4.4970047	-0.4526561	-2.2977957

C	-6.2298294	0.4112317	-3.7830197
C	-4.5435106	0.7457160	-1.5596376
O	-2.3058780	-1.0239128	-1.4681924
H	-6.9799005	2.4001777	-3.3226105
H	-5.2589867	-1.5163796	-4.0351450
H	-5.4603600	2.6998179	-1.3518823
H	-6.8703575	0.2853406	-4.6690795
H	-3.8447472	0.8932466	-0.7214433
Br	-0.2978897	-2.5863596	-3.4364057
Zn	-0.9000865	-2.4173265	-1.1339511
H	-6.0509484	-3.4454411	-0.3505766
C	-4.1223418	-2.4409679	-0.7234440
C	-5.3432568	-3.2597245	-1.1853738
C	-3.1648084	-3.5268400	-0.3688411
C	-2.0796325	-3.5218818	0.4626187
C	-3.5867025	-4.7640224	-1.1343643
O	-4.8278369	-4.5294296	-1.6435146
O	-2.9789397	-5.7982098	-1.2786171
H	-5.8960613	-2.7921493	-2.0216225
H	-1.8794582	-2.6740495	1.1390783
H	-1.5120080	-4.4569881	0.6100231
H	-3.3911334	-2.2328288	-2.7803806
H	-4.3399193	-1.7542701	0.1178697

15 ν -2-mi; COSMO



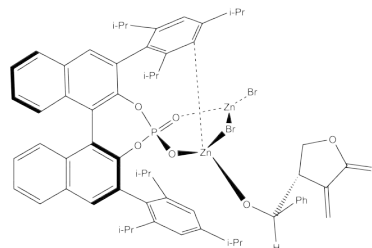
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C	0.3979951	-0.3877130	91.7806652
C	1.4598654	-1.2356870	92.2168685
C	-0.5942037	0.0214773	92.7474613
C	-0.5172466	-0.4865003	94.0795499
C	-1.6109728	0.9477863	92.3736359
H	-2.3671650	1.2337299	93.1199188
C	-1.6449084	1.5299940	91.1115405
C	2.5345247	0.1537557	87.2991092
C	2.7347497	-1.2007177	87.0672231
H	3.3149220	-1.5212281	86.1886929
C	2.1264432	-2.1955397	87.8877482
C	2.2802879	-3.5819960	87.5846741
C	1.2640258	-1.8010978	88.9791701
C	0.5267549	-2.8207792	89.6532342
C	1.1585296	-0.3984142	89.3134512
C	1.8163581	0.5117564	88.4813365
O	-0.7600458	1.6412307	88.8944061
O	1.7660798	1.8684622	88.8033657
P	0.3940655	2.6862870	88.4321485
O	0.4429335	3.9532494	89.3073400
O	0.1919458	2.8441364	86.9273821
C	0.5129860	-1.3320073	94.4630565
C	1.5170867	-1.6947645	93.5257599
H	-1.2866633	-0.1771990	94.8042324
H	0.5642334	-1.7092897	95.4957046
H	2.2474063	-1.5165549	91.5035049
H	2.3509516	-2.3406133	93.8404842
C	0.6833833	-4.1594752	89.3197509
C	1.5821299	-4.5492270	88.2916517
H	-0.1811793	-2.5387467	90.4438645

H	0.0997753	-4.9241350	89.8546496
H	1.7050737	-5.6143554	88.0433943
H	2.9511399	-3.8671005	86.7591414
C	-2.5094396	3.8969792	91.3132994
C	-2.6173324	2.6038370	90.7254543
C	-3.4484835	4.8835131	90.9542654
C	-3.6219620	2.3522559	89.7462792
C	-4.5194913	3.3822040	89.4116186
C	-4.4650878	4.6515256	90.0144854
H	-3.3799756	5.8814268	91.4164503
C	-3.7876145	0.9968935	89.0585667
H	-5.2898814	3.1831364	88.6501023
C	-3.6292635	1.1035420	87.5293123
H	-4.3722360	1.7912306	87.0765420
H	-3.7563061	0.1070152	87.0575567
H	-2.6248030	1.4823879	87.2596804
C	-5.1296536	0.3455059	89.4443455
H	-2.9883840	0.3231195	89.4299130
H	-5.9898143	0.9467453	89.0830270
H	-5.2278290	0.2446937	90.5445840
H	-5.2166099	-0.6659286	88.9960846
C	-5.4687291	5.7413763	89.6584199
C	-5.3419817	6.1776846	88.1877531
H	-6.0527861	6.9985616	87.9586018
H	-5.5585465	5.3383003	87.4957340
H	-4.3172575	6.5354950	87.9611003
C	-6.9095518	5.3115944	89.9897147
H	-5.2261145	6.6207744	90.2950591
H	-7.6225225	6.1382381	89.7903675
H	-7.0098431	5.0182001	91.0543735
H	-7.2224694	4.4455857	89.3696974
C	-1.4022294	4.2591079	92.3039988
C	-0.7418649	5.6114462	91.9830998
H	0.1719129	5.7549566	92.5938325
H	-1.4172896	6.4670342	92.1902214
H	-0.4445426	5.6659129	90.9180370
C	-1.9173644	4.2504769	93.7561218
H	-0.6124470	3.4850613	92.2162408
H	-1.0985570	4.4892222	94.4661226
H	-2.3399619	3.2666810	94.0406484
H	-2.7176723	5.0078862	93.8928876
H	2.4083017	4.8755005	83.2035903
H	6.6543077	2.6424025	86.7170692
H	0.6668108	-1.4408288	83.5688443
C	3.4258902	4.4784920	83.4212722
H	5.3132407	3.2847502	89.5231655
H	4.3042374	6.4391985	83.0888067
H	-1.1697460	0.1635711	84.1832504
C	3.2299632	3.3955918	84.4773132
C	6.2350702	1.8189128	87.3319998
C	4.3131100	5.6460102	83.8628698
H	5.3687845	5.3308476	84.0008022
C	4.0527930	3.2398623	85.6065035
C	1.4225019	-0.6544858	83.7709932
H	3.2950364	3.0434319	81.7471880
C	2.1912368	2.4455527	84.2889152
C	3.9549215	3.8548484	82.1133437
H	4.0175626	4.6256422	81.3184270
H	1.5534342	2.5401704	83.3958815
C	4.6854352	3.3786626	88.6143200
H	6.8800717	1.7069686	88.2273175
H	6.3037553	0.8850350	86.7383488
C	3.8692312	2.1871649	86.5265600
C	-0.4286167	0.9655884	84.3752047
C	1.9968489	1.3494194	85.1604389
H	2.3585880	-1.1523683	84.0934152
H	1.6342174	-0.1307167	82.8153415
C	4.7808889	2.1109583	87.7473156
C	2.8494224	1.2251479	86.2979956
C	0.8998844	0.3376366	84.8312664
H	3.6444458	3.5443881	88.9563096

H	-0.8481262	1.6365402	85.1484738
H	5.0176982	4.2864322	88.0703336
H	3.9643167	6.0969852	84.8129868
H	-0.3270092	1.5538623	83.4411839
H	4.9694906	3.4288105	82.2616496
H	4.4382291	1.2566680	88.3669200
H	0.6864233	-0.2369405	85.7546936
H	4.8546745	3.9688902	85.7907491
Zn	1.6711292	5.4392793	89.1227619
Br	2.9646479	6.4145489	90.7356796
C	1.0840820	8.1161261	80.8071080
C	-0.9935871	5.3470414	83.4612995
C	1.4942057	7.9668631	82.1446981
C	-0.6922600	6.4963451	81.1904707
C	-0.2913358	6.3386162	82.5303779
C	-0.0123795	7.3794705	80.3328001
C	0.8115858	7.0858950	82.9951213
O	-0.1054982	4.3796240	83.9030675
H	1.6201815	8.8062172	80.1373167
H	-1.5442676	5.9086054	80.8106250
H	2.3521990	8.5421242	82.5269744
H	-0.3388787	7.4867889	79.2865321
H	1.1449226	6.9696826	84.0386854
Br	1.8182924	5.9964646	86.7566634
Zn	0.7646000	4.0451738	85.4980016
H	-2.9342556	7.0412334	82.9148827
C	-1.7645369	6.1416023	84.5893458
C	-3.0297141	6.7845365	83.9876002
C	-2.3977303	5.2558587	85.6242340
C	-1.9754726	4.9079012	86.8557726
C	-3.7631916	4.9041816	85.1184555
O	-4.0705893	5.7817829	84.1112409
O	-4.5392595	4.0478897	85.4925331
H	-3.3431874	7.6900752	84.5487991
H	-2.5979762	4.2668165	87.5010285
H	-1.0277869	5.2822935	87.2692163
H	-1.0812332	6.8888472	85.0404463
H	-1.7925969	4.8396253	82.8614787

15 ν -2-mi



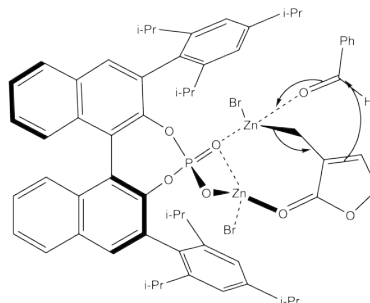
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C	0.3919510	-0.3891550	91.7870925
C	1.4415897	-1.2503935	92.2259767
C	-0.5960382	0.0347850	92.7518328
C	-0.5257353	-0.4712575	94.0844825
C	-1.6031125	0.9698922	92.3737160
H	-2.3603074	1.2637966	93.1158418
C	-1.6305752	1.5477249	91.1099200
C	2.5316013	0.1348039	87.3008427
C	2.7114806	-1.2211852	87.0617313
H	3.2794829	-1.5441075	86.1760516
C	2.0968783	-2.2123113	87.8818843
C	2.2318339	-3.5990120	87.5731271
C	1.2457981	-1.8124225	88.9802268
C	0.5015830	-2.8260915	89.6551809
C	1.1574709	-0.4100567	89.3197803
C	1.8249077	0.4949976	88.4897682
O	-0.7362473	1.6510749	88.8981830

O	1.7915151	1.8493782	88.8184841	H	1.5458338	2.5494387	83.4171347
P	0.4309961	2.6850949	88.4458857	C	4.6927307	3.3465952	88.6404582
O	0.4949696	3.9491156	89.3228059	H	6.8847660	1.6781379	88.2212398
O	0.2382322	2.8468853	86.9403915	H	6.2971694	0.8725205	86.7279538
C	0.4924067	-1.3292594	94.4707979	C	3.8635486	2.1751392	86.5429735
C	1.4915208	-1.7077480	93.5353265	C	-0.4346160	0.9759362	84.3998696
H	-1.2913284	-0.1500323	94.8079992	C	1.9990885	1.3395523	85.1649860
H	0.5378103	-1.7044378	95.5044171	H	2.3413756	-1.1485007	84.0522459
H	2.2248508	-1.5428757	91.5126517	H	1.6107816	-0.1023920	82.7989909
H	2.3161966	-2.3643461	93.8518183	C	4.7813167	2.0885850	87.7592037
C	0.6410947	-4.1648507	89.3161482	C	2.8497692	1.2088939	86.3034471
C	1.5277917	-4.5607568	88.2807884	C	0.8969050	0.3349069	84.8295432
H	-0.1970750	-2.5376390	90.4515972	H	3.6567909	3.4995660	89.0030482
H	0.0526092	-4.9247217	89.8524214	H	-0.8414837	1.6351485	85.1895743
H	1.6369119	-5.6261289	88.0274145	H	5.0098976	4.2632278	88.1025051
H	2.8936849	-3.8887707	86.7419439	H	3.9411977	6.1010113	84.8643407
C	-2.4880469	3.9226071	91.2657690	H	-0.3425538	1.5808341	83.4754895
C	-2.6029881	2.6166858	90.709520	H	4.9650815	3.4595422	82.2936651
C	-3.4319107	4.8997207	90.8950331	H	4.4422022	1.2280473	88.3722175
C	-3.6140020	2.3437662	89.7431330	H	0.6910007	-0.2551907	85.7448413
C	-4.5143255	3.3659250	89.3934012	H	4.8349056	3.9727052	85.8284454
C	-4.4573699	4.6465707	89.9707219	Zn	1.7621535	5.4074125	89.1685073
H	-3.3590250	5.9079152	91.3331970	Br	3.0324680	6.3846965	90.7839998
C	-3.7785912	0.9758820	89.0806600	C	1.0411236	8.1887426	80.8404143
H	-5.2870176	3.1518224	88.6385186	C	-0.9727033	5.3528287	83.4705591
C	-3.6141589	1.0545093	87.5503397	C	1.4593401	8.0308834	82.1740487
H	-4.3538446	1.7335930	87.0800974	C	-0.7007056	6.5300313	81.2095069
H	-3.7383700	0.0494940	87.0963142	C	-0.2925508	6.3644982	82.5457749
H	-2.6086051	1.4284776	87.2781056	C	-0.0417080	7.4366483	80.3608855
C	-5.1220127	0.3321274	89.4735585	C	0.7976519	7.1266993	83.0158546
H	-2.9811417	0.3087258	89.4680483	O	-0.0582705	4.4157425	83.9220627
H	-5.9808660	0.9257754	89.0974271	H	1.5609880	8.8972363	80.1772809
H	-5.2253385	0.2526924	90.5749246	H	-1.5404328	5.9278579	80.8251003
H	-5.2079675	-0.6874582	89.0441407	H	2.3075559	8.6177155	82.5603988
C	-5.4665998	5.7270761	89.6022660	H	-0.3731464	7.5497038	79.3169101
C	-5.3538566	6.1365998	88.1228576	H	1.1376399	7.0015180	84.0563058
H	-6.0693777	6.9506180	87.8842914	Br	1.8123149	6.0414807	86.8118278
H	-5.5723788	5.2846174	87.4472232	Zn	0.7597390	4.0981777	85.5444623
H	-4.3323020	6.4939745	87.8820081	H	-2.9771851	6.9656711	82.9108161
C	-6.9031080	5.3001148	89.9545362	C	-1.7750610	6.1271353	84.5925385
H	-5.2209272	6.6187995	90.2206913	C	-3.0662862	6.7123569	83.9852346
H	-7.6204569	6.1209612	89.7474164	C	-2.3728543	5.2287189	85.6363596
H	-6.9927270	5.0243572	91.0246322	C	-1.9373860	4.9080586	86.8709573
H	-7.2197977	4.4228145	89.3529027	C	-3.7271070	4.8194579	85.1365519
C	-1.3630524	4.3075393	92.2274639	O	-4.0647503	5.6742174	84.1165397
C	-0.7342680	5.6702033	91.8853160	O	-4.4681102	3.9431911	85.5272238
H	0.2107332	5.8190091	92.4447594	H	-3.4126575	7.6119620	84.5381477
H	-1.4060941	6.5164657	92.1376522	H	-2.5373470	4.2497818	87.5204744
H	-0.5002134	5.7400955	90.8049015	H	-1.0066433	5.3239842	87.2840913
C	-1.8381740	4.2980156	93.6929333	H	-1.1193993	6.9047288	85.0338686
H	-0.5629590	3.5460799	92.1213459	H	-1.7516792	4.8194808	82.8671730
H	-1.0070963	4.5629279	94.3788574				
H	-2.2277138	3.3067234	93.9968093				
H	-2.6536523	5.0357980	93.8453846				
H	2.3936847	4.8856627	83.2392674				
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H	0.6438728	-1.4204272	83.5374779				
C	3.4124727	4.4922851	83.4573653				
H	5.3344309	3.2500459	89.5391699				
H	4.2795209	6.4612432	83.1440051				
H	-1.1827394	0.1816300	84.2033809				
C	3.2185580	3.3995011	84.5044040				
C	6.2328068	1.7997221	87.3322216				
C	4.2927204	5.6606488	83.9103607				
H	5.3506257	5.3512354	84.0452863				
C	4.0391561	3.2391863	85.6354351				
C	1.4044000	-0.6408658	83.7475440				
H	3.2946633	3.0701256	81.7719471				
C	2.1910002	2.4420862	84.3031418				
C	3.9489174	3.8821256	82.1463627				
H	4.0093221	4.6588320	81.3571613				

6.3 Transition States for Product formation

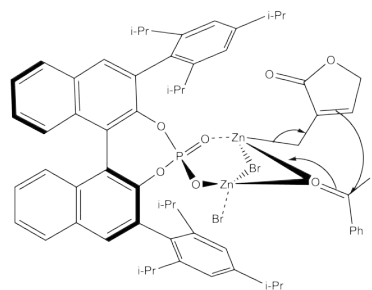
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C	4.2490916	3.8795874	0.5624857
C	2.0556642	4.9554730	0.8812788
C	2.7199216	6.2176554	0.9183985
C	0.6388975	4.8637179	0.9983287
H	0.0573523	5.7785463	1.1906544
C	-0.0267183	3.6500236	0.8849274
C	3.5302613	-0.9129349	-0.5011205
C	4.5403596	-1.1406097	0.4235302
H	5.2109957	-2.0020506	0.2862951
C	4.7261245	-0.2951821	1.5558578
C	5.7013722	-0.6010056	2.5506358
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C	4.0773355	1.6748482	2.8873567
C	2.9321400	1.1951193	0.6980606
C	2.7246122	0.2463026	-0.3004811
O	0.0665883	1.2776045	0.5616291
O	1.7111159	0.4640910	-1.2433973
P	0.1562710	0.3784343	-0.7973623
O	-0.6460400	0.8699501	-2.0230772
O	-0.4020862	-1.0160439	-0.3730760
C	4.0963050	6.3043053	0.7777671
C	4.8622058	5.1243298	0.5851012
H	2.1119759	7.1266308	1.0493164
H	4.5949344	7.2851577	0.8017298
H	4.8527715	2.9753283	0.4046277
H	5.9518086	5.1961338	0.4472781
C	5.0221792	1.3376736	3.8460471
C	5.8518385	0.1987680	3.6729710
H	3.4300884	2.5495497	3.0402144
H	5.1218195	1.9539025	4.7525401
H	6.6007395	-0.0562706	4.4381006
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C	-1.5042027	3.5077902	1.0934187
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C	-1.9815889	3.2792149	2.4103370
C	-3.3646024	3.0854815	2.6071683
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C	-0.9782405	1.8540933	4.2701487
H	-1.9779822	1.5165820	4.6164734
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H	-0.5760810	1.0936584	3.5720530
C	-1.4210215	4.3346854	4.6426316
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H	-1.4390987	5.3398652	4.1743213
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C	-5.7755641	2.8737584	1.7284789
C	-6.1505556	1.4585645	1.2429054
H	-7.2436050	1.2841628	1.3254091
H	-5.6329852	0.6915699	1.8572061
H	-5.8589121	1.3020079	0.1853725
C	-6.2821493	3.1114146	3.1561816
H	-6.2983855	3.5969510	1.0623339
H	-7.3874920	3.0332932	3.1944297
H	-5.9963764	4.1143507	3.5320538
H	-5.8787308	2.3571280	3.8640435
C	-1.9170363	3.8584798	-1.4161458
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H	-2.2558553	3.2976086	-3.4960873
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H	-2.9600341	2.1480744	-2.3140722
C	-1.7990202	5.3789678	-1.6416060
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H	-2.7904537	5.8671361	-1.5362103
H	1.9353756	-4.9701987	-5.0168007
H	5.8387309	-0.5974748	-4.7669205
H	2.7545149	-4.7653608	1.3660614
C	2.2698201	-3.9589067	-5.3382889
H	4.2432368	2.0469986	-3.9588344
H	0.6864134	-3.8162674	-6.8601657
H	0.3145745	-4.4321407	0.6253104
C	2.6975391	-3.2180364	-4.0777506
C	5.9033164	-0.1966127	-3.7337996
C	1.0572532	-3.2532965	-5.9781504
H	1.3330792	-2.2326546	-6.3178628
C	3.4303582	-2.0210919	-4.1353964
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C	2.2879474	-3.6764481	-2.8146947
C	3.4101263	-4.1470678	-6.3507325
H	3.0732610	-4.7621772	-7.2103867
H	1.7076167	-4.6103216	-2.7614945
C	3.7049056	1.0768996	-3.9278527
H	6.4731155	0.7545809	-3.7811242
H	6.4892083	-0.9196780	-3.1309910
C	3.7348005	-1.2768529	-2.9814374
C	0.7117152	-4.2221481	-0.3868632
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H	4.0837849	-3.9294148	0.5070901
H	3.2821699	-5.3355158	-0.2568864
C	4.5074120	0.0335605	-3.1277396
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C	2.0676307	-3.5076875	-0.2887178
H	2.7089348	1.2467335	-3.4738628
H	-0.0323312	-3.6059001	-0.9302403
H	3.5480888	0.7479412	-4.9764700
H	0.2224003	-3.1492498	-5.2556336
H	0.7917256	-5.1960910	-0.9132727
H	3.7568305	-3.1761857	-6.7622313
H	4.6640220	0.4486950	-2.1108553
H	1.9348552	-2.6361521	0.3879617
H	3.7609403	-1.6377734	-5.1136837
Zn	-1.9089371	-0.6725160	-2.0916382
Br	-2.4690500	-2.5328277	-3.2921219
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C	-2.6699205	-3.6727510	0.8808706
C	-3.9350220	-6.8415709	2.5623145
C	-4.0374362	-5.6038887	0.0431418
C	-3.3506151	-4.9785929	1.1061960
C	-4.6792897	-6.8360389	0.2447498
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O	-1.6627121	-3.3601490	1.6241961
H	-5.1378488	-8.4195807	1.6633329
H	-4.0348889	-5.1346437	-0.9547541
H	-3.8860965	-7.3339717	3.5458277
H	-5.2053410	-7.3226532	-0.5908300
H	-2.7211400	-5.1305621	3.1726431
Br	1.1477006	-1.2869008	2.9127659
Zn	-0.7264457	-1.6409707	1.5790091
H	-5.4283367	-3.4339682	-0.0430915
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C	-4.2209394	-2.3978413	1.5011177
C	-5.3148318	-2.4571578	0.4705293
H	-4.3690596	-2.8448348	2.4942793
C	-3.5461114	-1.1621710	1.3060038
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H	-6.3085803	-2.1532772	0.8667630
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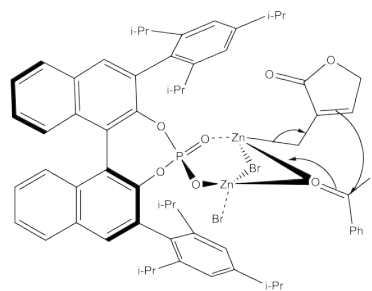
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H	0.5372410	5.2453247	1.5124084
C	0.4619313	3.1164956	1.1874956
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H	5.2226667	-2.8280170	1.2342063
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C	4.6004907	1.3323179	3.1774339
C	3.4090127	0.6764588	1.0451680
C	3.1281462	-0.3627943	0.1532217
O	0.5822778	0.7579636	0.8099144
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P	0.6402023	-0.0154814	-0.6312746
O	0.0911407	0.8308110	-1.7914949
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C	4.5582901	5.8135249	0.9996146
C	5.3326884	4.6418879	0.7834965
H	2.5740012	6.6157713	1.3290292
H	5.0470961	6.7996068	1.0115626
H	5.3383931	2.4906275	0.5991512
H	6.4172704	4.7268846	0.6160443
C	5.5350203	1.0499206	4.1647257
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H	4.0363389	2.2733326	3.2221060
H	5.7025653	1.7742715	4.9764733
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C	-1.8892568	3.6336405	0.4053118
C	-1.0226099	2.9973178	1.3387903
C	-3.2768245	3.6052693	0.6395766
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H	0.3451008	1.6516149	3.1831064
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H	-0.6150005	3.2351862	4.8610871
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C	-5.3480553	2.9782314	1.9772279
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C	-5.7182706	4.2167277	2.8178261	H	-2.7756476	-4.1954919	-2.0337266
H	-5.8299114	3.1073711	0.9812424	C	-4.4540486	-2.0628034	-1.0416625
H	-6.8171853	4.2927287	2.9540837	C	-5.3135917	-1.5633513	0.0880613
H	-5.3631578	5.1505393	2.3375050	H	-4.8570948	-2.2047930	-2.0542069
H	-5.2511081	4.1568037	3.8231268	C	-3.4519925	-2.8653966	-0.4792493
C	-1.3723500	4.2974100	-0.8702173	C	-2.4897665	-3.7248963	-1.0764532
C	-1.9963284	3.6592054	-2.1232531	C	-3.4482142	-2.5620729	1.0008348
H	-1.5323467	4.0615386	-3.0460441	O	-4.5293459	-1.7641799	1.2770258
H	-3.0891281	3.8409110	-2.1896375	O	-2.6701542	-2.9315044	1.8519294
H	-1.8377651	2.5640224	-2.1307631	H	-6.2559341	-2.1487503	0.1752396
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H	-0.2813121	4.1090505	-0.9260837	H	-3.0221398	-0.0760692	-0.5278478
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H	-2.6640498	6.0768280	-0.8054582				
H	1.7495737	-6.9613834	-2.4525534				
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H	2.6031993	-4.6234498	3.3407925				
C	1.4875440	-6.0266224	-3.0005677				
H	4.5324884	-0.3749718	-4.2192455				
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C	2.0983405	-4.8791108	-2.1948653				
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C	-0.0523146	-5.9393678	-3.0265457				
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C	2.8196112	-4.6831972	2.2539761				
H	3.1429047	-6.2654459	-4.4341740				
C	1.7772657	-4.7501855	-0.8279084				
C	2.0397428	-6.1566337	-4.4245127				
H	1.6081117	-7.0461653	-4.9259226				
H	1.1050775	-5.4926172	-0.3685700				
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C	4.4827974	-1.8939912	-2.6441711				
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H	-0.1829942	-3.2067087	1.2151093				
H	3.5120390	-1.7913757	-4.6202340				
H	-0.4819777	-5.9071532	-2.0054430				
H	0.1370948	-4.9546465	1.4873126				
H	1.7792285	-5.2704040	-5.0405721				
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C	-3.2301021	-0.3193725	-1.5953541				
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C	-4.9942096	1.4415644	-1.5044762				
C	-4.2553902	0.5024498	-2.2589396				
C	-5.9428021	2.2602046	-2.1305759				
C	-4.4717329	0.4005328	-3.6527451				
O	-2.2728471	-0.8354662	-2.3069548				
H	-6.8996045	2.7950511	-4.0096259				
H	-4.7796225	1.5598143	-0.4324136				
H	-5.5739433	1.1497396	-5.3605893				
H	-6.5053974	2.9991403	-1.5395787				
H	-3.8757950	-0.3133921	-4.2396483				
Br	0.1419658	-2.1230926	-3.8381952				

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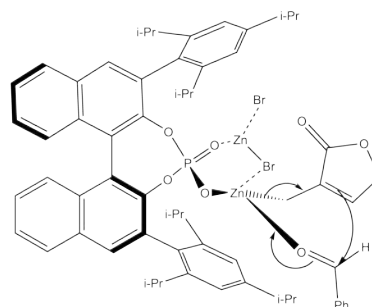


Energy (Hartree) = -11970.02641285
number of imaginary frequencies: 1

C	1.2627635	1.9578165	0.9564340
C	2.6632001	1.9641860	0.9660505
C	3.3222412	3.2468265	0.9736295
C	4.7286430	3.3872393	0.7786685
C	2.5311412	4.4407750	1.1539713
C	3.1844029	5.7094011	1.1776707
C	1.1190427	4.3325029	1.3058369
H	0.5327562	5.2424223	1.5063528
C	0.4588407	3.1144825	1.1831273
C	3.7143041	-1.6646657	0.2341737
C	4.7105457	-1.8550213	1.1828068
H	5.2176721	-2.8301755	1.2392239
C	5.0469493	-0.8491662	2.1326456
C	6.0152749	-1.0980505	3.1508538
C	4.3463664	0.4135166	2.1141008
C	4.5951621	1.3313249	3.1794267
C	3.4053503	0.6738981	1.0470345
C	3.1250469	-0.3657347	0.1551768
O	0.5783293	0.7565526	0.8067468
O	2.2511027	-0.1291992	-0.9021923
P	0.6387044	-0.0199021	-0.6334469
O	0.0867310	0.8186872	-1.7956872
O	-0.0141898	-1.3801670	-0.3313379
C	4.5560259	5.8095982	1.0019563
C	5.3299895	4.6378678	0.7887039
H	2.5715198	6.6125988	1.3250070
H	5.0450065	6.7955280	1.0142589
H	5.3341315	2.4862756	0.6057526
H	6.4149968	4.7219928	0.6239730
C	5.5289028	1.0500482	4.1671576
C	6.2623103	-0.1651330	4.1456125
H	4.0309117	2.2722998	3.2215151
H	5.6960309	1.7755352	4.9779063
H	7.0072991	-0.3726304	4.9287335
H	6.5494384	-2.0611686	3.1406558
C	-1.8917395	3.6300668	0.3995355
C	-1.0255897	2.9958259	1.3345205

C	-3.2788406	3.6038043	0.6354634	H	4.7666474	-1.1457500	-1.8692301
C	-1.5758190	2.2777688	2.4356171	H	2.1918477	-2.6819679	1.8438376
C	-2.9724995	2.2598070	2.6047440	H	3.2456370	-3.9931692	-3.8117302
C	-3.8443147	2.9344255	1.7347735	Zn	-0.7968883	0.1787844	-3.4611894
H	-3.9484249	4.1086072	-0.0804592	Br	-1.3926031	1.4983791	-5.2487464
C	-0.7218003	1.5380788	3.4655783	C	-6.1554397	2.1591176	-3.5054654
H	-3.3866619	1.7050793	3.4598173	C	-3.2324417	-0.3244513	-1.5922923
C	-1.0299808	0.0281991	3.4778826	C	-5.4102412	1.2405336	-4.2674474
H	-2.0756000	-0.1806088	3.7853341	C	-4.9978604	1.4388928	-1.4956146
H	-0.3637259	-0.4980797	4.1923677	C	-4.2568693	0.5046853	-2.2534205
H	-0.8776190	-0.4228373	2.4790857	C	-5.9453075	2.2602800	-2.1196242
C	-0.8705397	2.1617867	4.8661301	C	-4.4664385	0.4144559	-3.6484633
H	0.3428411	1.6548190	3.1813213	O	-2.2777541	-0.8374556	-2.3098388
H	-1.9072592	2.0629000	5.2502349	H	-6.8942085	2.8095322	-3.9983765
H	-0.6177527	3.2415138	4.8557700	H	-4.7840823	1.5530141	-0.4229157
H	-0.1980833	1.6575915	5.5905537	H	-5.5552955	1.1802258	-5.3563336
C	-5.3491169	2.9846139	1.9778858	H	-6.5094324	2.9951110	-1.5248673
C	-5.9132611	1.7058862	2.6156819	H	-3.8612379	-0.2881568	-4.2393101
H	-7.0219270	1.7228183	2.6132308	Br	0.1323295	-2.1320093	-3.8430601
H	-5.5943341	1.6038747	3.6735797	Zn	-1.0235472	-2.3824990	-1.6840828
H	-5.5741077	0.7915189	2.0878970	H	-5.5836632	-0.4857944	0.0334414
C	-5.7153163	4.2275447	2.8133766	H	-2.7676317	-4.1905060	-2.0373311
H	-5.8323458	3.1099297	0.9817099	C	-4.4429267	-2.0500294	-1.0409076
H	-6.8136202	4.3081340	2.9522641	C	-5.3018636	-1.5568919	0.0945749
H	-5.3574331	5.1581261	2.3292647	H	-4.8519719	-2.1954262	-2.0507838
H	-5.2457969	4.1711779	3.8175598	C	-3.4448521	-2.8616111	-0.4800962
C	-1.3747134	4.2871444	-0.8794036	C	-2.4870873	-3.7216296	-1.0777757
C	-1.9999965	3.6442505	-2.1291707	C	-3.4340501	-2.5571908	1.0015613
H	-1.5359138	4.0384831	-3.0550936	O	-4.5167683	-1.7574161	1.2796150
H	-3.0924717	3.8271428	-2.1976291	O	-2.6522162	-2.9253857	1.8465491
H	-1.8427776	2.5490482	-2.1315408	H	-6.2440013	-2.1442850	0.1814362
C	-1.5840294	5.8115105	-0.8699286	H	-1.9430880	-4.3744570	-0.3704616
H	-0.2840620	4.0965686	-0.9350303	H	-3.0167217	-0.0740242	-0.5275846
H	-1.1709824	6.2697753	-1.7919758				
H	-1.0898641	6.2887204	0.0007512				
H	-2.6628163	6.0699411	-0.8219643				
H	1.7638796	-6.9645291	-2.4597856				
H	5.5615822	-3.3422756	-3.8891590				
H	2.6099462	-4.6455839	3.3389510				
C	1.4954423	-6.0288790	-3.0033926				
H	4.5181040	-0.3642631	-4.2144447				
H	-0.4796728	-6.8257501	-3.5460567				
H	0.2532073	-3.8160774	2.8387399				
C	2.1037226	-4.8814022	-2.1957370				
C	5.7676803	-2.5873818	-3.1016577				
C	-0.0448466	-5.9480129	-3.0250649				
H	-0.3795752	-5.0335512	-3.5577641				
C	2.9767337	-3.9309917	-2.7478139				
C	2.8254382	-4.7011338	2.2518632				
H	3.1464504	-6.2553448	-4.4432492				
C	1.7862015	-4.7580966	-0.8279518				
C	2.0430174	-6.1512422	-4.4297040				
H	1.6140750	-7.0403896	-4.9340208				
H	1.1195122	-5.5052747	-0.3682047				
C	3.8122974	-1.1087220	-3.7916518				
H	6.4847950	-1.8527671	-3.5229328				
H	6.2645250	-3.1097558	-2.2590184				
C	3.5195852	-2.8785306	-1.9839039				
C	0.4640602	-3.9381683	1.7572148				
C	2.3052573	-3.7337272	-0.0182499				
H	3.9073530	-4.5110109	2.1075628				
H	2.6237457	-5.7405850	1.9175502				
C	4.4755767	-1.8868579	-2.6424359				
C	3.1854446	-2.7813449	-0.6115287				
C	1.9531594	-3.6988929	1.4698547				
H	2.9119141	-0.5706652	-3.4382324				
H	-0.1748613	-3.2149737	1.2205137				
H	3.5015644	-1.7819420	-4.6173965				
H	-0.4718135	-5.9208004	-2.0026268				
H	0.1410520	-4.9651531	1.4845626				
H	1.7764303	-5.2637877	-5.0411212				

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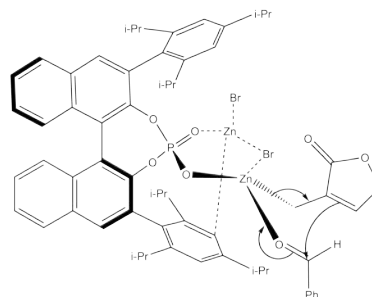


Energy (Hartree) = -11970.014802
number of imaginary frequencies: 1

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C	2.4740009	2.3024069	0.4522644
C	3.1292712	3.5900874	0.4719602
C	4.5362579	3.7422311	0.2862484
C	2.3321861	4.7810106	0.6460181
C	2.9791665	6.0518697	0.6959189
C	0.9145989	4.6739381	0.7408168
H	0.3230101	5.5855451	0.9143005
C	0.2616110	3.4560851	0.6059758
C	3.6479938	-1.1598576	-0.7566559
C	4.7289590	-1.3945577	0.0825769
H	5.3262277	-2.3101834	-0.0478750
C	5.0534193	-0.5065446	1.1509211
C	6.1079969	-0.8108336	2.0629090
C	4.2750851	0.6942849	1.3522850
C	4.5492879	1.4909681	2.5038116
C	3.2396650	1.0238233	0.3999290
C	2.9471474	0.0762991	-0.5827767
O	0.3989631	1.0671167	0.3482954

O	1.9570614	0.3554524	-1.5167770	H	0.8686111	-4.7564881	-1.7510708
P	0.3735498	0.3831811	-1.1422466	C	3.0499499	0.3274366	-4.5838610
O	-0.2380678	1.3236529	-2.1943947	H	5.7077439	-0.4348909	-4.8472642
O	-0.2511465	-1.0103198	-0.9936952	H	5.6562178	-1.8952155	-3.8008619
C	4.3525665	6.1607431	0.5421611	C	2.9931403	-1.7727337	-3.1169266
C	5.1320530	4.9952329	0.3190878	C	1.2828546	-2.9941789	1.0390769
H	2.3592989	6.9503951	0.8425826	C	2.3455367	-3.2506306	-1.2485223
H	4.8373498	7.1482655	0.5748584	H	3.1301136	-5.7044695	-0.2143684
H	5.1506869	2.8504251	0.1023145	H	1.3731218	-5.6356482	0.1429439
H	6.2180748	5.0849331	0.1643838	C	3.8451989	-0.6467877	-3.6991074
C	5.5695039	1.1543500	3.3831676	C	3.0619398	-2.1219947	-1.7385068
C	6.3689127	0.0037774	3.1543918	C	2.3961103	-3.6781095	0.2215973
H	3.9340263	2.3806415	2.6965639	H	2.1731102	0.7390951	-4.0483604
H	5.7557594	1.7833956	4.2669613	H	1.3828056	-1.8911732	1.0344045
H	7.1816872	-0.2487143	3.8522454	H	2.6785602	-0.1554357	-5.5108942
H	6.7020938	-1.7220820	1.8907032	H	-1.2620925	-2.7193411	-3.5789474
C	-2.0501181	3.5841268	-0.4498130	H	0.2921335	-3.2326191	0.6047435
C	-1.2268036	3.2987502	0.6762551	H	1.1583137	-3.9002757	-6.3083516
C	-3.4279442	3.3242869	-0.3538446	H	4.2562500	-0.0627422	-2.8489564
C	-1.8017464	2.7816368	1.8660038	H	3.3591329	-3.3260207	0.6413081
C	-3.1844057	2.5200145	1.9009904	H	2.0473333	-2.1939040	-5.0140679
C	-4.0155917	2.7712000	0.7991367	Zn	-1.3163193	0.8775853	-3.7352240
H	-4.0772425	3.5360191	-1.2182222	Br	-0.7828848	1.0702917	-5.9449483
C	-0.9599601	2.5030680	3.1097665	C	-4.1959463	-1.2593132	5.7289071
H	-3.6137169	2.0914316	2.8187117	C	-2.4815483	-1.9881578	1.8397304
C	-0.9835308	1.0151264	3.4949797	C	-4.8988998	-0.8862683	4.5679943
H	-1.9959245	0.6971050	3.8143980	C	-2.3943588	-2.1324062	4.3487832
H	-0.2910324	0.8145037	4.3386278	C	-3.0970357	-1.7660235	3.1821367
H	-0.6836727	0.3806665	2.6379120	C	-2.9424923	-1.8812641	5.6163382
C	-1.3919523	3.3975924	4.2858387	C	-4.3534203	-1.1365398	3.3031087
H	0.0902845	2.7683280	2.8723464	O	-2.8047019	-1.1819184	0.8781502
H	-2.4353192	3.1810601	4.5971472	H	-4.6241192	-1.0565439	6.7224007
H	-1.3382504	4.4719541	4.0167632	H	-1.3893404	-2.5762326	4.2612511
H	-0.7390116	3.2297270	5.1673773	H	-5.8774170	-0.3885521	4.6526246
C	-5.4933631	2.3946747	0.7805471	H	-2.3800280	-2.1589556	6.5206837
C	-5.6771963	1.0567218	0.0333317	H	-4.8826708	-0.8284130	2.3895791
H	-6.7447531	0.7531864	0.0102416	Br	-3.2619414	-0.2997817	-2.8215040
H	-5.0864514	0.2523654	0.5194839	Zn	-2.1512030	-1.5299635	-0.9371945
H	-5.3148065	1.1249541	-1.0114574	H	-2.3314421	-4.4858228	3.2475422
C	-6.1472125	2.3523121	2.1678581	H	-4.1023801	-3.0334189	-1.3000984
H	-6.0168892	3.1794977	0.1888823	C	-3.3239894	-3.8036275	1.3883882
H	-7.2384838	2.1778724	2.0772715	C	-2.7414159	-4.8692500	2.2904271
H	-5.9952878	3.3006571	2.7217175	H	-4.3548727	-3.4543405	1.5451194
H	-5.7354219	1.5314205	2.7906712	C	-2.8127816	-4.0553532	0.0926095
C	-1.4675809	4.1548914	-1.7426295	C	-3.0904436	-3.4445721	-1.1422809
C	-2.1869010	3.6518554	-3.0069902	C	-1.7108555	-5.0685011	0.2415091
H	-1.5488697	3.7671918	-3.9063692	O	-1.6659521	-5.4691537	1.5470166
H	-3.1325745	4.1971189	-3.2074564	O	-0.9782064	-5.5184199	-0.6141568
H	-2.4888847	2.5858931	-2.8952579	H	-3.4849364	-5.6593498	2.5371538
C	-1.4612166	5.6959003	-1.7325214	H	-2.6123949	-3.8994160	-2.0278480
H	-0.4167783	3.8061756	-1.8026104	H	-1.4294220	-2.3627543	1.8883623
H	-1.0267940	6.0949020	-2.6725384				
H	-0.8685727	6.0982293	-0.8890052				
H	-2.4939770	6.0913486	-1.6362514				
H	-0.1992942	-4.9980388	-3.7487392				
H	4.7114359	-1.8500206	-5.3204060				
H	2.5556515	-5.4619545	1.4682422				
C	0.2283611	-4.1517735	-4.3297751				
H	3.6905032	1.1777891	-4.8955044				
H	-1.7627964	-3.5661227	-5.0792361				
H	1.2965473	-3.3414621	2.0933892				
C	1.3222424	-3.5347679	-3.4692702				
C	5.0495211	-1.2391212	-4.4573113				
C	-0.8972693	-3.1201481	-4.5464905				
H	-0.5464697	-2.2516828	-5.1435557				
C	2.1282956	-2.4910383	-3.9568578				
C	2.3595473	-5.2047229	0.4068993				
H	1.5465544	-5.4559027	-5.5085502				
C	1.4844486	-3.9293226	-2.1319291				
C	0.7454159	-4.7061598	-5.6664359				
H	-0.0738937	-5.1916093	-6.2357454				

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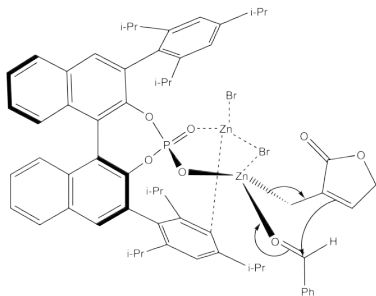


Energy (Hartree) = -11970.03284193

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C	2.1787239	2.6588361	1.3892155
C	2.8507511	3.9375472	1.4313797
C	4.2656654	4.0784105	1.2987613
C	2.0618925	5.1373392	1.5827984

C	2.7182806	6.4011861	1.6803603	C	2.2497843	-3.8851171	-4.8076250
C	0.6407356	5.0509788	1.5592436	H	3.2827857	2.3932605	-3.6880713
H	0.0513933	5.9772702	1.6361784	H	0.8604283	-3.8686448	-6.5042786
C	-0.0123805	3.8386423	1.3811228	H	0.7207532	-4.3228876	1.3440674
C	3.4647946	-0.6356224	-0.0852884	C	2.5915315	-3.0477193	-3.5824415
C	4.5437333	-0.9012778	0.7506609	C	5.2853214	0.4515404	-3.4931354
H	5.2076354	-1.7464237	0.5144734	C	1.1424591	-3.2227898	-5.6465673
C	4.8018906	-0.1302391	1.9200641	H	1.4741706	-2.2465168	-6.0588750
C	5.8531932	-0.4792026	2.8205816	C	3.0805320	-1.7356710	-3.7074071
C	3.9793893	1.0193471	2.2098631	C	3.4799458	-4.3637384	0.6819452
C	4.2156324	1.7340495	3.4226211	H	4.2802070	-4.6987748	-5.0541666
C	2.9341193	1.3808205	1.2837671	C	2.3980216	-3.5541384	-2.2876595
C	2.6596209	0.5011525	0.2293616	C	3.4981612	-4.1904903	-5.6543119
O	0.1078319	1.4318694	1.3534264	H	3.2431381	-4.8454812	-6.5133746
O	1.5808359	0.7670799	-0.6196031	H	1.9886353	-4.5697514	-2.1833430
P	0.0787573	0.5132386	-0.0167060	C	2.9046297	1.3535597	-3.5985860
O	-0.8985802	1.0695923	-1.0621509	H	5.6903291	1.4788081	-3.6056904
O	-0.1175164	-0.9370395	0.4540110	H	6.0109727	-0.1418566	-2.9003334
C	4.0984518	6.4961444	1.5881706	C	3.3665454	-0.9327553	-2.5897056
C	4.8728286	5.3244301	1.3759014	C	0.9985031	-4.0946482	0.2951543
H	2.1016504	7.3045526	1.8097341	C	2.6578017	-2.7920602	-1.1341826
H	4.5929178	7.4769580	1.6574976	H	4.4689154	-3.8659536	0.7229994
H	4.8806639	3.1854485	1.1245322	H	3.5642783	-5.2133340	-0.0279223
H	5.9650598	5.4038585	1.2651800	C	3.9027994	0.4805916	-2.8154470
C	5.2342122	1.3572099	4.2874537	C	3.1594524	-1.4702605	-1.2883464
C	6.0706159	0.2504100	3.9799697	C	2.3672436	-3.3949226	0.2397389
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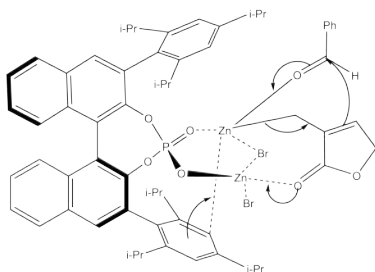
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TS ξ -ma; woelfling data



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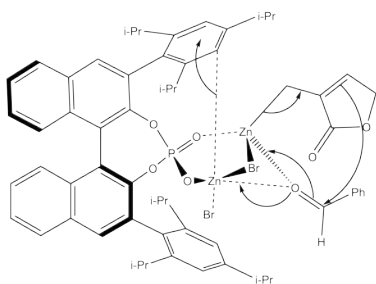
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H	-2.002017	-5.551961	-0.388891
C	-2.282894	-3.415174	-2.097766
H	-3.115096	-4.347540	-4.404905
H	-3.586999	-6.743317	-5.013094
H	-3.278554	-8.536341	-3.289166
O	-1.842594	-2.951747	-1.036749
H	-2.541842	-2.723446	-2.937536

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C	4.5947583	5.7075108	1.0989005
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H	2.6195113	6.5380725	1.4152052
H	5.1013026	6.6840857	1.1329157
H	5.3214538	2.3817913	0.6394292
H	6.4349095	4.5939125	0.7021650
C	5.6505916	0.8163429	4.0334754
C	6.4336460	-0.3572376	3.8670746
H	4.0517671	2.0432295	3.2714878
H	5.8307951	1.4760781	4.8959728
H	7.2276985	-0.5953629	4.5911379
H	6.7526984	-2.1424821	2.6829523
C	-1.7156035	3.6287058	-0.0283441
C	-1.0465235	3.0617173	1.0953101
C	-3.1181246	3.7333380	0.0047664
C	-1.7962372	2.5591181	2.1913906
C	-3.1989410	2.7011099	2.1793329
C	-3.8805852	3.3116144	1.1117285
H	-3.6428678	4.1792383	-0.8551057
C	-1.1232861	1.9171325	3.4031150
H	-3.7675128	2.3548619	3.0564882
C	-1.5385602	0.4445342	3.5707917
H	-2.6189767	0.3492843	3.8072156
H	-0.9751517	-0.0265682	4.4025599
H	-1.3348902	-0.1353912	2.6491246
C	-1.3736179	2.7287625	4.6871386
H	-0.0290669	1.9289660	3.2252857
H	-2.4509605	2.7486140	4.9545152
H	-1.0368924	3.7789997	4.5708399
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C	-5.3717111	3.6311627	1.1566092
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H	-5.9462227	2.7330729	3.0874132
H	-6.0774408	1.6156848	1.6931045
C	-5.5704528	5.0876292	1.6256022
H	-5.7443568	3.5596312	0.1128660
H	-6.6439203	5.3688712	1.6026479
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H	-5.2029500	5.2186894	2.6653677
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H	-2.5074720	3.9521092	-2.8012248
H	-1.4863617	2.5078253	-2.5656409
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H	0.1005185	3.8288718	-1.1449285
H	-0.3631817	6.0895953	-2.1158474
H	-0.5297366	6.1322002	-0.3308671
H	-1.9908646	6.0952909	-1.3629657
H	0.4418516	-5.9672857	-3.0413209
H	5.2144226	-2.6996528	-4.4659686
H	3.2978658	-5.1623778	2.7580705
C	1.4608370	-5.8008877	-3.4598437
H	3.8463025	0.1759303	-4.4034340
H	0.7531260	-6.2449935	-5.4744166
H	0.9103728	-4.3584172	2.7436717
C	2.0807667	-4.6975260	-2.6086002
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C	1.3021359	-5.4423161	-4.9417265
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C	2.8032832	-3.6219040	-3.1480166
C	3.3348943	-5.0658823	1.6529575
H	2.3307801	-7.4156874	-2.2333722
C	1.9423429	-4.7573309	-1.2071930
C	2.2509237	-7.1152449	-3.2973747
H	1.7607735	-7.9431839	-3.8505533
H	1.3711191	-5.5912125	-0.7708856
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H	6.0199343	-1.1491841	-4.0686788

TS γ -mi; COSMO



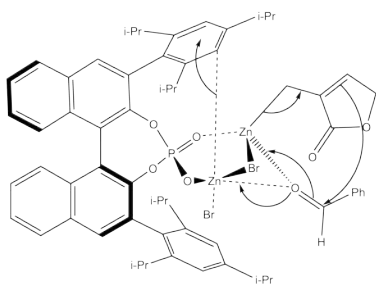
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C	4.7262649	3.2853578	0.8304558
C	2.5478779	4.3691005	1.2091322
C	3.2200955	5.6277055	1.2614632
C	1.1304934	4.2861161	1.2945380
H	0.5527719	5.2109633	1.4425525
C	0.4495074	3.0826684	1.1412340
C	3.7404213	-1.6325322	-0.0292766
C	4.8042012	-1.8505545	0.8384692
H	5.3607620	-2.7979785	0.7754913
C	5.1439305	-0.9224157	1.8633369
C	6.1764924	-1.2119738	2.8058023
C	4.3872366	0.2994336	1.9961072
C	4.6536082	1.1365357	3.1217771
C	3.3781520	0.6042352	1.0082872
C	3.0782576	-0.3695767	0.0514858
O	0.5392850	0.6846730	0.9453273
O	2.1054114	-0.0900120	-0.9094700
P	0.5235349	-0.1342345	-0.4776441
O	-0.2222697	0.6582453	-1.5702255

H	6.0701445	-2.5155154	-2.9035106
C	3.3607780	-2.6140093	-2.3370744
C	0.9315664	-4.2715646	-1.6375830
C	2.4977809	-3.7927282	-0.3493978
H	4.3820824	-4.8463986	1.3625066
H	3.0694927	-6.0516175	1.2161974
C	4.1348853	-1.4720026	-2.9914038
C	3.2112415	-2.7014388	-0.9302147
C	2.3630432	-3.9726828	1.1646948
H	2.3596698	-0.2918621	-3.5071038
H	0.2375185	-3.4604833	1.3465923
H	2.9602901	-1.3145845	-4.8494936
H	0.7389130	-4.4970310	-5.0759523
H	0.5358703	-5.2200732	1.2219537
H	3.2825458	-7.0021718	-3.6930010
H	4.4346000	-0.7676530	-2.1880053
H	2.6638847	-3.0202559	1.6450059
H	2.9254218	-3.5447694	-4.2382078
Zn	-0.9433808	-2.8192527	-1.2900002
Br	-1.6986680	-5.0012026	-1.0022227
H	-5.1220670	-4.6856686	1.2972981
H	-5.8345423	-3.4880917	3.3857166
C	-4.9441141	-3.6046716	1.4019469
C	-5.3395583	-2.9328267	2.5742225
C	-4.3146979	-2.9053708	0.3654860
C	-5.0966120	-1.5557302	2.7119554
H	-3.9917306	-3.4346924	-0.5432831
H	-5.3925160	-1.0285632	3.6318024
C	-4.0684859	-1.5217736	0.4989388
C	-4.4645631	-0.8515126	1.6772398
H	-6.1311359	0.0952147	-0.1033204
H	-5.0005961	-1.5116562	-2.1332931
C	-6.0958202	0.2451140	-1.2019125
C	-4.9421161	-0.4409111	-1.8896522
H	-4.2401002	0.2205470	1.7868661
C	-3.3839152	-0.7454056	-0.5587766
O	-2.4930933	-1.3167830	-1.3262050
H	-7.0744629	-0.0742070	-1.6215949
Br	-0.4296880	-2.1121429	-3.6581230
C	-4.3606451	0.5052770	-2.7630236
O	-5.9214064	1.6499741	-1.4634628
H	-3.3672373	-0.5795161	-4.3278930
Zn	-1.6037391	-0.1268077	-2.7418620
C	-3.3648699	0.3694494	-3.7606365
C	-4.9508167	1.8450850	-2.4040422
H	-3.1776541	1.2769441	-4.3620872
O	-4.6938252	2.9379432	-2.8638131
H	-3.2053311	0.3238249	-0.2922743

H	0.5483663	5.2094461	1.4425567
C	0.4492422	3.0821417	1.1421716
C	3.7380268	-1.6293795	-0.0303588
C	4.8002633	-1.8504923	0.8381701
H	5.3526322	-2.8002814	0.7742279
C	5.1425934	-0.9244434	1.8636754
C	6.1742389	-1.2163437	2.8056838
C	4.3888519	0.2989273	1.9975197
C	4.6578441	1.1345691	3.1233340
C	3.3802123	0.6067368	1.0103786
C	3.0794393	-0.3645854	0.0512444
O	0.5419048	0.6843482	0.9483818
O	2.1077467	-0.0816719	-0.9094232
P	0.5273112	-0.1301689	-0.4774172
O	-0.2242135	0.6669375	-1.5638325
O	0.0546285	-1.5501909	-0.1323842
C	4.5917415	5.7106630	1.1103293
C	5.3465526	4.5301501	0.8771945
H	2.6153719	6.5391064	1.4214011
H	5.0970892	6.6877397	1.1459604
H	5.3212031	2.3860087	0.6510202
H	6.4334436	4.5990753	0.7178904
C	5.6546764	0.8119872	4.0336777
C	6.4343396	-0.3630300	3.8666717
H	4.0580291	2.0425518	3.2726207
H	5.8371557	1.4713375	4.8959227
H	7.2282314	-0.6035565	4.5900311
H	6.7476821	-2.1484626	2.6823038
C	-1.7129138	3.6267449	-0.0336446
C	-1.0466116	3.0607516	1.0920953
C	-3.1151773	3.7330246	-0.0034133
C	-1.7988600	2.5594875	2.1867225
C	-3.2012678	2.7022742	2.1712583
C	-3.8801350	3.3129184	1.1022562
H	-3.6382010	4.1775501	-0.8650365
C	-1.1286116	1.9186109	3.4005180
H	-3.7716765	2.3575395	3.0478659
C	-1.5446229	0.4466125	3.5698381
H	-2.6253629	0.3510871	3.8048060
H	-0.9830582	-0.0243319	4.4027809
H	-1.3395837	-0.1355888	2.6500822
C	-1.3797644	2.7330655	4.6824121
H	-0.0341743	1.9293312	3.2241567
H	-2.4572817	2.7553903	4.9487432
H	-1.0424016	3.7826977	4.5643504
H	-0.8339554	2.2905465	5.5411331
C	-5.3708212	3.6351352	1.1432581
C	-6.2092979	2.6790647	2.0003720
H	-7.2866190	2.9245529	1.9099774
H	-5.9509420	2.7489393	3.0779888
H	-6.0793026	1.6232676	1.6898890
C	-5.5679752	5.0939105	1.6050788
H	-5.7426759	3.5587222	0.0996099
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H	-5.0097202	5.7997862	0.9583387
H	-5.2012158	5.2301070	2.6443114
C	-0.9462349	4.1584542	-1.2461406
C	-1.4729425	3.6071758	-2.5803380
H	-0.8124646	3.9246545	-3.4131175
H	-2.5004062	3.9487740	-2.8105028
H	-1.4852390	2.5008588	-2.5660137
C	-0.9479263	5.6993368	-1.2693057
H	0.1048614	3.8202498	-1.1489854
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H	-0.5207071	6.1275189	-0.3409799
H	-1.9810990	6.0915384	-1.3731281
H	0.4218671	-5.9445789	-3.0510686
H	5.2129580	-2.7031390	-4.4642648
H	3.2846803	-5.1696038	2.7466559
C	1.4427026	-5.7831768	-3.4669028
H	3.8643354	0.1822110	-4.4012926

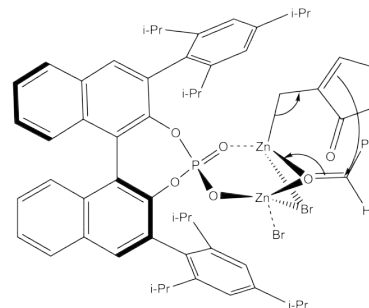
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C	4.7258686	3.2896152	0.8406957
C	2.5460188	4.3708786	1.2149586
C	3.2172985	5.6293651	1.2692700
C	1.1288407	4.2859851	1.2967311

H	0.7378133	-6.2239854	-5.4831066
H	0.9011281	-4.3537910	2.7408017
C	2.0662449	-4.6831248	-2.6143049
C	5.4338102	-1.9938686	-3.6392931
C	1.2892510	-5.4240204	-4.9490298
H	2.2740282	-5.3162486	-5.4509943
C	2.7952752	-3.6110145	-3.1512643
C	3.3192099	-5.0684871	1.6419419
H	2.3033193	-7.4012755	-2.2383836
C	1.9256522	-4.7436016	-1.2131256
C	2.2267384	-7.1007299	-3.3024195
H	1.7344901	-7.9269789	-3.8561243
H	1.3493859	-5.5749554	-0.7787804
C	3.2858133	-0.6717055	-3.9918366
H	6.0286216	-1.1590361	-4.0647881
H	6.0666434	-2.5269837	-2.9010386
C	3.3572022	-2.6072466	-2.3387526
C	0.9203854	-4.2612102	1.6352474
C	2.4864164	-3.7838933	-0.3533789
H	4.3668908	-4.8545497	1.3493429
H	3.0480170	-6.0509545	1.2018289
C	4.1393040	-1.4692361	-2.9905259
C	3.2057977	-2.6956949	-0.9323435
C	2.3523759	-3.9679965	1.1603139
H	2.3745582	-0.2730904	-3.5060856
H	0.2300060	-3.4442557	1.3524305
H	2.9664160	-1.3000148	-4.8491033
H	0.7299069	-4.4769076	-5.0853452
H	0.5161474	-5.2044736	1.2161886
H	3.2598924	-6.9926199	-3.6949972
H	4.4427299	-0.7682249	-2.1855315
H	2.6596253	-3.0192578	1.6439278
H	2.9196765	-3.5339007	-4.2411344
Zn	-0.9161081	-2.8355585	-1.2984059
Br	-1.6985238	-5.0037534	-1.0224252
H	-5.0675664	-4.7046262	1.3362095
H	-5.8095304	-3.4970211	3.4095665
C	-4.9107667	-3.6194726	1.4303900
C	-5.3207371	-2.9424066	2.5938603
C	-4.2885288	-2.9214728	0.3888491
C	-5.0973794	-1.5612037	2.7192950
H	-3.9479435	-3.4569142	-0.5102055
H	-5.4023114	-1.0292176	3.6334104
C	-4.0631641	-1.5336383	0.5098754
C	-4.4708032	-0.8579663	1.6808801
H	-6.1243915	0.0724011	-0.0940149
H	-4.9884881	-1.5294845	-2.1230227
C	-6.0864228	0.2266990	-1.1920629
C	-4.9280152	-0.4594636	-1.8757815
H	-4.2581879	0.2173851	1.7825433
C	-3.3854364	-0.7580156	-0.5549243
O	-2.4924599	-1.3317034	-1.3192432
H	-7.0639060	-0.0943648	-1.6151723
Br	-0.4198472	-2.0907088	-3.6677911
C	-4.3532738	0.4885670	-2.7544895
O	-5.9134090	1.6298937	-1.4491604
H	-3.3495603	-0.5920454	-4.3184134
Zn	-1.6000375	-0.1418371	-2.7167949
C	-3.3596214	0.3574516	-3.7527515
C	-4.9411740	1.8294852	-2.3910835
H	-3.1753891	1.2682019	-4.3501572
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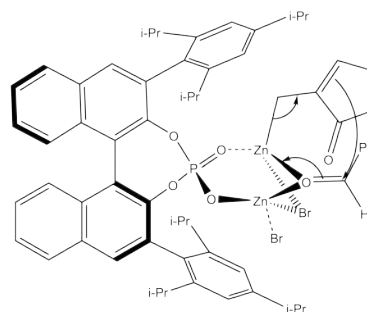
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C	4.8806302	3.3635650	0.6501929
C	2.7583532	4.5787725	0.9681544
C	3.4866766	5.8027297	0.8764078
C	1.3461076	4.5697896	1.1604712
H	0.8221085	5.5257353	1.3123892
C	0.6151476	3.3878701	1.1589402
C	3.6160875	-1.6077947	0.4031176
C	4.6087175	-1.8009466	1.3567215
H	5.0876916	-2.7884947	1.4391733
C	4.9878333	-0.7756444	2.2694176
C	5.9510100	-1.0240186	3.2933980
C	4.3490295	0.5174859	2.1974116
C	4.6557857	1.4755511	3.2110444
C	3.4063140	0.7687782	1.1318585
C	3.0629556	-0.2960725	0.2948843
O	0.5820629	0.9965352	0.9705791
O	2.1615966	-0.0655788	-0.7410851
P	0.5667622	0.1139627	-0.4103081
O	0.0053286	0.8983628	-1.6105761
O	-0.1128567	-1.2044331	-0.0120522
C	4.8588604	5.8028546	0.6732038
C	5.5568507	4.5716657	0.5480243
H	2.9326383	6.7510277	0.9584237
H	5.4068538	6.7543207	0.5967084
H	5.4283245	2.4163173	0.5438259
H	6.6417993	4.5748646	0.3625630
C	5.5829543	1.1956131	4.2058349
C	6.2518257	-0.0569413	4.2404620
H	4.1420262	2.4463918	3.2068938
H	5.7964423	1.9510005	4.9775126
H	6.9919717	-0.2634810	5.0284809
H	6.4388338	-2.0109436	3.3257670
C	-1.7877034	3.7276119	0.4155430
C	-0.8595243	3.3555908	1.4224717
C	-3.1606092	3.7378542	0.7327483
C	-1.3206410	2.9521544	2.7075885
C	-2.7023933	2.9633931	2.9656587
C	-3.6413278	3.3646104	1.9984852
H	-3.8843801	4.0414884	-0.0400819
C	-0.3660487	2.5004791	3.8125047
H	-3.0561964	2.6515459	3.9616983
C	-0.5558465	1.0064879	4.1377488
H	-1.5665012	0.8101749	4.5539612
H	0.1877934	0.6732483	4.8911947
H	-0.4303847	0.3849016	3.2295234
C	-0.4898588	3.3775249	5.0710913
H	0.6703288	2.6244931	3.4379808
H	-1.4942464	3.2897541	5.5356079
H	-0.3219543	4.4478425	4.8340144
H	0.2561979	3.0730549	5.8340136
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H	-6.7647799	1.9810130	2.7641969	Br	-0.0839836	-2.1887447	-3.4468288
H	-5.1963347	1.5374606	3.5067416	Zn	-1.1872992	-2.3026925	-1.2501277
H	-5.4577172	1.2739870	1.7566913	H	-6.5649783	-3.5868508	-1.9886903
C	-5.4675012	4.3484581	3.4598860	H	-1.9911251	-4.6239807	-0.5179633
H	-5.6482666	3.7600551	1.3998673	C	-4.6844774	-2.6361010	-1.4393725
H	-6.5627410	4.3953586	3.6322080	C	-5.6614583	-3.1452639	-2.4656440
H	-5.1077804	5.3737810	3.2401631	H	-4.9958133	-1.9806572	-0.6146402
H	-4.9941497	4.0229781	4.4097956	C	-3.6415179	-3.5620235	-1.3571450
C	-1.3330472	4.1056722	-0.9914508	C	-2.5292860	-3.6586954	-0.4765867
C	-2.1860917	3.4376610	-2.0795642	C	-3.7913248	-4.4862421	-2.5402739
H	-1.7333075	3.5808311	-3.0804359	O	-4.9622839	-4.1775024	-3.1801850
H	-3.2162894	3.8483525	-2.1235020	O	-3.0555854	-5.3771997	-2.9039696
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C	-1.3009539	5.6337562	-1.1813457	H	-2.6665852	-3.2474754	0.5398192
H	-0.2976029	3.7243702	-1.1123437	H	-3.5284562	-1.5880466	-3.4278500
H	-0.9506385	5.8954115	-2.2012256				
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H	-2.3138537	6.0688203	-1.0476326				
H	1.8479978	-6.9984533	-2.1940925				
H	5.5033420	-3.1904801	-3.7287485				
H	2.4817659	-4.6495253	3.5055719				
C	1.6301270	-6.0984066	-2.8144905				
H	4.3017934	-0.2782248	-4.0697360				
H	-0.2897093	-6.9361591	-3.4874978				
H	0.1515144	-3.8252481	2.9646642				
C	2.1505436	-4.9037714	-2.0171377				
C	5.6742916	-2.4219666	-2.9460914				
C	0.1016622	-6.0259253	-2.9892371				
H	-0.1887660	-5.1526611	-3.6074594				
C	2.9702788	-3.9080343	-2.5708504				
C	2.7142022	-4.7038106	2.4217169				
H	3.4221220	-6.3607124	-4.0709212				
C	1.7974338	-4.7749601	-0.6587790				
C	2.3195496	-6.2949745	-4.1695824				
H	1.9640876	-7.2286798	-4.6500194				
H	1.1598276	-5.5512938	-0.2047653				
C	3.6387439	-1.0535672	-3.6330527				
H	6.3500223	-1.6530890	-3.3747296				
H	6.2020815	-2.9129664	-2.1032010				
C	3.4458182	-2.8188324	-1.8137402				
C	0.3734971	-3.9048431	1.8806155				
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C	4.3507784	-1.7861126	-2.4822029				
C	3.0972822	-2.7288791	-0.4428483				
C	1.8739728	-3.6843368	1.6277700				
H	2.7149160	-0.5591423	-3.2755283				
H	-0.2253417	-3.1379108	1.3551333				
H	3.3560374	-1.7515395	-4.4483108				
H	-0.4281257	-5.9268842	-2.0221734				
H	0.0343741	-4.9089232	1.5509619				
H	2.0879186	-5.4612747	-4.8652509				
H	4.6102865	-1.0239818	-1.7187656				
H	2.1179499	-2.6733305	2.0136256				
H	3.2578275	-3.9712757	-3.6301903				
Zn	-0.9748716	0.1396536	-3.1292122				
Br	-1.9375790	1.1066052	-4.9897382				
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C	-5.5607903	0.1373882	-3.5577846				
C	-4.6823292	0.0182782	-2.4565815				
C	-6.5735077	1.1062783	-3.5492638				
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H	-7.5123949	2.7201557	-2.4334537				
H	-5.4151950	-0.5034571	-4.4415069				
H	-5.9389791	2.5345871	-0.4922507				
H	-7.2449355	1.2054324	-4.4153696				
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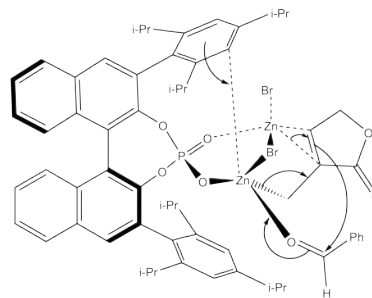


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C	2.7539867	4.5769995	0.9667968
C	3.4821817	5.8005334	0.8754242
C	1.3418369	4.5666643	1.1576961
H	0.8161680	5.5218074	1.3088782
C	0.6113034	3.3847379	1.1562236
C	3.6149705	-1.6084766	0.4027460
C	4.6069356	-1.8007605	1.3569236
H	5.0856372	-2.7884823	1.4388609
C	4.9854754	-0.7759028	2.2699749
C	5.9479665	-1.0230772	3.2942219
C	4.3462372	0.5167885	2.1975975
C	4.6525556	1.4750704	3.2108392
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C	3.0613572	-0.2968842	0.2939669
O	0.5796725	0.9938472	0.9679816
O	2.1617292	-0.0667926	-0.7421807
P	0.5661669	0.1117477	-0.4141939
O	0.0035025	0.8953230	-1.6130843
O	-0.1094661	-1.2089813	-0.0153241
C	4.8541582	5.8013871	0.6743876
C	5.5525109	4.5708649	0.5509569
H	2.9275742	6.7486353	0.9557209
H	5.4016738	6.7530862	0.5980896
H	5.4243196	2.4154692	0.5476834
H	6.6376963	4.5743155	0.3672217
C	5.5793762	1.1957032	4.2055502
C	6.2482963	-0.0561541	4.2408428
H	4.1385642	2.4457135	3.2053452
H	5.7926384	1.9515212	4.9768034
H	6.9882442	-0.2624265	5.0290523
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C	-1.7915920	3.7263827	0.4143825	H	0.0331723	-4.9089026	1.5515846
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C	-3.1635605	3.7416598	0.7345498	H	4.6106474	-1.0254447	-1.7176331
C	-1.3230864	2.9528880	2.7067118	H	2.1177523	-2.6743942	2.0131867
C	-2.7039336	2.9692421	2.9672149	H	3.2583690	-3.9718965	-3.6296864
C	-3.6429281	3.3726398	2.0016369	Zn	-0.9752914	0.1394305	-3.1353630
H	-3.8875006	4.0463849	-0.0377278	Br	-1.9629976	1.1029203	-4.9798973
C	-0.3679662	2.4983049	3.8098549	C	-6.7158439	1.9550014	-2.4250768
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C	-0.5621442	1.0051265	4.1357754	C	-5.8352845	1.8422407	-1.3327569
H	-1.5725010	0.8120160	4.5541001	C	-5.5531998	0.1466126	-3.5545686
H	0.1818146	0.6690661	4.8875715	C	-4.6779194	0.0179800	-2.4525287
H	-0.4413545	0.3829375	3.2274984	C	-6.5678688	1.1129465	-3.5394645
C	-0.4852472	3.3767829	5.0679372	C	-4.8153867	0.8853910	-1.3448726
H	0.6679875	2.6183674	3.4330170	O	-2.5176879	-0.7790721	-1.8035315
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H	-0.3141803	4.4461524	4.8296410	H	-5.4004531	-0.4825732	-4.4454495
H	0.2611906	3.0703034	5.8296156	H	-5.9422111	2.5136011	-0.4682785
C	-5.1336495	3.3971046	2.3180726	H	-7.2364961	1.2198157	-4.4067890
C	-5.6758821	1.9858291	2.6090861	H	-4.1026501	0.8069018	-0.5094113
H	-6.7724621	2.0065939	2.7787963	Br	-0.0856153	-2.1910915	-3.4537012
H	-5.2045042	1.5566797	3.5175637	Zn	-1.1798289	-2.3050072	-1.2564114
H	-5.4712571	1.2909892	1.7694911	H	-6.5553051	-3.5907686	-2.0085861
C	-5.4602464	4.3693315	3.4654890	H	-1.9832116	-4.6271000	-0.5280995
H	-5.6491755	3.7774277	1.4074305	C	-4.6765218	-2.6390166	-1.4478323
H	-6.5546040	4.4232963	3.6414136	C	-5.6485852	-3.1481099	-2.4803291
H	-5.0947045	5.3916497	3.2426144	H	-4.9917159	-1.9851725	-0.6232131
H	-4.9858822	4.0440115	4.4147625	C	-3.6334483	-3.5645853	-1.3638016
C	-1.3387209	4.0987330	-0.9947192	C	-2.5227807	-3.6629297	-0.4828741
C	-2.1962800	3.4304680	-2.0790477	C	-3.7767669	-4.4873270	-2.5513166
H	-1.7462027	3.5677186	-3.0817295	O	-4.9481721	-4.1754770	-3.1950731
H	-3.2253288	3.8441091	-2.1228597	O	-3.0387501	-5.3744923	-2.9112432
H	-2.2869202	2.3407441	-1.9050435	H	-5.9953820	-2.3824456	-3.2057232
C	-1.3017788	5.6260292	-1.1891994	H	-2.6580085	-3.2537531	0.5345537
H	-0.3049585	3.7133736	-1.1170043	H	-3.5195681	-1.5814951	-3.4326540
H	-0.9528421	5.8833785	-2.2104903				
H	-0.6244112	6.1181239	-0.4631701				
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H	2.4816796	-4.6505376	3.5054911				
C	1.6326925	-6.0999684	-2.8150718				
H	4.3030899	-0.2783652	-4.0683540				
H	-0.2867396	-6.9400852	-3.4892912				
H	0.1510702	-3.8250522	2.9645757				
C	2.1514523	-4.9048936	-2.0175123				
C	5.6745540	-2.4237673	-2.9444895				
C	0.1043372	-6.0299924	-2.9911347				
H	-0.1878736	-5.1576006	-3.6094279				
C	2.9706726	-3.9088116	-2.5704711				
C	2.7134008	-4.7048295	2.4215147				
H	3.4257409	-6.3597627	-4.0706274				
C	1.7980575	-4.7759093	-0.6594973				
C	2.3231901	-6.2954756	-4.1696384				
H	1.9692469	-7.2292450	-4.6508083				
H	1.1612812	-5.5530350	-0.2056059				
C	3.6398433	-1.0536251	-3.6320990				
H	6.3512439	-1.6557030	-3.3729339				
H	6.2013608	-2.9154561	-2.1016041				
C	3.4458525	-2.8197458	-1.8135235				
C	0.3732087	-3.9048542	1.8806036				
C	2.2504230	-3.7157228	0.1444677				
H	3.7999994	-4.5287105	2.2955418				
H	2.5042843	-5.7401521	2.0796306				
C	4.3511639	-1.7871408	-2.4815433				
C	3.0969835	-2.7299228	-0.4429681				
C	1.8736625	-3.6853435	1.6273038				
H	2.7166284	-0.5584133	-3.2746790				
H	-0.2248188	-3.1372163	1.3552569				
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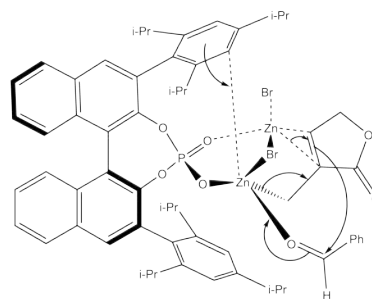


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C	2.6089693	5.0043083	1.2229077
C	3.3502820	6.2239238	1.2435703
C	1.1840007	5.0088223	1.2518229
H	0.6585909	5.9713584	1.3439135
C	0.4425082	3.8384237	1.1473474
C	3.3466180	-1.1313927	0.2453506
C	4.3038756	-1.4603506	1.1977842
H	4.7121551	-2.4827229	1.2197917
C	4.7092069	-0.5353799	2.2038187
C	5.6374299	-0.9169617	3.2191657
C	4.1161593	0.7819190	2.2491961
C	4.4277522	1.6230934	3.3598064
C	3.2126668	1.1754079	1.1939544
C	2.8760975	0.2160023	0.2357626
O	0.4160955	1.4321561	0.9607223

O	2.0337560	0.5783173	-0.8113388	H	0.4086215	-4.7025205	-0.4560529
P	0.4327430	0.8180834	-0.5496967	C	3.1632848	-0.2854075	-3.7939860
O	0.0194929	1.8877444	-1.5783667	H	5.7949261	-1.1741496	-3.7185817
O	-0.3611575	-0.4919919	-0.5787727	H	5.5850851	-2.4653878	-2.4874794
C	4.7347929	6.2191377	1.1610125	C	2.8709294	-2.1166607	-2.0501372
C	5.4327050	4.9873234	1.0436076	C	-0.0101228	-2.9696669	1.7709013
H	2.7966441	7.1735586	1.3109271	C	1.7770206	-3.0678560	-0.0559189
H	5.2932077	7.1675593	1.1701902	H	3.1908420	-4.4140987	1.9270018
H	5.2930864	2.8369038	0.9375464	H	1.6444944	-5.2805146	1.6857873
H	6.5292723	4.9871227	0.9484904	C	3.8425036	-1.1440072	-2.7149759
C	5.3217584	1.2143662	4.3403700	C	2.6856619	-2.1392806	-0.6417062
C	5.9472948	-0.0586073	4.2634684	C	1.4888622	-3.1003863	1.4468023
H	3.9455422	2.6069110	3.4393392	H	2.2824384	0.2404847	-3.3744279
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H	6.6607785	-0.3682469	5.0422606	H	2.8070103	-0.8923904	-4.6515048
H	6.0904202	-1.9194254	3.1653197	H	-0.6898627	-3.5506167	-4.2237224
C	-1.7993010	4.1989522	-0.0017927	H	-0.5828546	-3.8630531	1.4431248
C	-1.0559266	3.8117466	1.1483776	H	2.3564444	-5.8779784	-4.0508339
C	-3.2040548	4.1052721	0.0446232	H	4.2157892	-0.4532449	-1.9314785
C	-1.7307340	3.3508308	2.3129008	H	1.9833087	-2.2196995	1.9022443
C	-3.1331523	3.2769227	2.3022356	H	2.3088722	-3.0105471	-3.9377053
C	-3.8918484	3.6397368	1.1776323	Zn	0.3282054	2.0327264	-3.4761763
H	-3.7917480	4.3988815	-0.8398875	Br	1.5984686	3.5246560	-4.6458253
C	-0.9787107	2.9530686	3.5823685	C	-3.7155528	-7.4161177	-2.0172436
H	-3.6475829	2.9016378	3.2008162	C	-2.3711149	-3.3876207	-1.3000663
C	-1.2277884	1.4859909	3.9737520	C	-3.8550497	-6.4356096	-3.0183119
H	-2.2921991	1.3082489	4.2314823	C	-2.7200464	-5.7608301	-0.5397738
H	-0.6150793	1.2142754	4.8586982	C	-2.8678158	-4.7711902	-1.5354959
H	-0.9802968	0.8036993	3.1391950	C	-3.1438156	-7.0774374	-0.7799683
C	-1.3060437	3.9158594	4.7392500	C	-3.4320089	-5.1224983	-2.7815019
H	0.1068830	3.0575483	3.3803921	O	-2.0199824	-2.6889942	-2.3304174
H	-2.3800221	3.8647822	5.0162687	H	-4.0450518	-8.4490941	-2.2076393
H	-1.0798775	4.9669467	4.4661374	H	-2.2396029	-5.5044492	0.4183520
H	-0.7144895	3.6597903	5.6428623	H	-4.2918833	-6.7036199	-3.9927476
C	-5.4093462	3.5026103	1.1697111	H	-3.0161045	-7.8445501	-0.0010275
C	-5.8318208	2.0212772	1.1775283	H	-3.5136661	-4.3482461	-3.5591169
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H	-5.4073740	1.4789299	0.3093986	H	-3.7828552	-3.9419233	1.1128535
C	-6.0706980	4.2790819	2.3215451	H	-4.1361288	-0.2827072	-2.4281255
H	-5.7684665	3.9485764	0.2156763	C	-4.1227560	-2.4894013	-0.5251276
H	-7.1767612	4.2213252	2.2521532	C	-4.2499698	-2.9567555	0.9057664
H	-5.7795714	5.3489213	2.3072457	H	-4.7861798	-2.8889113	-1.3053498
H	-5.7792044	3.8644689	3.3091824	C	-3.7421815	-1.1302252	-0.4740690
C	-1.1270276	4.7266919	-1.2690684	C	-3.5678355	-0.1702549	-1.4898437
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H	-1.1288229	4.4277402	-3.4371019	O	-3.5754534	-1.9631685	1.6991381
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H	-1.9375478	3.0976105	-2.5103753	H	-5.3115948	-3.0147323	1.2339466
C	-1.1036793	6.2673550	-1.2915816	H	-3.3662204	0.8633553	-1.1506581
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H	-0.5822998	6.6826990	-0.4070148				
H	-2.1356263	6.6771259	-1.2936427				
H	-0.3001606	-5.3831618	-2.5508792				
H	4.7711583	-2.6016315	-4.0772486				
H	1.9222446	-4.3538816	3.1961669				
C	0.5516280	-5.0029419	-3.1559578				
H	3.8553839	0.4854898	-4.1887426				
H	-0.6378314	-5.1782590	-4.9790017				
H	-0.1643885	-2.8728966	2.8649067				
C	1.2739307	-3.9740301	-2.2946178				
C	5.0672104	-1.8879765	-3.2800410				
C	-0.0336481	-4.4139382	-4.4481023				
H	0.7609016	-4.0798734	-5.1477256				
C	2.1602911	-3.0322713	-2.8469397				
C	2.0969734	-4.3548506	2.1001830				
H	1.8600950	-6.6551464	-2.5156832				
C	1.1064761	-3.9730563	-0.8992590				
C	1.4782170	-6.1986599	-3.4513771				
H	0.9422339	-6.9834377	-4.0250213				

TS ν -2-mi



Energy (Hartree) = -11970.01637317
number of imaginary frequencies: 1

C	1.1725174	2.6067242	1.0819063
C	2.5676817	2.5167485	1.1466925
C	3.3180005	3.7487990	1.1531678
C	4.7406009	3.7841346	1.0466891

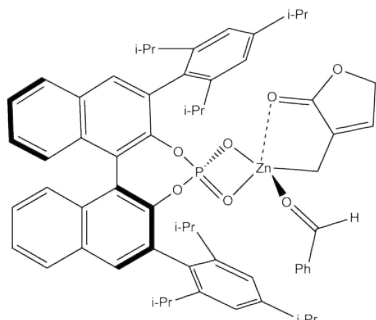
C	2.6047871	5.0016107	1.2262520	H	1.9251035	-4.3500549	3.1957459
C	3.3443411	6.2216298	1.2504859	C	0.5558569	-5.0034664	-3.1568297
C	1.1800683	5.0030959	1.2522070	H	3.8601467	0.4853222	-4.1909808
H	0.6517403	5.9640009	1.3443271	H	-0.6318853	-5.1818964	-4.9811288
C	0.4401897	3.8321805	1.1451044	H	-0.1633872	-2.8685175	2.8612642
C	3.3516453	-1.1321027	0.2430417	C	1.2777344	-3.9737406	-2.2961323
C	4.3079839	-1.4605572	1.1962473	C	5.0720881	-1.8900637	-3.2814853
H	4.7158508	-2.4831165	1.2175691	C	-0.0284461	-4.4168722	-4.4504800
C	4.7119343	-0.5363300	2.2031379	H	0.7662400	-4.0845174	-5.1505651
C	5.6394373	-0.9167821	3.2188669	C	2.1644071	-3.0326586	-2.8483502
C	4.1176471	0.7802298	2.2487186	C	2.0998852	-4.3516764	2.0998187
C	4.4278335	1.6209581	3.3597293	H	1.8642800	-6.6537572	-2.5125246
C	3.2149051	1.1739309	1.1929778	C	1.1103618	-3.9721394	-0.9010280
C	2.8804943	0.2150709	0.2334520	C	1.4826912	-6.1995828	-3.4491973
O	0.4184224	1.4267348	0.9541571	H	0.9480501	-6.9857147	-4.0220982
O	2.0405368	0.5768293	-0.8148583	H	0.4121008	-4.7012471	-0.4576634
P	0.4389919	0.8158292	-0.5575480	C	3.1688314	-0.2858037	-3.7956214
O	0.0268783	1.8845930	-1.5863822	H	5.8006471	-1.1773054	-3.7202246
O	-0.3540051	-0.4954066	-0.5889928	H	5.5890503	-2.4680880	-2.4890317
C	4.7285227	6.2195223	1.1718351	C	2.8759270	-2.1176518	-2.0521032
C	5.4283995	4.9895045	1.0546535	C	-0.0069773	-2.9670609	1.7678461
H	2.7888592	7.1702249	1.3170026	C	1.7812467	-3.0673186	-0.0580144
H	5.2851016	7.1689250	1.1835835	H	3.1935843	-4.4115414	1.9268398
H	5.2919037	2.8389781	0.9450096	H	1.6486400	-5.2781033	1.6860152
H	6.5251604	4.9910770	0.9624794	C	3.8476823	-1.1453166	-2.7171252
C	5.3213941	1.2127327	4.3402665	C	2.6906737	-2.1399438	-0.6438807
C	5.9479283	-0.0590810	4.2633887	C	1.4920526	-3.0982171	1.4445901
H	3.9444209	2.6041416	3.4383398	H	2.2889567	0.2410550	-3.3759546
H	5.5406612	1.8801399	5.1875720	H	-0.4408841	-2.0738212	1.2784664
H	6.6611800	-0.3685570	5.0423875	H	2.8115151	-0.8917886	-4.6533754
H	6.0931815	-1.9188875	3.1648880	H	-0.6843345	-3.5523769	-4.2302594
C	-1.8025812	4.1912947	-0.0028957	H	-0.5793151	-3.8610111	1.4403710
C	-1.0581522	3.8032363	1.1461652	H	2.3617171	-5.8798617	-4.0476485
C	-3.2068520	4.0953598	0.0447938	H	4.2210529	-0.4550035	-1.9332301
C	-1.7312418	3.3399468	2.3105788	H	1.9858825	-2.2169516	1.8995944
C	-3.1332063	3.2635976	2.3002497	H	2.3123437	-3.0107124	-3.9391439
C	-3.8930542	3.6268485	1.1770991	Zn	0.3357181	2.0338797	-3.4860520
H	-3.7956733	4.3906749	-0.8383920	Br	1.5763023	3.5384913	-4.6598980
C	-0.9786969	2.9449120	3.5806364	C	-3.7421535	-7.4034805	-1.9932546
H	-3.6460647	2.8856613	3.1985257	C	-2.3668180	-3.3817243	-1.3006359
C	-1.2231991	1.4777123	3.9745200	C	-3.8734044	-6.4281922	-2.9998952
H	-2.2866586	1.2953900	4.2327773	C	-2.7322244	-5.7481807	-0.5266174
H	-0.6097073	1.2092188	4.8597279	C	-2.8724446	-4.7630923	-1.5277480
H	-0.9729578	0.7941729	3.1419963	C	-3.1670994	-7.0622401	-0.7587098
C	-1.3095664	3.9085784	4.7357022	C	-3.4392892	-5.1176128	-2.7714543
H	0.1066944	3.0527599	3.3790794	O	-2.0153800	-2.6894966	-2.3329000
H	-2.3833939	3.8552290	5.0122849	H	-4.0804021	-8.4346546	-2.1772973
H	-1.0870331	4.9598890	4.4611909	H	-2.2471678	-5.4888723	0.4283942
H	-0.7182744	3.6557505	5.6403163	H	-4.3123001	-6.6986213	-3.9726388
C	-5.4103398	3.4875338	1.1704458	H	-3.0451556	-7.8260533	0.0243176
C	-5.8313834	2.0058157	1.1758958	H	-3.5117715	-4.3469726	-3.5535105
H	-6.9365548	1.9069230	1.1418498	Br	-0.8406942	0.0444364	-4.2981046
H	-5.4684976	1.4925124	2.0902841	Zn	-1.6070334	-0.8046549	-2.1002608
H	-5.4071730	1.4656497	0.3063318	H	-3.7899079	-3.9156792	1.1152789
C	-6.0715109	4.2617896	2.3236261	H	-4.1232179	-0.2705611	-2.4429188
H	-5.7709639	3.9348207	0.2174266	C	-4.1262260	-2.4698240	-0.5280113
H	-7.1776282	4.2033431	2.2561207	C	-4.2510447	-2.9275553	0.9065957
H	-5.7807687	5.3314793	2.3107366	H	-4.7881528	-2.8744959	-1.3067322
H	-5.7784519	3.8467480	3.3104454	C	-3.7359872	-1.1140426	-0.4864488
C	-1.1324725	4.7239220	-1.2693492	C	-3.5538190	-0.1591851	-1.5052499
C	-1.7775705	4.1951691	-2.5642365	C	-3.2938012	-0.8314575	0.9270290
H	-1.1340407	4.4327199	-3.4377340	O	-3.5693111	-1.9367084	1.6920366
H	-2.7658111	4.6589294	-2.7644794	O	-2.7941520	0.1758647	1.3728510
H	-1.9410418	3.0983592	-2.5160460	H	-5.3124831	-2.9789024	1.2388857
C	-1.1119280	6.2645457	-1.2873698	H	-3.3468979	0.8744544	-1.1692641
H	-0.0810375	4.3717529	-1.2609954	H	-1.8093826	-3.2409595	-0.3469819
H	-0.5936860	6.6397976	-2.1941308				
H	-0.5908405	6.6781192	-0.4019719				
H	-2.1443334	6.6729110	-1.2863602				
H	-0.2964563	-5.3830789	-2.5518306				
H	4.7764501	-2.6040496	-4.0784088				

7 Other Pathways

7.1 Complexes 10, 11, 14 and 15

7.1.1 Educt Complexes 10

10a-ma



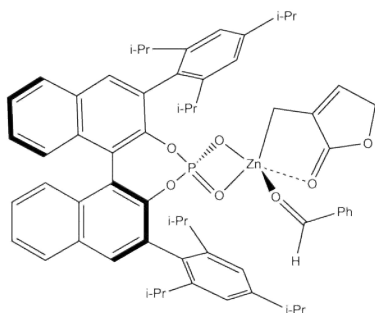
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C	0.0820768	1.0839813	269.2506785
C	0.9642521	0.1331794	269.7703697
C	0.5641854	-0.5896974	270.9527336
C	1.4354248	-1.4738467	271.6575587
C	-0.7695490	-0.3898014	271.4699044
C	-1.1883705	-1.1273271	272.6176231
C	-1.6273468	0.5716419	270.8614013
H	-2.6335279	0.7231727	271.2807849
C	-1.2124934	1.3569371	269.7922895
C	4.4959879	0.9133484	268.4875409
C	4.9533697	-0.3579484	268.1612288
H	6.0032679	-0.4862222	267.8551192
C	4.1044459	-1.4999849	268.2097599
C	4.5641080	-2.7846899	267.7923969
C	2.7509042	-1.3557517	268.6883229
C	1.9045925	-2.5056367	268.6748412
C	2.2939019	-0.0591334	269.1246654
C	3.1419813	1.0410135	268.9272663
O	0.4588462	1.7812805	268.1183924
O	2.6973246	2.3185016	269.2375941
P	1.5427265	3.0181604	268.2622113
O	0.9785588	4.1871172	269.1080839
O	1.9751505	3.4197730	266.8664420
C	-0.3261279	-2.0029594	273.2596148
C	1.0013437	-2.1631611	272.7814349
H	-2.2116063	-0.9723329	272.9948712
H	-0.6618666	-2.5604988	274.1472917
H	2.4675696	-1.6014340	271.3030885
H	1.6949480	-2.8360129	273.3086664
C	2.3774906	-3.7380872	268.2468679
C	3.7219401	-3.8857756	267.8133537
H	0.8594133	-2.4020634	268.9980841
H	1.7016445	-4.6068959	268.2378174
H	4.0875283	-4.8696915	267.4820410
H	5.6029705	-2.8805622	267.4391209
C	-2.2034570	3.6683663	270.0342352
C	-2.0338801	2.4874194	269.2514793
C	-2.9721201	4.7197229	269.5069829
C	-2.6087236	2.4105089	267.9556893
C	-3.3842844	3.4882489	267.4838504
C	-3.5866034	4.6508904	268.2435670
H	-3.0898873	5.6400953	270.1014263
C	-2.4273473	1.1911924	267.0543061
H	-3.8368046	3.4075268	266.4845062
C	-1.7422027	1.5643849	265.7265838

H	-2.3764539	2.2425896	265.1176897
H	-1.5505155	0.6561475	265.1184661
H	-0.7718584	2.0665584	265.9072663
C	-3.7640663	0.4632984	266.8214220
H	-1.7601627	0.4783770	267.5796094
H	-4.4906818	1.1091098	266.2850370
H	-4.2301862	0.1609425	267.7811694
H	-3.6133861	-0.4498586	266.2089420
C	-4.4602568	5.8105399	267.7723035
C	-4.6921631	5.8488423	266.2570900
H	-5.2180384	6.7818586	265.9680539
H	-5.3263991	5.0021349	265.9208787
H	-3.7381327	5.8044259	265.6953059
C	-5.8031545	5.8128207	268.5303425
H	-3.9205832	6.7429428	268.0564795
H	-6.4216243	6.6903590	268.2475685
H	-5.6500442	5.8387222	269.6275908
H	-6.3821919	4.8952876	268.2956089
C	-1.5882672	3.8255346	271.4254289
C	-0.8850156	5.1782302	271.6274783
H	-0.3727185	5.1931116	272.6118909
H	-1.5980320	6.0284185	271.6189867
H	-0.1359561	5.3533077	270.8347862
C	-2.6506616	3.5965049	272.5184256
H	-0.8127980	3.0404193	271.5346669
H	-2.1977661	3.6641075	273.5295450
H	-3.1355482	2.6041060	272.4275531
H	-3.4516542	4.3629250	272.4539664
H	7.9591996	6.1899340	268.1900526
H	7.7405901	2.0186818	272.0546434
H	5.2057044	1.2878478	264.2163171
C	8.4756220	5.2301345	268.4263435
H	4.6900882	2.0544438	272.8400300
H	9.9725759	6.2555165	269.6394593
H	3.9061286	3.5006754	264.3442805
C	7.3857477	4.1580070	268.4908849
C	7.0921794	1.1837957	271.7154228
C	9.2401335	5.4290972	269.7401654
H	9.8059372	4.5151365	270.0181264
C	7.1060985	3.4212348	269.6532541
C	5.7472032	1.5400662	265.1516149
H	8.9713116	4.8596520	266.3002002
C	6.6217281	3.8707602	267.3429103
C	9.4720013	4.9465993	267.2841118
H	10.2250511	5.7580423	267.2073793
H	6.7950390	4.4582666	266.4285930
C	4.9781426	2.5890759	271.9110656
H	6.8178026	0.5980409	272.6167580
H	7.7004642	0.5333395	271.0550068
C	6.1334586	2.4012118	269.6792559
C	4.5659780	3.7810157	265.1895036
C	5.6589312	2.8473655	267.3066798
H	5.9430488	0.5941204	265.6941083
H	6.7290464	1.9774723	264.8718913
C	5.8306082	1.6874233	270.9960365
C	5.4299528	2.0878990	268.4872778
C	4.9290035	2.5299551	266.0035018
H	4.0494840	2.9100313	271.3978981
H	4.0117622	4.5105099	265.8095755
H	5.5454886	3.4972462	272.2087485
H	8.5682166	5.6805466	270.5829457
H	5.4618987	4.2757316	264.7578898
H	10.0128999	3.9947392	267.4679192
H	5.2168491	0.7948518	270.7573972
H	3.9702572	2.0427380	266.2735400
H	7.6602719	3.6349133	270.5780074
C	6.2009409	8.5458506	268.9507891
C	5.0564264	7.8730580	268.5163748
C	4.5226642	6.8220528	269.2987039
C	5.1484469	6.4474949	270.5085552
C	6.2828935	7.1392294	270.9489707

C	6.8081068	8.1845152	270.1704727
H	6.6258978	9.3617005	268.3467614
H	4.5493742	8.1396584	267.5769937
C	3.2958909	6.1331724	268.9046940
H	6.7641323	6.8609858	271.8983430
H	7.7066825	8.7209112	270.5125481
O	2.6274106	6.4428388	267.9037445
H	-2.0239905	10.2048655	266.7022920
H	-0.2926038	5.8958132	265.0959794
Zn	0.7760872	5.4960924	267.5409123
C	-1.9942134	8.1366794	265.9447177
C	-2.3906118	9.1814320	266.9426303
H	-2.3156779	8.1564243	264.8941082
C	-1.2441518	7.1842233	266.5590853
C	-0.6046356	5.9108481	266.1575999
C	-1.0710877	7.6479139	267.9660141
O	-1.7905896	8.7783802	268.1868534
O	-0.3521253	7.1414029	268.8236925
H	-3.4941610	9.2444627	267.0814270
H	-1.3293465	5.0755915	266.3029855
H	4.7343667	5.6132275	271.0959475
H	2.9444211	5.3019311	269.5654820

10a-mi



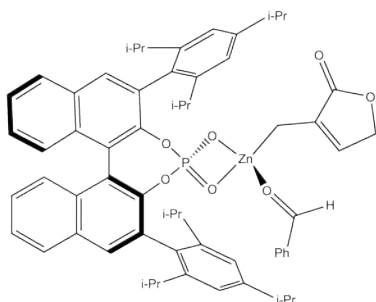
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C	0.0582654	-0.5938803	329.7995218
C	0.7056064	-1.7233705	330.3873307
C	-1.3140071	-0.3372527	330.1683093
C	-1.9962663	-1.2575756	331.0190669
C	-1.9337297	0.8763061	329.7559245
H	-2.9515296	1.1023879	330.1101147
C	-1.2591606	1.8198663	328.9928159
C	4.4729787	0.9960800	328.5149546
C	4.9307497	-0.2400109	328.0714282
H	6.0133412	-0.4006332	327.9581794
C	4.0415313	-1.2946837	327.7174692
C	4.5268640	-2.5181865	327.1657580
C	2.6202851	-1.1171841	327.8917189
C	1.7477615	-2.1541975	327.4447807
C	2.1388095	0.1074226	328.4796363
C	3.0634165	1.1355615	328.7062873
O	0.6148313	2.3432488	327.5854568
O	2.6043452	2.3664507	329.1621827
P	1.8978472	3.3000512	327.9871090
O	1.5307578	4.6593023	328.5778092
O	2.7996607	3.4357175	326.7403808
C	-1.3490514	-2.3702304	331.5331477
C	0.0200598	-2.5891557	331.2282078
H	-3.0467900	-1.0510124	331.2778187
H	-1.8850103	-3.0689115	332.1934752
H	1.7673037	-1.9047105	330.1744529
H	0.5474268	-3.4498665	331.6672150
C	2.2512955	-3.3240516	326.8934666

C	3.6527325	-3.5170908	326.7650954
H	0.6617009	-2.0110317	327.5348316
H	1.5579288	-4.1062437	326.5485089
H	4.0408808	-4.4523477	326.3336990
H	5.6145925	-2.6457284	327.0482033
C	-1.4374322	4.1759045	329.8165360
C	-1.7776933	3.2148781	328.8191102
C	-1.8878557	5.4938232	329.6546357
C	-2.5753149	3.5850470	327.7111777
C	-3.0295617	4.9184768	327.6139967
C	-2.6833190	5.8946095	328.5647186
H	-1.6137585	6.2481237	330.4082254
C	-2.9142453	2.5720433	326.6197597
H	-3.6856371	5.1878775	326.7726823
C	-2.0441789	2.7944608	325.3672245
H	-2.2770839	3.7672313	324.8855129
H	-2.2248801	1.9986458	324.6149833
H	-0.9667805	2.7878180	325.6248784
C	-4.4102741	2.5499089	326.2673595
H	-2.6560567	1.5692725	327.0213077
H	-4.7382326	3.5003097	325.7959294
H	-5.0377129	2.3878218	327.1669965
H	-4.6279714	1.7373090	325.5441116
C	-3.1035127	7.3604595	328.4695821
C	-1.9033298	8.2588952	328.1016721
H	-2.1753011	9.3312176	328.1885277
H	-1.5821902	8.0835109	327.0546552
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H	-3.4227930	7.6512188	329.4962263
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H	0.9786750	5.1886687	330.7298644
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H	-2.2832283	2.5426814	331.8987521
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H	6.8472711	1.1248251	324.6645765
C	8.4356610	5.1874007	329.5944220
H	3.3510258	2.7324139	332.7791713
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H	5.4174732	3.2489406	324.3286250
C	7.3465354	4.1591847	329.3113650
C	5.7517555	1.3445910	332.3042217
C	7.9053226	6.4312169	330.3275641
H	7.5158947	6.1726806	331.3348847
C	6.5685317	3.6084996	330.3441302
C	7.0397204	1.4132496	325.7187838
H	10.0176993	3.6738972	329.8113141
C	7.1049099	3.7061599	328.0049420
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H	7.6854605	4.1505078	327.1804292
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H	5.1644866	0.9054783	333.1372009
H	6.3176181	0.5264961	331.8141818
C	5.6075987	2.6085447	330.1106027
C	5.7656868	3.5570387	325.3351183
C	6.1465691	2.7173715	327.7098751
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C	4.8263337	2.0597376	331.3031929
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C	5.9187068	2.3274536	326.2485278
H	3.3359936	3.6697146	331.2481202
H	5.0214059	4.2657265	325.7465069
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H	6.7217019	4.1050528	325.2031428
H	9.2831793	4.1892085	331.3592280
H	4.1156577	1.2981017	330.9261157
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H	6.7240959	3.9571495	331.3779378
Zn	3.1487472	5.4527311	327.1339646
H	2.3765441	6.6708767	332.0807660
H	4.6491217	7.4603761	327.4240351
C	4.0073001	6.8929397	330.6380642
C	2.8545877	7.4339245	331.4262619
H	4.9109845	6.4686627	331.0955891
C	3.7388849	7.0044092	329.3111348
C	4.4619302	6.5916666	328.0907500
C	2.3657484	7.5892226	329.2012916
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C	-1.5350110	6.5022823	324.7379093
C	-2.3780312	6.9088627	323.6964183
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H	1.5155466	7.0409520	323.2502522
C	0.7269282	6.1081910	325.6696394
H	-1.9474743	6.1322066	325.6878658
H	-3.4704275	6.8670474	323.8238969
H	-2.4843369	7.6912852	321.6713053
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10b-ma



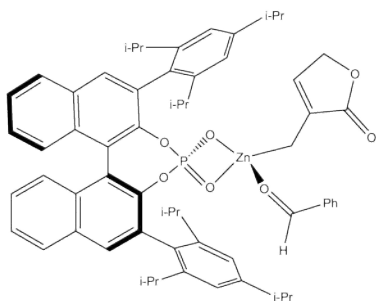
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C	17.6619421	-2.1538324	660.8822407
C	17.1648682	-0.0705083	659.6247666
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C	23.0439868	0.9002115	656.7671079
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H	24.3508162	-0.2683354	655.5190446
C	22.5844008	-1.4161659	656.0854864
C	22.9428698	-2.5692373	655.3247323
C	21.3275522	-1.3989391	656.7964505
C	20.4545298	-2.5179844	656.6381651
C	20.9910128	-0.2456447	657.6001579

C	21.8466791	0.8620605	657.5444002
O	19.2254516	1.9179899	657.3540544
O	21.5765277	1.9885393	658.3059848
P	20.3146827	2.9890712	657.9772294
O	19.8810527	3.5674236	659.3480713
O	20.5411547	4.0852935	656.9369422
C	18.5422652	-3.1612859	661.2464625
C	19.8519239	-3.1877799	660.6979711
H	16.6521670	-2.1077959	661.3197021
H	18.2344273	-3.9305900	661.9709053
H	21.2686024	-2.2555339	659.3630730
H	20.5596705	-3.9709021	661.0099737
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H	23.9112422	-2.5695345	654.7998832
C	16.3889175	3.1042976	659.5319950
C	16.6812278	2.1582260	658.5079674
C	15.5528440	4.1954264	659.2249308
C	16.1606121	2.3522811	657.1967245
C	15.3385564	3.4646828	656.9457279
C	15.0148759	4.3990699	657.9440104
H	15.3200037	4.9291226	660.0130802
C	16.4423963	1.3820760	656.0505539
H	14.9329278	3.6013745	655.9304831
C	17.1360246	2.0823711	654.8674973
H	16.4720896	2.8352604	654.3927975
H	17.4111595	1.3445447	654.0856361
H	18.0599663	2.5944891	655.1997245
C	15.1589807	0.6539735	655.6102012
H	17.1381433	0.6041644	656.4238996
H	14.4062976	1.3642469	655.2084740
H	14.6907630	0.1156256	656.4590667
H	15.3803312	-0.0860716	654.8133078
C	14.0912437	5.5777520	657.6590424
C	14.5713687	6.4355792	656.4752578
H	13.9040645	7.3096564	656.3283390
H	14.5700517	5.8574994	655.5274721
H	15.5996037	6.8159659	656.6380013
C	12.6419816	5.0994850	657.4498746
H	14.1049263	6.2223173	658.5656013
H	11.9560691	5.9591226	657.3004304
H	12.2810359	4.5160193	658.3205701
H	12.5647976	4.4466364	656.5551166
C	16.9512288	2.9776923	660.9481699
C	17.4834731	4.3108611	661.5014191
H	18.0312924	4.1421715	662.4504015
H	16.6688786	5.0334900	661.7152800
H	18.1842340	4.7851534	660.7884580
C	15.9054974	2.3855108	661.9130167
H	17.8139737	2.2831257	660.8982643
H	16.3312457	2.2650777	662.9307737
H	15.5430536	1.3942584	661.5771092
H	15.0208410	3.0519487	661.9912682
H	25.6642079	6.3468532	655.1011978
H	26.8289342	2.3363938	659.3556339
H	22.9384850	1.4834042	652.2360162
C	26.1657774	5.7875950	655.9225233
H	24.1727817	2.4371937	661.1206348
H	26.8098745	7.6708733	656.8283515
H	21.1022105	3.0959962	653.0461265
C	25.3067932	4.5586676	656.1966956
C	26.0900681	1.5091260	659.3086237
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H	26.8571085	6.2873358	657.9534849
C	25.3272707	3.8894054	657.4317836
C	23.6139809	1.8506143	653.0362732
H	27.4784856	4.7163914	654.5158753
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C	27.5572020	5.3624304	655.4132825
H	28.1753822	6.2464560	655.1511374
H	24.4449011	4.5590830	654.2151621
C	24.1742569	2.9671954	660.1458279
H	26.1245578	0.9743746	660.2804258
H	26.4238192	0.8071510	658.5177436
C	24.5920257	2.7107646	657.6578904
C	21.8247285	3.4993888	653.7856112
C	23.7228729	2.8658084	655.3589010
H	24.2702114	1.0105983	653.3414024
H	24.2630121	2.6366605	652.5957952
C	24.6716164	2.0361715	659.0248999
C	23.8054234	2.1784582	656.6030721
C	22.8068624	2.3982089	654.2267021
H	23.1424101	3.3166763	659.9462586
H	21.2551281	3.8880875	654.6532187
H	24.8267785	3.8589294	660.2540971
H	25.2826765	7.0235006	657.5087746
H	22.3506994	4.3461261	653.2946204
H	28.0983715	4.7858792	656.1925857
H	23.9971831	1.1559143	659.0051217
H	22.1900658	1.5650714	654.6197087
H	25.9422891	4.2908265	658.2518313
C	22.6821726	7.0848655	655.3620561
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C	22.4935382	7.6508379	657.7163298
C	23.0796383	8.9132127	657.4625378
C	23.4534003	9.2609214	656.1611045
C	23.2541995	8.3459649	655.1116871
H	22.5393762	6.3634038	654.5448437
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C	22.0536891	7.3480348	659.0767273
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H	23.5506368	8.6186372	654.0867479
O	21.3533571	6.3815138	659.4192510
H	20.1030802	8.1399361	654.4006810
H	17.3253330	6.0875587	657.9660610
Zn	19.6695048	5.4494984	658.6627138
C	18.5225024	7.4132150	655.7258119
C	19.2736017	8.5148086	655.0451549
H	17.9811637	6.6220442	655.1885617
C	18.6602616	7.5387191	657.0737550
C	18.2091982	6.7097909	658.2042376
C	19.5114445	8.7462023	657.3096632
O	19.8451613	9.3002663	656.0963188
O	19.9116808	9.2090675	658.3624409
H	18.6319893	9.1719249	654.4143390
H	18.0116783	7.3305654	659.1010326
H	23.2077506	9.6266973	658.2910734
H	22.3953735	8.0589392	659.8719283

10b-mi



Energy (Hartree) = -5044.0638992

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C	0.3309346	-0.2172889	330.0050490
C	1.1231296	-1.2709627	330.5517837
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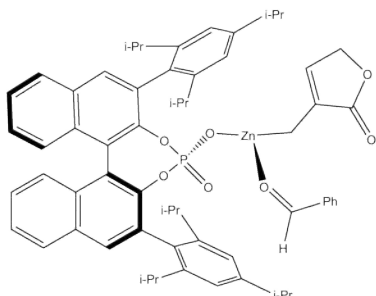
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C	-1.3179221	1.9567409	329.1099307
C	4.4702479	1.5377892	328.0138497
C	4.8146499	0.3471230	327.3843121
H	5.8388319	0.2280495	326.9984528
C	3.8792087	-0.7073878	327.1920812
C	4.2306697	-1.8857323	326.4680395
C	2.5395862	-0.5654914	327.7071524
C	1.5934466	-1.5931056	327.4092957
C	2.2056887	0.6153501	328.4680233
C	3.1524678	1.6422481	328.5548778
O	0.6071513	2.8824200	327.9858724
O	2.8434495	2.7961089	329.2621587
P	1.7145852	3.8723748	328.7300426
O	1.1465189	4.5956974	329.9677253
O	2.2145206	4.8735460	327.6809985
C	-0.7976623	-2.1228936	331.7905850
C	0.5729700	-2.1982722	331.4254228
H	-2.6502871	-1.0217280	331.5796721
H	-1.2239284	-2.8680436	332.4794058
H	2.1865171	-1.3337040	330.2808931
H	1.2063580	-2.9958797	331.8428202
C	1.9616020	-2.7188306	326.6858295
C	3.2946464	-2.8782753	326.2229554
H	0.5553854	-1.4826276	327.7514788
H	1.2101737	-3.4923167	326.4649244
H	3.5764573	-3.7795264	325.6574788
H	5.2615680	-1.9819093	326.0923684
C	-2.6129264	4.1255511	329.3690641
C	-2.2000302	3.0358616	328.5568209
C	-3.5421148	5.0441447	328.8415847
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C	-3.6064115	3.8592456	326.7451681
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C	-2.2095107	1.7947485	326.2947087
H	-3.9872946	3.7540777	325.7163001
C	-1.3071200	2.3504518	325.1768497
H	-1.8726247	3.0334981	324.5077128
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H	-4.0339319	1.5833817	325.0706331
H	-4.0114375	0.5586332	326.5389475
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C	-4.6029699	6.6664471	325.7644171
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H	-4.4206605	5.9680211	324.9203643
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C	-6.4482026	5.2302675	326.7574401
H	-5.2503919	6.6744122	327.8168041
H	-7.2140510	5.9664851	326.4366732
H	-6.8195629	4.7197698	327.6684540
H	-6.3621089	4.4652885	325.9575334
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H	-2.6476197	6.3949304	331.2290057
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H	4.7063066	2.5225673	323.8052409
C	8.7173513	5.5676567	328.0983642

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H	3.5871343	4.7360047	324.4329391
C	7.5652047	4.5667302	328.1597917
C	7.3437608	1.1675859	330.9653597
C	9.4519271	5.7769709	329.4280087
H	9.9833607	4.8562822	329.7484410
C	7.3507354	3.7023988	329.2458368
C	5.3714750	2.5908834	324.6911819
H	9.2227733	5.0577066	326.0113527
C	6.6706194	4.4897393	327.0743320
C	9.7192362	5.1681473	326.9955974
H	10.5198805	5.9295466	326.8908291
H	6.7905615	5.2001553	326.2422950
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H	7.1127990	0.4968275	331.8184552
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C	4.3586383	4.8479328	325.2217793
C	5.6337347	3.5454800	327.0171661
H	5.5677975	1.5605104	325.0469098
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C	6.0747713	1.8929521	330.4889638
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C	4.7327047	3.4693863	325.7849086
H	4.5020438	3.2109655	331.2705992
H	3.9448318	5.5053233	326.0077179
H	6.1367488	3.5506807	331.9314865
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H	5.2279927	5.3593470	324.7578420
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H	8.0096649	3.7594854	330.1246846
Zn	1.4286532	6.4468969	328.9931077
H	6.8576615	7.9372404	330.0433086
H	2.0112375	8.9216837	328.9824251
C	4.7364818	7.5217246	330.4297311
C	6.0266063	7.2705442	329.7186059
H	4.6163418	7.4243928	331.5177136
C	3.7749299	7.8392287	329.5232140
C	2.3273419	8.0899926	329.6453320
C	4.4274265	7.8121093	328.1771024
O	5.7574514	7.5123680	328.3319917
O	3.9249487	8.0038270	327.0834981
H	6.3767487	6.2177883	329.8224893
H	2.0209472	8.3066325	330.6871006
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C	0.0009601	6.4568158	325.5991258
C	-0.5805264	6.0683471	324.3666146
C	0.1107486	6.2772680	323.1690074
C	1.3803020	6.8847965	323.1950179
H	2.9541490	7.7504949	324.4499062
H	1.7584888	7.3841489	326.5498141
C	-0.7576272	6.2050069	326.8196090
H	-1.5747269	5.5938135	324.3670798
H	-0.3346477	5.9673819	322.2118140
H	1.9260392	7.0469292	322.2523165
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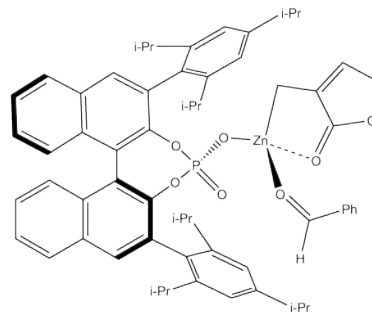
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C	-0.9246024	-0.3098340	330.7254753
C	-1.4060174	-1.0957430	331.8148549
C	-1.7281068	0.7207178	330.1562984
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C	3.0792711	1.2031108	328.3686965
O	0.4214657	1.9581652	327.4878322
O	2.5930018	2.4566361	328.6900565
P	1.5718427	3.1653424	327.5820091
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C	-0.5848092	-2.0108915	332.4552281
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H	-2.4438095	-0.9439035	332.1516160
H	-0.9680777	-2.6060228	333.2980558
H	2.3056661	-1.5420786	330.6638105
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H	0.9018074	-2.3104167	328.3228591
H	1.8579964	-4.4883741	327.6253363
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H	5.7349976	-2.6327046	327.0264256
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10c-mi



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H	5.4499053	7.0422353	323.9193846
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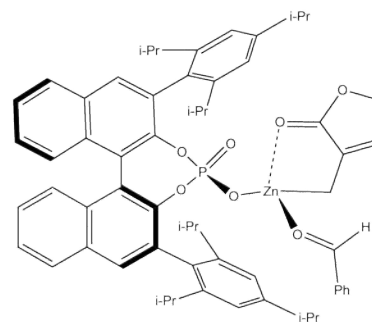
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P	1.9662520	3.8980964	328.7624074
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10f-ma

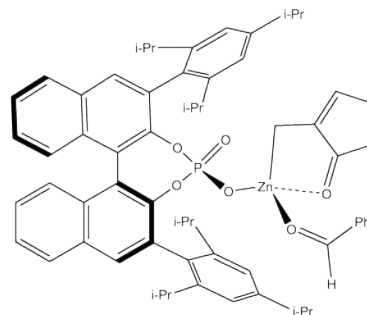


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C	2.8270611	0.8497457	268.9019974
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P	1.2440020	2.8474787	268.2158051
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H	-2.6011358	3.7830597	273.7745452				
H	-3.6217879	2.8560944	272.6245096				
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H	7.2530395	5.0759271	265.1241752				
H	7.3308084	3.2700814	270.7497504				
H	5.0057863	-0.4871179	263.8974834				
C	7.3578673	5.0954219	266.2324199				
H	4.3925065	3.8235567	271.8497518				
H	7.5819335	7.2759368	266.2469705				
H	3.0036705	1.1082206	263.7075856				
C	6.4614841	3.9887601	266.7769476				
C	6.6193475	2.4308055	270.8983150				
C	6.9436386	6.4967525	266.7122798				
H	7.0518084	6.5972593	267.8124456				
C	6.2263022	3.8423241	268.1556051				
C	5.4921781	0.2154662	264.6056137				
H	9.1483368	3.8179968	266.1758573				
C	5.8729812	3.0506355	265.9147865				
C	8.8358575	4.8096040	266.5601637				
H	9.5007920	5.5795346	266.1159412				
H	6.0359130	3.1578505	264.8290414				
C	4.5708740	3.9399812	270.7607105				
H	6.4714071	2.3074561	271.9913132				
H	7.1019469	1.5105922	270.5111115				
C	5.4552309	2.7886407	268.6784720				
C	3.5201204	1.8152572	264.3899213				
C	5.0831539	1.9826631	266.3820124				
H	6.1166480	-0.3798837	265.3025620				
H	6.1770108	0.8627599	264.0180855				
C	5.2764589	2.6948576	270.1925095				
C	4.8942533	1.8332114	267.7853503				
C	4.4387625	1.0480253	265.3576095				
H	3.5904042	4.0953391	270.2700277				
H	2.7566615	2.3758497	264.9646212				
H	5.1814531	4.8565508	270.6189335				
H	5.8870801	6.7194205	266.4631745				
H	4.0947382	2.5244634	263.7561139				
H	9.0032885	4.8099985	267.6576346				
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10f-mi



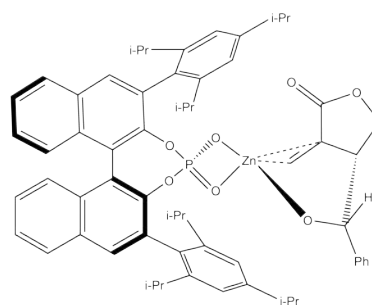
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C	0.8200721	-1.3343912	330.6865899
C	-1.2245459	0.0376664	330.6588672
C	-1.8733020	-0.9777533	331.4229339
C	-1.9008353	1.2392171	330.3012590
H	-2.9620622	1.3532156	330.5708952
C	-1.2543929	2.2730877	329.6363919
C	4.4989038	1.4321911	328.6240702
C	4.7965541	0.2731070	327.9160143
H	5.8300344	0.1025422	327.5755928
C	3.7957294	-0.6802199	327.5749086
C	4.1037435	-1.8190555	326.7718703
C	2.4373411	-0.4745926	328.0186414
C	1.4395062	-1.3946762	327.5751247
C	2.1409642	0.6602426	328.8595258
C	3.1553413	1.5985195	329.0889851
O	0.7218566	3.0938621	328.5550871
O	2.8892149	2.7024384	329.8654223
P	1.9434875	3.9534917	329.3023851
O	1.5413949	4.7687035	330.4957426
O	2.6252348	4.6023380	328.0680731
C	-1.1969715	-2.1257199	331.8066946
C	0.1658646	-2.2950052	331.4451977

H	-2.9237546	-0.8223551	331.7158861	C	6.0845519	3.2081820	327.7748389
H	-1.7079030	-2.8974734	332.4024410	H	7.2050769	1.4881236	325.9121668
H	1.8773248	-1.4738962	330.4212747	H	7.6374301	3.1442130	325.3964884
H	0.7112265	-3.1930142	331.7738031	C	5.4427699	2.0202436	331.4158266
C	1.7689786	-2.4826701	326.7787951	C	5.5317986	2.4859477	328.8725774
C	3.1142904	-2.7095003	326.3844264	C	5.6442583	2.9842465	326.3265342
H	0.3929693	-1.2275343	327.8649163	H	3.9952632	3.5752449	331.9631354
H	0.9781141	-3.1724928	326.4463769	H	4.1076125	4.5270074	326.2210344
H	3.3652263	-3.5805626	325.7600263	H	5.5521147	3.6788107	332.8626900
H	5.1473388	-1.9677007	326.4520085	H	7.6482944	6.7419535	330.9296441
C	-2.1203884	4.5804968	330.2245468	H	5.7430754	5.1151154	325.7351110
C	-1.9593428	3.5433326	329.2671014	H	10.1667993	3.9435116	330.2173500
C	-2.8295347	5.7365893	329.8479234	H	4.6470727	1.3303818	331.0727519
C	-2.4704736	3.6976778	327.9494391	H	4.8374395	2.2256124	326.3314079
C	-3.1637517	4.8785807	327.6224268	H	7.3385143	3.9188170	331.4133098
C	-3.3682230	5.9061365	328.5619847	Zn	3.6481081	6.2791339	328.0964363
H	-2.9701734	6.5423566	330.5852153	H	2.1031816	6.1236833	332.8151054
C	-2.2798696	2.6141741	326.8884788	H	5.2845157	7.9428816	329.1458252
H	-3.5761392	4.9860023	326.6053357	C	3.9750719	6.8013218	331.9382028
C	-1.2857144	3.0591093	325.7997508	C	2.6168152	7.0637304	332.5118254
H	-1.6886612	3.9082194	325.2086979	H	4.8108983	6.3941103	332.5234935
H	-1.0817954	2.2292326	325.0914979	C	3.9601802	7.0882475	330.6104837
H	-0.3224065	3.3736995	326.2475489	C	4.9108456	6.9517899	329.4823041
C	-3.6156150	2.1521809	326.2814100	C	2.5658051	7.5159444	330.3041864
H	-1.8345659	1.7332837	327.3942997	O	1.8414583	7.6234676	331.4333365
H	-4.1159097	2.9664525	325.7161081	O	2.0977332	7.6953777	329.1760556
H	-4.3188396	1.8095355	327.0671961	H	2.6077786	7.7719334	333.3686540
H	-3.4539036	1.3124452	325.5742697	H	5.7640792	6.2894366	329.7084659
C	-4.1846109	7.1491132	328.2246489	C	0.5165476	7.3229855	322.6929245
C	-3.6080837	7.9362951	327.0368837	C	1.3183289	7.1930969	323.8287063
H	-4.1830844	8.8690917	326.8623647	C	0.7280893	6.8401368	325.0664063
H	-3.6559453	7.3438364	326.0992297	C	-0.6651933	6.6179397	325.1541547
H	-2.5489733	8.2147313	327.2088970	C	-1.4619574	6.7462815	324.0096966
C	-5.6645395	6.7933183	327.9905150	C	-0.8724431	7.0985077	322.7839514
H	-4.1366441	7.8126059	329.1159399	H	0.9662665	7.5970118	321.7266744
H	-6.2707874	7.7050044	327.8079519	H	2.4059769	7.3550209	323.7901896
H	-6.0928028	6.2625085	328.8642218	C	1.5376409	6.6709425	326.2682220
H	-5.7803814	6.1295013	327.1079518	H	-1.1130477	6.3318591	326.1196061
C	-1.5698300	4.4490671	331.6435228	H	-2.5459347	6.5681589	324.0712237
C	-1.0035468	5.7662544	332.1942953	H	-1.5004043	7.1983443	321.8850339
H	-0.4887497	5.5769378	333.1592216	O	2.7759043	6.8148622	326.2851531
H	-1.8004887	6.5121178	332.3991112	H	0.9950816	6.3888288	327.2024913
H	-0.2679794	6.2083727	331.4976146				
C	-2.6360925	3.8753546	332.5968773				
H	-0.7229733	3.7337427	331.5950094				
H	-2.2242500	3.7595633	333.6210300				
H	-3.0005126	2.8835590	332.2655789				
H	-3.5138713	4.5530449	332.6576633				
H	8.6492690	6.1508764	328.6777913				
H	7.3727282	1.7689550	332.4532705				
H	6.4525202	2.1963761	324.4447035				
C	8.7077225	5.4249824	329.5197915				
H	4.3606334	2.4114848	333.2786713				
H	9.4232972	6.9940553	330.8637445				
H	4.7851063	4.0816568	324.6325966				
C	7.5628534	4.4370256	329.3213478				
C	6.5375626	1.1508155	332.0619636				
C	8.6242497	6.2259679	330.8275295				
H	8.7609558	5.5758375	331.7167335				
C	6.9885583	3.7260320	330.3875991				
C	6.7975713	2.4223628	325.4749595				
H	10.1489974	4.1565000	328.4412232				
C	7.0831082	4.1667544	328.0285434				
C	10.0609725	4.6943900	329.4064080				
H	10.9090180	5.4062266	329.4856240				
H	7.5112133	4.7292403	327.1817606				
C	4.8018439	2.9804531	332.4343001				
H	6.1253093	0.5690821	332.9124041				
H	6.9652021	0.4345194	331.3313557				
C	5.9804174	2.7633870	330.1941359				
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7.1.2 Product Complexes 11

11a-ma

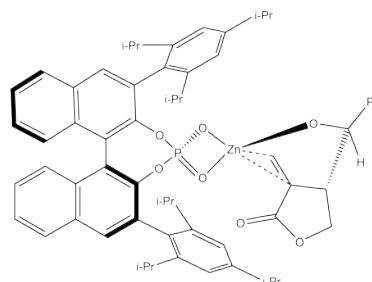


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C	0.2908818	-1.2797624	810.7802288
C	1.0311199	-2.3427168	811.3796948
C	-1.0664376	-1.0592668	811.2223790
C	-1.6376504	-1.9456790	812.1840479
C	-1.8007355	0.0563276	810.7261942
H	-2.8334501	0.2114986	811.0738396
C	-1.2327104	0.9781180	809.8555228

C	4.4602670	0.3329244	808.6518955	C	6.6058227	4.0972523	808.4586712
C	4.8502858	-0.9024713	808.1507105	C	6.9528609	1.0395332	811.6735432
H	5.8702616	-1.0259107	807.7562550	C	6.6086016	6.4807931	809.3342064
C	3.9459921	-2.0019048	808.0740754	H	6.7834021	6.2193203	810.3992020
C	4.3425187	-3.2358711	807.4767105	C	6.4178039	3.4344902	809.6843359
C	2.5909503	-1.8557402	808.5539113	C	6.2042128	0.9133753	805.2772679
C	1.6806538	-2.9341254	808.3414558	H	9.2736646	4.6619862	807.9312959
C	2.2062610	-0.6175480	809.1905030	C	6.1518357	3.4567275	807.2951191
C	3.1397924	0.4222763	809.1919141	C	8.7888527	5.3576720	808.6458442
O	0.6192748	1.6211549	808.4842590	H	9.2782709	6.3493114	808.5507988
O	2.7916837	1.6389066	809.7771832	H	6.2943731	3.9659187	806.3286546
P	1.8058410	2.6440792	808.9500079	C	4.8979692	2.4667258	812.1518836
O	1.4147535	3.7767894	809.9361829	H	6.8295219	0.5229855	812.6481556
O	2.3711331	3.2866610	807.6637646	H	7.4262010	0.3301972	810.9647537
C	-0.8996576	-2.9882459	812.7226609	C	5.7637698	2.1940229	809.7712636
C	0.4509876	-3.1752712	812.3265212	C	4.3162917	2.5945140	805.0771546
H	-2.6772966	-1.7722627	812.5034701	C	5.4959150	2.2115182	807.3207030
H	-1.3515910	-3.6595898	813.4685800	H	6.6946816	0.1476643	805.9113258
H	2.0803624	-2.4927535	811.0903074	H	6.9798130	1.6591578	805.0032349
H	1.0465393	-3.9832664	812.7781392	C	5.5967935	1.5400178	811.1413459
C	2.0947187	-4.1143148	807.7394007	C	5.2912301	1.5768761	808.5794852
C	3.4405776	-4.2766648	807.3176835	C	5.0266051	1.5927389	806.0035734
H	0.6337148	-2.8197953	808.6542313	H	3.9301727	2.8304747	811.7549592
H	1.3704752	-4.9283265	807.5832199	H	3.4852782	3.0924903	805.6112932
H	3.7600135	-5.2200530	806.8493527	H	5.5234174	3.3498781	812.3986657
H	5.3816729	-3.3375882	807.1262487	H	5.5150937	6.5225668	809.1601383
C	-2.1398605	3.2888140	810.3377394	H	5.0094310	3.3726114	804.6944773
C	-1.9306368	2.2267380	809.4116554	H	8.9911883	4.9795326	809.6701279
C	-2.7737674	4.4600561	809.8864891	H	4.9521314	0.6463162	811.0134356
C	-2.3381338	2.3755606	808.0571504	H	4.2851283	0.8055361	806.2499668
C	-2.9670076	3.5705201	807.6598086	H	6.7767866	3.9094872	810.6109715
C	-3.1961821	4.6279999	808.5568178	C	5.6917623	9.3740716	806.4646024
H	-2.9180322	5.2945491	810.5888371	C	4.6704659	8.5244714	806.9095183
C	-2.1373148	1.2722205	807.0197608	C	3.9478156	8.8283323	808.0806107
H	-3.2860983	3.6731766	806.6111238	C	4.2782138	9.9864899	808.8073011
C	-1.2938777	1.7519547	805.8245515	C	5.3015957	10.8409381	808.3616712
H	-1.8151957	2.5458154	805.2494432	C	6.0079721	10.5383429	807.1878128
H	-1.0964099	0.9137479	805.1247309	H	6.2550128	9.1226964	805.5524239
H	-0.3180465	2.1519781	806.1629819	H	4.4405048	7.5881585	806.3783307
C	-3.4873431	0.6875017	806.5647047	C	2.8533412	7.8742616	808.5465092
H	-1.5782193	0.4466617	807.5050107	H	5.5556587	11.7402711	808.9435976
H	-4.1093717	1.4533256	806.0558227	H	6.8141027	11.2030102	806.8410660
H	-4.0693913	0.3033969	807.4267314	O	3.2582542	6.5775085	808.3688909
H	-3.3349279	-0.1490674	805.8515214	H	1.5975554	10.2417917	808.6023539
C	-3.9128518	5.9109268	808.1510150	Zn	2.1139377	5.1429741	808.5828923
C	-3.5929438	6.3769260	806.7232190	C	1.4970021	8.2031831	807.7129643
H	-4.0557188	7.3652394	806.5246700	C	0.8657664	9.5210630	808.1904626
H	-3.9882489	5.6757538	805.9586516	C	0.4355830	7.2276996	808.0570697
H	-2.5003182	6.4733165	806.5598262	C	0.2078960	5.9690541	807.5726904
C	-5.4331136	5.7581532	808.3540345	C	-0.3800562	7.8365145	809.1702567
H	-3.5536282	6.6989548	808.8479563	O	-0.0489681	9.1604951	809.2480613
H	-5.9647370	6.7054193	808.1253824	O	-1.2049970	7.3144036	809.8856965
H	-5.6719811	5.4721601	809.3978882	H	0.2936433	10.0219863	807.3811754
H	-5.8406137	4.9675533	807.6891434	H	3.7495231	10.2091090	809.7487600
C	-1.7029180	3.2076300	811.8004606	H	-0.6175675	5.3621919	807.9861303
C	-0.8865340	4.4341294	812.2456906	H	0.6825130	5.6294396	806.6352945
H	-0.5473675	4.3040149	813.2942164	H	2.6015901	8.1197704	809.6127256
H	-1.4773298	5.3716888	812.2008828	H	1.7793984	8.2025431	806.6428048
H	0.0052621	4.5581658	811.6037468				
C	-2.9208586	2.9880932	812.7186232				
H	-1.0406314	2.3239228	811.9052328				
H	-2.6033906	2.8811186	813.7765949				
H	-3.4909741	2.0792124	812.4381333				
H	-3.6199450	3.8485950	812.6602932				
H	7.1328315	5.8365874	807.3509042				
H	7.6596455	1.8821745	811.8251418				
H	5.8627127	0.4190545	804.3439257				
C	7.2742000	5.4646336	808.3902188				
H	4.7009516	1.9283944	813.1019009				
H	7.0219320	7.4975519	809.1699365				
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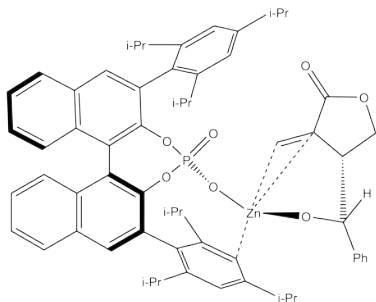
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C	0.7161587	-0.0665729	989.4493181	H	-3.6684001	4.4017996	991.9518702
C	0.1450635	-0.8363540	990.5307935	H	8.3805871	5.3788193	987.4127180
C	0.8886541	-1.7984007	991.2781415	H	6.8708900	2.4671068	992.2466370
C	-1.2306608	-0.5996252	990.9038650	H	6.4367032	0.4095430	984.4259889
C	-1.8147982	-1.3837542	991.9434257	C	8.0462014	5.2564482	988.4668676
C	-1.9647778	0.4513640	990.2810825	H	3.7540628	2.9275599	992.7089693
H	-2.9971482	0.6454057	990.6097742	H	8.1564611	7.4039160	988.9027324
C	-1.3899006	1.2804720	989.3260270	H	4.6300296	2.1572932	984.0092205
C	4.3857994	0.6717141	988.5653128	C	7.0495254	4.1030604	988.4829018
C	4.8569295	-0.6034520	988.2736832	C	6.1445652	1.6595640	992.0173876
H	5.9251193	-0.7406131	988.0454777	C	7.4079258	6.5848308	988.9108351
C	3.9897383	-1.7316779	988.2172166	H	6.9913767	6.5143440	989.9365960
C	4.4747697	-3.0150000	987.8236305	C	6.4455405	3.6812455	989.6809636
C	2.5896049	-1.5742213	988.5328591	C	6.7060959	0.9236028	985.3717849
C	1.7307210	-2.7030100	988.3738615	H	9.7638619	3.9801849	988.9792787
C	2.1079083	-0.2817278	988.9585029	C	6.7154352	3.4127419	987.3067698
C	3.0017599	0.7948048	988.8949568	C	9.2905935	4.9259718	989.3115940
O	0.4604659	1.7203596	987.8627815	H	10.0457666	5.7357109	989.2378523
O	2.5638975	2.0763441	989.2227696	H	7.1633779	3.7452739	986.3557999
P	1.5643001	2.8714988	988.2011088	C	4.1971676	3.2840005	991.7561403
O	1.0639524	4.1266893	988.9550114	H	5.7301311	1.2997366	992.9817983
O	2.1657244	3.3186763	986.8433782	H	6.7068602	0.8248699	991.5513179
C	-1.0732564	-2.3376261	992.6231395	C	5.5713943	2.5820021	989.7360073
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H	-2.8677848	-1.1999279	992.2086551	C	5.8271059	2.3184453	987.2978212
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H	-3.3351924	6.1080609	985.1437732	O	1.1491741	6.8525947	986.5989367
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11b-ma



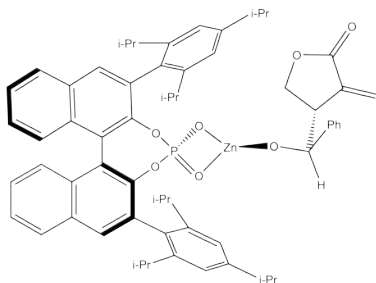
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H	5.7449278	-0.9503118	267.5867004
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C	4.2160895	-3.1676206	267.7665419
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C	1.6580078	-2.7277266	268.8560926
C	2.2849786	-0.3489231	269.4130796
C	3.2163058	0.6800676	269.2237865
O	0.7119052	1.8382914	268.6352601
O	2.9790699	1.9244547	269.7601415
P	1.8812047	2.9496262	269.0179707
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O	2.4416957	3.3204676	267.6141797
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C	0.7591314	-2.5620034	272.9210336
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C	3.2970448	-4.2043569	267.8143419
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C	-3.6309929	6.4722619	266.7556051
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H	6.2298080	1.3334306	264.3634377
C	5.9643266	2.0755519	270.5625778
C	5.2056508	1.7379217	268.1267108
C	4.4644642	1.3900401	265.6749649
H	4.3766993	3.4264282	271.2569057
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C	3.4991169	10.0325820	270.0370443
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O	3.8975528	6.2192886	268.1937653
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H	2.0082872	5.8337951	268.9727571
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11b-mi



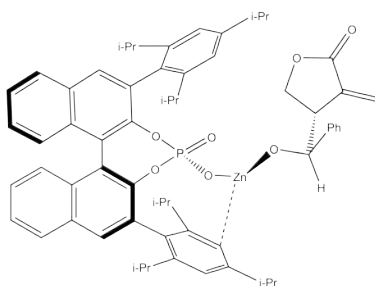
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C	4.0492431	-1.0757183	987.0802159
C	4.5908749	-2.1933832	986.3769042
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C	2.1388297	0.0040950	988.2538316
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O	0.3520077	2.0621062	987.6631995
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P	1.3475027	3.1918041	988.2942469
O	0.6961452	4.1163177	989.3633419
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H	-1.1962568	-3.8116803	992.0888036
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C	5.2349721	2.0718674	990.6350199
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H	6.1183653	7.2828607	989.6430776
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C	0.4208361	6.5777434	985.3869458
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H	1.4565424	5.5825844	982.2719047
O	0.6014865	7.4866564	988.0224742
H	2.6888526	11.2248358	987.3195232
H	4.4119160	11.2868676	986.5342910
H	1.0017334	9.1926684	986.9828737
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11c-mi



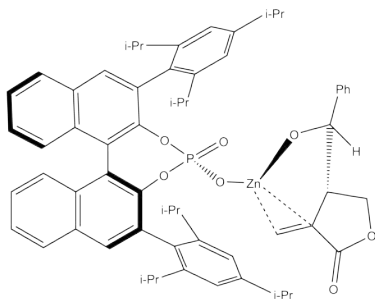
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C	-0.8444158	-0.3881523	990.9025661
C	-1.3222316	-1.0588180	992.0681302
C	-1.6774732	0.5269782	990.1944153
H	-2.7010543	0.7038633	990.5603851
C	-1.2013706	1.2438065	989.1045913
C	4.5050272	0.9388976	987.9780277
C	5.0753767	-0.3205839	987.8442196
H	6.1236874	-0.4042199	987.5189204
C	4.3239441	-1.5127366	988.0581995
C	4.9020783	-2.7966044	987.8257151
C	2.9419267	-1.4269902	988.4703217
C	2.1895915	-2.6370181	988.5567187
C	2.3708173	-0.1277720	988.7357883
C	3.1532030	0.9987120	988.4409438
O	0.5190539	1.5506664	987.4612446
O	2.6292096	2.2643143	988.6404921
P	1.5362923	2.8669153	987.5588793
O	0.8505274	3.9448547	988.4648780
O	1.9822129	3.2232178	986.1778041
C	-0.4809708	-1.8543582	992.8305075
C	0.8827360	-1.9931420	992.4608420
H	-2.3738254	-0.9143904	992.3625441
H	-0.8615046	-2.3605447	993.7306242
H	2.4328647	-1.4821346	991.0524386

H	1.5601829	-2.5944234	993.0861003
C	2.7780646	-3.8689233	988.3054973
C	4.1506644	-3.9548459	987.9530795
H	1.1231856	-2.5858709	988.8167302
H	2.1722273	-4.7854468	988.3738521
H	4.6095556	-4.9371494	987.7637297
H	5.9599959	-2.8465275	987.5234052
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H	-2.7388192	3.6408034	985.3863851
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C	-3.6136273	0.6654059	986.0481255
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H	-1.1610238	5.8192465	990.8573927
H	0.1847877	4.6239970	990.6808329
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H	-1.3313444	2.7373400	991.0656756
H	-2.9609923	3.8161079	992.6095814
H	-3.8255943	3.0010986	991.2646046
H	-3.6452162	4.7812283	991.2643596
H	6.7991885	6.1402380	985.3551392
H	7.2626894	3.7383497	990.7629917
H	6.0499371	0.1124300	983.7600298
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H	6.7822881	8.1853719	986.7409139
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C	6.3455159	4.7073431	986.8590621
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C	6.3755881	7.2409482	987.1565556
H	6.5886704	7.2510462	988.2439758
C	6.1054927	4.3930070	988.2077157
C	6.3163196	0.8500713	984.5456584
H	8.9663606	5.1173709	986.0968062
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C	8.5147255	5.9666658	986.6487197
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H	6.1792461	3.9845239	984.8328724
C	4.4371074	3.9414276	990.7634818
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H	7.3386817	1.9999995	990.3436055
C	5.5398821	3.1679126	988.6005882
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C	5.4227227	2.5085825	986.2286328
H	6.8816903	0.3185817	985.3379617
H	7.0049756	1.5940108	984.0926547

C	5.3439859	2.8941412	990.0913893
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C	5.0563898	1.5374006	985.1056043
H	3.4384724	3.9542117	990.2857159
H	3.3312177	2.6788457	984.4025282
H	4.8620027	4.9636456	990.6916308
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H	8.7610990	5.8374799	987.7236102
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H	4.4111707	0.7482473	985.5424441
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C	2.3752078	6.8479995	989.5888061
C	2.5024446	9.2063352	989.4529504
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C	3.8786774	8.6094349	989.4499285
O	3.7518845	7.2451697	989.4526993
O	4.9532147	9.1678879	989.4506824
H	2.2079622	5.9967697	988.9004252
C	3.0280355	6.3513865	985.2296883
C	2.0749178	6.5528887	986.2396943
C	1.7811451	7.8376653	986.7335134
C	2.4620767	8.9338146	986.1604064
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C	3.2412341	5.3233610	984.9014231
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H	2.2434386	9.9512914	986.5202216
H	3.9274216	9.6157741	984.7134957
H	4.4502302	7.3023963	983.8852137
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H	0.3999414	9.1095037	987.7548153
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11d-mi



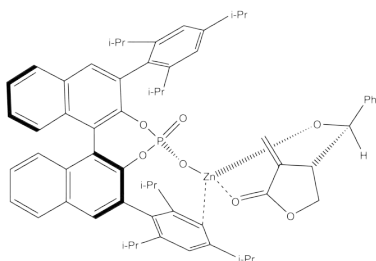
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C	0.6602392	-1.5267319	1000.6792236
C	-1.3728956	-0.1478539	1000.5076137
C	-2.0421930	-1.0946419	1001.3394871
C	-2.0275537	1.0407645	1000.0737482
H	-3.0819162	1.1956449	1000.3483900
C	-1.3648831	2.0165300	999.3400811
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C	4.7360862	-0.0371381	997.8871807
H	5.7806331	-0.1898912	997.5749854
C	3.7853849	-1.0678704	997.6339402
C	4.1653012	-2.2686224	996.9624598
C	2.4046932	-0.8813649	998.0163853
C	1.4605053	-1.8841321	997.6414803

C	2.0347289	0.3196815	998.7258601
C	3.0135309	1.3069561	998.8890118
O	0.5812994	2.6728262	998.1114345
O	2.6762362	2.4802960	999.5387669
P	1.7902724	3.6112841	998.7287837
O	1.2213247	4.4253965	999.9507369
O	2.4622852	4.3507234	997.6135293
C	-1.3811563	-2.2124166	1001.8248062
C	-0.0133044	-2.4173757	1001.5033978
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H	1.7208308	-1.6935083	1000.4461199
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C	1.8608575	-3.0322674	996.9721468
C	3.2267121	-3.2374175	996.6423881
H	0.3988797	-1.7346640	997.8820065
H	1.1108693	-3.7870106	996.6900874
H	3.5340601	-4.1554611	996.1187792
H	5.2233878	-2.4019765	996.6871043
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C	-2.4556199	3.5111238	997.6178153
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C	-1.3416425	2.9606973	995.4076439
H	-1.7944647	3.8221564	994.8721048
H	-1.1642314	2.1616941	994.6583878
H	-0.3597379	3.2760835	995.8115338
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H	-1.7533455	1.5829424	997.0014371
H	-4.1745608	2.7532150	995.4834804
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C	-5.5332541	6.7351743	997.6021421
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C	7.1743963	4.4815827	998.7538894
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C	6.3618824	1.8919760	995.1910688
H	9.9060738	4.2459821	999.1550316

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C	5.7559433	2.7929159	999.8521035
C	4.6941304	3.8119724	995.2331753
C	5.7602671	2.9865737	997.3954932
H	6.7373678	0.9884737	995.7127366
H	7.2314137	2.5615845	995.0226287
C	5.2969281	2.1565222	1001.1634872
C	5.3154048	2.3307630	998.5789280
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H	3.6606178	3.5630526	1001.5611736
H	3.8798043	4.2877960	995.8126255
H	5.2055887	4.0325005	1002.3337771
H	6.7493733	7.2502691	998.8489742
H	5.4748251	4.5724431	995.0203016
H	9.2415732	4.9436780	1000.6642961
H	4.5773633	1.3494537	1000.9172826
H	4.4247590	1.8886723	996.1297051
H	7.0103902	4.2089296	1000.8987147
Zn	1.4664319	6.2662437	999.9699471
H	3.9191497	10.6481476	1000.8249957
C	3.2789408	8.8642135	999.6450271
C	3.4212752	9.6680593	1000.9630942
C	3.9026139	7.5389497	1000.0063560
C	3.9954836	6.3734397	999.3168355
C	4.4718626	7.6442710	1001.3983049
O	4.2227942	8.8934431	1001.8750425
O	5.0800171	6.8039241	1002.0253837
H	2.4282896	9.8164983	1001.4346687
C	2.2668608	7.3695198	995.6507791
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C	1.5510605	8.0601772	997.8857321
C	0.3920963	7.2613277	997.7195326
C	0.1923639	6.5016778	996.5536555
C	1.1373940	6.5435506	995.5222443
H	3.0159513	7.4048374	994.8449857
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O	1.0769145	8.0651433	1000.2637834
H	3.8548378	9.3510674	998.8311133
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11f-ma



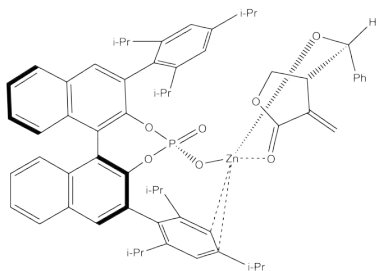
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C	-1.8730327	0.3589591	821.0474867

H	-2.8637134	0.5507943	821.4881818
C	-1.5052447	1.0105409	819.8784601
C	4.1495466	0.8502968	818.5349334
C	4.7674354	-0.3889528	818.4289410
H	5.8228527	-0.4411144	818.1212145
C	4.0621292	-1.6035746	818.6721636
C	4.6838676	-2.8717181	818.4689070
C	2.6864088	-1.5568497	819.1082180
C	1.9836594	-2.7897101	819.2604670
C	2.0682565	-0.2739130	819.3353801
C	2.7893653	0.8743531	818.9789248
O	0.0500737	1.2370277	818.0683599
O	2.1914406	2.1164988	819.1040515
P	1.0957107	2.5313181	817.9200895
O	0.4283953	3.7748409	818.5783019
O	1.6145953	2.5622666	816.5179254
C	-0.4136939	-1.8367608	823.7122077
C	0.9169479	-1.9752359	823.2368669
H	-2.3579165	-0.9560988	823.3506375
H	-0.7070069	-2.2937003	824.6695706
H	2.3343203	-1.5231637	821.6789180
H	1.6569830	-2.5272859	823.8362073
C	2.6133759	-4.0063853	819.0373329
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H	0.9233393	-2.7659329	819.5489946
H	2.0464586	-4.9427082	819.1541250
H	4.4709052	-5.0224088	818.4841747
H	5.7367723	-2.8930995	818.1461460
C	-2.3146096	3.3903478	819.8994340
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H	-2.2276206	-0.2480187	815.3868857
H	-1.3065678	1.2030286	815.9052265
C	-4.3376888	-0.0012447	817.2255481
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H	-3.5993502	6.3520235	817.4128929
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H	-5.2541023	6.1231784	819.2950430
H	-6.3010686	5.1001778	818.2614610
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H	-1.3081891	5.8073481	821.0717348
H	0.0910700	4.7355310	820.7211005
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H	-1.0906079	2.7513825	821.5322926
H	-2.4362767	3.8023817	823.3472059
H	-3.4950331	2.8057067	822.2959497
H	-3.5032648	4.5884213	822.1391899
H	7.2628893	5.9106160	816.4828697
H	6.7757353	3.5280622	821.5029094
H	5.9520141	0.1187545	814.4645629
C	6.4774622	6.0791244	817.2548030
H	3.7119035	3.3366788	822.4710168

H	5.7688012	7.9142564	816.2684969
H	3.9266865	1.4702798	813.7221357
C	5.9384391	4.7000793	817.6281629
C	6.2240316	2.5646902	821.4830686
C	5.3703523	6.9334213	816.6018521
H	4.5506133	7.1261942	817.3247521
C	5.6680754	4.3160312	818.9513655
C	6.1438414	0.8557779	815.2720314
H	7.9146159	6.2354251	818.9158302
C	5.6594590	3.7702704	816.6097227
C	7.1279573	6.8375925	818.4181143
H	7.5929610	7.7769509	818.0565955
H	5.8800531	4.0505874	815.5668627
C	3.9378352	3.6847683	821.4418819
H	6.0585547	2.2507328	822.5347582
H	6.8806374	1.8138965	820.9986555
C	5.1160283	3.0597198	819.2666891
C	4.1547647	2.2264057	814.5014116
C	5.0999421	2.5066792	816.8661788
H	6.6272213	0.3219889	816.1148440
H	6.8768444	1.5966557	814.8886205
C	4.8851832	2.7004612	820.7342172
C	4.8217790	2.1495286	818.2165969
C	4.8373811	1.5514726	815.7023158
H	2.9813731	3.7755252	820.8908394
H	3.2027807	2.6934645	814.8147544
H	4.3897997	4.6949558	821.5326610
H	4.9360948	6.4235707	815.7184704
H	4.8012715	2.9946170	814.0274804
H	6.3783282	7.1219431	819.1858151
H	4.3992367	1.7042676	820.7643417
H	4.1379163	0.7724887	816.0678756
H	5.8942822	5.0101596	819.7743429
C	2.9084145	7.0524921	819.6402611
C	1.6851311	6.8843812	818.9709296
C	0.9705917	7.9966968	818.4838830
C	1.5152835	9.2815932	818.6910508
C	2.7349757	9.4551106	819.3617639
C	3.4379147	8.3366212	819.8401832
H	3.4491410	6.1638843	819.9968867
H	1.3081805	5.8627207	818.8266718
C	-0.3324361	7.8569024	817.6952933
H	3.1348757	10.4689826	819.5191394
H	4.3947567	8.4665847	820.3693489
O	-1.1938422	6.8462822	818.1090245
H	-2.0443175	8.5234583	815.7418466
Zn	-0.9928468	4.9711902	818.1222204
C	0.0102907	7.7610954	816.1438024
C	-1.2511691	7.9089866	815.2716235
C	0.3933841	6.3399153	815.8484412
C	1.5774021	5.6962148	815.8939839
C	-0.9081101	5.6643278	815.5860775
O	-1.7969862	6.5671509	815.1283605
O	-1.2364633	4.4977202	815.8236599
H	-1.0286201	8.3043362	814.2587927
H	0.9646067	10.1649583	818.3256193
H	0.7859309	8.5067850	815.8854796
H	-0.8720075	8.8326001	817.8065248
H	1.6302495	4.6012479	815.7611353
H	2.5078054	6.2453743	816.1027346

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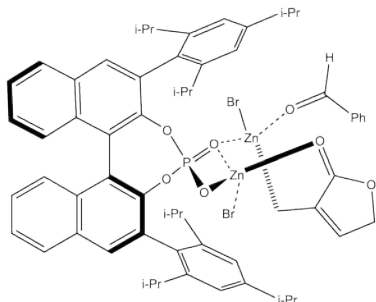


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C	0.1358818	1.6758066	989.4620599	H	-3.5008596	2.7058252	992.1387930
C	0.6979748	0.4051455	989.6643141	H	-3.7613163	4.4074101	992.6223390
C	-0.1036330	-0.5806210	990.3467489	H	6.8546991	6.7220858	988.2792845
C	0.4203155	-1.8359778	990.7789347	H	7.8167795	2.0958907	991.9576572
C	-1.4842314	-0.2779919	990.6446391	H	5.6033494	2.1078610	984.3130399
C	-2.2855351	-1.2615630	991.2975935	C	7.3659962	6.0447869	989.0018954
C	-2.0185139	0.9998475	990.3048214	H	4.9674486	2.0092196	993.4698664
H	-3.0814013	1.2014390	990.5073201	H	7.9046577	7.7491807	990.2439727
C	-1.2263507	1.9992479	989.7559129	H	3.2924621	3.0073655	984.9345980
C	4.4067825	0.9615178	988.8475304	C	6.5695828	4.7391795	989.0155501
C	4.7152769	-0.1693331	988.1027721	C	7.0791734	1.2905651	991.7564300
H	5.7226655	-0.2796394	987.6706956	C	7.4177671	6.7597736	990.3568643
C	3.7291401	-1.1540914	987.8051444	H	8.0157782	6.1891207	991.0974266
C	4.0422790	-2.2751316	986.9794099	C	6.4024161	3.9450031	990.1691899
C	2.3691588	-0.9637607	988.2585886	C	5.9951394	2.5307341	985.2600289
C	1.3738131	-1.8653741	987.7730707	H	8.7554406	5.3034843	987.4521484
C	2.0721426	0.1355936	989.1476189	C	6.0763363	4.2115256	987.7850060
C	3.1024969	1.0397990	989.4415976	C	8.7826227	5.7698244	988.4572227
O	0.9030175	2.6795872	988.9081189	H	9.3613336	6.7128157	988.3826677
O	2.8863699	2.0406243	990.3528896	H	6.2581804	4.7806002	986.8575496
P	1.9990454	3.4043069	989.9458832	C	5.1066787	2.6736287	992.5932291
O	1.4426298	3.9811474	991.2026604	H	7.0208098	0.6533391	992.6624328
O	2.8283377	4.2145186	988.9263721	H	7.4737419	0.6707953	990.9258013
C	-1.7513680	-2.4831732	991.6791271	C	5.7761242	2.6847847	990.1311247
C	-0.3819511	-2.7633694	991.4293128	C	3.6718965	3.3543413	985.9169803
H	-3.3397159	-1.0219771	991.5087545	C	5.4356746	2.9455119	987.7005645
H	-2.3808930	-3.2281942	992.1891669	H	6.8772566	1.9308203	985.5643550
H	1.4816096	-2.0590972	990.5998483	H	6.3444262	3.5598823	985.0336695
H	0.0497038	-3.7206403	991.7595688	C	5.6920137	1.8725219	991.4179563
C	1.7081087	-2.9342266	986.9530651	C	5.2705267	2.1834797	988.8953838
C	3.0560311	-3.1577360	986.5673335	C	4.8956452	2.5153504	986.3369807
H	0.3244635	-1.7031138	988.0527238	H	4.1223248	3.1104955	992.3368217
H	0.9174633	-3.6110057	986.5945847	H	2.8556889	3.2604024	986.6586071
H	3.3107271	-4.0148596	985.9255965	H	5.7807885	3.4958502	992.9123972
H	5.0864229	-2.4126513	986.6563418	H	6.4017836	6.9119269	990.7692978
C	-1.9618840	4.3227527	990.4672064	H	3.9132378	4.4353064	985.8280425
C	-1.7334080	3.3738670	989.4320626	H	9.3323540	5.0834418	989.1343875
C	-2.4415660	5.5992551	990.1146617	H	5.0148111	1.0174336	991.2258511
C	-1.9419250	3.7407999	988.0729567	H	4.5489530	1.4699044	986.4335100
C	-2.4164233	5.0322428	987.7771378	Hn	6.7660308	4.3257695	991.1331828
C	-2.6856273	5.9767319	988.7838129	Zn	4.2919390	5.3646667	988.5341734
H	-2.6321047	6.3350728	990.9120923	H	0.2762226	6.9496877	988.9640094
C	-1.6790562	2.7705201	986.9222310	C	2.0588842	8.1148478	988.2510451
H	-2.5937346	5.3008551	986.7230501	C	1.0473353	7.6620149	989.3183563
C	-0.6067489	3.3056894	985.9563320	C	3.2674353	8.3221277	989.1072854
H	-0.9508274	4.2135429	985.4181699	C	4.3104349	9.1650919	989.0143222
H	-0.3558673	2.5441742	985.1891490	C	3.1521699	7.2260634	990.1116469
H	0.3220198	3.5624287	986.5022993	O	1.8558475	6.9306665	990.2928195
C	-2.9816267	2.4085843	986.1858125	O	4.0618733	6.5496584	990.6043929
H	-1.2852734	1.8301567	987.3579950	H	0.5513773	8.5088561	989.8372939
H	-3.4395891	3.3000370	985.7080178	C	2.2570638	8.1691664	983.6130562
H	-3.7310031	1.9799965	986.8818415	C	2.7509007	7.8215266	984.8799512
H	-2.7882144	1.6634108	985.3863489	C	1.8998932	7.2439677	985.8404178
C	-3.2848809	7.3426396	988.4651467	C	0.5526321	7.0038021	985.5074086
C	-2.5160126	8.1110215	987.3787437	C	0.0572641	7.3524656	984.2414262
H	-2.9532442	9.1188498	987.2243838	C	0.9082830	7.9400443	983.2906100
H	-2.5516343	7.5877923	986.4007069	H	2.9311195	8.6177660	982.8661470
H	-1.4475774	8.2417305	987.6429339	H	3.8081446	7.9706957	985.1458860
C	-4.7741236	7.2035080	988.0941301	C	2.4188645	6.9007280	987.2248083
H	-3.2292260	7.9414955	989.4014531	H	-0.1104928	6.5208946	986.2429682
H	-5.2389278	8.1967124	987.9215451	H	-0.9968264	7.1518355	983.9920912
H	-5.3408446	6.6900174	988.8963713	H	0.5233596	8.2093860	982.2948404
H	-4.8947524	6.6063577	987.1658957	O	3.7849923	6.6130272	987.2053253
C	-1.7153295	3.9943180	991.9389150	H	1.8191010	6.0302417	987.5931441
C	-1.0356035	5.1421330	992.7044325	H	1.7335923	9.0141951	987.6959177
H	-0.7625995	4.8017412	993.7242749	H	4.3512747	9.9379062	988.2323903
H	-1.7057768	6.0196067	992.8248283	H	5.1464103	9.0973452	989.7283638
H	-0.1050685	5.4530891	992.1936497				
C	-3.0254296	3.5755330	992.6339668				
H	-1.0131862	3.1365480	991.9661021				
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7.1.3 Educt Complexes 14

14a-mi; COSMO



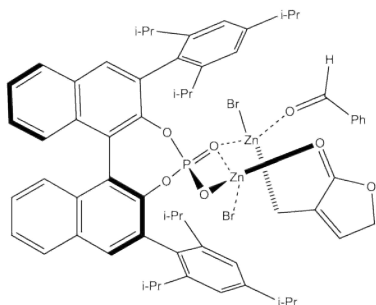
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Zn	-3.6953804	8.4476704	237.8317120
Br	-1.6947020	9.5621007	238.0315219
C	-7.7278394	6.8728595	231.2395471
C	-7.2478764	6.8740500	232.5527275
C	-8.0576703	7.3835148	233.5957368
C	-9.3534107	7.8713124	233.3042341
C	-9.8290490	7.8694196	231.9875693
C	-9.0136232	7.3729684	230.9546664
H	-7.1002413	6.4711527	230.4297938
H	-6.2567679	6.4525515	232.7841757
C	-7.5914452	7.4193631	234.9872079
H	-9.9866673	8.2438165	234.1238968
H	-10.8370396	8.2495512	231.7633154
H	-9.3858431	7.3673658	229.9184965
O	-6.4827606	7.0461595	235.3891124
C	-6.0910227	10.2897114	233.9038582
C	-5.2009587	9.6570564	234.7294969
C	-5.7197613	9.8862820	236.1001754
O	-6.8431800	10.6237896	236.0788661
C	-7.1560036	10.9503357	234.7086699
O	-5.2795766	9.5009068	237.1976918
C	-4.0348745	8.8123462	234.4624823
H	-6.0534060	10.3279977	232.8069693
H	-7.1721978	12.0589352	234.6164061
H	-8.1847659	10.5833569	234.4964861
Zn	-4.4426757	6.8285259	234.7487940
Br	-4.2902906	4.7262308	233.6907675
H	-3.2060021	9.0396780	235.1676108
H	-3.6595526	8.9482797	233.4299040
C	-6.4237365	4.1376195	238.2151618
C	-5.7240358	2.9333773	238.3355111
C	-6.2915480	1.8992262	239.1661892
C	-5.5854605	0.7027197	239.4948716
C	-7.6076193	2.0923200	239.7248047
C	-8.1726784	1.0744363	240.5504176
C	-8.3235977	3.2857215	239.4250258
H	-9.3599599	3.3897704	239.7827248
C	-7.7624285	4.3163925	238.6780773
C	-2.0410398	3.3921299	237.3582497
C	-1.8404540	2.2818058	236.5465935
H	-0.8282839	2.0654723	236.1734118
C	-2.9107440	1.4221994	236.1637817
C	-2.7030938	0.3452048	235.2510390
C	-4.2329174	1.6430445	236.6980065
C	-5.2965212	0.8017098	236.2562046
C	-4.4309979	2.7274476	237.6265021
C	-3.3650824	3.5959020	237.8485222
O	-5.8509239	5.2047990	237.5232107
O	-3.5835709	4.7211409	238.6550928
P	-4.4684933	5.9290057	238.0128004
O	-4.5880047	7.0319594	239.0777893
O	-3.8435017	6.5700741	236.7345532
C	-7.4653183	-0.0832878	240.8379907
C	-6.1572910	-0.2623075	240.3126936
H	-9.1819435	1.2317078	240.9622631
H	-7.9095867	-0.8587951	241.4803791

H	-4.5688279	0.5557128	239.1042081
H	-5.5887747	-1.1716627	240.5604906
C	-5.0636386	-0.2263896	235.3529729
C	-3.7553898	-0.4665410	234.8539628
H	-6.3148769	0.9869777	236.6263796
H	-5.9012158	-0.8559627	235.0156079
H	-3.5823163	-1.2880043	234.1420549
H	-1.6888464	0.1808297	234.8545666
C	-8.5653154	6.7102456	238.9842850
C	-8.5953385	5.4907246	238.2571278
C	-9.4328784	7.7461064	238.5976197
C	-9.4738392	5.3360465	237.1469939
C	-10.3320125	6.4047981	236.8098148
C	-10.3348432	7.6158416	237.5254600
H	-9.4265183	8.6868013	239.1700447
C	-9.4781481	4.0466934	236.3201431
H	-11.0231715	6.2754775	235.9657450
C	-8.3749643	4.0573257	235.2411252
H	-8.6084886	4.7999310	234.4506640
H	-8.2978311	3.0642814	234.7524086
H	-7.3769122	4.3108430	235.6461216
C	-10.8401199	3.7181411	235.6913510
H	-9.2367672	3.2185738	237.0183366
H	-11.1074364	4.4313530	234.8833495
H	-11.6562811	3.7320942	236.4419956
H	-10.8130919	2.7095010	235.2315084
C	-11.2614992	8.7873074	237.1990316
C	-10.4761801	9.9807593	236.6173887
H	-11.1226414	10.8782741	236.5321717
H	-10.1017018	9.7465148	235.5987380
H	-9.5964381	10.2440198	237.2373594
C	-12.4482023	8.4230697	236.2991434
H	-11.6771288	9.1255398	238.1751580
H	-13.1313171	9.2892292	236.1898617
H	-13.0326892	7.5755525	236.7098854
H	-12.1195434	8.1382681	235.2769423
C	-7.6757983	6.8748525	240.2127106
C	-7.1423009	8.3037032	240.3937088
H	-6.3630514	8.3185270	241.1813825
H	-7.9412151	9.0081748	240.7071226
H	-6.6846391	8.6848571	239.4603219
C	-8.4125057	6.3936360	241.4784300
H	-6.7933895	6.2181890	240.0724442
H	-7.7569836	6.4800757	242.3695437
H	-8.7287053	5.3350019	241.3897081
H	-9.3212351	7.0052938	241.6600416
H	2.4328398	7.7200882	238.1437700
H	0.9020166	2.8617974	241.1342392
H	-0.4208931	4.5631842	233.4068826
C	2.1597255	7.1184803	239.0385401
H	-2.1276153	3.3263920	242.0342529
H	2.3534793	8.8583835	240.3640514
C	1.0978176	6.1226215	238.5903140
C	0.0732858	2.3330936	240.6183752
C	1.6001942	8.0886257	240.0955204
H	1.3252305	7.5495608	241.0266386
C	0.5474539	5.1909647	239.4877451
C	-0.0001269	4.5404424	234.4336017
H	3.8538073	5.7412766	238.7615999
C	0.6119922	6.1298340	237.2732958
C	3.4355211	6.4162213	239.5357654
H	4.2155448	7.1584681	239.8047860
H	1.0249964	6.8663971	236.5665910
C	-1.6693296	4.0512429	241.3296194
H	-0.3479206	1.5942466	241.3315697
H	0.5104544	1.7770447	239.7641736
C	-0.4655354	4.2939226	239.1068158
C	-1.0632756	6.7805575	234.9049427
C	-0.4002979	5.2542073	236.8370681
H	0.0974207	3.4790131	234.7353478
H	1.0220757	4.9735798	234.3994167

C	-1.0135325	3.3162251	240.1459670
C	-0.9417623	4.3237586	237.7660677
C	-0.9006869	5.3343925	235.3981064
H	-2.4613199	4.7404708	240.9766733
H	-0.9255443	4.6463673	241.8997974
H	0.6911166	8.6024957	239.7227206
H	3.2323556	5.8050742	240.4402623
H	-1.8034589	2.7081734	239.6591469
H	-1.9078439	4.8702043	235.3687010
H	0.9103104	5.1681171	240.5280936
H	-0.0874038	7.2712771	234.7078284
H	-1.5999388	7.3985064	235.6497905
H	-1.6333036	6.7928232	233.9524770
H	-8.3161058	7.8248295	235.7376024

14a-mi



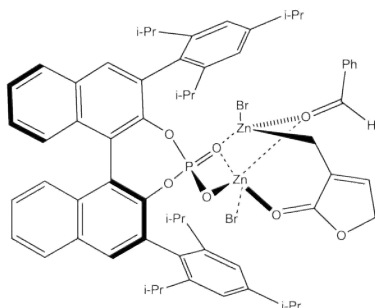
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C	-7.2535779	6.8315701	232.5691316
C	-8.0516441	7.3684703	233.6068028
C	-9.3425854	7.8670191	233.3144223
C	-9.8243630	7.8513300	232.0001296
C	-9.0205786	7.3287574	230.9713220
H	-7.1223625	6.3906658	230.4540408
H	-6.2679849	6.3971090	232.8033898
C	-7.5761689	7.4185998	234.9967582
H	-9.9670708	8.2555327	234.1334850
H	-10.8292571	8.2393589	231.7748613
H	-9.3983932	7.3113120	229.9372228
O	-6.4683157	7.0421153	235.3933942
C	-6.0807059	10.2771688	233.9180679
C	-5.1869114	9.6461645	234.7411022
C	-5.7065480	9.8685747	236.1154314
O	-6.8341693	10.6052421	236.0942690
C	-7.1478306	10.9321409	234.7268212
O	-5.2673567	9.4786877	237.2079189
C	-4.0198863	8.8075653	234.4745985
H	-6.0439310	10.3157361	232.8212587
H	-7.1693377	12.0416408	234.6371091
H	-8.1756051	10.5610096	234.5146917
Zn	-4.4141518	6.8152392	234.7537741
Br	-4.2830228	4.7372546	233.6640645
H	-3.1946277	9.0303753	235.1850963
H	-3.6410568	8.9448896	233.4436227
C	-6.4213614	4.1371391	238.2114131
C	-5.7266907	2.9294321	238.3286703
C	-6.2994811	1.8948396	239.1550199
C	-5.5987572	0.6942284	239.4791096
C	-7.6149186	2.0907685	239.7136537
C	-8.1836437	1.0720421	240.5348216
C	-8.3254153	3.2879220	239.4172669
H	-9.3616923	3.3965158	239.7741170
C	-7.7599034	4.3186065	238.6740434

C	-2.0426489	3.3875860	237.3550011
C	-1.8438433	2.2807248	236.5385227
H	-0.8320792	2.0685453	236.1621785
C	-2.9136941	1.4220482	236.1533805
C	-2.7071555	0.3492872	235.2361531
C	-4.2355150	1.6402881	236.6892576
C	-5.2986533	0.7997492	236.2454422
C	-4.4330678	2.7217241	237.6212582
C	-3.3665014	3.5883526	237.8474299
O	-5.8461435	5.2046548	237.5240470
O	-3.5849099	4.7094208	238.6588685
P	-4.4599248	5.9238538	238.0164365
O	-4.5792194	7.0262179	239.0809556
O	-3.8293040	6.5603450	236.7392389
C	-7.4816841	-0.0894081	240.8178428
C	-6.1748881	-0.2715726	240.2921672
H	-9.1921663	1.2320525	240.9474583
H	-7.9294486	-0.8654203	241.4571035
H	-4.5830600	0.5456971	239.0869524
H	-5.6102797	-1.1843730	240.5359462
C	-5.0657870	-0.2247158	235.3386839
C	-3.7586156	-0.4615936	234.8371764
H	-6.3163631	0.9833065	236.6180100
H	-5.9032947	-0.8535280	234.9999446
H	-3.5856632	-1.2793733	234.1211424
H	-1.6935618	0.1885246	234.8367576
C	-8.5520532	6.7154262	238.9831046
C	-8.5885958	5.4965885	238.2553198
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C	-9.4798397	4.0565892	236.3195334
H	-11.0175125	6.2911248	235.9691328
C	-8.3730145	4.0568039	235.2442650
H	-8.5998023	4.7964533	234.4493774
H	-8.2983649	3.0619180	234.7591654
H	-7.3745782	4.3064176	235.6505024
C	-10.8419510	3.7377904	235.6862592
H	-9.2476037	3.2275780	237.0198193
H	-11.1002379	4.4511964	234.8754580
H	-11.6613096	3.7595634	236.4331080
H	-10.8218546	2.7284930	235.2276821
C	-11.2468170	8.8018092	237.2077412
C	-10.4630997	9.9941568	236.6221050
H	-11.1067180	10.8944648	236.5429673
H	-10.0975587	9.7591872	235.6002336
H	-9.5764654	10.2530772	237.2339343
C	-12.4398421	8.4407050	236.3150280
H	-11.6566155	9.1402414	238.1863615
H	-13.1227605	9.3074906	236.2091374
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H	-12.1175092	8.1545772	235.2911468
C	-7.6598948	6.8761774	240.2099619
C	-7.1255597	8.3040008	240.3953177
H	-6.3396822	8.3135676	241.1760873
H	-7.9215447	9.0066553	240.7204827
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C	-8.3939260	6.3900490	241.4752254
H	-6.7774290	6.2207513	240.0658010
H	-7.7373196	6.4758500	242.3654062
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H	-9.3038948	6.9987407	241.6601009
H	2.3849169	7.7581368	238.1504305
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H	-0.3960716	4.5411197	233.4057938
C	2.1216665	7.1488330	239.0430298
H	-2.1327844	3.3269098	242.0362245
H	2.2959953	8.8855581	240.3749392
C	1.0727054	6.1410998	238.5915749

C	0.0683626	2.3407298	240.6123951	O	1.7854033	4.3034155	88.9230276
C	1.5521906	8.1071149	240.1051395	O	2.0755746	3.3913144	86.5931292
H	1.2872956	7.5614416	241.0352277	C	0.1871018	-1.9897973	93.1053902
C	0.5255147	5.2079778	239.4887213	C	1.4138792	-2.2270119	92.4294155
C	0.0179910	4.5274798	234.4351695	H	-1.6491520	-0.8417201	93.1354268
H	3.8317285	5.7937714	238.7544448	H	-0.0494999	-2.5464564	94.0249591
C	0.5963491	6.1373763	237.2715801	H	2.6793851	-1.7270595	90.7560262
C	3.4072709	6.4595597	239.5329251	H	2.1293039	-2.9582025	92.8357089
H	4.1791499	7.2089868	239.8054610	C	1.7129120	-3.7593728	87.6407822
H	1.0069111	6.8750662	236.5648562	C	2.9540970	-4.0686717	87.0231397
C	-1.6761866	4.0536696	241.3325074	H	0.5191792	-2.2688583	88.6455002
H	-0.3470948	1.6004861	241.3275319	H	0.9186312	-4.5202868	87.6825944
H	0.5030476	1.7866816	239.7558632	H	3.1221101	-5.0713280	86.6012305
C	-0.4776767	4.3015977	239.1059965	H	4.9018077	-3.3224324	86.4404881
C	-1.0602249	6.7634284	234.8859468	C	-2.0166929	3.7616586	89.5092975
C	-0.4048727	5.2512635	236.8320975	C	-1.9979776	2.3787649	89.1875495
H	0.1209614	3.4686004	234.7435884	C	-2.9602584	4.5875249	88.8690990
H	1.0378098	4.9662719	234.4065350	C	-2.9193873	1.8439814	88.2432270
C	-1.0220823	3.3225572	240.1457781	C	-3.8447099	2.7138964	87.6381263
C	-0.9463069	4.3222718	237.7625378	C	-3.8820476	4.0877204	87.9332468
C	-0.8943262	5.3209098	235.3888235	H	-2.9838275	5.6622835	89.1065784
H	-2.4688844	4.7438489	240.9836687	C	-2.8862122	0.3701380	87.8370138
H	-0.9326155	4.6479024	241.9036683	H	-4.5536509	2.3029975	86.9028028
H	0.6353044	8.6102313	239.7375214	C	-2.1247911	0.1797801	86.5114460
H	3.2136658	5.8400156	240.4337158	H	-2.6546520	0.6826882	85.6751639
H	-1.8121111	2.7133173	239.6604906	H	-2.0353078	-0.8966615	86.2578213
H	-1.8988540	4.8513992	235.3526832	H	-1.0986737	0.5938654	86.5520723
H	0.8820164	5.1927484	240.5313226	C	-4.2840700	-0.2668910	87.7746193
H	-0.0857980	7.2561546	234.6870597	H	-2.3191069	-0.1763522	88.6178733
H	-1.5973257	7.3861929	235.6264767	H	-4.8993770	0.1577807	86.9540527
H	-1.6279595	6.7670547	233.9320319	H	-4.8401419	-0.1232622	88.7234466
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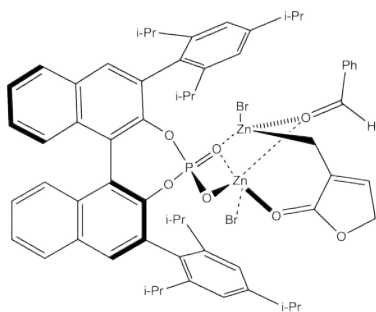


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C	0.8227437	-0.5754397	90.7178233	C	7.3699395	3.7807115	87.5754118
C	1.7226885	-1.5400389	91.2632371	C	7.3271346	0.6663860	90.7095051
C	-0.4070951	-0.3102804	91.4255836	C	7.6181212	6.1953232	88.2362890
C	-0.7019415	-1.0464897	92.6122103	H	7.4756741	5.9853344	89.3175129
C	-1.3097588	0.6693995	90.9207103	C	7.1459044	3.0761775	88.7708385
H	-2.2836257	0.8039410	91.4163155	C	5.7867911	0.8911038	84.3455638
C	-1.0029732	1.4458386	89.8095603	H	10.1669699	3.8613493	87.5831128
C	4.5151799	0.5223174	87.7643678	C	6.6687013	3.3703542	86.4294789
C	4.7385449	-0.7829254	87.3456235	C	9.6842511	4.7157729	88.0994766
H	5.7090345	-1.0471028	86.8993055	H	10.3407952	5.6031101	87.9857877
C	3.7384651	-1.7915738	87.4652017	H	6.8307067	3.9231485	85.4911163
C	3.9437751	-3.1007212	86.9363751	C	5.4053804	2.2570818	91.2275805
C	2.4921982	-1.4896189	88.1269310				
C	1.4888362	-2.5014221	88.1831430				
C	2.2945175	-0.1675946	88.6681309				
C	3.2584260	0.7958029	88.3801343				
O	0.5615396	2.0332133	88.0845105				
O	3.0404958	2.1161001	88.7939167				
P	1.8777311	3.0051356	88.0909673				

H	7.1419193	0.1154298	91.6549370	C	-1.3181364	0.6603669	90.9172397
H	7.7482692	-0.0470638	89.9722036	H	-2.2937098	0.7964034	91.4091780
C	6.2399499	2.0030581	88.8460455	C	-1.0066958	1.4395119	89.8095859
C	4.6127222	3.1239930	84.3139949	C	4.5128678	0.5186827	87.7729953
C	5.7489417	2.3051755	86.4489659	C	4.7368681	-0.7856910	87.3523619
H	6.0307877	-0.0178788	84.9292866	H	5.7067784	-1.0456014	86.9024676
H	6.7434622	1.3264728	83.9863958	C	3.7387651	-1.7959928	87.4698710
C	6.0268724	1.3046916	90.1886555	C	3.9451756	-3.1032940	86.9382176
C	5.5353941	1.6158647	87.6731319	C	2.4916161	-1.4968542	88.1308948
C	4.9969968	1.9167452	85.1804806	C	1.4895587	-2.5098024	88.1836602
H	4.4604134	2.6944636	90.8496460	C	2.2921204	-0.1760086	88.6742044
H	4.1289323	3.9109603	84.9251416	C	3.2560975	0.7885831	88.3901769
H	6.0946707	3.0925500	91.4714726	O	0.5620222	2.0293023	88.0908340
H	6.6201710	6.4117426	87.8034826	O	3.0373735	2.1069993	88.8078203
H	5.4918233	3.5754620	83.8079974	P	1.8796590	3.0005361	88.1039604
H	9.6423670	4.4749949	89.1824060	O	1.7853623	4.2957414	88.9396944
H	5.3054496	0.4773110	90.0283805	O	2.0809498	3.3896816	86.6068858
H	4.0486600	1.4295038	85.4902085	C	0.1665897	-2.0082921	93.0977971
H	7.6797610	3.3827608	89.6846930	C	1.3940818	-2.2459114	92.4245364
C	1.2878922	6.6020626	80.2539854	H	-1.6665270	-0.8562824	93.1265768
C	1.3377808	5.6020597	81.2281438	H	-0.0739459	-2.5671378	94.0149629
C	1.7541718	5.9262400	82.5421196	H	2.6645911	-1.7430551	90.7554680
C	2.1205779	7.2537970	82.8688940	H	2.1066495	-2.9803094	92.8299206
C	2.0665582	8.2511845	81.8856795	C	1.7157708	-3.7659237	87.6390426
C	1.6517020	7.9251462	80.5824659	C	2.9571512	-4.0723087	87.0218679
H	0.9660957	6.3596209	79.2298877	H	0.5193818	-2.2784834	88.6452893
H	1.0564401	4.5624870	81.0019022	H	0.9219968	-4.5274000	87.6778812
C	1.7792834	4.9172774	83.5982398	H	3.1263741	-5.0732904	86.5967091
H	2.4446626	7.4892983	83.8964508	H	4.9031458	-3.3219412	86.4410057
H	2.3502027	9.2848109	82.1338902	C	-2.0105993	3.7592816	89.5102284
H	1.6108126	8.7088933	79.8102571	C	-1.9974316	2.3766683	89.1874306
O	1.4528532	3.7296665	83.4493299	C	-2.9479939	4.5894161	88.8672259
Zn	2.0287110	5.5185567	87.3240326	C	-2.9191105	1.8461344	88.2412002
Br	3.6946889	6.9284859	86.5912279	C	-3.8383613	2.7207254	87.6339893
H	-0.7373594	7.3079996	83.0037342	C	-3.8694097	4.0943980	87.9289645
Br	1.4593301	0.3355612	84.8160750	H	-2.9667539	5.6640728	89.1053871
H	-1.8106445	2.8899947	84.9617335	C	-2.8928302	0.3716334	87.8365716
Zn	0.7441082	2.5558865	85.0992572	H	-4.5482766	2.3129134	86.8979669
C	-1.6066298	5.4686853	83.8293486	C	-2.1222766	0.1718930	86.5177878
C	-1.3662576	6.9365524	83.8446826	H	-2.6408067	0.6768011	85.6758071
C	-1.0860711	4.8907768	84.9626739	H	-2.0395010	-0.9052159	86.2655711
C	-1.0293176	3.5131156	85.4360811	H	-1.0925186	0.5761142	86.5637446
C	-0.4622705	6.0104812	85.6999917	C	-4.2945837	-0.2555048	87.7645393
O	-0.6383781	7.1819444	85.0659632	H	-2.3363859	-0.1771936	88.6234714
O	0.1675883	5.9758431	86.7741367	H	-4.8992347	0.1680277	86.9355130
H	-2.2950548	7.5486848	83.8676095	H	-4.8594966	-0.1023682	88.7064744
H	-1.1467638	3.4642355	86.5374673	H	-4.2181571	-1.3468209	87.5818167
H	-2.1436956	4.9556883	83.0203386	C	-4.8948994	5.0203403	87.2853091
H	2.1261273	5.2861237	84.5987419	C	-4.8835301	4.9430755	85.7493977
				H	-5.5900269	5.6794374	85.3131208
				H	-5.1928773	3.9393224	85.3903879
				H	-3.8726230	5.1441367	85.3418649
				C	-6.3039868	4.7521466	87.8466554
				H	-4.6125200	6.0579892	87.5708993
				H	-7.0454814	5.4607374	87.4221298
				H	-6.3226837	4.8519622	88.9504212
				H	-6.6389747	3.7231788	87.5986404
				C	-1.0709759	4.3248363	90.5723058
				C	-0.6769844	5.7895666	90.3341755
				H	0.1495142	6.0754159	91.0148048
				H	-1.5205329	6.4837074	90.5322981
				H	-0.3354073	5.9510709	89.2942656
				C	-1.6772388	4.1484366	91.9788346
				H	-0.1349298	3.7298511	90.5331226
				H	-0.9847798	4.5339035	92.7555285
				H	-1.8834271	3.0843185	92.2067823
				H	-2.6340921	4.7047354	92.0649747
				H	8.3899663	5.2559768	86.4036995
				H	8.0776760	1.4757652	90.9127806
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				C	8.2697376	5.0013135	87.4800550

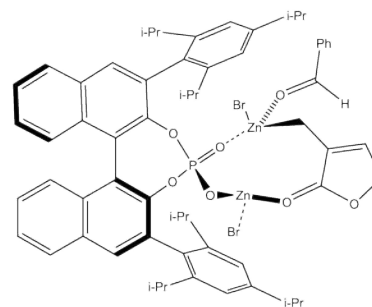
14b-ma



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C	0.8118640	-0.5874880	90.7172267
C	1.7077851	-1.5557814	91.2620989
C	-0.4194018	-0.3224306	91.4221450
C	-0.7184720	-1.0617873	92.6051695

H	5.1631658	1.8222147	92.1756522
H	8.2317767	7.1198000	88.0690060
H	3.8906552	2.7262848	83.5156696
C	7.3565180	3.7838073	87.5431580
C	7.2890105	0.7171396	90.7261066
C	7.6055590	6.2086881	88.1698329
H	7.4637355	6.0148203	89.2539910
C	7.1199216	3.1075723	88.7520994
C	5.8255333	0.8510007	84.3378896
H	10.1511911	3.8630485	87.5454044
C	6.6701318	3.3438055	86.4000438
C	9.6703255	4.7246973	88.0509421
H	10.3282709	5.6095288	87.9263894
H	6.8411107	3.8741203	85.4502836
C	5.3903653	2.3429680	91.2221800
H	7.1020643	0.1882484	91.6837492
H	7.6961518	-0.0164315	90.0010787
C	6.2171980	2.0337417	88.8427956
C	4.6042682	3.0587916	84.2948717
C	5.7531858	2.2768128	86.4341179
H	6.0879503	-0.0496912	84.9264444
H	6.7740613	1.3036733	83.9787567
C	5.9958069	1.3643911	90.1986487
C	5.5279998	1.6155506	87.6713882
C	5.0131177	1.8632442	85.1667535
H	4.4521768	2.7891072	90.8382718
H	4.1150620	3.8418923	84.9065487
H	6.0919105	3.1716847	91.4532923
H	6.6071052	6.4208738	87.7366404
H	5.4724845	3.5206931	83.7793771
H	9.6295896	4.4967940	89.1366251
H	5.2629063	0.5439815	90.0552505
H	4.0738292	1.3584688	85.4757342
H	7.6421493	3.4377349	89.6644205
C	1.2941488	6.6405261	80.3038662
C	1.3529527	5.6326248	81.2693106
C	1.7756045	5.9461194	82.5830566
C	2.1394275	7.2709787	82.9197957
C	2.0759364	8.2766320	81.9450391
C	1.6553144	7.9616490	80.6415363
H	0.9687328	6.4056251	79.2790334
H	1.0752589	4.5927211	81.0396464
C	1.8093899	4.9233575	83.6295431
H	2.4677537	7.4963694	83.9485784
H	2.3580014	9.3089224	82.2009410
H	1.6085230	8.7519479	79.8762810
O	1.4737608	3.7420824	83.4664901
Zn	2.0326018	5.5166498	87.3503566
Br	3.6520574	6.9740936	86.6212823
H	-0.7075758	7.3077191	83.0394366
Br	1.4663400	0.3183958	84.8223284
H	-1.7804513	2.8453820	84.9042591
Zn	0.7746019	2.5341172	85.1074809
C	-1.5880554	5.4530696	83.8218321
C	-1.3480913	6.9218479	83.8655080
C	-1.0826741	4.8564788	84.9526122
C	-1.0221325	3.4754116	85.4055883
C	-0.4681259	5.9654584	85.7171735
O	-0.6376221	7.1481243	85.0986449
O	0.1489404	5.9085642	86.7945595
H	-2.2781542	7.5333495	83.8879198
H	-1.1560563	3.4074492	86.5040268
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Energy (Hartree) = -11970.03608095

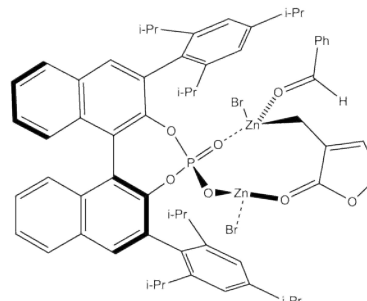
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C	3.0579142	1.5652728	102.8074847
C	3.9572922	1.3243574	103.8896898
C	2.0785006	2.5968977	102.8808584
H	1.9887705	3.1774246	103.8113727
C	1.2557092	2.9104488	101.8041427
C	2.3079051	-0.1732109	96.8685310
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H	2.3317687	-2.1991734	96.1413171
C	2.0470633	-2.1560574	98.3021270
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C	2.1611983	0.1003097	99.3428700
C	2.2585160	0.6264488	98.0492702
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O	2.3915590	2.0029009	97.8823357
P	1.1117741	2.9821328	98.2019238
O	1.7538183	4.3536084	98.4641336
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C	4.9475046	0.3582681	103.7925428
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H	3.8581879	1.9353749	104.8006698
H	5.6394808	0.1878554	104.6313271
H	4.3287352	-0.7929801	100.6154537
H	5.8851873	-1.1466326	102.5123874
C	1.5149630	-3.3267894	100.8192641
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H	1.5693122	-1.3299819	101.6282998
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H	1.5151959	-5.2382190	99.7528713
H	1.9668509	-4.1908417	97.5261928
C	0.7891102	5.3897059	101.8982654
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H	-1.8264700	8.3161469	102.5517536
H	-3.9784752	8.1344891	103.7922535
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C	2.2686900	5.7071653	101.6807706
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H	3.5021347	6.8972485	100.3044392
H	2.2396075	7.8534422	101.1226818
H	1.7455885	6.7650092	99.8302643
C	3.0087958	6.0272551	102.9919630
H	2.7357726	4.8058881	101.2330697
H	4.0760083	6.2589162	102.7952536
H	2.9708849	5.1788474	103.7020703
H	2.5553254	6.9073034	103.4944272
H	1.9919182	1.6785405	90.8965150
H	6.4998133	0.3604454	94.4780993
H	-1.4340175	-1.5624451	95.0475461
C	2.9975033	1.7213582	91.3694316
H	6.2938549	2.2563920	97.0027055
H	3.6135977	3.4163957	90.1245394
H	-2.1179512	0.9160537	95.1042391
C	2.8088758	1.3323977	92.8315929
C	6.0979034	-0.0384571	95.4328780
C	3.5253629	3.1556622	91.1994931
H	4.5313858	3.2741702	91.6538240
C	3.8937031	1.2854790	93.7275429
C	-0.4172970	-1.2924673	94.6947865
H	3.4982697	-0.3244770	90.7316969
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C	3.8964814	0.7061099	90.6393376
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H	0.6776085	1.0417811	92.6392025
C	5.4458722	2.2720005	96.2873497
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C	3.7456019	0.8525889	95.0594251
C	-1.1511930	1.1214541	94.6039314
C	1.3358983	0.5364533	94.6432869
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C	4.9621382	0.8413917	95.9836449
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H	5.7986666	2.7840919	95.3670968
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H	-1.3195447	1.0315043	93.5104152
H	4.9249545	0.7078210	91.0578166
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H	-0.0740544	0.2053709	96.2134858
H	4.8952378	1.5838103	93.3768357
Zn	2.5289391	5.9980029	97.8721457
Br	4.7743018	6.3543485	97.5574962
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Br	-3.5058060	3.6712724	96.1688737
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C	-2.2563776	7.8718316	97.3685141
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C	-1.2365802	7.0539782	97.7926334
C	-1.2400220	5.7697952	98.4841075
C	-0.0062961	7.6922181	97.2836237
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C	3.2569247	4.7798561	94.3731260
C	4.4058700	5.4691674	93.9717390
C	4.3538279	6.8597844	93.7827781
H	3.1276519	8.6595324	93.8496437
H	1.0631927	7.4287174	94.5862569
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H	5.3472487	4.9231688	93.8120646
H	5.2592683	7.4027315	93.4712329
O	-0.1652491	5.2602972	95.4634229
H	-3.3296235	7.7146293	97.5388053
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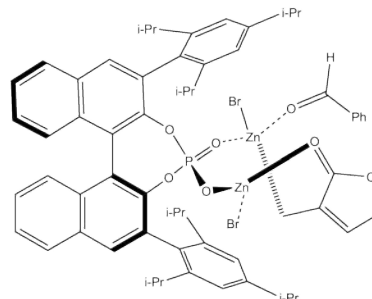
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C	2.0823325	2.5989880	102.8828807
H	1.9884651	3.1767274	103.8147549
C	1.2642550	2.9182236	101.8046422
C	2.3079699	-0.1599853	96.8656041
C	2.2414778	-1.5392093	97.0235742
H	2.3232869	-2.1833746	96.1349762
C	2.0434498	-2.1438509	98.2969710
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C	1.9716914	-1.3136242	99.4750312
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H	3.8545847	1.9270051	104.8059951
H	5.6295018	0.1738264	104.6382500
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H	1.5047318	-5.2256433	99.7445204
H	1.9550453	-4.1766914	97.5190803
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H	3.5074357	6.9117933	100.3116799
H	2.2493220	7.8653558	101.1409509
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H	2.7408047	4.8175454	101.2312168
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H	6.4968347	0.3397056	94.4678081
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H	6.3117198	2.2390903	96.9933662
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C	3.5652987	3.1543946	91.1946644
H	4.5781564	3.2442301	91.6403791
C	3.8960933	1.2894364	93.7230269
C	-0.4292728	-1.2572314	94.7124339
H	3.4341536	-0.3227746	90.7250205
C	1.5390608	1.0071448	93.3235825
C	3.8618549	0.6954518	90.6305705
H	3.9407131	0.9389224	89.5507520
H	0.6747438	1.0782609	92.6446979
C	5.4621874	2.2611939	96.2802550
H	6.9366086	-0.1088227	96.1417363
H	5.7346796	-1.0871900	95.2350403
C	3.7477046	0.8562735	95.0545050
C	-1.1520415	1.1576771	94.5987016
C	1.3339222	0.5615139	94.6444487
H	0.2747195	-1.9944936	95.1448687
H	-0.4079404	-1.3777933	93.6088468
C	4.9659329	0.8350476	95.9763314
C	2.4612686	0.4510716	95.5046779
C	-0.0738914	0.1892674	95.1088951
H	4.6640453	2.8835773	96.7300591
H	-0.8937674	2.2128391	94.8049923
H	5.8177257	2.7711860	95.3598177
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H	-1.3300046	1.0502216	93.5082569
H	4.8919533	0.6651592	91.0436266
H	4.6471664	0.3886211	96.9403937

H	-0.0785060	0.2533084	96.2169350
H	4.8996220	1.5783532	93.3700547
Zn	2.5464540	6.0042948	97.8456843
Br	4.7823773	6.3979094	97.5592858
H	-2.0654452	8.8834797	95.4489802
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H	-2.1252568	5.6043850	99.1462461
Zn	-1.4520425	4.3306877	97.0304445
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C	-1.2535271	7.0143363	97.7911790
C	-1.2397041	5.7435623	98.4995198
C	-0.0282652	7.6588477	97.2748322
O	-0.3135615	8.7498033	96.5438485
O	1.1734697	7.3613579	97.4279372
H	-1.9702958	9.9420737	96.8975118
H	-0.3175505	5.5782707	99.0844956
C	3.1714281	7.5662293	94.0453314
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C	2.0461508	5.4863444	94.6132609
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H	3.1547844	8.6584027	93.9143989
H	1.0752715	7.4361952	94.6206008
C	0.8738194	4.7388194	95.0720921
H	3.2639711	3.6793906	94.5260979
H	5.3416274	4.9036902	93.8473829
H	5.2787648	7.3887115	93.5365897
O	-0.1740024	5.2694085	95.4731856
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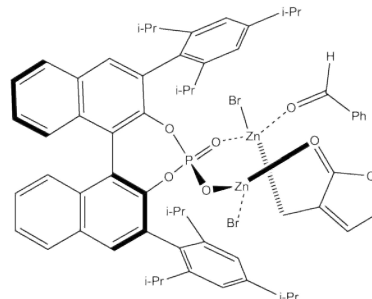


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C	0.7419965	-1.9185244	88.3694909
C	0.8438232	-3.3421757	88.3951302
C	-0.4915892	-1.2684710	88.6540992
H	-1.3755688	-1.8840510	88.8793936
C	-0.5892973	0.1151833	88.7221935
C	4.6843413	2.7481910	88.6043172
C	5.5220877	2.3721858	87.5552586
H	6.5524976	2.7599865	87.5378452
C	5.0920327	1.5249529	86.4977767
C	5.9231505	1.2527880	85.3690840
C	3.7885519	0.9162547	86.5765026
C	3.3563862	0.0938308	85.4927806
C	2.9697685	1.1689393	87.7355147
C	3.3732629	2.1712754	88.6333517
O	0.4136492	2.2670761	88.2613747
O	2.5367096	2.5305759	89.6854342
P	1.0656796	3.2266893	89.4393174
O	0.3259478	3.0308160	90.7764635

O	1.1144784	4.6325141	88.8411607	H	6.8956536	0.9047468	91.0919521
C	2.0689255	-3.9712934	88.2356292	C	5.3230099	3.1930292	91.0120646
C	3.2432082	-3.1911049	88.0632379	C	4.0830628	6.2884797	87.8860030
H	-0.0709556	-3.9309407	88.5672341	C	5.6472094	4.9710417	89.3336149
H	2.1372331	-5.0694063	88.2651898	H	7.5684677	5.9801663	87.5546223
H	4.0942005	-1.2220498	87.8865682	H	6.6346750	7.4206552	88.0689366
H	4.2217039	-3.6877856	87.9774782	C	4.9107670	1.7864111	91.4466612
C	4.1788877	-0.1344925	84.3978902	C	5.1964152	3.6609363	89.6727082
C	5.4786966	0.4379386	84.3384285	C	5.4397483	5.5679566	87.9401646
H	2.3510129	-0.3502231	85.5263277	H	2.9483834	2.4192300	92.2014697
H	3.8194504	-0.7609649	83.5671622	H	3.2580391	5.5996420	88.1507078
H	6.1249264	0.2420763	83.4691680	H	4.2018485	2.2697025	93.4749379
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C	-1.9743704	0.9156877	90.6614344	H	4.0465319	7.1281109	88.6101806
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C	-2.7908056	1.3212121	88.3664591	H	5.3849446	4.7337884	87.2134714
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C	-4.0770119	2.1833620	90.2792259	Zn	-1.5512141	3.5028421	91.1523744
H	-3.2746492	1.6872715	92.2339958	Br	-2.2600932	4.5126336	93.1365500
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H	-2.1497719	2.3842119	85.1017072	C	-0.0920505	8.6051915	83.8931252
H	-1.3804884	2.9522292	86.6259921	C	0.1245193	9.9827552	84.0728830
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H	3.8872805	6.6971490	86.8715981				
C	6.3464376	5.3335366	91.6677510				
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H	5.6783061	5.6207767	94.4141757				
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H	9.0010976	5.4587795	92.4806922				
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H	8.7302305	6.3379974	94.0243056				
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14c-mi

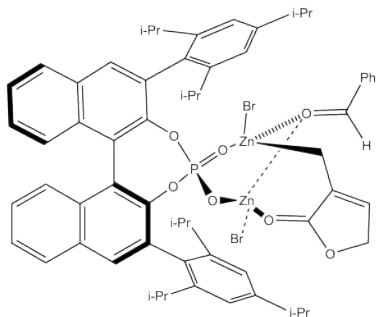


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C	3.3686341	2.1747266	88.6231662	C	8.2506934	5.6441503	93.2927269
O	0.4083696	2.2642035	88.2541998	H	8.7135275	6.3349188	94.0280725
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C	2.0761571	-3.9698281	88.2438919	C	5.3169372	3.1944988	91.0020812
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H	-4.6483142	2.4144217	88.2076579	C	0.8261251	9.5897118	86.3836104
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H	-1.3750241	2.9596017	86.6292345	C	0.1378597	9.9784007	84.0833990
C	-3.8737261	0.5279149	86.2185167	H	0.7662958	11.5488426	85.4552226
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C	-1.0783766	0.1540118	91.6460533	H	-2.2335565	6.8073424	86.1146180
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H	-0.1585877	1.8211517	92.7571395	H	-0.7857415	8.0104064	90.7385283
C	-1.7369232	-1.2044757	91.9699565	H	-1.7179941	8.6687710	88.0762550
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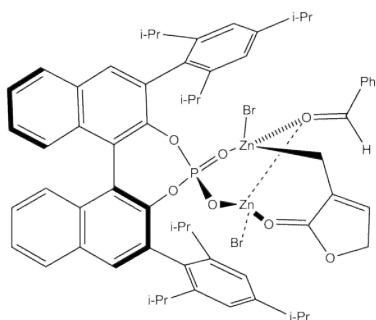
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Zn	1.8767187	5.3578025	86.5875758
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O	-0.8585183	8.7459410	88.8356229
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C	3.9186825	-1.7896877	87.8761836
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C	2.5696284	-1.6017776	88.3557694
C	1.6454683	-2.6786110	88.2012756
C	2.2063291	-0.3301509	88.9375471
C	3.1428368	0.7069282	88.8722017
O	0.6040758	1.8848975	88.1976781
O	2.8211125	1.9433441	89.4223335
P	1.7833175	2.9416155	88.6438283
O	1.2574295	3.8949445	89.7286214
O	2.3691679	3.5394332	87.3660103
C	-0.7892033	-2.6232337	92.5976222
C	0.5593727	-2.7958017	92.1874305
H	-2.5895967	-1.4412684	92.3748096
H	-1.2183519	-3.2825632	93.3673896
H	2.1584953	-2.1193616	90.9101037
H	1.1764857	-3.5793403	92.6529905
C	2.0423819	-3.8933671	87.6594702
C	3.3846252	-4.0948253	87.2426471
H	0.6009878	-2.5359546	88.5103346
H	1.3069735	-4.7046343	87.5470612
H	3.6905104	-5.0651934	86.8228191
H	5.3349163	-3.1884869	86.9922844
C	-2.1472884	3.5492786	90.2606896
C	-1.9317718	2.5370066	89.2777293
C	-2.7931466	4.7354461	89.8719592
C	-2.3848718	2.7378477	87.9464736
C	-3.0559784	3.9329120	87.6229061
C	-3.2660571	4.9512233	88.5651421
H	-2.9374499	5.5291670	90.6233189
C	-2.2071214	1.6804909	86.8582851
H	-3.4111331	4.0675617	86.5909533
C	-1.4089795	2.2121875	85.6543538
H	-1.9450198	3.0373843	85.1400710
H	-1.2484812	1.4072411	84.9078549
H	-0.4158683	2.5857868	85.9700114
C	-3.5671915	1.1013549	86.4259638
H	-1.6252098	0.8426092	87.2921713
H	-4.2114270	1.8787946	85.9643883
H	-4.1181022	0.6811442	87.2916088
H	-3.4309611	0.2923804	85.6786177
C	-4.0040388	6.2485215	88.2409205
C	-4.1500226	6.5332510	86.7415166
H	-4.5904718	7.5381958	86.5788822
H	-4.8250414	5.8004010	86.2523016
H	-3.1730976	6.4981821	86.2200455
C	-5.3819341	6.2739620	88.9331948
H	-3.3982134	7.0733902	88.6840733
H	-5.8976896	7.2418011	88.7624747
H	-5.2929785	6.1210902	90.0269659
H	-6.0292705	5.4650971	88.5347023
C	-1.7619944	3.3781775	91.7321690
C	-0.8590396	4.4989044	92.2722337
H	-0.7075069	4.3875200	93.3650536
H	-1.2730963	5.5121865	92.0952134
H	0.1448983	4.4426758	91.8109386
C	-3.0315447	3.2282355	92.5945556
H	-1.1859566	2.4369461	91.8267353
H	-2.7671439	3.0174064	93.6513649
H	-3.6773789	2.4035326	92.2300970
H	-3.6417162	4.1556525	92.5777185
H	7.4694248	5.6355637	86.1872643
H	7.7509122	2.4928525	91.1537066
H	5.7074096	0.2579178	83.8629069
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H	4.8812306	2.7584885	92.5365987

14d-ma

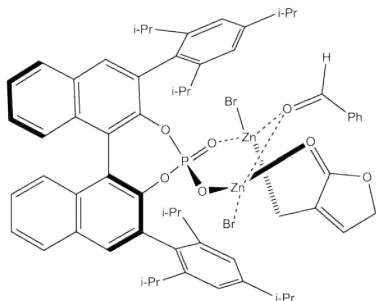


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Br	2.7162412	6.4510362	92.0989296
H	-0.4912759	10.1208094	87.2989007
Br	3.4239409	6.0949373	84.9606145
H	-0.5916133	5.3311654	85.9574212
Zn	1.8888645	5.3339107	86.5595257
C	-0.8651574	8.0840774	86.5571026
C	-1.1343458	9.2281127	87.4735308
C	-0.4514138	6.9949239	87.2782819
C	-0.0866216	5.6347265	86.8953640
C	-0.4139007	7.4560613	88.6888860
O	-0.8357896	8.7323598	88.7907257
O	-0.0767159	6.8471832	89.7152974
H	-2.1945774	9.5687249	87.4638238
H	-0.3728442	4.9220358	87.6938806
H	-1.0202402	8.1283413	85.4707000
C	3.0556469	10.0488012	85.9304318
C	2.8021676	8.9377256	86.7391756
C	3.5378236	8.7620147	87.9380345
C	4.5196647	9.7124968	88.3146794
C	4.7721377	10.8167914	87.4967391
C	4.0398672	10.9819911	86.3052513
H	2.4938652	10.1822472	84.9941223
H	2.0385607	8.1995799	86.4606375
C	3.3006964	7.6297673	88.8117899
H	5.0837756	9.5647292	89.2488904
H	5.5380184	11.5533881	87.7810578
H	4.2393164	11.8522966	85.6608276
O	2.5195598	6.6843902	88.5475560
C	0.1014333	1.0113816	89.1604538
C	0.8726972	-0.0893158	89.5573725
C	0.3430296	-0.9472907	90.5913467
C	1.1108508	-1.9798786	91.2096548
C	-1.0082655	-0.7369761	91.0519588
C	-1.5523635	-1.6074197	92.0436231
C	-1.7568270	0.3646684	90.5504658

H	6.8137398	7.7186994	87.4293572	P	1.8430588	2.8789165	88.5170418
H	3.6140838	1.7194644	83.7774281	O	1.3739886	3.9610318	89.5115933
C	6.6382488	4.2368872	87.5619067	O	2.5426150	3.2912961	87.2341182
C	7.0309557	1.6478765	91.1353145	C	-1.2567291	-2.7590094	92.1213594
C	6.3654866	6.7310828	87.6689061	C	0.1101445	-2.9665222	91.7949465
H	6.1484625	6.7123663	88.7589564	H	-2.9824587	-1.4769395	91.8581511
C	6.4552714	3.7656865	88.8739732	H	-1.7672808	-3.4450747	92.8143035
C	6.0880597	0.8585234	84.7152098	H	1.8240779	-2.2893473	90.6817596
H	9.3567655	4.8829883	87.6846664	H	0.6599702	-3.8042431	92.2505969
C	6.1326639	3.4608845	86.5084505	C	1.9263862	-3.8824580	87.3978760
C	8.6790882	5.7129863	87.9690062	C	3.3037974	-4.1495811	87.1749309
H	9.1669167	6.6688356	87.6862785	H	0.4506773	-2.4711616	88.0920803
H	6.2537442	3.8307272	85.4779240	H	1.1733189	-4.6428765	87.1403859
C	5.0147337	3.1559376	91.5095597	H	3.6149949	-5.1207346	86.7607267
H	6.9417766	1.2584375	92.1708533	H	5.3180201	-3.3586872	87.2614670
H	7.4692619	0.8495408	90.5026296	C	-2.0170909	3.5924722	90.3295419
C	5.7795565	2.5648120	89.1487981	C	-1.9051424	2.7010693	89.2217990
C	4.0243095	2.3377378	84.6028453	C	-2.6903876	4.8124966	90.1454025
C	5.4490568	2.2500558	86.7235277	C	-2.4111869	3.0812855	87.9503505
H	6.7102353	0.1964869	85.3518001	C	-3.0759919	4.3184438	87.8226294
H	6.7563601	1.6433423	84.3029061	C	-3.2454028	5.1924440	88.9122510
C	5.6585389	2.0975541	90.5980718	C	-2.2927407	2.1698535	86.7311865
C	5.2696991	1.7996736	88.0635963	H	-3.5011008	4.5878054	86.8417986
C	4.9244505	1.4818081	85.5091755	C	-1.4757318	2.8279073	85.6062808
H	4.0188361	3.4627054	91.1372343	H	-1.9741825	3.7397617	85.2143831
H	3.1805794	2.7629262	85.1779582	H	-1.3477287	2.1344988	84.7501088
H	5.6376760	4.0704850	91.5926267	H	-0.4607781	3.1085931	85.9479077
H	5.4076944	6.6483404	87.1158740	C	-3.6760131	1.7091427	86.2360403
H	4.5691467	3.1880470	84.1451643	H	-1.7423169	1.2600618	87.0460741
H	8.5865514	5.7059085	89.0751783	H	-4.2874606	2.5652534	85.8809295
H	5.0001221	1.2049308	90.6117625	H	-4.2440735	1.2024886	87.0426774
H	4.2968343	0.6480150	85.8803550	H	-3.5720479	0.9993538	85.3894984
H	6.8478838	4.3544452	89.7182977	C	-4.0605017	6.4768199	88.8119682
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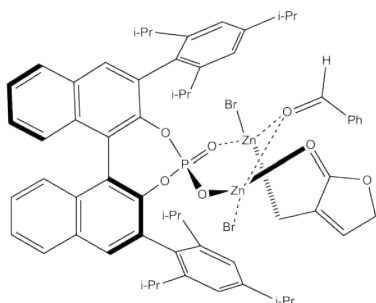


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C	0.7166305	-0.1243518	89.3583305	C	6.3822691	1.2018103	91.9716143
C	0.0865352	-1.0155645	90.3068659	C	7.1035461	6.3772161	89.2481682
C	0.7640385	-2.1178587	90.9119001	H	7.0839185	6.1951145	90.3427711
C	-1.2818219	-0.7694135	90.6937903	C	6.4472810	3.4387646	89.7517720
C	-1.9335484	-1.6739110	91.5858569	C	7.0699615	0.7605523	85.4885362
C	-1.9357818	0.4101916	90.2410296	H	9.7233730	4.1859558	88.4284554
H	-2.9636100	0.6101996	90.5800568	C	6.7185732	3.1971938	87.3752919
C	-1.2876581	1.3564403	89.4550190	C	9.2158790	4.9846100	89.0062281
C	4.4482808	0.4043180	88.5976325	H	9.8252806	5.9091380	88.9276797
C	4.8204368	-0.8722793	88.1896354	H	7.1302590	3.5682241	86.4220687
H	5.8787076	-1.0783695	87.9659470	C	4.4397425	2.8474141	91.9728687
C	3.8625777	-1.9065484	87.9850302				
C	4.2498155	-3.1757844	87.4581233				
C	2.4692150	-1.6544426	88.2653474				
C	1.5200722	-2.6669197	87.9316993				
C	2.0904217	-0.3866731	88.8442774				
C	3.0725432	0.6068232	88.9358518				
O	0.5930815	1.9076826	88.0656261				
O	2.7275397	1.8551545	89.4427874				

H	6.0410029	0.7891675	92.9438360	C	-1.9367279	0.4175056	90.2216200
H	6.8912449	0.3903205	91.4125850	H	-2.9659299	0.6208206	90.5545082
C	5.6665025	2.2722074	89.8079064	C	-1.2816872	1.3652191	89.4434812
C	5.0113758	2.1781627	85.0023550	C	4.4553704	0.3994408	88.6110740
C	5.9446433	2.0204296	87.3704111	C	4.8261523	-0.8786862	88.2073041
H	7.5680713	0.0938605	86.2224309	H	5.8854597	-1.0863715	87.9897161
H	7.7781529	1.5823649	85.2523290	C	3.8672414	-1.9106967	87.9985496
C	5.1940945	1.7716547	91.1720706	C	4.2530393	-3.1815229	87.4757322
C	5.3894298	1.5655694	88.6021294	C	2.4732126	-1.6537874	88.2697986
C	5.7361021	1.3021926	86.0358099	C	1.5232553	-2.6631359	87.9302770
H	3.5930617	3.2585455	91.3897023	C	2.0947934	-0.3853671	88.8473786
H	3.9947738	2.4332258	85.3577513	C	3.0789100	0.6054874	88.9447376
H	5.1053888	3.6884480	92.2587978	O	0.6076332	1.9176612	88.0679578
H	6.0551192	6.5123831	88.9162853	O	2.7358672	1.8532230	89.4537831
H	5.5571586	3.1208366	84.7887376	P	1.8584186	2.8831564	88.5276966
H	9.2067334	4.6741223	90.0723434	O	1.3875990	3.9636395	89.5233102
H	4.4907453	0.9317777	91.0030332	O	2.5684870	3.2995413	87.2524302
H	5.0796405	0.4293560	86.2146178	C	-1.2776668	-2.7594675	92.0947770
H	6.6512114	3.9821907	90.6874699	C	0.0903250	-2.9684391	91.7766973
Zn	1.1887522	5.8436400	89.1286682	H	-2.9981501	-1.4725092	91.8253340
Br	-0.2489398	7.5214138	89.8302592	H	-1.7943920	-3.4468033	92.7817732
C	0.7765181	7.8902652	83.2090518	H	1.8128767	-2.2902328	90.6774234
C	0.9235793	7.2933120	84.4620199	H	0.6355610	-3.8088944	92.2326832
C	-0.2152686	6.7814538	85.1356423	C	1.9289166	-3.8802488	87.4007710
C	-1.4938971	6.8689275	84.5321284	C	3.3062638	-4.1522928	87.1874566
C	-1.6306552	7.4479890	83.2671664	H	0.4538949	-2.4626677	88.0839950
C	-0.4964111	7.9606566	82.6101064	H	1.1748664	-4.6381254	87.1389849
H	1.6555770	8.2927034	82.6843985	H	3.6171438	-5.1247789	86.7762960
C	-0.0949725	6.1671379	86.4405309	H	5.3218837	-3.3678046	87.2858903
H	-2.3711143	6.4698023	85.0626728	C	-2.0169668	3.5951529	90.3266843
H	-2.6198489	7.5063254	82.7898793	C	-1.8969057	2.7112995	89.2138178
H	-0.6055894	8.4231074	81.6169276	C	-2.6935466	4.8134356	90.1470689
O	1.0066701	5.8945009	86.9805003	C	-2.3968132	3.0981861	87.9422678
C	4.1249526	8.4387668	86.1807937	C	-3.0666744	4.3331394	87.8202297
C	4.0969548	7.1773723	86.7151313	C	-3.2454534	5.1986511	88.9145041
C	3.4072801	7.3231602	88.0152537	C	-2.2663635	2.1966566	86.7169533
O	3.0694459	8.6000822	88.2518598	H	-3.4880952	4.6064058	86.8388979
C	3.4794186	9.3996004	87.1227148	C	-1.4415226	2.8645326	85.6037557
O	3.1218312	6.4163563	88.8191959	H	-1.9366659	3.7797435	85.2153047
C	4.4825251	5.8567728	86.2227529	H	-1.3051085	2.1799120	84.7421911
H	4.1560564	10.1998705	87.4960035	H	-0.4284712	3.1408442	85.9538375
H	2.5685730	9.8933041	86.7159351	C	-3.6443040	1.7356615	86.2078838
Zn	2.8746548	4.6970673	85.8265206	H	-1.7159660	1.2860898	87.0294098
Br	1.7652505	4.0321770	83.8503958	H	-4.2562080	2.5918629	85.8538004
H	4.9729976	5.2555656	87.0157067	H	-4.2177722	1.2223398	87.0062170
H	5.1310037	5.9081251	85.3275458	H	-3.5322939	1.0324672	85.3569894
H	1.9099814	7.2287383	84.9444270	C	-4.0687301	6.4784787	88.8239460
H	4.5420940	8.7361190	85.2090585	C	-3.7358036	7.3495247	87.6052466
H	-1.0363315	5.9329958	86.9936406	H	-4.3233227	8.2902226	87.6252415
H	-2.7855334	5.5046157	90.9964509	H	-3.9885128	6.8349468	86.6537166
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				C	-5.5726450	6.1456282	88.8764212
				H	-3.8202089	7.0751311	89.7284421
				H	-6.1874242	7.0699296	88.8812824
				H	-5.8227863	5.5591683	89.7830971
				H	-5.8736720	5.5405123	87.9951755
				C	-1.4519661	3.2656227	91.7104706
				C	-0.5533483	4.3829900	92.2684583
				H	-0.1199969	4.0730454	93.2416464
				H	-1.1076505	5.3289221	92.4345468
				H	0.2819717	4.5982133	91.5770064
				C	-2.5812629	2.9292251	92.7030334
				H	-0.8148995	2.3642834	91.6082964
				H	-2.1647845	2.6493737	93.6927749
				H	-3.2068288	2.0868037	92.3462783
				H	-3.2514860	3.8014647	92.8527009
				H	7.8262382	5.5218832	87.4237897
				H	7.1489775	1.9837811	92.1874199
				H	6.9212296	0.2162334	84.5399533
				C	7.7772251	5.2222742	88.4943785
				H	4.0454272	2.4137977	92.9239037

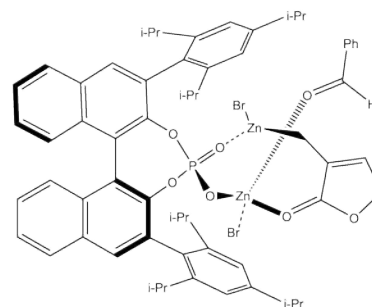
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C	0.0808692	-1.0124984	90.2958856
C	0.7518226	-2.1180592	90.9017307
C	-1.2892229	-0.7650047	90.6747543
C	-1.9480474	-1.6712344	91.5590309

H	7.6490949	7.3272502	89.0940680
H	4.8554565	1.6129500	84.0667339
C	6.9636746	3.9351935	88.5480389
C	6.3921308	1.1988949	91.9777870
C	7.1102305	6.3730811	89.2667886
H	7.1142272	6.1875765	90.3608918
C	6.4482886	3.4391729	89.7577126
C	7.0866743	0.8012038	85.4681760
H	9.7175895	4.1902649	88.3877708
C	6.7218358	3.1907687	87.3829240
C	9.2197359	4.9846818	88.9792106
H	9.8274292	5.9100510	88.8974434
H	7.1318394	3.5607555	86.4285008
C	4.4501260	2.8455009	91.9854388
H	6.0543112	0.7867316	92.9513440
H	6.8986915	0.3873909	91.4169858
C	5.6722150	2.2699855	89.8171173
C	4.9644865	2.1423198	85.0351416
C	5.9537605	2.0105769	87.3809326
H	7.6287121	0.1562296	86.1901037
H	7.7577078	1.6479258	85.2129363
C	5.2021219	1.7701837	91.1822389
C	5.3978569	1.5592610	88.6135353
C	5.7462092	1.2901921	86.0470561
H	3.6032004	3.2592858	91.4047946
H	3.9414980	2.3424020	85.4069795
H	5.1163258	3.6855130	92.2729511
H	6.0542778	6.5061615	88.9588616
H	5.4620750	3.1126385	84.8265736
H	9.2293768	4.6654665	90.0425711
H	4.4978111	0.9309006	91.0142334
H	5.1279386	0.3918281	86.2345486
H	6.6492173	3.9859861	90.6919312
Zn	1.1816110	5.8440276	89.1404420
Br	-0.2693623	7.5182987	89.8053956
C	0.7713162	7.8390209	83.1800700
C	0.9253931	7.2541583	84.4386402
C	-0.2141520	6.7874321	85.1413403
C	-1.5001518	6.9051102	84.5608217
C	-1.6448018	7.4726848	83.2917477
C	-0.5092066	7.9414670	82.6054357
H	1.6530163	8.2020446	82.6316990
C	-0.0869795	6.1836413	86.4530795
H	-2.3766591	6.5401276	85.1161856
H	-2.6411358	7.5552943	82.8330479
H	-0.6239835	8.3927935	81.6076833
O	1.0150218	5.8979482	86.9805907
C	4.1092893	8.4151000	86.1579272
C	4.1003233	7.1605353	86.7093933
C	3.3981053	7.3123488	88.0048915
O	3.0360618	8.5879964	88.2194704
C	3.4353131	9.3759763	87.0819848
O	3.1225727	6.4136272	88.8173345
C	4.5077093	5.8407749	86.2408681
H	4.0898422	10.1988626	87.4473140
H	2.5151195	9.8416919	86.6616791
Zn	2.9099531	4.6685652	85.8145671
Br	1.7983158	4.0525546	83.8389133
H	4.9779524	5.2473818	87.0511129
H	5.1741576	5.8845402	85.3586733
H	1.9178983	7.1649696	84.9032435
H	4.5290130	8.7049109	85.1851368
H	-1.0258539	5.9724175	87.0196991
H	-2.7927093	5.5009310	91.0013739



Energy (Hartree) = -11970.05099434

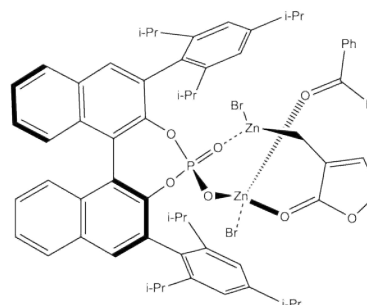
Zn	0.2397668	5.8683202	88.9829512
Br	-0.5245686	7.7397933	90.1389522
H	2.3424574	7.8011837	84.9115250
Br	1.3109886	0.4055935	85.0028242
H	-1.1937631	3.9514411	84.8235547
Zn	0.8981798	2.6822836	85.3458068
C	0.9779658	6.3807809	83.9418749
C	1.2588936	7.5899458	84.7671234
C	0.3041436	5.4517357	84.6874999
C	-0.1786027	4.0989680	84.3996127
C	0.1686896	6.0539126	86.0311799
O	0.6959778	7.2932854	86.0626838
O	-0.3435477	5.5438343	87.0411061
H	0.7798180	8.5197813	84.3888710
H	-0.1986020	3.8835461	83.3143386
H	1.2785684	6.2866159	82.8896888
C	5.4027729	7.3106974	85.7662380
C	4.3675693	6.9270967	86.6224230
C	3.8426657	7.8635558	87.5467745
C	4.3784700	9.1695378	87.6212759
C	5.4307246	9.5397322	86.7739141
C	5.9356750	8.6131845	85.8438035
H	5.8071988	6.5935947	85.0364821
H	3.9457866	5.9110619	86.5991479
C	2.7051559	7.4973104	88.3884190
H	3.9609698	9.8881308	88.3444020
H	5.8561050	10.5527472	86.8304023
H	6.7564031	8.9072147	85.1715060
O	2.2010776	6.3652794	88.3672369
C	-0.2073160	0.9465509	89.2849824
C	0.6849476	-0.0932719	89.5597303
C	0.3476336	-1.0049656	90.6276388
C	1.2429471	-2.0128915	91.0980299
C	-0.9366905	-0.8781176	91.2771261
C	-1.2915800	-1.8007036	92.3071231
C	-1.8055776	0.1951017	90.9231243
H	-2.7665475	0.2960174	91.4500934
C	-1.4431916	1.1440002	89.9763351
C	4.0997251	0.8922996	88.1080360
C	4.5156369	-0.3125011	87.5525861
H	5.5182499	-0.3785873	87.1035148
C	3.6678773	-1.4546720	87.5071078
C	4.0746430	-2.6484301	86.8392313
C	2.3606465	-1.3965891	88.1136189
C	1.4956452	-2.5213347	87.9651106
C	1.9625769	-0.1930879	88.7994483
C	2.8100799	0.9179219	88.7197307
O	0.0910075	1.8399888	88.2626412
O	2.4068397	2.1230159	89.2988940
P	1.2649252	2.9764406	88.4835747
O	0.8234263	4.0677837	89.4695968
O	1.7022531	3.3738887	87.0721311
C	-0.4098486	-2.7903121	92.7157208
C	0.8739994	-2.8832707	92.1149612
H	-2.2789808	-1.6988775	92.7844971

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H	-0.6949397	-3.4913252	93.5150208
H	2.2422968	-2.0924773	90.6488193
H	1.5857065	-3.6484513	92.4609862
C	1.9129532	-3.6605634	87.2911061
C	3.2183163	-3.7340856	86.7350660
H	0.4781526	-2.4716718	88.3770902
H	1.2227777	-4.5108337	87.1793446
H	3.5399349	-4.6452506	86.2077976
H	5.0791956	-2.6819797	86.3886745
C	-2.1397396	3.4809515	90.6149508
C	-2.2123180	2.3966255	89.6959671
C	-2.7360211	4.7055866	90.2537195
C	-2.9030524	2.5457715	88.4634506
C	-3.4792928	3.7892805	88.1512077
C	-3.3986285	4.8882300	89.0261582
H	-2.6822773	5.5560435	90.9502818
C	-3.0810181	1.3647061	87.5114238
H	-4.0134499	3.9019604	87.1938943
C	-2.5921530	1.6591562	86.0868080
H	-3.1688247	2.4779427	85.6080407
H	-2.6844218	0.7606681	85.4434303
H	-1.5240912	1.9478288	86.0950629
C	-4.5458730	0.8868739	87.5190764
H	-2.4649237	0.5271281	87.8988411
H	-5.2273611	1.6771545	87.1396653
H	-4.8762802	0.6235169	88.5444454
H	-4.6724336	-0.0078962	86.8748157
C	-4.0465861	6.2251092	88.6844248
C	-3.4579477	6.8526385	87.4091149
H	-3.9552651	7.8191561	87.1846168
H	-3.5941213	6.1901680	86.5285216
H	-2.3739282	7.0431718	87.5277000
C	-5.5777786	6.0909855	88.5904175
H	-3.8161332	6.9150566	89.5250135
H	-6.0507968	7.0793788	88.4136615
H	-6.0035776	5.6667415	89.5222710
H	-5.8725726	5.4240013	87.7529430
C	-1.4929172	3.3305143	91.9923941
C	-0.6200726	4.5209097	92.4185495
H	-0.1561134	4.3137518	93.4048422
H	-1.2005418	5.4605744	92.5187545
H	0.1929074	4.6974461	91.6896483
C	-2.5806689	3.0516786	93.0500504
H	-0.8289783	2.4429364	91.9521860
H	-2.1260792	2.8726523	94.0467108
H	-3.1935565	2.1661055	92.7878850
H	-3.2699455	3.9175927	93.1399971
H	7.7019620	5.9000530	86.9089944
H	7.2979870	2.1698264	91.4580166
H	5.1003592	1.1761984	83.7095171
C	7.7403203	5.4900990	87.9423482
H	4.3219600	2.4881250	92.5588069
H	8.0823159	7.4860438	88.7798763
H	3.3718401	3.0713877	83.9002808
C	6.7418321	4.3400921	87.9970942
C	6.5373207	1.3869730	91.2547314
C	7.3830577	6.6338628	88.9062364
H	7.4467113	6.3085479	89.9654314
C	6.4061647	3.7202900	89.2129990
C	5.6091885	1.5481737	84.6228680
H	9.4494307	4.1892182	87.4621189
C	6.1504558	3.8376838	86.8258723
C	9.1742465	4.9822435	88.1864404
H	9.9109356	5.8074105	88.0932442
H	6.3977564	4.3158184	85.8638775
C	4.5796872	2.9836299	91.5997634
H	6.3116702	0.8822067	92.2169624
H	6.9964804	0.6407158	90.5747547
C	5.5364595	2.6170202	89.2791763
C	3.9646204	3.4653469	84.7539850
C	5.2556574	2.7502920	86.8357371

H	6.0515185	0.6751413	85.1422963
H	6.4450517	2.2079877	84.3065151
C	5.2577889	1.9864754	90.6424836
C	4.9684348	2.1120583	88.0757978
C	4.6147410	2.3008546	85.5241678
H	3.6464420	3.3821186	91.1562256
H	3.2893266	4.0487479	85.4110743
H	5.2470863	3.8390390	91.8357041
H	6.3543598	7.0051376	88.7281962
H	4.7143430	4.1653425	84.3276105
H	9.2733211	4.5537622	89.2059306
H	4.5520098	1.1454554	90.4912013
H	3.7962975	1.5969855	85.7761787
H	6.8489801	4.0984490	90.1482748
H	2.2638465	8.2929605	89.0435033

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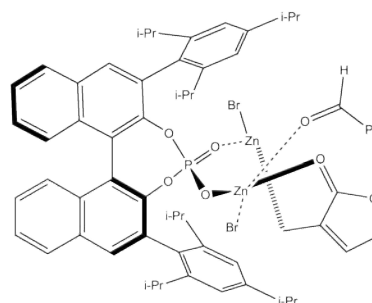


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Zn	0.1878177	5.8463869	89.0341560
Br	-0.5339325	7.7498830	90.1505391
H	2.3504679	7.7761043	84.9404869
Br	1.3494363	0.4134026	84.9750660
H	-1.2004883	3.9426422	84.8792557
Zn	0.8989795	2.6653016	85.3458523
C	0.9721219	6.3671831	83.9690627
C	1.2648433	7.5722316	84.7980731
C	0.2943918	5.4401213	84.7141756
C	-0.1974041	4.0931673	84.4295251
C	0.1652765	6.0408070	86.0611117
O	0.7048867	7.2774469	86.0931760
O	-0.3517175	5.5353482	87.0677249
H	0.7903005	8.5073956	84.4251627
H	-0.2418205	3.8792008	83.3449075
H	1.2664900	6.2724731	82.9153096
C	5.3636796	7.2722441	85.8017958
C	4.3371624	6.8935497	86.6711622
C	3.7932931	7.8474228	87.5651852
C	4.3025108	9.1648171	87.5980164
C	5.3467302	9.5305586	86.7389652
C	5.8698122	8.5864350	85.8374360
H	5.7811611	6.5387006	85.0964721
H	3.9361365	5.8685744	86.6796264
C	2.6568229	7.4828550	88.4143793
H	3.8697892	9.8968024	88.2986563
H	5.7516467	10.5532292	86.7640598
H	6.6842790	8.8762790	85.1556868
O	2.1789419	6.3423992	88.4248224
C	-0.2029191	0.9437329	89.2683680
C	0.6877368	-0.0971265	89.5435039
C	0.3501341	-1.0068806	90.6128459
C	1.2422004	-2.0186135	91.0802912
C	-0.9309270	-0.8736091	91.2671192
C	-1.2854289	-1.7936043	92.2988333
C	-1.7955121	0.2036176	90.9160532
H	-2.7525528	0.3122129	91.4486457

C	-1.4343614	1.1488769	89.9653885	H	3.4012597	3.0483637	83.8864522
C	4.1054194	0.8914282	88.1021920	C	6.7451074	4.3411459	87.9973227
C	4.5239600	-0.3129497	87.5481905	C	6.5191046	1.3979622	91.2595040
H	5.5282079	-0.3768085	87.1025929	C	7.3898531	6.6359865	88.9051055
C	3.6776140	-1.4555581	87.4986447	H	7.4480901	6.3127868	89.9650878
C	4.0867350	-2.6485079	86.8318670	C	6.3975978	3.7286293	89.2131838
C	2.3680879	-1.3984117	88.0999817	C	5.6420845	1.5405722	84.6213616
C	1.5043448	-2.5233183	87.9481366	H	9.4522132	4.1813606	87.4733875
C	1.9666911	-0.1958381	88.7850579	C	6.1657353	3.8306874	86.8239423
C	2.8135797	0.9160008	88.7088942	C	9.1779748	4.9771736	88.1945898
O	0.0972439	1.8343075	88.2433964	H	9.9186451	5.7989625	88.1032345
O	2.4090045	2.1205067	89.2875939	H	6.4251074	4.2997338	85.8604276
P	1.2652089	2.9747546	88.4761180	C	4.5629587	2.9992727	91.5937648
O	0.8148872	4.0511455	89.4741746	H	6.2895306	0.8959707	92.2221550
O	1.7027600	3.3865799	87.0684671	H	6.9792491	0.6496022	90.5828603
C	-0.4075129	-2.7870857	92.7042273	C	5.5295063	2.6242361	89.2776337
C	0.8727496	-2.8866501	92.0983971	C	3.9869243	3.4487661	84.7417139
H	-2.2702271	-1.6862682	92.7802878	C	5.2704515	2.7439551	86.8313573
H	-0.6929951	-3.4861561	93.5050127	H	6.0882411	0.6723648	85.1452076
H	2.2388462	-2.1029329	90.6263161	H	6.4757825	2.2034668	84.3056030
H	1.5819299	-3.6554501	92.4413686	C	5.2430242	1.9988271	90.6416197
C	1.9250579	-3.6616779	87.2758102	C	4.9727517	2.1120731	88.0721040
C	3.2317779	-3.7341462	86.7244205	C	4.6398153	2.2892303	85.5167933
H	0.4854504	-2.4729878	88.3562145	H	3.6327368	3.3999634	91.1463083
H	1.2354801	-4.5118249	87.1605981	H	3.3034182	4.0282390	85.3940064
H	3.5554596	-4.6443344	86.1969390	H	5.2307163	3.8534992	91.8328502
H	5.0922300	-2.6805888	86.3835325	H	6.3629718	7.0109277	88.7242466
C	-2.1181987	3.4895946	90.6062593	H	4.7348338	4.1532076	84.3186415
C	-2.1973836	2.4057072	89.6874977	H	9.2715758	4.5491221	89.2145464
C	-2.7049158	4.7186285	90.2434717	H	4.5364119	1.1588329	90.4895064
C	-2.8888715	2.5583583	88.4559249	H	3.8225725	1.5819889	85.7631836
C	-3.4538506	3.8063158	88.1415840	H	6.8310674	4.1119520	90.1506684
C	-3.3653289	4.9056019	89.0150723	H	2.1898945	8.2883701	89.0409867
H	-2.6505269	5.5676106	90.9417376				
C	-3.0861773	1.3734081	87.5123297				
H	-3.9895850	3.9211833	87.1853712				
C	-2.5966380	1.6459006	86.0838863				
H	-3.1558934	2.4745801	85.6013042				
H	-2.7129840	0.7458051	85.4470007				
H	-1.5215886	1.9068724	86.0841221				
C	-4.5584771	0.9193160	87.5288669				
H	-2.4826569	0.5294563	87.9055790				
H	-5.2290326	1.7160314	87.1437594				
H	-4.8902772	0.6726968	88.5577099				
H	-4.7017668	0.0201495	86.8944507				
C	-4.0124152	6.2442284	88.6780757				
C	-3.4349265	6.8733748	87.3987898				
H	-3.9422333	7.8344418	87.1738707				
H	-3.5678265	6.2081037	86.5197527				
H	-2.3532093	7.0772551	87.5145661				
C	-5.5444686	6.1108545	88.5986612				
H	-3.7729951	6.9337940	89.5163309				
H	-6.0192730	7.0996031	88.4292522				
H	-5.9611037	5.6836796	89.5330535				
H	-5.8485057	5.4459970	87.7629066				
C	-1.4822549	3.3344468	91.9882450				
C	-0.5928087	4.5113642	92.4177320				
H	-0.1545748	4.3076363	93.4163095				
H	-1.1515555	5.4662204	92.4927838				
H	0.2415055	4.6585052	91.7066019				
C	-2.5840478	3.0780007	93.0370620				
H	-0.8335260	2.4354582	91.9571612				
H	-2.1418559	2.8917890	94.0378647				
H	-3.2117680	2.2042504	92.7704434				
H	-3.2582164	3.9561758	93.1201697				
H	7.7135456	5.8973560	86.9104784				
H	7.2812634	2.1790538	91.4637096				
H	5.1380503	1.1613537	83.7086422				
C	7.7464764	5.4888939	87.9450045				
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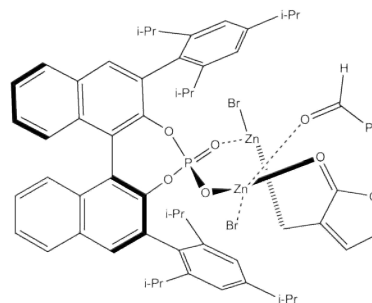


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Br	3.3419816	6.2323828	91.9648647
C	-0.0169652	5.9454900	85.9045792
C	0.0356956	6.2247945	87.2722085
C	-0.0881784	7.5615683	87.7177193
C	-0.3111030	8.6041060	86.7853104
C	-0.3252869	8.3205308	85.4138776
C	-0.1651125	6.9925171	84.9748150
H	0.0521973	4.9086532	85.5462143
H	0.1443742	5.4175237	88.0094196
C	0.0483208	7.8893585	89.1329575
H	-0.4440963	9.6368312	87.1457229
H	-0.4683927	9.1306424	84.6832729
H	-0.1672812	6.7559370	83.8997282
O	0.5677837	7.1632836	89.9973392
C	3.8377083	8.4136597	85.7341759
C	3.9057457	7.1321332	86.2077236
C	3.3038918	7.1851220	87.5538016
O	2.9326215	8.4346295	87.8837185
C	3.2208030	9.3014220	86.7630928
O	3.1248530	6.2217991	88.3114131

C	4.3735833	5.8584926	85.6543047	C	-1.4392241	3.5604120	91.6714451
H	3.8887206	10.1150999	87.1214769	C	-0.4495923	4.6153651	92.1893354
H	2.2594239	9.7624349	86.4436512	H	-0.1759855	4.4071829	93.2436407
Zn	2.9011807	4.5103471	85.3773833	H	-0.8579736	5.6457025	92.1489672
Br	1.6611267	3.7814849	83.5051729	H	0.4870758	4.5932389	91.6028716
H	5.0057200	5.3222419	86.3944303	C	-2.6584702	3.4409261	92.6076451
H	4.9331095	5.9939739	84.7092420	H	-0.9067617	2.5890825	91.6953649
H	4.1791920	8.7758687	84.7552671	H	-2.3387626	3.1916326	93.6406535
C	0.0726050	1.1627079	88.9705101	H	-3.3607580	2.6537588	92.2654827
C	0.8058887	0.0174684	89.3002934	H	-3.2251850	4.3949749	92.6492789
C	0.2703017	-0.8530395	90.3239926	H	8.0135224	5.6080139	87.4901361
C	1.0040106	-1.9440848	90.8812782	H	7.2088983	1.8022682	91.9126416
C	-1.0519969	-0.5922750	90.8424778	H	7.0463809	0.8662538	84.0620140
C	-1.6069721	-1.4706215	91.8215784	C	7.6771273	5.3803257	88.5259857
C	-1.7602857	0.5671801	90.4160597	H	4.1251410	2.0700083	92.7495592
H	-2.7570038	0.7658329	90.8391745	H	7.2669669	7.4894810	88.9847698
C	-1.2014976	1.4836269	89.5339575	H	4.5620242	1.5392029	84.0383160
C	4.4839301	0.4911128	88.2836782	C	6.9416011	4.0473813	88.4703249
C	4.8113688	-0.7958391	87.8722048	C	6.4704195	1.0185493	91.6419340
H	5.8589103	-1.0396243	87.6372556	C	6.7356119	6.5153262	88.9707426
C	3.8211700	-1.8088736	87.7149475	H	6.3246237	6.3342585	89.9857676
C	4.1544956	-3.0904406	87.1816826	C	6.4196323	3.4620032	89.6370596
C	2.4521435	-1.5324559	88.0797204	C	7.1743179	1.4843576	84.9740279
C	1.4695730	-2.5365008	87.8290403	H	9.6169636	4.5055006	89.0848036
C	2.1270679	-0.2525158	88.6640948	C	6.7659722	3.3608303	87.2569622
C	3.1222529	0.7320455	88.6625732	C	8.9297733	5.3096189	89.4173877
O	0.5647527	2.0288078	88.0015143	H	9.4849698	6.2702544	89.3942257
O	2.8298587	1.9956228	89.1583474	H	7.2075447	3.7909458	86.3438254
P	1.8323113	3.0162256	88.3456699	C	4.4899320	2.6009988	91.8462014
O	1.4305807	4.0691917	89.3917769	H	6.1620407	0.5060817	92.5769700
O	2.3696422	3.4571121	86.9958275	H	6.9867592	0.2785510	90.9968182
C	-0.8795273	-2.5443405	92.3120830	C	5.6898884	2.2633903	89.6073012
C	0.4445416	-2.7672605	91.8493574	C	4.7084614	2.0704815	85.0005669
H	-2.6224156	-1.2643944	92.1951515	C	6.0392647	2.1559571	87.1666867
H	-1.3162230	-3.2098814	93.0722483	H	8.0287908	1.0760630	85.5509639
H	2.0337920	-2.1264915	90.5459982	H	7.4512314	2.5049056	84.6367036
H	1.0371217	-3.5962561	92.2656542	C	5.2490326	1.6320274	90.9277187
C	1.8224645	-3.7646098	87.2858546	C	5.4499476	1.6303227	88.3525588
C	3.1779166	-4.0533723	86.9738066	C	5.8792414	1.4793854	85.8020998
H	0.4166714	-2.3230977	88.0614539	H	3.6165361	3.0437232	91.3321259
H	1.0440734	-4.5182616	87.0915839	H	3.7591205	2.0004916	85.5670591
H	3.4476796	-5.0340510	86.5530682	H	5.1284820	3.4388296	92.1930307
H	5.2051413	-3.2932930	86.9205573	H	5.8716355	6.6016344	88.2843464
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C	-2.4579832	5.0527913	89.9037766	H	4.5638922	0.7922030	90.6939440
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C	-2.9037444	4.3323492	87.6516983	H	6.5804172	3.9583209	90.6068056
C	-2.9700733	5.3423334	88.6253268	H	-0.3414664	8.8892891	89.4547487
H	-2.4974039	5.8365792	90.6783593				
C	-2.3576411	2.0039505	86.8249068				
H	-3.2948615	4.5267295	86.6422303				
C	-1.5885703	2.4395736	85.5662087				
H	-2.0355100	3.3427296	85.1005413				
H	-1.6043414	1.6357517	84.8018824				
H	-0.5278145	2.6560469	85.7955455				
C	-3.8026929	1.5873465	86.4890879				
H	-1.8491510	1.1029143	87.2244084				
H	-4.3797314	2.4348579	86.0630105				
H	-4.3408328	1.2349786	87.3926404				
H	-3.8102898	0.7673103	85.7414783				
C	-3.6102643	6.7038338	88.3689313				
C	-3.7425429	7.0709111	86.8866017				
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H	-4.4759038	6.4171451	86.3699051				
H	-2.7764203	6.9847573	86.3519862				
C	-4.9765385	6.7966365	89.0786241				
H	-2.9408141	7.4588255	88.8436309				
H	-5.4198059	7.8070626	88.9587440				
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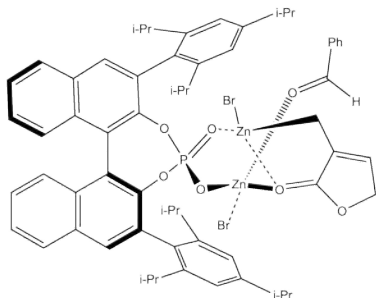


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C	0.0335063	6.2076671	87.2854739
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C	-0.3052495	8.5826402	86.7779256
C	-0.3308921	8.2859388	85.4095887

C	-0.1766212	6.9531725	84.9821171	H	-1.8672244	1.1073363	87.2361702
H	0.0420466	4.8759163	85.5698976	H	-4.3947528	2.4480619	86.0778074
H	0.1476329	5.4086122	88.0307986	H	-4.3579477	1.2551565	87.4124996
C	0.0756923	7.8860242	89.1311718	H	-3.8356060	0.7767824	85.7618047
H	-0.4305585	9.6196531	87.1297470	C	-3.6120296	6.7121864	88.3813089
H	-0.4774023	9.0893698	84.6720071	C	-3.7506934	7.0803671	86.8998203
H	-0.1792828	6.7024386	83.9102136	H	-4.1122169	8.1229748	86.7914415
O	0.5939488	7.1636312	89.9952058	H	-4.4862210	6.4267338	86.3862586
C	3.8584162	8.3547102	85.6757974	H	-2.7874320	6.9946287	86.3601818
C	3.9262530	7.0843788	86.1795721	C	-4.9754889	6.8020926	89.0963223
C	3.3134259	7.1673363	87.5220544	H	-2.9413565	7.4683024	88.8532270
O	2.9358658	8.4266971	87.8171805	H	-5.4225914	7.8112271	88.9796767
C	3.2295726	9.2644737	86.6794013	H	-4.8834522	6.5888974	90.1798853
O	3.1301693	6.2259917	88.3010570	H	-5.6840220	6.0616888	88.6700311
C	4.3966206	5.8006322	85.6609944	C	-1.4168176	3.5703845	91.6708455
H	3.8912719	10.0900076	87.0241247	C	-0.4392409	4.6337471	92.1937782
H	2.2677242	9.7128948	86.3415425	H	-0.1547330	4.4183588	93.2435096
Zn	2.9042633	4.4737855	85.3509447	H	-0.8616025	5.6588748	92.1692890
Br	1.6315953	3.7966786	83.5013067	H	0.4941171	4.6331144	91.6022191
H	4.9905356	5.2613770	86.4291555	C	-2.6316724	3.4310319	92.6100497
H	4.9866005	5.9133825	84.7317459	H	-0.8726277	2.6052386	91.6864077
H	4.2075736	8.6927149	84.6911324	H	-2.3065566	3.1797516	93.6407912
C	0.0757038	1.1747069	88.9669460	H	-3.3268669	2.6387898	92.2657610
C	0.8063660	0.0253051	89.2887060	H	-3.2094143	4.3780221	92.6585898
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C	1.0003261	-1.9476640	90.8554808	H	7.1958961	1.7954511	91.9208361
C	-1.0519704	-0.5910865	90.8280412	H	7.0473064	0.9529595	84.0390802
C	-1.6076251	-1.4751075	91.8008696	C	7.6866622	5.3845947	88.5640345
C	-1.7575340	0.5725216	90.4096727	H	4.1106308	2.0534132	92.7565760
H	-2.7536955	0.7714198	90.8338712	H	7.2719917	7.4996959	88.9914832
C	-1.1976710	1.4932873	89.5333413	H	4.5163500	1.4621914	84.0945210
C	4.4856038	5.028424	88.2804646	C	6.9468334	4.0543398	88.4977574
C	4.8127321	-0.7826995	87.8650094	C	6.4583829	1.0132235	91.6439410
H	5.8615417	-1.0260677	87.6351906	C	6.7325899	6.5306087	88.9507312
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C	4.1564230	-3.0738990	87.1622706	C	6.4096143	3.4692545	89.6568993
C	2.4532687	-1.5190744	88.0612226	C	7.1610947	1.5824847	84.9449778
C	1.4711143	-2.5211700	87.8032193	H	9.5932837	4.5062803	89.2222359
C	2.1277126	-0.2426224	88.6522665	C	6.7822904	3.3708068	87.2808829
C	3.1231852	0.7412812	88.6589031	C	8.9009646	5.3239005	89.5072835
O	0.5672829	2.0475820	88.0045372	H	9.4657056	6.2788801	89.4853546
O	2.8301386	2.0003340	89.1640535	H	7.2380367	3.8007937	86.3751391
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O	1.4400106	4.0809658	89.4003893	H	6.1499397	0.4940360	92.5751485
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C	-0.8830143	-2.5539201	92.2827074	C	5.6815897	2.2698770	89.6175177
C	0.4394915	-2.7764722	91.8172803	C	4.6687987	2.0128263	85.0447016
H	-2.6220721	-1.2686250	92.1769485	C	6.0508556	2.1703094	87.1791271
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H	1.0304950	-3.6099162	92.2267145	C	5.2370241	1.6305309	90.9329025
C	1.8248278	-3.7469453	87.2564674	C	5.4513217	1.6416720	88.3589553
C	3.1804578	-4.0351611	86.9474591	C	5.8958199	1.4947310	85.8125236
H	0.4182151	-2.3070373	88.0344692	H	3.6010652	3.0358963	91.3472180
H	1.0465580	-4.4992473	87.0569526	H	3.7414784	1.9125561	85.6415992
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C	-1.8897858	3.8158008	90.2364512	H	4.8133812	3.0817758	84.7688615
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C	-2.4467440	5.0639069	89.9088528	H	4.5537000	0.7911604	90.6922178
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C	-2.9685832	5.3515051	88.6341756	H	-0.3004877	8.8956843	89.4459309
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C	-2.3719476	2.0096959	86.8348155				
H	-3.3091116	4.5333399	86.6547145				
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H	-1.6315440	1.6324910	84.8082334				
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14l-ma; COSMO



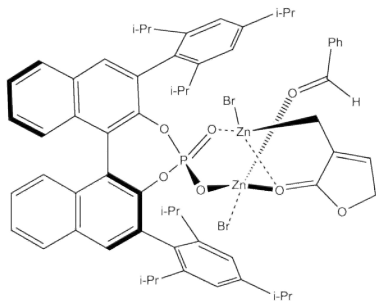
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C	-1.7754653	0.5311092	90.8608969
H	-2.7966460	0.6849209	91.2414014
C	-1.3250304	1.2831554	89.7830463
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C	4.7086255	-0.7615381	88.0540983
H	5.7110152	-0.9593595	87.6446677
C	3.8548794	-1.8633883	88.3389425
C	4.2642017	-3.2031254	88.0631616
C	2.5342948	-1.6189175	88.8664257
C	1.6554337	-2.7350682	89.0150311
C	2.1443825	-0.2643727	89.1853678
C	3.0104549	0.7754954	88.8141253
O	0.3727280	1.6108382	88.1042361
O	2.6602157	2.0945467	89.0757765
P	1.4750681	2.8233412	88.1825833
O	0.9703269	3.9590225	89.0817816
O	1.9110603	3.1035131	86.7526317
C	-0.5136375	-1.8948469	93.4303623
C	0.8297852	-2.0615432	93.0004842
H	-2.4049233	-0.9092233	93.0541418
H	-0.8668481	-2.4039751	94.3401459
H	2.3272688	-1.5696248	91.5281231
H	1.5184520	-2.6883532	93.5875207
C	2.0748910	-4.0243192	88.7165028
C	3.3963310	-4.2673583	88.2547125
H	0.6263704	-2.5653224	89.3593801
H	1.3732229	-4.8644551	88.8327416
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C	-2.1910642	3.6475581	89.9727858
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H	-4.3309598	0.5372523	87.8182835
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H	-2.2940765	5.7753649	91.9912089
H	8.3487788	4.3503059	85.4093698
H	7.7328926	2.6696322	90.7941897
H	5.1228559	-0.5843893	83.9191049
C	7.9423711	4.7535695	86.3636309
H	4.8552680	3.3870810	91.9714617
H	7.9319112	6.8164911	85.5980157
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C	6.9557417	3.7095017	86.8805671
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C	7.2242104	6.0727435	86.0201719
H	6.7573406	6.5197135	86.9219865
C	6.6929360	3.5219669	88.2488593
C	5.6447675	0.0612177	84.6553936
H	9.6567306	4.0443030	87.5449508
C	6.2597837	2.8987489	85.9659408
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C	5.0451029	3.5814508	90.8954389
H	6.7945008	1.6882001	91.9620167
H	7.3427953	0.9632272	90.4135151
C	5.8092088	2.5270124	88.7124695
C	3.9535949	1.8978948	84.2377775
C	5.3577442	1.8991402	86.3731370
H	6.1256329	-0.5973626	85.4060652
H	6.4534932	0.6010321	84.1191041
C	5.6322750	2.3321427	90.2171260
C	5.1538658	1.6926785	87.7682698
C	4.6600827	1.0502228	85.3086556
H	4.0875095	3.8740849	90.4238088
H	3.2074070	2.5687763	84.7025676
H	5.7413001	4.4443455	90.8337485
H	6.4117738	5.9065916	85.2864922
H	4.6634831	2.5208745	83.6554068
H	8.8228233	5.4528360	88.2608228
H	4.9045393	1.5092656	90.3650607
H	3.8733774	0.4577933	85.8178422
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Zn	1.0089269	5.8699531	89.2559733
Br	-0.0918895	7.4666046	90.5537099
C	7.3829322	8.6602894	90.6650948
C	3.4254028	7.0876443	90.5338876
C	7.0607613	7.6730583	89.7112851
C	5.1174120	8.5953237	91.5306428
C	4.7903404	7.6019797	90.5784210
C	6.4147418	9.1211308	91.5744822
C	5.7706367	7.1388935	89.6657727
O	3.0566493	6.2086834	89.7358296
H	8.4025473	9.0742955	90.6961552
H	4.3451322	8.9492031	92.2319544
H	7.8280362	7.3252388	89.0038011
H	6.6744520	9.8920624	92.3150383
H	5.4942870	6.3614294	88.9364621
H	4.3888295	9.3595523	87.5395333

Br	-0.1858409	4.5372362	84.1572007
H	4.1876997	4.8388404	85.9603789
Zn	1.8080576	4.6037379	85.3797989
C	4.1657615	8.0440885	85.8076509
C	3.6282135	9.0191069	86.8024574
C	3.5136454	6.8489083	85.9326346
C	3.6047341	5.5212878	85.2995487
C	2.5066877	7.0763812	86.9833987
O	2.5959554	8.2971634	87.5190479
O	1.6282425	6.2590548	87.3320261
H	3.1508319	9.9212429	86.3616044
H	4.1115375	5.5554338	84.3168878
H	2.6829930	7.5369486	91.2418768
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14l-ma



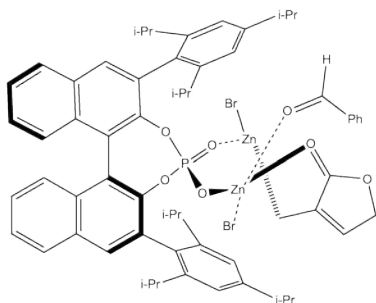
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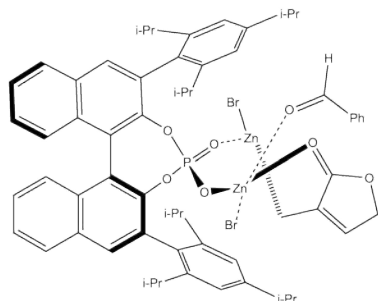
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H	5.6113689	-1.5987471	87.4926088
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H	6.3062446	2.8990139	92.0298603
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H	5.5937684	2.6925720	84.2909748
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H	5.1655841	0.3455465	90.7061638
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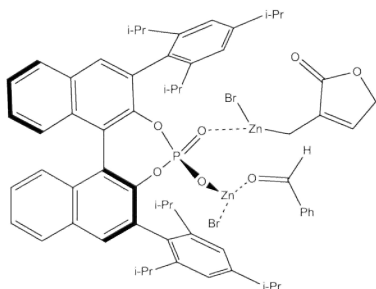
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H	7.0303019	3.1657416	85.8731214
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H	7.0686037	-0.0970241	92.2586922
H	7.5286026	-0.4094540	90.5495845
C	6.2019382	1.7142656	89.4086287
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C	-39.0924874	-58.5586459	389.4598008
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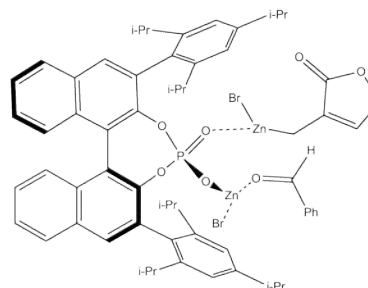
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H	-29.7321858	-57.4438061	391.1087029
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H	-33.3144877	-56.0244406	390.9381521
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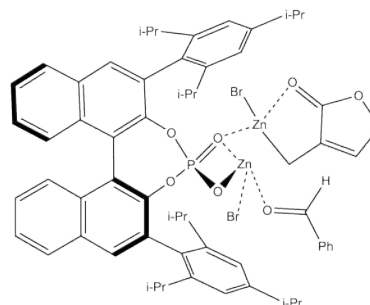


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O	-34.4905115	-56.7989394	388.7760060
P	-35.4802147	-55.6650026	388.1259817
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C	-38.2227181	-61.9940934	390.6960853
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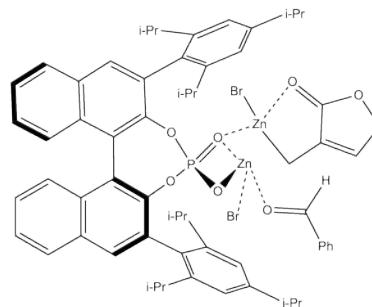
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C	4.1422779	9.5337010	266.9181111
C	4.1127279	8.5159980	267.9019739
C	5.3688748	9.9858447	266.4193896
C	5.3198196	7.9488898	268.3792144
O	2.7021279	7.1561096	269.2522626
H	7.5307753	9.7816426	266.5138933
H	3.1961486	9.9607837	266.5495215
H	7.4826364	7.9771651	268.2469236
H	5.3983251	10.7738846	265.6525724
H	5.2729126	7.1379271	269.1213850
Br	1.8127820	2.6659871	265.2277604
C	-0.1725616	1.6100408	269.2230934
C	0.7472239	0.5623159	269.2518497
C	0.4165416	-0.5941582	270.0525167
C	1.3403761	-1.6539624	270.3001100
C	-0.8917655	-0.6728315	270.6587702
C	-1.2348409	-1.8246216	271.4289846
C	-1.8130517	0.4022833	270.4952737
H	-2.8216100	0.3087303	270.9257414
C	-1.4695036	1.5645131	269.8165057
C	4.2689390	1.7288936	268.2731423
C	4.6759948	0.6828706	267.4532932
H	5.7194213	0.6509686	267.1039700
C	3.7769065	-0.3390594	267.0364731
C	4.1776383	-1.3447320	266.1069238
C	2.4363839	-0.3656854	267.5682883
C	1.5432371	-1.3775981	267.1067704
C	2.0354547	0.6511338	268.5090975

C	2.9155780	1.7144145	268.7229206
O	0.1461994	2.7680392	268.5088810
O	2.5189480	2.7999844	269.5091151
P	1.2789006	3.7706321	269.0974666
O	0.9125003	4.5297869	270.3968185
O	1.5224568	4.8367316	267.9909298
C	-0.3209246	-2.8483974	271.6290605
C	0.9815505	-2.7516806	271.0707173
H	-2.2406932	-1.8767108	271.8746144
H	-0.5968828	-3.7279331	272.2305543
H	2.3539501	-1.5908789	269.8805698
H	1.7154794	-3.5515338	271.2530966
C	1.9578877	-2.3303938	266.1863582
C	3.2888328	-2.3241198	265.6894435
H	0.5068737	-1.3840346	267.4725775
H	1.2459947	-3.0916711	265.8324770
H	3.6071358	-3.0879141	264.9636196
H	5.2062954	-1.3175206	265.7143395
C	-2.5712145	3.6944392	270.6477748
C	-2.4113379	2.7148639	269.6294252
C	-3.4576855	4.7625204	270.4157285
C	-3.1147321	2.8334598	268.3999637
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C	-4.1717557	4.9005535	269.2135613
H	-3.5916758	5.5299742	271.1936839
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C	-2.2649585	2.4190860	266.0445115
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H	-2.1364335	1.6531167	265.2516467
H	-1.2651394	2.8182756	266.2967641
C	-4.3048960	1.1605934	266.9113675
H	-2.3027349	0.9962689	267.6518364
H	-5.0155842	1.9027028	266.4910985
H	-4.7862606	0.6993958	267.7981409
H	-4.1615589	0.3695188	266.1463309
C	-5.0955703	6.0919919	268.9922831
C	-4.4859683	7.0748440	267.9772231
H	-5.1331089	7.9687205	267.8519939
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C	-6.5154381	5.6648962	268.5826236
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H	-7.1825376	6.5479292	268.4995919
H	-6.9585335	4.9662990	269.3212856
H	-6.5171367	5.1568695	267.5955694
C	-1.8262902	3.5951695	271.9787134
C	-1.4197616	4.9624619	272.5526416
H	-0.7158542	4.8270446	273.3987527
H	-2.2938616	5.5258793	272.9406964
H	-0.9225171	5.5898893	271.7888884
C	-2.6486230	2.8070979	273.0174645
H	-0.8892890	3.0318424	271.7854189
H	-2.0949040	2.7207674	273.9757210
H	-2.8841137	1.7829572	272.6684617
H	-3.6109679	3.3212438	273.2237671
H	8.5952316	6.1918752	269.1703769
H	6.9387220	1.5023841	272.2719653
H	6.0328645	3.3532173	264.3399354
C	8.3259699	5.5690843	270.0528823
H	3.8669661	1.8716890	272.9813933
H	8.6749025	7.2305142	271.4437111
H	4.3290546	5.1783842	265.0178805
C	7.2172928	4.6244020	269.6032045
C	6.1675697	0.9245593	271.7206642
C	7.8688317	6.5165145	271.1760606
H	7.6046961	5.9534015	272.0951620
C	6.6137312	3.7304449	270.5062682
C	6.4195395	3.3369788	265.3798264
H	9.9417230	4.1342314	269.6409239
C	6.7821950	4.5964610	268.2685407

C	9.5895760	4.7898134	270.4625846
H	10.4139565	5.4826668	270.7310354
H	7.2322535	5.2999968	267.5488204
C	4.3174829	2.5911760	272.2665704
H	5.7329471	0.1883471	272.4282201
H	6.6807978	0.3638102	270.9131931
C	5.6340220	2.8049169	270.1063297
C	4.7929590	5.1771274	266.0254314
C	5.7904380	3.7023659	267.8175519
H	6.7717374	2.3076882	265.5950982
H	7.3031506	4.0087162	265.4241193
C	5.0698879	1.8421392	271.1510544
C	5.2305414	2.7779646	268.7394409
C	5.3253251	3.7765655	266.3669198
H	3.5030070	3.2138873	271.8474463
H	4.0207823	5.4914947	266.7560605
H	4.9985828	3.2518784	272.8431870
H	6.9764174	7.1038817	270.8791675
H	5.5911325	5.9489659	266.0327207
H	9.3910593	4.1455504	271.3445316
H	4.3356524	1.1817859	270.6477838
H	4.4684149	3.0828680	266.2472350
Zn	0.8439783	6.3377074	269.5430728
Br	-0.7544569	7.9945315	269.4668064
H	6.9314608	3.7378574	271.5614446
H	-1.6923623	9.2464101	266.9326371
H	1.7409861	6.6030311	264.0889544
Zn	1.4427345	4.8930684	265.8912877
C	-0.0033027	8.7800574	265.6178081
C	-1.4666980	8.8138219	265.9324875
H	0.6011400	9.6902534	265.4946630
C	0.4030468	7.4879559	265.4871064
C	1.6682242	6.7802551	265.1869724
C	-0.8002066	6.6558262	265.7697343
O	-1.8858814	7.4350671	265.9565632
O	-0.8305703	5.4280210	265.8642686
H	-2.0686036	9.3587201	265.1724451
H	2.5680036	7.3585034	265.4739874
H	1.9106192	8.5166349	267.9424833

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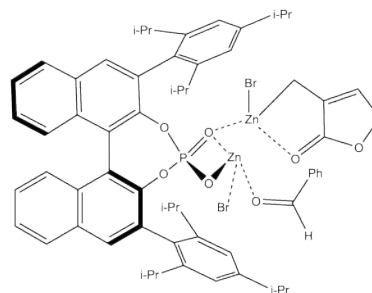


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C	6.1321882	8.2640595	267.1735356
C	4.0327654	10.0352114	267.7958996
C	3.9500152	8.6704823	268.1602547
C	5.1659875	10.5109242	267.1273212
C	5.0074474	7.7815150	267.8471750
O	2.6228660	7.0025876	269.2039044
H	7.1015787	9.9959236	266.2836531
H	3.2008778	10.7144015	268.0427847
H	6.9530512	7.5770653	266.9204127
H	5.2375675	11.5711739	266.8427670
H	4.9217480	6.7202398	268.1276802
Br	1.8107724	2.6102537	265.2223506
C	-0.2029289	1.4819896	269.1815421

C	0.7190983	0.4388517	269.2484381	H	-3.8237002	3.2707556	273.1719156
C	0.3813184	-0.6910069	270.0849943	H	8.2672234	6.3907119	268.8265421
C	1.3012467	-1.7425393	270.3760622	H	6.8360086	1.8468904	272.2306444
C	-0.9321837	-0.7484539	270.6829687	H	6.3672725	2.6018306	264.2936358
C	-1.2831418	-1.8759049	271.4841381	C	7.9939619	5.8487316	269.7598554
C	-1.8479569	0.3266947	270.4901319	H	3.7476250	2.1689288	272.9449377
H	-2.8535545	0.2546863	270.9308818	H	8.0995311	7.6897028	270.9500004
C	-1.4969548	1.4693776	269.7838189	H	4.6368453	4.5349138	264.4783580
C	4.2425663	1.5965783	268.2361430	C	6.9999830	4.7631604	269.3648782
C	4.6683119	0.5032528	267.4913952	C	6.0738535	1.2029206	271.7439043
H	5.7161863	0.4570195	267.1593633	C	7.3802819	6.8740652	270.7292888
C	3.7832232	-0.5476813	267.1215159	H	7.1065642	6.4023658	271.6957669
C	4.2052504	-1.6022068	266.2585124	C	6.3829697	3.9518753	270.3329157
C	2.4334434	-0.5497324	267.6285574	C	6.6355065	2.7462212	265.3604317
C	1.5519822	-1.5872662	267.2030886	H	9.7488695	4.5300627	269.6192768
C	2.0142175	0.5097460	268.5138446	C	6.6856445	4.5198279	268.0191032
C	2.8843373	1.5915162	268.6792810	C	9.2864773	5.2398401	270.3341012
O	0.1180891	2.6166150	268.4308998	H	10.0298376	6.0298259	270.5688849
O	2.4858404	2.7075241	269.4160640	H	7.1721936	5.1340407	267.2431222
P	1.2087000	3.6432207	269.0476998	C	4.1776739	2.8484070	272.1804909
O	0.8300405	4.3537280	270.3703322	H	5.6705125	0.5168498	272.5172440
O	1.4056087	4.7606602	267.9796008	H	6.5921895	0.5912486	270.9779136
C	-0.3736879	-2.8944683	271.7235978	C	5.4871927	2.9237657	269.9934984
C	0.9336745	-2.8156386	271.1760957	C	5.0342465	4.7022124	265.4996122
H	-2.2925002	-1.9119173	271.9233484	C	5.7742589	3.5214634	267.6200169
H	-0.6571144	-3.7548350	272.3487928	H	6.9261368	1.7597532	265.7741125
H	2.3187522	-1.6926789	269.9649225	H	7.5342453	3.3978294	265.3997287
H	1.6652608	-3.6096782	271.3901798	C	4.9429577	2.0409170	271.1171620
C	1.9875119	-2.5877302	266.3456384	C	5.1725974	2.7056894	268.6189471
C	3.3282021	-2.6061154	265.8780857	C	5.4593721	3.3688112	266.1336966
H	0.5084372	-1.5761910	267.5471937	H	3.3450096	3.4202464	271.7271567
H	1.2837939	-3.3682685	266.0186829	H	4.2309748	5.1838506	266.0913630
H	3.6631744	-3.4077443	265.2024209	H	4.8420482	3.5623686	272.7111740
H	5.2412378	-1.5916702	265.8849646	H	6.4618805	7.3306877	270.3086912
C	-2.5882054	3.5781223	270.6710245	H	5.8749426	5.4243016	265.4224897
C	-2.3968485	2.6533982	269.6065475	H	9.0806010	4.6826746	271.2718059
C	-3.4038732	4.7024009	270.4429289	H	4.2266270	1.3208426	270.6751201
C	-3.0037313	2.8807597	268.3405600	H	4.5870752	2.6911277	266.0366344
C	-3.8039469	4.0229688	268.1689880	Zn	0.7587367	6.1835820	269.5442225
C	-4.0198551	4.9471620	269.2050477	Br	-0.7351538	7.9063611	269.8689903
H	-3.5534723	5.4316012	271.2541294	H	6.6208007	4.1116595	271.3967680
C	-2.8288960	1.9145877	267.1702653	H	-1.1047124	9.3280912	267.4100667
H	-4.2658169	4.1998928	267.1847612	H	2.0431338	6.6746158	264.2475368
C	-2.2181697	2.6002685	265.9369100	Zn	1.5646798	4.8406437	265.8820641
H	-2.8813297	3.3931643	265.5338417	C	0.5766044	8.8507724	266.0809865
H	-2.0427428	1.8617516	265.1280833	C	-0.8853410	9.0254012	266.3613827
H	-1.2474608	3.0714075	266.1766222	H	1.2996273	9.6785204	266.1062262
C	-4.1593765	1.2134167	266.8376231	C	0.8230628	7.5535666	265.7487669
H	-2.1212015	1.1207679	267.4868784	C	1.9976444	6.7496564	265.3583228
H	-4.9260301	1.9428380	266.5020650	C	-0.4859801	6.8473296	265.8756883
H	-4.5685709	0.6809682	267.7205757	O	-1.4724059	7.7259628	266.1640876
H	-4.0204202	0.4739646	266.0217762	O	-0.6684313	5.6352950	265.7852620
C	-4.8771177	6.1877296	268.9891154	H	-1.3791252	9.7497985	265.6758286
C	-4.2571861	7.1174271	267.9321189	H	2.9539615	7.1950503	265.6937814
H	-4.8584405	8.0439564	267.8180769	H	1.8974295	8.8975695	268.9600313
H	-4.2025012	6.6263916	266.9387504				
H	-3.2231927	7.4002470	268.2083760				
C	-6.3309945	5.8219673	268.6411828				
H	-4.8909298	6.7397867	269.9549733				
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H	-6.7837986	5.1755189	269.4200151				
H	-6.3876231	5.2744276	267.6771410				
C	-1.9460542	3.3756619	272.0436686				
C	-1.4430762	4.6821143	272.6802940				
H	-0.8426019	4.4584406	273.5855682				
H	-2.2787156	5.3396390	272.9977972				
H	-0.8072168	5.2525576	271.9786190				
C	-2.9141020	2.6567087	273.0040052				
H	-1.0602718	2.7226169	271.8980137				
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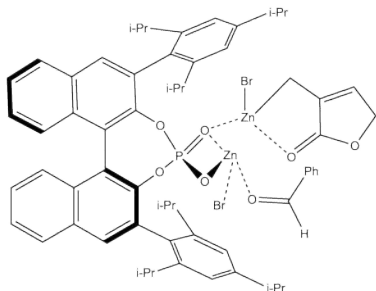


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C	-2.9932997	-4.8331121	469.3527070	H	-7.5466315	-4.2079447	461.2688275
C	-3.3740595	-4.4154329	468.0545077	C	-10.1774500	-2.1268082	460.2226651
C	-3.1172327	-6.1784894	469.7180540	H	-9.6938917	-3.1442672	462.0409527
C	-3.8597825	-5.3625247	467.1232154	H	-9.6940847	-1.6589001	459.3396541
O	-3.6073322	-2.4584734	466.6574029	H	-10.8067646	-1.3540137	460.7092344
H	-3.7222891	-8.1665520	469.0734192	H	-10.8451564	-2.9330645	459.8536836
H	-2.6248332	-4.0886084	470.0753204	C	-5.6336634	0.8823803	460.3541552
H	-4.3716461	-7.4359119	466.7715211	C	-4.6714856	-0.0909278	459.6511696
H	-2.8288208	-6.5054625	470.7283558	H	-3.9453169	0.4624451	459.0202507
H	-4.1483541	-5.0543434	466.1089529	H	-5.2188337	-0.7929504	458.9875328
C	-6.8401209	-4.9991909	471.2306438	H	-4.1062250	-0.6938775	460.3897995
C	-6.8248713	-4.4518898	469.9837331	C	-6.4254463	1.7243622	459.3363961
C	-5.8202392	-3.3599604	470.0356085	H	-5.0180420	1.5796791	460.9636381
O	-5.2042652	-3.3249733	471.2403296	H	-5.7407066	2.2849243	458.6662542
C	-5.8159960	-4.3222396	472.0864693	H	-7.0865601	2.4556084	459.8442670
O	-5.5669943	-2.5495286	469.1404658	H	-7.0659364	1.0787567	458.6989861
C	-7.5344826	-4.6733766	468.7084299	C	-7.4847913	0.3592225	465.0456739
H	-8.5046975	-5.1910211	468.8332811	C	-6.0851792	0.4503673	465.6716081
H	-7.4676470	-5.8270795	471.5882134	H	-6.1726526	0.6381705	466.7607330
H	-6.2346780	-3.7994387	472.9748623	H	-5.4612030	1.2507139	465.2233994
H	-5.0230038	-5.0159516	472.4457369	H	-5.5251879	-0.4977612	465.5476144
Zn	-7.5351160	-2.8645748	467.7944022	C	-8.2250103	1.7003676	465.2016543
H	-6.9005287	-5.2933831	468.0393096	H	-8.0378146	-0.3903056	465.6431839
Br	-8.6697633	-0.8586019	468.2517608	H	-8.3100525	1.9681636	466.2748934
C	-8.9951297	-3.2723163	464.3774101	H	-9.2495310	1.6558718	464.7796608
C	-9.8055538	-4.0427810	465.2122299	H	-7.6867199	2.5195399	464.6793333
C	-10.8108975	-3.3558772	465.9840606	H	-2.9697047	-10.8080972	465.1940696
C	-11.5495305	-3.9931024	467.0235004	H	-7.9238032	-10.9252074	468.5835095
C	-11.0538540	-1.9604626	465.7151663	H	-7.3879450	-8.3719437	461.3413486
C	-12.0551520	-1.2755844	466.4651879	C	-3.5491371	-10.8824087	466.1402698
C	-10.2745501	-1.2824256	464.7347400	H	-7.7911479	-8.1618359	470.1728286
H	-10.4955939	-0.2257784	464.5235889	H	-1.7214984	-11.1088553	467.3302114
C	-9.2054074	-1.8932088	464.0861966	H	-5.4102216	-6.7642224	461.5923695
C	-8.3463321	-7.6159516	465.4146403	C	-4.7516708	-9.9573561	465.9913579
C	-9.4864721	-8.3662964	465.1547905	C	-8.5866163	-10.0743591	468.3196722
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14o-mi



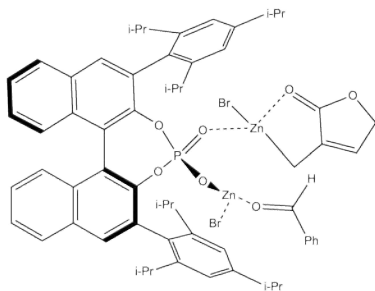
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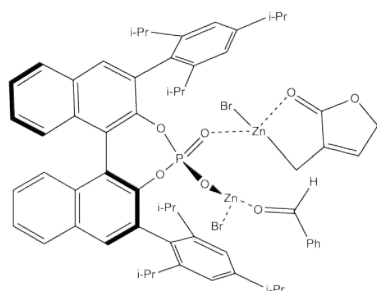
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H	1.2488203	-4.6442038	87.9245556
H	3.6135854	-5.0235969	87.1494171
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H	8.4774090	7.1590818	87.5858910
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C	6.2362134	3.3100118	86.6170033
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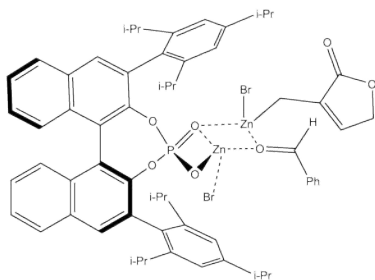
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C	-1.0635228	-0.7221815	91.3075121
C	-1.6275483	-1.5987988	92.2820163
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C	3.8799362	-1.7444473	88.1802373
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C	2.5466535	-1.5459599	88.6959965
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P	1.7229981	3.0198997	89.1644888
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H	6.2237652	0.1947438	85.2338496
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C	5.9120363	2.0467898	90.7524405
C	5.2759851	1.8099677	88.2728237
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H	4.1249208	3.4321418	84.6684714
H	9.6729059	4.3169582	88.3783326
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H	3.9863595	0.7629291	86.2133049
Zn	1.3762886	5.0706800	91.6938582
Br	2.4552248	5.2435021	93.7008725
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H	4.4893652	5.7051179	87.5467680
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H	3.5416330	10.6179771	86.0372886
Zn	2.2566575	5.3241025	86.5724609
H	4.8009038	5.8841965	85.7929283
Br	0.3745197	5.1547630	85.2039132
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H	5.7713150	5.8565787	90.2499115
H	6.9142285	8.0769782	90.5163459
H	5.5599194	8.7586957	85.8124383
H	1.0205322	8.7750825	90.2503624

H	7.6222075	5.7166226	95.7104314
H	4.0947474	3.1923727	95.7886917
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H	6.2248328	3.9832943	96.8601472
H	4.7898520	5.8886108	92.4382834
Br	0.1119305	1.9039439	93.0680181
Zn	0.1763750	4.0821528	92.2219049
H	3.2878827	8.4448541	92.9880530
H	-0.9706608	6.3838029	91.8452370
C	1.1775470	7.9670229	92.7084348
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H	0.8303256	8.5457104	91.8432726
C	0.6628716	6.7947033	93.1744277
C	-0.4353241	5.9317242	92.7024750
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C	-1.0308820	3.4771116	86.8681342
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C	3.4737806	-0.8621199	86.8387979
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O	1.2353531	3.4431355	87.6663812
O	1.4363982	1.6834396	89.4963699
P	1.6928027	3.2746688	89.2190958
O	0.8663161	4.1344778	90.2079456
O	3.1723398	3.7212150	89.2718053
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H	1.2136673	0.4552521	84.5724129
H	2.5621184	-0.9272280	83.0179403
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H	5.0735526	-2.2427431	86.3054113
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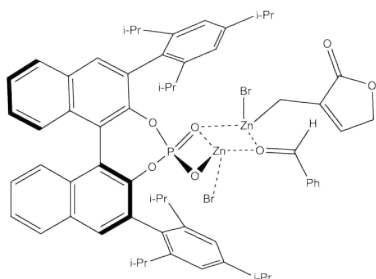
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C	6.6529730	0.8557669	89.8405688
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C	4.6581224	0.9006215	92.5143351
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C	5.8384211	3.0376526	90.8099740
C	4.4773546	0.8863518	91.1173037
H	6.3762847	-0.0891120	89.3333986
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H	7.6117727	5.7253778	95.7297617
H	4.0777224	3.2075979	95.7968467
H	6.9044495	6.6673327	93.5169310
H	6.2031839	4.0028623	96.8807829
H	4.8013432	5.8778088	92.4368348
Br	0.1357738	1.8861458	93.0509613
Zn	0.1857599	4.0680143	92.2328039
H	3.2615097	8.4728025	92.9415648
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C	1.5351941	6.4070163	94.3332898
O	2.4899359	7.3743036	94.5256818
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H	2.1674562	9.3742926	94.0515352
H	-1.1286725	5.7118384	93.5694634
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C	-0.8082474	0.6605679	86.3279741
C	-0.8332995	-0.7573742	86.1703381
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C	-3.0650762	0.7287976	85.3106087
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H	-2.9611244	3.3591436	85.9273962
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C	3.1571518	0.0332704	89.1070292
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C	3.4669446	-0.8702527	86.8389622
C	4.2100538	-1.6726039	85.9224047
C	2.3378192	-0.1123698	86.3569363
C	2.0420090	-0.1531648	84.9611320
C	1.5786966	0.6868317	87.2884530
O	2.0675440	0.8041424	88.5961710
O	1.2374547	3.4415522	87.6666418
O	1.4362693	1.6818867	89.4948677
P	1.6931847	3.2746372	89.2210095
O	0.8634654	4.1350090	90.2062113
O	3.1728524	3.7183101	89.2760620
C	-3.0404733	-0.6466053	85.1384034
C	-1.9213255	-1.3945111	85.5898420
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H	-3.8936444	-1.1617440	84.6714749
H	0.0214263	-1.3504382	86.5231694
H	-1.9173783	-2.4901293	85.4849656
C	2.7963935	-0.9293143	84.0927383
C	3.8815508	-1.7076096	84.5760801
H	1.2110781	0.4523240	84.5733300
H	2.5540283	-0.9364397	83.0191416
H	4.4675354	-2.3255230	83.8788453
H	5.0616726	-2.2557516	86.3065925
C	-2.0433548	5.0800483	88.5224694
C	-1.1533185	4.8596548	87.4286440
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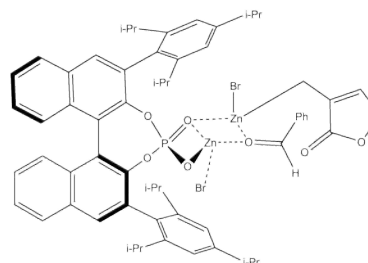
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H	0.6141747	4.6742665	85.4865586
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H	0.1985102	9.9296657	88.3147471
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H	-1.3500400	8.4752459	90.5634263
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H	4.1992993	-2.0186168	95.1728415
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Zn	2.8945557	5.2357958	90.5622305
Br	3.6817364	7.3552552	90.1765641
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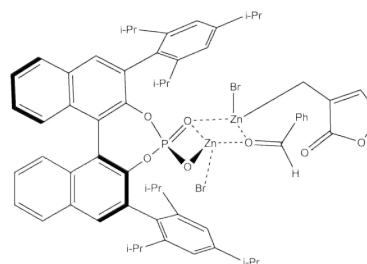
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C	1.1225355	0.4521551	166.7267453
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C	0.8467971	-4.0511872	169.8633338
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H	3.2117687	1.1283357	166.7742271
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C	-0.9713918	-2.6528640	165.8006302
C	-0.5286837	-3.4148770	169.5799167
C	-1.1195647	-3.2813669	167.0750629
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H	-1.9663597	-2.0574444	170.5441694
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H	-0.2584753	-1.6623073	170.8963311
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H	-1.6157547	1.2098307	165.6747722
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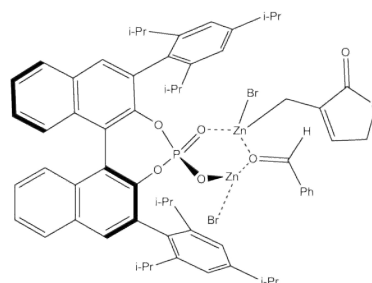


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P	-4.3175858	-1.8602358	168.2416149
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H	-9.3796123	-6.0183444	171.0064127
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H	-4.7064591	-7.1214910	169.5527852
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H	-7.9268123	-2.7190412	164.0891580	C	-6.3971332	3.3213350	166.4582826
H	-7.6812187	-4.4788041	164.3697222	O	-4.6232842	1.7454947	168.0238600
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H	-6.5670697	0.6659432	171.3447467	H	-2.0574967	0.7062699	163.9250893
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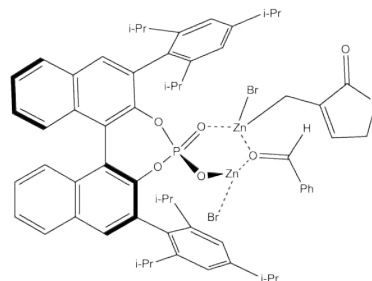


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C	-39.0724254	-58.0421810	1189.6131227
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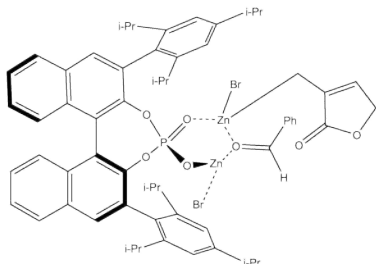


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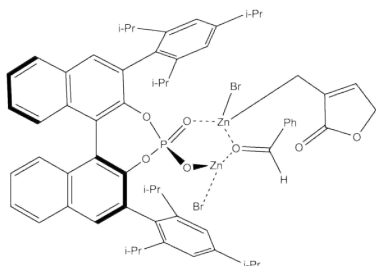
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O	1.0568537	6.2214593	77.8101083
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H	5.9959703	10.0524341	79.3384425
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C	4.5186265	8.5035502	78.8818516
C	5.0245944	9.6476202	79.7023786
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C	4.4096674	7.4100191	79.6729496
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C	4.8588368	7.8017936	81.0429086
O	5.2045205	9.1298274	81.0263147
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H	3.1927844	-4.6989697	75.9758083
H	4.9495699	-2.9631474	76.3700911
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C	-2.6003947	5.6946721	79.5374016
H	-1.9207921	5.8459773	81.5856470
C	-2.4076346	2.6175795	77.2446180
H	-3.1258821	5.2015904	77.4899427
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H	-2.0669421	4.1800184	75.7244058
H	-1.7053215	2.5185623	75.1700420
H	-0.5774079	3.3527774	76.2885492
C	-3.8892729	2.3644644	76.9093775
H	-1.9542922	1.6310364	77.4727904
H	-4.4142636	3.3104293	76.6596939
H	-4.4211115	1.9017068	77.7653755
H	-3.9857895	1.6860143	76.0363010
C	-3.0739493	7.1469829	79.5135810
C	-3.5499971	7.6314686	78.1396094
H	-3.7852259	8.7144464	78.1704587
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C	-4.1741332	7.3887506	80.5669881
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H	-4.4664635	8.4588049	80.5920412
H	-3.8432924	7.1059468	81.5854615
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C	-1.0695301	3.3552021	82.1830545
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H	-0.5560867	5.2849550	83.1367889
H	0.7611517	4.5645938	82.1643706
C	-2.2297900	3.0398751	83.1491032
H	-0.5180251	2.4112852	81.9973357
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H	-2.9385282	2.3026380	82.7223743
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H	6.7204745	6.2833415	77.2171987
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H	5.4921814	0.7621698	73.7832834
C	7.4283330	5.5889892	77.7285580
H	4.9216148	2.2505836	82.6258771
H	8.2695263	7.2370164	78.8841257
H	3.5668859	2.4040142	73.7658190
C	6.6732074	4.2690993	77.8764502
C	7.0135605	1.2408528	81.0977241
C	7.8377289	6.2313136	79.0594086
H	8.6083639	5.6272422	79.5825097
C	6.5336481	3.5990423	79.1031624
C	5.8974767	1.2533626	74.6922339
H	8.3754028	5.0152417	75.8171717
C	6.0580928	3.6912728	76.7464389
C	8.6541426	5.4243357	76.8084220
H	9.1558416	6.4000560	76.6440195
H	6.1433675	4.2075300	75.7777922
C	5.0334132	2.7488956	81.6410739
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H	7.4378276	0.5147454	80.3747652
C	5.7806120	2.4141487	79.2320637
C	3.9786539	2.9099460	74.6633583
C	5.3339892	2.4874506	76.8092269
H	6.4483498	0.4903276	75.2785825
H	6.6351025	2.0166721	74.3663551
C	5.6536543	1.7806667	80.6155972
C	5.1824979	1.8454790	78.0773358

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H	4.0287210	3.0810883	81.3151034
H	3.1355174	3.3362566	75.2387107
H	5.6603407	3.6514955	81.7967086
H	6.9804730	6.3509928	79.7509886
H	4.6074925	3.7519383	74.3093964
H	9.3924370	4.7318220	77.2645673
H	4.9720375	0.9098677	80.5268034
H	4.0544081	1.0985327	75.7928950
Zn	1.8028801	6.0107827	79.7983585
Br	0.8563983	7.7683927	80.9824405
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14r-mi



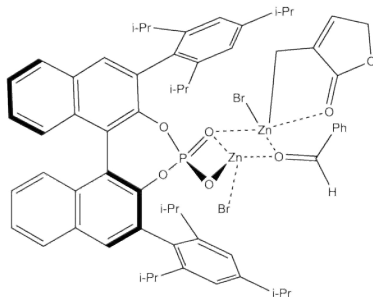
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C	-0.8943811	8.1413813	75.4241253
C	-0.0817260	7.0885933	75.9124924
C	-1.2151185	8.1998388	74.0647068
C	0.4079465	6.0962266	75.0252559
O	1.0432869	6.1967019	77.8002387
H	-0.9877611	7.2522880	72.1219755
H	-1.2637125	8.9105927	76.1201951
H	0.4537686	5.3901092	72.9790571
H	-1.8429963	9.0164215	73.6787676
H	1.0353894	5.2863682	75.4222460
Br	3.8920313	6.6424446	75.6070137
Zn	3.2412437	5.4740101	77.5114034
H	6.0103307	10.0269044	79.3268322
H	3.8887641	5.4806057	80.4336101
C	4.5108955	8.4881249	78.9039582
C	5.0507172	9.6210786	79.7218657
H	4.2393654	8.5665742	77.8407711
C	4.4192569	7.3901766	79.6892444
C	3.9473710	6.0028235	79.4468001
C	4.9193692	7.7640272	81.0494022
O	5.2738378	9.0924542	81.0306866
O	5.0365408	7.0560545	82.0274718
H	4.3335580	10.4709867	79.7921220
H	4.7733459	5.3835441	79.0053327
C	0.0188685	1.2329876	79.1810357
C	0.7015475	0.0299785	79.4008021
C	0.1198530	-0.9081758	80.3328600
C	0.7967114	-2.0842644	80.7760348
C	-1.1904759	-0.6338209	80.8741590
C	-1.7935339	-1.5802910	81.7559956
C	-1.8294736	0.6052753	80.5831520
H	-2.8061073	0.8188387	81.0429427
C	-1.2193056	1.5804675	79.8038534
C	4.2956356	0.6393603	78.1769444
C	4.5983207	-0.5807852	77.5847985
H	5.5928305	-0.7298708	77.1372983
C	3.6279741	-1.6167516	77.4607375

C	3.9297687	-2.8245309	76.7626514
C	2.2955345	-1.4173780	77.9814309
C	1.3084078	-2.4096962	77.7019671
C	2.0101774	-0.2150371	78.7285946
C	3.0080454	0.7653571	78.7847177
O	0.5499372	2.1649074	78.2885415
O	2.7622158	1.9411201	79.4871474
P	1.8091375	3.0800789	78.7911454
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O	2.4197634	3.6653230	77.5044927
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H	-2.7985737	-1.3622676	82.1501798
H	-1.5975191	-3.4510447	82.8198244
H	1.8180605	-2.2798054	80.4223294
H	0.7380827	-3.8704504	81.9810567
C	1.6298418	-3.5638828	77.0013017
C	2.9552125	-3.7855244	76.5424986
H	0.2768331	-2.2480956	78.0434589
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C	-2.2599573	3.4861802	78.4834807
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H	-1.9286736	5.8468957	81.5760843
C	-2.3924455	2.6128192	77.2377825
H	-3.1245427	5.1921112	77.4800182
C	-1.6252472	3.2002368	76.0396214
H	-2.0462565	4.1765039	75.7197689
H	-1.6773499	2.5163012	75.1671988
H	-0.5579466	3.3513060	76.2926378
C	-3.8711372	2.3551213	76.8941009
H	-1.9372675	1.6277513	77.4683119
H	-4.3985195	3.2990870	76.6423340
H	-4.4062486	1.8911273	77.7471024
H	-3.9616728	1.6767272	76.0203559
C	-3.0864176	7.1392275	79.5037965
C	-3.5565739	7.6231375	78.1276018
H	-3.7964745	8.7052926	78.1572070
H	-4.4758099	7.0908706	77.8040254
H	-2.7935814	7.4659674	77.3402622
C	-4.1947300	7.3737743	80.5499615
H	-2.2083215	7.7558506	79.8098986
H	-4.4929185	8.4421833	80.5763726
H	-3.8689658	7.0901039	81.5695753
H	-5.0949198	6.7717753	80.3051777
C	-1.0745045	3.3605300	82.1811831
C	-0.0839278	4.3356849	82.8383511
H	0.3304710	3.8865073	83.7638237
H	-0.5587529	5.2959397	83.1251108
H	0.7592038	4.5660597	82.1622941
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H	-0.5233777	2.4154374	82.0005191
H	-1.8548230	2.6455371	84.1067083
H	-2.9459455	2.3126068	82.7220776
H	-2.8138272	3.9718171	83.3712008
H	6.6880930	6.2925536	77.2259182
H	7.7618876	2.0750020	81.2165068
H	5.4757748	0.7668497	73.7809089
C	7.4085025	5.5970256	77.7179210
H	4.9408380	2.2532149	82.6283476
H	8.2646871	7.2384726	78.8726929
H	3.5420896	2.3966394	73.7731899
C	6.6611335	4.2730776	77.8690189
C	7.0278780	1.2516854	81.0918080
C	7.8402516	6.2293497	79.0463599
H	8.6241300	5.6246195	79.5486422

C	6.5307571	3.6023087	79.0961155
C	5.8814885	1.2607292	74.6881844
H	8.3228111	5.0453133	75.7838819
C	6.0403730	3.6939148	76.7429897
C	8.6174490	5.4457288	76.7738799
H	9.1129013	6.4245415	76.6091490
H	6.1162505	4.2116318	75.7744054
C	5.0405688	2.7489410	81.6410299
H	6.9289077	0.7412523	82.0719850
H	7.4545943	0.5284114	80.3676598
C	5.7818349	2.4155189	79.2296441
C	3.9497476	2.9029613	74.6723990
C	5.3217660	2.4872003	76.8096331
H	6.4420758	0.5020342	75.2708606
H	6.6120761	2.0292037	74.3590913
C	5.6631720	1.7833232	80.6144866
C	5.1795711	1.8447099	78.0783689
C	4.7495618	1.8988677	75.5181874
H	4.0296743	3.0683443	81.3222418
H	3.1027953	3.3158211	75.2517395
H	5.6567079	3.6598811	81.7904618
H	6.9974414	6.3391720	79.7566849
H	4.5667131	3.7547190	74.3211453
H	9.3666608	4.7515497	77.2088734
H	4.9863180	0.9084025	80.5284877
H	4.0459651	1.0904866	75.7986088
Zn	1.7919758	6.0068879	79.8018942
Br	0.8161244	7.7840370	80.9235767
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H	-0.2195216	7.7754011	78.0201588

14s-mi; COSMO



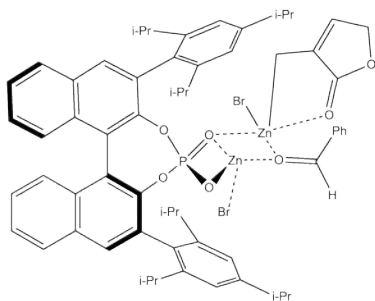
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Br	-0.4751902	4.1294148	96.0326076
C	0.1071542	1.0996844	99.5734608
C	0.8561831	-0.0632712	99.7798255
C	0.3776384	-1.0003427	100.7679850
C	1.1481364	-2.1234099	101.1945767
C	-0.9088285	-0.7769643	101.3826783
C	-1.3826792	-1.7009751	102.3616221
C	-1.6914925	0.3437715	100.9810385
H	-2.7149021	0.4484420	101.3733796
C	-1.2117113	1.2929446	100.0859837
C	4.3431652	0.4358341	98.2303500
C	4.5131003	-0.7677684	97.5547144
H	5.4562397	-0.9523494	97.0173660
C	3.4792677	-1.7470494	97.4894011
C	3.6419249	-2.9373392	96.7179494
C	2.2276665	-1.5189597	98.1742980
C	1.1758299	-2.4673230	97.9976540
C	2.0829517	-0.3269444	98.9758533
C	3.1156142	0.6081700	98.9356207
O	0.6213838	2.1176897	98.7476848
O	2.9855568	1.7777427	99.6836658

P	1.9163250	2.9348347	99.3004540
O	1.7165230	3.7370345	100.6118326
O	2.4175202	3.9136734	98.1978883
C	-0.6144178	-2.7906531	102.7439883
C	0.6653309	-2.9945239	102.1616985
H	-2.3707820	-1.5253411	102.8151371
H	-0.9888907	-3.4922842	103.5048423
H	2.1439692	-2.2861799	100.7588712
H	1.2826211	-3.8471593	102.4833328
C	1.3612317	-3.6052595	97.2240030
C	2.6084104	-3.8534498	96.5909163
H	0.2021534	-2.2836606	98.4725594
H	0.5316859	-4.3173067	97.0962054
H	2.7461111	-4.7631993	95.9869418
H	4.6043751	-3.1053258	96.2096437
C	-2.1464139	3.6651090	100.0825250
C	-2.0837590	2.3681691	99.5116228
C	-2.9338452	4.6423045	99.4454841
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C	-3.6109640	3.0666035	97.7528949
C	-3.6624903	4.3696845	98.2751674
H	-2.9806471	5.6585522	99.8679275
C	-2.7687443	0.6704879	97.6949202
H	-4.1768149	2.8317919	96.8390124
C	-1.7596368	0.6438314	96.5304394
H	-2.0906239	1.3092968	95.7063770
H	-1.6560597	-0.3853510	96.1270480
H	-0.7596853	1.0003285	96.8442591
C	-4.1454902	0.1529948	97.2468087
H	-2.3971446	-0.0374613	98.4639217
H	-4.5597378	0.7463785	96.4052762
H	-4.8817873	0.1814839	98.0757640
H	-4.0646007	-0.8955736	96.8937398
C	-4.5045158	5.4568625	97.6188493
C	-4.3215051	5.5118222	96.0929487
H	-4.8320909	6.4013283	95.6682567
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H	-3.2483744	5.5453870	95.8146766
C	-5.9900061	5.3060603	97.9983685
H	-4.1501735	6.4257741	98.0363154
H	-6.6000212	6.1235815	97.5599707
H	-6.1290865	5.3226542	99.0982866
H	-6.3940617	4.3421537	97.6233506
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C	-0.8881024	5.4145491	101.4656454
H	-0.2190073	5.5313155	102.3423905
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H	-0.3125221	5.6644038	100.5544502
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H	-3.2480192	4.3051871	102.5717934
H	7.7805804	5.5336082	97.1256991
H	7.9870424	1.1844361	101.2067641
H	5.2934346	1.1766879	93.6514779
C	8.0090513	5.0047230	98.0749367
H	5.2265138	1.5833118	102.7752095
H	8.4139602	6.8962767	99.0920648
H	3.4153671	2.7826029	94.2272573
C	7.0728623	3.8047351	98.1294046
C	7.1416713	0.4798743	101.0602316
C	7.7667589	6.0034421	99.2171061
H	8.0025934	5.5635591	100.2091339
C	6.8579903	3.0846499	99.3176274
C	5.8250564	1.4887166	94.5743226
H	9.6636922	3.8611653	97.1772634
C	6.4111288	3.3654650	96.9723957
C	9.4784800	4.5437504	98.0316124
H	10.1647097	5.4111370	97.9350006
H	6.5536291	3.9367871	96.0431050

C	5.4024759	2.1639991	101.8461658
H	7.0170835	-0.0987040	101.9992702
H	7.4299727	-0.2267100	100.2555001
C	5.9991373	1.9737972	99.3757332
C	3.9089998	3.0488689	95.1846345
C	5.5375326	2.2627660	96.9706344
H	6.4577500	0.6415584	94.9104489
H	6.5029841	2.3250803	94.3043397
C	5.8455512	1.2326093	100.7032872
C	5.3299864	1.5572083	98.1897654
C	4.8226275	1.9062705	95.6658432
H	4.4638186	2.6937612	101.5909879
H	3.1165980	3.2465950	95.9327005
H	6.1734952	2.9287188	102.0746299
H	6.7141400	6.3464349	99.2356028
H	4.4705638	3.9942081	95.0418171
H	9.7505269	3.9989335	98.9607730
H	5.0549267	0.4646755	100.5782091
H	4.1682320	1.0328424	95.8574403
H	7.3731419	3.4023631	100.2376889
C	-2.2121933	9.7720337	97.2555408
C	1.0588138	7.6334559	98.9336765
C	-2.0685888	8.3995095	96.9780358
C	-0.2186375	9.7240924	98.6378941
C	-0.0627711	8.3415117	98.3553173
C	-1.2904682	10.4334072	98.0909274
C	-1.0057381	7.6768796	97.5289245
O	1.2423022	6.3831872	98.7686808
H	-3.0538110	10.3321086	96.8198269
H	0.5130353	10.2312399	99.2868709
H	-2.7943866	7.8884478	96.3292341
H	-1.4134429	11.5043981	98.3103106
H	-0.9044036	6.5978230	97.3281930
H	1.7305816	8.1765333	99.6349900
C	3.0169462	8.7513547	97.2367991
C	3.2251013	7.5483597	96.6087207
C	4.6458286	7.1563619	96.8963370
O	5.2212170	8.1191319	97.6829727
C	4.2720986	9.1595806	97.9493701
O	5.2600563	6.1882548	96.4947652
C	2.3764108	6.6875719	95.8133165
H	2.1468851	9.4101628	97.1271349
H	4.6857950	10.1238086	97.5772537
H	4.1535711	9.2434918	99.0535706
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14s-mi

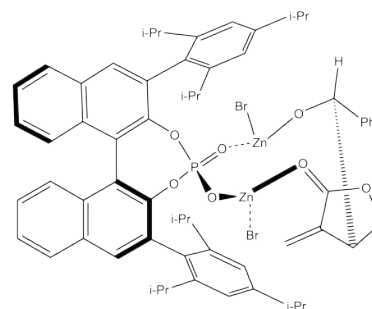


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Zn	1.4359426	5.1554549	96.8331413
Br	-0.5210341	4.1668163	96.0326724
C	0.1122898	1.1029389	99.5604344
C	0.8590958	-0.0615153	99.7672299
C	0.3793187	-0.9968260	100.7563277
C	1.1470403	-2.1218089	101.1821854
C	-0.9055961	-0.7701496	101.3726241
C	-1.3798798	-1.6929009	102.3518866

C	-1.6850754	0.3526678	100.9718427
H	-2.7076202	0.4620511	101.3652664
C	-1.2049874	1.3002022	100.0754588
C	4.3507083	0.4331946	98.2264267
C	4.5203577	-0.7704872	97.5513661
H	5.4649105	-0.9545789	97.0164960
C	3.4860945	-1.7487940	97.4832886
C	3.6489556	-2.9394475	96.7133302
C	2.2333259	-1.5198895	98.1654667
C	1.1821475	-2.4685051	97.9883654
C	2.0870712	-0.3271015	98.9654439
C	3.1208136	0.6069347	98.9272901
O	0.6266712	2.1182333	98.7331359
O	2.9894571	1.7778011	99.6721883
P	1.9247221	2.9353341	99.2799342
O	1.7261297	3.7468065	100.5851341
O	2.4255170	3.9027129	98.1673771
C	-0.6147302	-2.7844489	102.7331489
C	0.6631094	-2.9916250	102.1492509
H	-2.3666963	-1.5141998	102.8069987
H	-0.9902313	-3.4848032	103.4946049
H	2.1414529	-2.2863821	100.7442358
H	1.2785839	-3.8459296	102.4697702
C	1.3688938	-3.6071306	97.2168190
C	2.6162945	-3.8556321	96.5856632
H	0.2083526	-2.2834968	98.4623430
H	0.5396947	-4.3195286	97.0890855
H	2.7550971	-4.7657555	95.9825937
H	4.6120701	-3.1075494	96.2063482
C	-2.1361377	3.6736717	100.0771213
C	-2.0778174	2.3771564	99.5054246
C	-2.9325208	4.6492417	99.4492800
C	-2.8366244	2.0641543	98.3426380
C	-3.6229516	3.0742553	97.7625509
C	-3.6733179	4.3759790	98.2874238
H	-2.9771697	5.6650064	99.8731234
H	-2.7721788	0.6818369	97.6903650
H	-4.1970085	2.8392489	96.8539201
C	-1.7653922	0.6609789	96.5237097
H	-2.0975705	1.3294634	95.7028249
H	-1.6610135	-0.3660985	96.1153748
H	-0.7648381	1.0171289	96.8354026
C	-4.1488306	0.1633523	97.2436135
H	-2.3983007	-0.0279320	98.4567262
H	-4.5641568	0.7555260	96.4018508
H	-4.8851762	0.1916334	98.0723437
H	-4.0680164	-0.8849211	96.8898886
C	-4.5264887	5.4609458	97.6420500
C	-4.3484834	5.5286423	96.1159912
H	-4.8690165	6.4158247	95.6980551
H	-4.7813814	4.6380335	95.6149918
H	-3.2769317	5.5713545	95.8330592
C	-6.0091259	5.2955032	98.0256763
H	-4.1780801	6.4296352	98.0655509
H	-6.6285967	6.1103194	97.5955332
H	-6.1441328	5.3021017	99.1259861
H	-6.4064835	4.3307899	97.6461773
C	-1.4007624	3.9898896	101.3765372
C	-0.8608158	5.4263051	101.4392628
H	-0.1760669	5.5437660	102.3037044
H	-1.6713467	6.1757460	101.5569113
H	-0.3016719	5.6745280	100.5171875
C	-2.2975461	3.6876233	102.5926506
H	-0.5215665	3.3160839	101.4326856
H	-1.7577315	3.8870579	103.5416639
H	-2.6230453	2.6285381	102.6031196
H	-3.2104900	4.3193612	102.5758830
H	7.8003544	5.5279264	97.1443840
H	7.9874765	1.1678449	101.2122237
H	5.3084813	1.1210144	93.6762064
C	8.0129830	5.0043503	98.1003113

H	5.222571	1.5600639	102.7774186
H	8.3892263	6.9023708	99.1171465
H	3.4589259	2.7927332	94.2095102
C	7.0815863	3.8003911	98.1443251
C	7.1421647	0.4642872	101.0616641
C	7.7435744	6.0073740	99.2327426
H	7.9603689	5.5736428	100.2317138
C	6.8623502	3.0766286	99.3292985
C	5.8363153	1.4234878	94.6044223
H	9.6894462	3.8634931	97.2405996
C	6.4252904	3.3638401	96.9835212
C	9.4849710	4.5503265	98.0868832
H	10.1689524	5.4202435	97.9985330
H	6.5718149	3.9380067	96.0566271
C	5.3999168	2.1442972	101.8509411
H	7.0166793	-0.1182981	101.9980814
H	7.4326507	-0.2381297	100.2543390
C	6.0045089	1.9651623	99.3811934
C	3.9804096	3.0761983	95.1468499
C	5.5497613	2.2632300	96.9763029
H	6.4227251	0.5540793	94.9662745
H	6.5588974	2.2219214	94.3358670
C	5.8469658	1.2185610	100.7052063
C	5.3391034	1.5532085	98.1918745
C	4.8368620	1.9090346	95.6701134
H	4.4607901	2.6735571	101.5969239
H	3.2135279	3.3532756	95.8957505
H	6.1688210	2.9093155	102.0850335
H	6.6901974	6.3479795	99.2286479
H	4.5885312	3.9821469	94.9506881
H	9.7428863	4.0116967	99.0234698
H	5.0567591	0.4509806	100.5742640
H	4.1418952	1.0698427	95.8731336
H	7.3734408	3.3927454	100.2521651
C	-2.2311667	9.7785022	97.3152259
C	1.0995003	7.6375379	98.8827866
C	-2.0869023	8.4106207	97.0209873
C	-0.1976906	9.7274367	98.6378557
C	-0.0410824	8.3490530	98.3387430
C	-1.2887836	10.4360979	98.1299756
C	-1.0040915	7.6885613	97.5342662
O	1.2629708	6.3816130	98.7256806
H	-3.0882454	10.3382693	96.9102227
H	0.5495407	10.2326229	99.2708777
H	-2.8265205	7.8980052	96.3891837
H	-1.4112681	11.5040203	98.3647223
H	-0.9039500	6.6120799	97.3182495
H	1.7820268	8.1701610	99.5814713
C	2.9519057	8.7324230	97.1864098
C	3.1897900	7.5229933	96.5751659
C	4.6019002	7.1374595	96.9216399
O	5.1503967	8.1232981	97.6992276
C	4.1921486	9.1628180	97.9171128
O	5.2228874	6.1567195	96.5706853
C	2.3757531	6.6455025	95.7737018
H	2.0898852	9.3905056	97.0231597
H	4.6088938	10.1200944	97.5287811
H	4.0527241	9.2742283	99.0168230
H	2.9787736	6.0267510	95.0796262
H	1.5229974	7.1334918	95.2660675



Energy (Hartree) = -11970.03645194

Zn	-4.3002833	8.2016430	719.4406272
Br	-2.7136973	8.5701692	721.0346776
C	-7.7531924	8.4125238	711.0420015
C	-6.7016991	8.2871174	711.9628379
C	-6.9722407	8.0992959	713.3321823
C	-8.3115153	8.0178705	713.7584202
C	-9.3665603	8.1417767	712.8387920
C	-9.0893484	8.3446540	711.4771559
H	-7.5308021	8.5567438	709.9730248
H	-5.6523007	8.3093788	711.6310616
C	-5.8263212	7.9938532	714.3329280
H	-8.5293157	7.8285997	714.8220096
H	-10.4092586	8.0682660	713.1872083
H	-9.9128767	8.4380496	710.7524457
O	-4.7298149	7.3167770	713.8200731
C	-5.3186225	9.4299671	714.7653491
C	-4.4757904	9.2969667	716.0054304
C	-5.3084738	9.7547673	717.1305337
O	-6.4079377	10.3552046	716.6915864
C	-6.3954315	10.4224460	715.2277201
O	-5.1136422	9.6642930	718.3617849
C	-3.2431594	8.7669191	716.1528675
H	-6.1577535	11.4697704	714.9558103
H	-7.4198785	10.1833065	714.8896091
Zn	-4.4344826	5.5560758	714.3974021
Br	-4.5985846	3.3564622	713.7392477
C	-6.5418790	3.7396569	718.0338957
C	-5.8491357	2.5510829	718.2963196
C	-6.4445549	1.6150364	719.2196842
C	-5.7637479	0.4480088	719.6825602
C	-7.7691114	1.8776663	719.7304401
C	-8.3739267	0.9406283	720.6216226
C	-8.4391119	3.0786277	719.3615343
H	-9.4576160	3.2579337	719.7391150
C	-7.8375998	4.0348758	718.5517982
C	-2.1629791	3.0975449	717.3678072
C	-1.8616472	1.9046902	716.7213551
H	-0.8354112	1.7247550	716.3683557
C	-2.8569980	0.9200931	716.4532984
C	-2.5456851	-0.2513757	715.7003416
C	-4.2119334	1.1216852	716.9086225
C	-5.2037593	0.1673242	716.5362437
C	-4.5140467	2.2999813	717.6812553
C	-3.5031656	3.2478181	717.8394210
O	-5.9871247	4.6885989	717.1759824
O	-3.8160790	4.4343423	718.5133374
P	-4.6420343	5.5203427	717.6139229
O	-5.0125866	6.6545543	718.5807158
O	-3.9338192	5.8950705	716.3178967
C	-7.6945226	-0.1977120	721.0279777
C	-6.3727771	-0.4346023	720.5638666
H	-9.3899282	1.1492724	720.9921564
H	-8.1694782	-0.9095179	721.7202143
H	-4.7378033	0.2546222	719.3404665
H	-5.8232970	-1.3235162	720.9096165

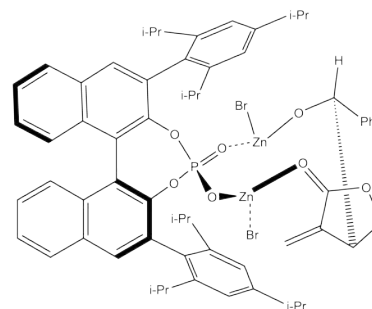
7.1.4 Product Complexes 15

15a-mi; COSMO

C	-4.8710631	-0.9523042	715.7861378
C	-3.5294008	-1.1734241	715.3752849
H	-6.2472574	0.3350388	716.8377098
H	-5.6552229	-1.6702735	715.5010689
H	-3.2767468	-2.0675576	714.7851741
H	-1.5073565	-0.3991917	715.3641823
C	-8.4719193	6.4374742	719.0615911
C	-8.5390960	5.3108328	718.1934459
C	-9.2182321	7.5825687	718.7337440
C	-9.2999736	5.3735523	716.9971217
C	-10.0279372	6.5481974	716.7149930
C	-10.0178148	7.6580994	717.5762902
H	-9.1945675	8.4524778	719.4098171
C	-9.3269400	4.2062862	716.0107538
H	-10.6345246	6.5800788	715.7979273
C	-8.4560262	4.4994773	714.7733723
H	-8.8697930	5.3380677	714.1767374
H	-8.3964443	3.6094910	714.1141176
H	-7.4197272	4.7635321	715.0613776
C	-10.7551637	3.8046658	715.6056327
H	-8.8787631	3.3315075	716.5253598
H	-11.2595230	4.6028532	715.0217669
H	-11.3832400	3.5864601	716.4932844
H	-10.7342692	2.8980713	714.9668037
C	-10.8156229	8.9314928	717.3020063
C	-9.9186474	10.0371366	716.7104443
H	-10.4673603	10.9995415	716.6471357
H	-9.5983570	9.7669792	715.6827201
H	-9.0052036	10.1970827	717.3166699
C	-12.0571194	8.7133702	716.4271292
H	-11.1652981	9.2929561	718.2952084
H	-12.6576995	9.6434820	716.3686394
H	-12.7063870	7.9078178	716.8253794
H	-11.7810442	8.4422781	715.3861059
C	-7.6336492	6.4056857	720.3405335
C	-6.9949059	7.7653466	720.6815544
H	-6.1497355	7.6333741	721.3912986
H	-7.7070137	8.4595280	721.1739879
H	-6.6538337	8.2920356	719.7649766
C	-8.4478223	5.8937670	721.5443650
H	-6.8051478	5.6901911	720.1635714
H	-7.8220172	5.8699050	722.4605894
H	-8.8325363	4.8704572	721.3707351
H	-9.3174538	6.5556832	721.7388425
H	1.8807538	7.9296303	717.2972974
H	0.7829158	3.8642100	721.0091233
H	-0.1932985	3.4195135	713.3453471
C	1.1121377	7.9007921	718.1026920
H	-2.2595889	4.0207555	722.0140776
H	0.7058631	10.0580357	717.9472418
C	0.3546992	6.5867391	717.9352519
C	0.0263331	3.1275219	720.6663021
C	0.1612348	9.0939758	717.8719815
H	-0.6471833	9.0975067	718.6340668
C	-0.0781414	5.8171142	719.0266371
C	0.0807471	3.7805314	714.3582840
H	2.5002167	7.1769423	719.6507199
C	0.0213695	6.1344939	716.6445320
C	1.8364800	8.0415810	719.4474879
H	2.4570061	8.9603581	719.4574870
H	0.3713971	6.7176673	715.7770247
C	-1.9324494	4.6700515	721.1758988
H	-0.2428239	2.4901472	721.5342313
H	0.5065575	2.4837150	719.9014989
C	-0.8464264	4.6493462	718.8616457
C	-1.4754602	5.7412112	714.0768712
C	-0.7556138	4.9840931	716.4221962
H	0.3638842	2.9010441	714.9695599
H	0.9828942	4.4211193	714.2633498
C	-1.2201207	3.8348412	720.0993367
C	-1.2084606	4.2362911	717.5502350

C	-1.0834296	4.5672872	714.9900723
H	-2.8247008	5.1770009	720.7612202
H	-1.2706021	5.4523150	721.6012143
H	-0.3098234	9.0478803	716.8695592
H	1.1170359	8.1251394	720.2887017
H	-1.9226787	3.0373801	719.7827069
H	-1.9618406	3.8911459	715.0318989
H	0.1801835	6.1334119	720.0472796
H	-0.6103254	6.3821373	713.8068734
H	-2.2158113	6.4122003	714.5609819
H	-1.9002960	5.3610798	713.1243727
H	-4.7522335	9.8200014	713.8971125
H	-6.2509187	7.5263895	715.2639259
H	-2.7718930	8.6635885	717.1437122
H	-2.6634732	8.4351168	715.2816282

15a-mi

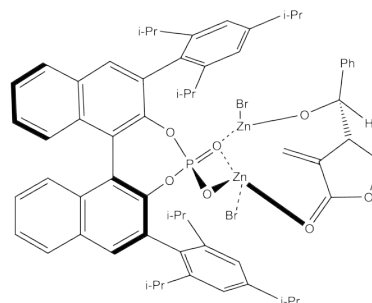


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Zn	-4.1760991	8.2016176	719.4243092
Br	-2.6369057	8.6050347	721.0457316
C	-7.7737504	8.3259806	711.0621498
C	-6.7238413	8.2068119	711.9848628
C	-6.9966376	8.0635956	713.3586834
C	-8.3365121	8.0163256	713.7880502
C	-9.3895181	8.1345315	712.8657907
C	-9.1098867	8.2956102	711.4995416
H	-7.5502072	8.4338383	709.9892261
H	-5.6735369	8.1949872	711.6558087
C	-5.8494726	7.9667892	714.3593563
H	-8.5569550	7.8539434	714.8554868
H	-10.4327122	8.0870654	713.2171615
H	-9.9321118	8.3833133	710.7727650
O	-4.7509734	7.2950324	713.8513985
C	-5.3480978	9.4109511	714.7780003
C	-4.4712547	9.2880403	715.9940452
C	-5.2755450	9.7392664	717.1419342
O	-6.3956305	10.3268867	716.7318328
C	-6.4247846	10.3890614	715.2700468
O	-5.0435819	9.6536752	718.3656783
C	-3.2348910	8.7570413	716.1041481
H	-6.2114128	11.4396429	714.9873401
H	-7.4541137	10.1340109	714.9593674
Zn	-4.4483999	5.5318310	714.4212154
Br	-4.5647270	3.3392935	713.7559376
C	-6.5325909	3.7603073	718.0348782
C	-5.8468343	2.5653687	718.2894334
C	-6.4538972	1.6221716	719.1979867
C	-5.7806844	0.4488213	719.6552674
C	-7.7823939	1.8824289	719.6987199
C	-8.3971384	0.9381436	720.5745560
C	-8.4457878	3.0874906	719.3333575
H	-9.4686235	3.2662976	719.6994992
C	-7.8344497	4.0508587	718.5397847
C	-2.1532183	3.0956034	717.3771155
C	-1.8575693	1.9042887	716.7256005

H	-0.8318159	1.7223864	716.3724480	H	-0.6507636	9.1161134	718.5927046
C	-2.8571832	0.9266255	716.4495005	C	-0.0817027	5.8264674	719.0336324
C	-2.5508106	-0.2415491	715.6903194	C	0.1126390	3.7660629	714.3761698
C	-4.2127365	1.1340430	716.8999720	H	2.4718163	7.2027743	719.6856206
C	-5.2089083	0.1893979	716.5158658	C	0.0336726	6.1286298	716.6512095
C	-4.5101992	2.3092318	717.6794498	C	1.8121604	8.0646726	719.4596721
C	-3.4933735	3.2483298	717.8479802	H	2.4330878	8.9831159	719.4693210
O	-5.9690400	4.7203036	717.1956525	H	0.3894360	6.7060936	715.7821800
O	-3.8012316	4.4314114	718.5300875	C	-1.9294403	4.6805338	721.1864032
P	-4.6099235	5.5301073	717.6323381	H	-0.2374972	2.5024749	721.5467597
O	-4.9595175	6.6693085	718.6035747	H	0.5090419	2.4935044	719.9127168
O	-3.9023332	5.8972552	716.3338644	C	-0.8440714	4.6547994	718.8705332
C	-7.7248111	-0.2054948	720.9757142	C	-1.4476041	5.7208314	714.0768458
C	-6.4000058	-0.4408237	720.5214361	C	-0.7391903	4.9756220	716.4299307
H	-9.4159575	1.1458236	720.9377963	H	0.3967578	2.8917280	714.9942594
H	-8.2080418	-0.9228010	721.6563569	H	1.0137785	4.4081723	714.2826046
H	-4.7524035	0.2568810	719.3198315	C	-1.2180912	3.8439007	720.1104811
H	-5.8558198	-1.3345596	720.8628959	C	-1.1975358	4.2332779	717.5594534
C	-4.8800330	-0.9269466	715.7600363	C	-1.0573574	4.5521953	714.9975261
C	-3.5385714	-1.1544643	715.3544370	H	-2.8235269	5.1852611	720.7733194
H	-6.2525319	0.3633852	716.8126647	H	-1.2692572	5.4646237	721.6105835
H	-5.6679644	-1.6366351	715.4652188	H	-0.2891762	9.0377725	716.8330343
H	-3.2890947	-2.0455458	714.7585745	H	1.0775484	8.1599185	720.2861944
H	-1.5122993	-0.3930260	715.3565904	H	-1.9204087	3.0453918	719.7958443
C	-8.4652125	6.4529034	719.0534690	H	-1.9351338	3.8750701	715.0349300
C	-8.5364027	5.3275321	718.1845132	H	0.1684574	6.1497073	720.0539513
C	-9.2162422	7.5963848	718.7319105	H	-0.5825255	6.3628905	713.8087216
C	-9.3074438	5.3886406	716.9942625	H	-2.1949024	6.3886980	714.5536851
C	-10.0412373	6.5613166	716.7202181	H	-1.8681417	5.3344671	713.1252587
C	-10.0263570	7.6702133	717.5824273	H	-4.8103887	9.8036999	713.8927486
H	-9.1889982	8.4654045	719.4088010	H	-6.2716541	7.5074343	715.2960513
C	-9.3338810	4.2225682	716.0060690	H	-2.7327871	8.6509926	717.0793756
H	-10.6563383	6.5920431	715.8091197	H	-2.6872023	8.4208634	715.2141571
C	-8.4121346	4.4914536	714.7997221				
H	-8.7829157	5.3403914	714.1898842				
H	-8.3519188	3.6008230	714.1416976				
H	-7.3795901	4.7280231	715.1221592				
C	-10.7555856	3.8586274	715.5474661				
H	-8.9281032	3.3363065	716.5363371				
H	-11.2113246	4.6625368	714.9324237				
H	-11.4269627	3.6701081	716.4097042				
H	-10.7354073	2.9445741	714.9196416				
C	-10.8321190	8.9409504	717.3186624				
C	-9.9479281	10.0521184	716.7181781				
H	-10.4990072	11.0140653	716.6692663				
H	-9.6458512	9.7882849	715.6833070				
H	-9.0246734	10.2105492	717.3099941				
C	-12.0834015	8.7185594	716.4591305				
H	-11.1719624	9.2991391	718.3165660				
H	-12.6894634	9.6455361	716.4080118				
H	-12.7237310	7.9096137	716.8643944				
H	-11.8186291	8.4492754	715.4147855				
C	-7.6223246	6.4200776	720.3293631				
C	-6.9953938	7.7828694	720.6783889				
H	-6.1524278	7.6537532	721.3909051				
H	-7.7173959	8.4674369	721.1702407				
H	-6.6429335	8.3121765	719.7692664				
C	-8.4286933	5.8893105	721.5302198				
H	-6.7871981	5.7141385	720.1447310				
H	-7.8021950	5.8670881	722.4459854				
H	-8.8000502	4.8621807	721.3509294				
H	-9.3067021	6.5383714	721.7301263				
H	1.8949755	7.9229253	717.3125166				
H	0.7865368	3.8754821	721.0166047				
H	-0.1550133	3.3975657	713.3643360				
C	1.1117486	7.9063303	718.1043689				
H	-2.2552167	4.0329587	722.0262672				
H	0.7125515	10.0623020	717.9097545				
C	0.3565301	6.5903777	717.9407976				
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C	0.1674309	9.0980340	717.8414278				

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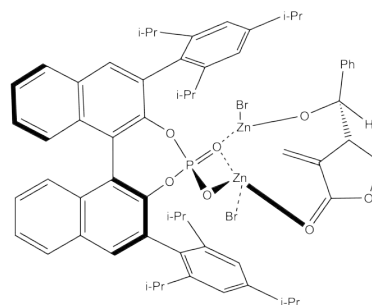


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C	0.8451192	-0.7072197	90.6661056
C	1.7750532	-1.6726463	91.1572244
C	-0.3848794	-0.5100192	91.3960050
C	-0.6526785	-1.3163571	92.5428795
C	-1.3099737	0.4824675	90.9607096
H	-2.2758333	0.5766552	91.4804478
C	-1.0268989	1.3278142	89.8953514
C	4.4498191	0.6355920	87.6759733
C	4.7025123	-0.6398840	87.1887240
H	5.6654782	-0.8496950	86.6991307
C	3.7440302	-1.6891110	87.3026969
C	3.9784437	-2.9662648	86.7115345
C	2.5117622	-1.4619785	88.0192264
C	1.5481527	-2.5123097	88.0625319
C	2.2819025	-0.1698134	88.6185985
C	3.2060480	0.8359708	88.3444041
O	0.4741845	2.0073739	88.1524228
O	2.9599950	2.1303380	88.8227060
P	1.7615517	3.0101190	88.1736767

O	1.6474757	4.2482827	89.0936711	H	7.3047177	-0.0338154	91.3878330
O	1.9291145	3.4722910	86.7007274	H	7.8817777	0.0235473	89.6882563
C	0.2639087	-2.2606710	92.9804854	C	6.1905996	2.0527318	88.8028196
C	1.4927477	-2.4275552	92.2875498	C	4.3534404	3.5802431	84.4572307
H	-1.6006768	-1.1637248	93.0821707	C	5.5599586	2.5874971	86.4808649
H	0.0480367	-2.8714266	93.8702797	H	5.7674940	0.3896833	84.7692434
H	2.7332994	-1.8065674	90.6364580	H	6.4611122	1.8038752	83.9154472
H	2.2308642	-3.1582375	92.6519166	C	6.0704226	1.2103398	90.0725756
C	1.7986750	-3.7369140	87.4588683	C	5.4356312	1.7643761	87.6330522
C	3.0283342	-3.9736862	86.7887161	C	4.7633616	2.3043553	85.2103175
H	0.5863709	-2.3366606	88.5641798	H	4.4249033	2.4075031	90.9020576
H	1.0339209	-4.5278072	87.4933478	H	3.8880261	4.3214203	85.1380569
H	3.2179750	-4.9507241	86.3187357	H	6.0430680	2.8678099	91.5202065
H	4.9261282	-3.1304836	86.1751625	H	6.2418120	6.5655267	87.9544489
C	-1.9992798	3.6785390	89.8100632	H	5.2232595	4.0696821	83.9725203
C	-2.0086148	2.3273460	89.3617148	H	9.3280944	4.8227556	89.4318608
C	-2.9001723	4.5833234	89.2261745	H	5.4063529	0.3512250	89.8459254
C	-2.9249722	1.9100624	88.3613476	H	3.8352475	1.7779139	85.5265404
C	-3.8033449	2.8631172	87.8033098	H	7.6167404	3.3979632	89.7168788
C	-3.8034659	4.2056452	88.2127616	C	1.3929643	5.5340956	79.6408369
H	-2.9005055	5.6310448	89.5640322	C	1.0620954	4.9505408	80.8724112
C	-2.9969630	0.4605741	87.8793927	C	1.4287297	5.5790322	82.0789359
H	-4.5047805	2.5334410	87.0226152	C	2.1495479	6.7880498	82.0336602
C	-2.5901435	0.3134485	86.4028172	C	2.4803426	7.3742672	80.7991614
H	-3.2427051	0.9167010	85.7366728	C	2.0988953	6.7504812	79.6006289
H	-2.6729823	-0.7450880	86.0808718	H	1.1049404	5.0341216	78.7028163
H	-1.5391116	0.6221484	86.2366278	H	0.5330162	3.9860649	80.9150004
C	-4.3863921	-0.1456336	88.1495984	C	1.0440620	4.9511402	83.4120095
H	-2.2679726	-0.1274605	88.4727681	H	2.4716598	7.2643345	82.9745029
H	-5.1782917	0.3658895	87.5632977	H	3.0481082	8.3173932	80.7759448
H	-4.6587610	-0.0664604	89.2218907	H	2.3605898	7.2058874	78.6329668
H	-4.4045969	-1.2186534	87.8679763	O	1.2167522	3.5902078	83.3989502
C	-4.7091247	5.2659728	87.5898384	Zn	1.6842177	5.7030216	87.7721764
C	-3.8976666	6.1941711	86.6624177	Br	3.0814446	7.2128997	86.7788687
H	-4.5330931	7.0106272	86.2611590	H	-0.0344024	7.4641847	83.4282298
H	-3.4938771	5.6207672	85.8012330	Br	1.2142071	0.2649160	85.0876785
H	-3.0431398	6.6562320	87.1955046	Zn	1.2885294	2.5829339	84.9869295
C	-5.9303962	4.6986126	86.8566296	C	-0.4998147	5.6001969	83.7266196
H	-5.0822751	5.8919990	88.4318461	C	-0.7320379	6.7954936	83.9656068
H	-6.6000418	5.5189831	86.5283279	C	-0.8110663	4.7296578	85.0669281
H	-6.5177567	4.0149427	87.5022093	C	-1.1156433	3.4563502	85.4362989
H	-5.6348230	4.1353802	85.9465301	C	-0.5199015	5.8171712	86.0213730
C	-1.0711204	4.1238433	90.9385216	O	-0.4853378	6.9903630	85.3969584
C	-0.6601839	5.6015470	90.8585533	O	-0.2713897	5.7251810	87.2405175
H	0.1555504	5.8097378	91.5793880	H	-1.7752570	7.1097026	83.7623354
H	-1.5014922	6.2805281	91.1100217	H	-1.1040768	4.8868871	82.8977432
H	-0.3019446	5.8664251	89.8458233	H	1.6436497	5.4699148	84.2090202
C	-1.7011268	3.8191894	92.3125567	H	-1.2283420	3.1933416	86.5004441
H	-0.1417782	3.5224526	90.8525179	H	-1.3964188	2.7047349	84.6829784
H	-1.0152007	4.1152710	93.1331297				
H	-1.9277910	2.7419024	92.4321033				
H	-2.6504084	4.3807631	92.4389640				
H	8.1677531	5.5957011	86.6672806				
H	8.1494943	1.4200900	90.7772940				
H	4.8909001	1.1080981	83.3817350				
C	8.0151033	5.2790706	87.7228273				
H	5.2598728	1.3660385	92.1058290				
H	7.7915110	7.3577826	88.4092809				
H	3.6274181	3.3469618	83.6521714				
C	7.1780988	4.0067338	87.6821752				
C	7.4267205	0.6237070	90.5022776				
C	7.2293159	6.4008311	88.4319639				
H	7.0467171	6.1379453	89.4954738				
C	7.0484964	3.1680276	88.8017630				
C	5.5141746	1.3443356	84.2687610				
H	9.9646435	4.2678094	87.8511416				
C	6.4357254	3.6871952	86.5325014				
C	9.4014660	5.0797417	88.3543751				
H	10.0005015	6.0106974	88.2822298				
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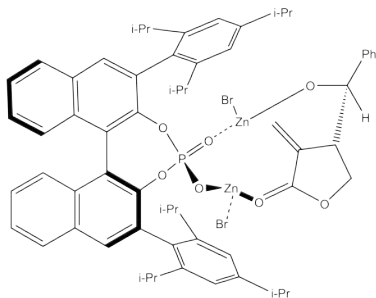


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C	0.8418123	-0.7038654	90.6721684
C	1.7702801	-1.6682310	91.1673616
C	-0.3895082	-0.5050118	91.3989740
C	-0.6587971	-1.3082411	92.5470646
C	-1.3132812	0.4860241	90.9585551

H	-2.2807257	0.5828545	91.4749555	H	7.7903540	7.3555063	88.3644502
C	-1.0281415	1.3288272	89.8920043	H	3.6309854	3.3214739	83.6310935
C	4.4489098	0.6289111	87.6764248	C	7.1768004	3.9992883	87.6602672
C	4.7006368	-0.6489217	87.1954438	C	7.4263666	0.6279454	90.4950271
H	5.6634955	-0.8590733	86.7058515	C	7.2271392	6.3993048	88.3912508
C	3.7433636	-1.6981895	87.3149170	H	7.0406758	6.1437903	89.4557327
C	3.9770514	-2.9776957	86.7297126	C	7.0479946	3.1673915	88.7844229
C	2.5118517	-1.4681841	88.0314893	C	5.5062149	1.3144960	84.2649622
C	1.5488163	-2.5185534	88.0800636	H	9.9614281	4.2584788	87.8318505
C	2.2822471	-0.1733157	88.6252856	C	6.4330696	3.6733357	86.5137996
C	3.2059857	0.8313338	88.3457298	C	9.3995471	5.0766874	88.3259190
O	0.4762009	2.0058182	88.1523789	H	10.0005350	6.0056118	88.2452488
O	2.9619320	2.1276100	88.8194250	H	6.5247754	4.3233741	85.6304850
P	1.7621437	3.0091728	88.1785551	C	5.4182936	2.0249643	91.2068752
O	1.6503383	4.2551127	89.0849750	H	7.3068799	-0.0233623	91.3854976
O	1.9250040	3.4797850	86.7018597	H	7.8752172	0.0214156	89.6825328
C	0.2562917	-2.2512802	92.9887835	C	6.1900619	2.0527027	88.7930798
C	1.4856694	-2.4201823	92.2985260	C	4.3557705	3.5557326	84.4368820
H	-1.6075176	-1.1536662	93.0845224	C	5.5574663	2.5736874	86.4687112
H	0.0386301	-2.8593506	93.8799095	H	5.7545809	0.3617820	84.7711337
H	2.7285944	-1.8032053	90.6472295	H	6.4556770	83.9096239	83.9096239
H	2.2228416	-3.1503456	92.6656482	C	6.0708856	1.2182335	90.0681179
C	1.7994953	-3.7454927	87.4822558	C	5.4343510	1.7575239	87.6258331
C	3.0280441	-3.9849126	86.8123627	C	4.7599203	2.2840294	85.2001290
H	0.5874601	-2.3400681	88.5812323	H	4.4340713	2.4279797	90.8972365
H	1.0347186	-4.5360759	87.5205342	H	3.8947988	4.3060799	85.1106955
H	3.2173999	-4.9635814	86.3458987	H	6.0551955	2.8831818	91.5075736
H	4.9236547	-3.1434058	86.1920357	H	6.2411318	6.5626758	87.9107158
C	-2.0013123	3.6785008	89.8011821	H	5.2281642	4.0377044	83.9494793
C	-2.0096717	2.3267480	89.3552683	H	9.3261480	4.8309906	89.4059723
C	-2.9061677	4.5798435	89.2186000	H	5.4025781	0.3604703	89.8486099
C	-2.9260714	1.9063632	88.3564755	H	3.8298867	1.7624567	85.5197885
C	-3.8089402	2.8561334	87.8007738	H	7.6174237	3.4023388	89.6974250
C	-3.8122517	4.1984358	88.2098338	C	1.4899313	5.5789640	79.6802772
H	-2.9068586	5.6280208	89.5548857	C	1.1449006	4.9764943	80.8981736
C	-2.9970971	0.4558447	87.8775980	C	1.4566860	5.6094014	82.1171256
H	-4.5122945	2.5234323	87.0230769	C	2.1422177	6.8393594	82.0993465
C	-2.6266177	0.3072112	86.3918065	C	2.4871894	7.4435029	80.8782464
H	-3.2972531	0.9062006	85.7398973	C	2.1566465	6.8171510	79.6666278
H	-2.7139727	-0.7518352	86.0732703	H	1.2455899	5.0757814	78.7316747
H	-1.5804646	0.6170419	86.1989161	H	0.6515941	3.9928697	80.9253914
C	-4.3747930	-0.1591258	88.1856721	C	1.0493112	4.9632998	83.4344265
H	-2.2487319	-0.1252531	88.4534563	H	2.4287200	7.3145885	83.0526012
H	-5.1857076	0.3485015	87.6225490	H	3.0279509	8.4025876	80.8757104
H	-4.6185543	-0.0810133	89.2647682	H	2.4299477	7.2871191	78.7092792
H	-4.3957585	-1.2321889	87.9045292	O	1.2211868	3.6052415	83.4094985
C	-4.7235234	5.2553233	87.5894731	Zn	1.7116594	5.6465732	87.6762963
C	-3.9202596	6.1799306	86.6516507	Br	3.0752504	7.2337769	86.7723834
H	-4.5592254	6.9933039	86.2494030	H	-0.0672865	7.4679615	83.4240525
H	-3.5201665	5.6016346	85.7919753	Br	1.1948232	0.2625047	85.1169001
H	-3.0626957	6.6462728	87.1758841	Zn	1.3039399	2.5688310	84.9751631
C	-5.9505937	4.6841924	86.8691570	C	-0.5051347	5.3003544	83.7212684
H	-5.0910617	5.8844753	88.4317338	C	-0.7601332	6.7921800	83.9594585
H	-6.6254828	5.5015550	86.5442076	C	-0.8258180	4.7257271	85.0571206
H	-6.5304191	4.0010058	87.5217301	C	-1.1169710	3.4487531	85.4234601
H	-5.6628693	4.1190453	85.9577708	C	-0.5414856	5.8141811	86.0128910
C	-1.0687384	4.1295553	90.9236060	O	-0.5259115	6.9909043	85.3893238
C	-0.6619693	5.6079764	90.8356175	O	-0.2762834	5.7225479	87.2270608
H	0.1631104	5.8184168	91.5448094	H	-1.8067362	7.0913909	83.7470849
H	-1.5009881	6.2854166	91.0992152	H	-1.0861856	4.8791817	82.8796690
H	-0.3178603	5.8718954	89.8181033	H	1.6295515	5.4772838	84.2494604
C	-1.6900889	3.8270716	92.3018053	H	-1.2288807	3.1812322	86.4865317
H	-0.1377402	3.5313688	90.8343461	H	-1.3823576	2.6929647	84.6688598
H	-1.0021739	4.1313294	93.1175665				
H	-1.9086206	2.7489943	92.4281386				
H	-2.6424499	4.3826072	92.4307340				
H	8.1678994	5.5796766	86.6343963				
H	8.1545593	1.4223265	90.7610075				
H	4.8818276	1.0751171	83.3798177				
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H	5.2675302	1.3885359	92.1035989				

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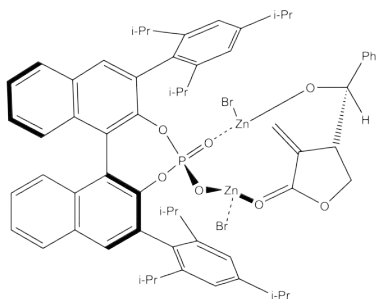
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C	2.8854345	-1.2751905	101.8848946
C	2.0433961	0.7322683	103.0358672
C	2.4625888	0.1568926	104.2732538
C	1.4829184	2.0406437	102.9887882
H	1.3338875	2.5912865	103.9303010
C	1.1427805	2.6459777	101.7854445
C	2.7022091	-0.2401698	96.9206099
C	2.2322340	-1.5408949	96.7911078
H	2.3809785	-2.0814873	95.8448992
C	1.5016579	-2.1836254	97.8344641
C	0.9450790	-3.4834075	97.6414622
C	1.2662103	-1.4986542	99.0838784
C	0.4256795	-2.1222420	100.0519382
C	1.8533339	-0.1962338	99.2803801
C	2.5113857	0.3814087	98.1956779
O	0.8756577	2.4966597	99.4145222
O	3.0400820	1.6630109	98.3609569
P	1.9843503	2.9019754	98.2696785
O	2.8027767	4.1214964	98.7178327
O	1.2011832	2.9900822	96.9624063
C	3.0730060	-1.0875029	104.3106848
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15c-ma



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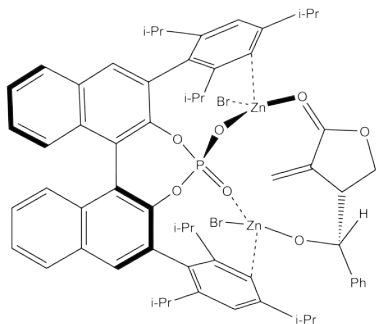
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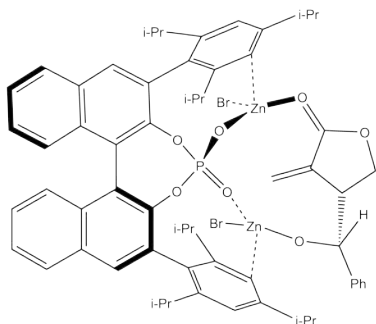
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H	3.3440017	6.7991882	267.1216324
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H	5.3517777	1.3993563	270.7218173
H	4.1939689	3.8474685	266.8238088
H	5.8275834	4.7271782	272.4282806
Zn	-1.3949481	3.0837171	271.3352683
Br	-2.0896306	3.8196942	273.4425912
C	1.9153757	10.8477948	267.0517477
C	1.6521690	9.7737889	267.9143886
C	1.1402962	8.5594188	267.4135674
C	0.9173264	8.4375094	266.0283164
C	1.1793963	9.5121879	265.1605962
C	1.6758117	10.7222200	265.6709789
H	2.3166127	11.7904472	267.4563753
H	1.8579661	9.8519775	268.9930918
C	0.8440239	7.4152998	268.3788691
H	0.5589053	7.4788891	265.6179834
H	1.0058122	9.3980944	264.0790779
H	1.8864688	11.5641343	264.9933059
O	1.8182447	7.3262195	269.3514812
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C	-1.5578240	5.5098289	269.4228391
O	-2.0166209	5.9038745	268.2282611
C	-1.7228048	7.3242763	268.0314275
O	-1.7523094	4.3392674	269.7871259
C	-0.4917394	6.6294799	271.3901769
H	-2.6539780	7.8882881	268.2419566
H	-1.4533886	7.4523650	266.9665927
Zn	2.2283560	5.6692567	270.1673210
Br	2.1801536	4.9814100	272.4273117
H	-0.7500968	5.8040525	272.0710855
H	0.0320936	7.4979968	271.8147004
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H	-1.6400079	-2.0614354	268.6494678
C	-0.6286007	-0.1619365	268.5851410
C	4.6705430	2.2936713	268.5699053
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H	6.5279053	2.3930182	267.4885973
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C	6.1184691	0.5003846	265.5998457
C	3.9464528	0.1994101	266.7539074
C	3.5769484	-0.7051566	265.7128176
C	3.0794158	0.5128152	267.8664550
C	3.4508500	1.5628961	268.7182913
O	0.6319392	1.8653271	268.2411542
O	2.6403160	1.8987596	269.7986323
P	1.2222155	2.6988583	269.5416529
O	0.3775286	2.4126576	270.7917885
O	1.4196620	4.1379607	269.0577295
C	1.5956821	-4.5160352	268.2699326
C	2.8596131	-3.8706451	268.2214579
H	-0.5482409	-4.2414147	268.3987364
H	1.5396743	-5.6149855	268.2898798
H	3.9326141	-2.0035965	268.1545086
H	3.7810164	-4.4726565	268.2215424
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C	5.7421124	-0.4127642	264.6273297
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H	4.1375683	-1.6987147	263.8840415
H	6.4308610	-0.6646924	263.8067115
H	7.1020801	0.9938437	265.5549456
C	-2.0822725	0.5795291	270.4906340
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C	-3.1320445	1.3926226	270.9899002
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H	-4.2111651	2.8531238	268.1011238
C	-1.8459825	3.0108491	266.3503123
H	-2.6635639	3.7358364	266.5395073
H	-1.5970335	3.0533622	265.2699356
H	-0.9611928	3.3477654	266.9226036
C	-3.4246015	1.0584672	265.9039588
H	-1.3788150	0.9193550	266.5395927
H	-4.3330950	1.6808598	266.0431489
H	-3.6870942	0.0154060	266.1735904
H	-3.1690053	1.0806733	264.8247168
C	-5.0941435	3.0019114	270.7116954
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H	-5.7701880	5.0678190	270.9542726
H	-4.7418695	4.8138521	269.5053479
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C	-6.4278356	2.5486609	270.0902480
H	-5.1317915	2.7816472	271.8004298
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H	-6.5847079	1.4581583	270.2141091
H	-6.4647683	2.7722689	269.0035382
C	-1.3906041	-0.4014882	271.4406502
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H	-1.7981960	-2.3861591	272.2802935
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H	-3.2354862	-1.3157468	272.2113918
H	6.1228976	7.8995796	270.8613483
H	7.3064949	2.8637582	272.5734421
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15c-mi

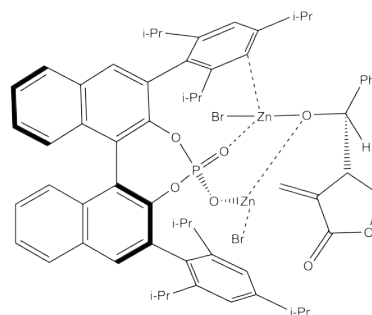


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C	2.9464324	-2.4860804	268.1820020
C	0.4942936	-2.3303399	268.3071017
C	0.4375383	-3.7563169	268.3215268

H	4.7587343	1.0303842	273.1014316
H	4.3241714	9.1556192	271.9986070
H	3.1924521	5.8124623	265.6523810
C	5.2143641	5.9895313	270.7915938
C	7.0168823	2.0804281	271.8421928
C	4.1145143	8.1428694	271.5972391
H	3.3943693	7.6429020	272.2769888
C	5.4688891	4.7463870	271.3908004
C	5.7461627	5.3473350	266.5075892
H	7.0337847	6.6535370	272.8537153
C	4.7752349	5.9883207	269.4448370
C	6.0641898	7.1902475	272.8914187
H	6.2514271	8.1930044	273.3249844
H	4.6005894	6.9515957	268.9404572
C	4.5940184	2.0232423	272.6340281
H	7.2054115	1.0957919	272.3176181
H	7.6895898	2.1742396	270.9654143
C	5.2834316	3.5277100	270.7075967
C	3.2601091	5.7693576	266.7585466
C	4.6564182	4.7977869	268.6921152
H	6.6035280	4.7004789	266.7830645
H	6.0016335	6.3843589	266.8095222
C	5.5380890	2.2108519	271.4337188
C	4.8872637	3.5524849	269.3488104
C	4.4374417	4.8855597	267.1812789
H	3.5346200	2.0965869	272.3225177
H	2.3113583	5.3522078	267.1445540
H	4.7642580	2.7957409	273.4120229
H	3.6129170	8.2585275	270.6155001
H	3.3512474	6.8100953	267.1260851
H	5.3948919	6.6471106	273.5905604
H	5.3260313	1.3925585	270.7139931
H	4.2178446	3.8643355	266.8136331
H	5.7957249	4.7102528	272.4386414
Zn	-1.3615802	3.1128481	271.3611359
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C	1.9322046	10.8120619	266.9985082
C	1.6702949	9.7509276	267.8764498
C	1.1394516	8.5369293	267.3960402
C	0.8980645	8.4019058	266.0152979
C	1.1590255	9.4639089	265.1326758
C	1.6730732	10.6740238	265.6232020
H	2.3488758	11.7546733	267.3870337
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C	0.8444042	7.4063109	268.3775086
H	0.5289369	7.4405189	265.6209421
H	0.9717365	9.3394570	264.0546794
H	1.8833717	11.5061178	264.9335825
O	1.8222526	7.3225029	269.3457221
C	-0.5863247	7.6484271	269.0288990
C	-0.8512139	6.6309803	270.1005519
C	-1.5579307	5.5232885	269.4394383
O	-2.0236865	5.9199103	268.2461064
C	-1.7258007	7.3372490	268.0501273
O	-1.7491271	4.3521882	269.8009313
C	-0.4893407	6.6431727	271.4047934
H	-2.6525741	7.9064112	268.2699345
H	-1.4634072	7.4688464	266.9838070
Zn	2.2308069	5.6682142	270.1697616
Br	2.1555269	4.9783145	272.4226214
H	-0.7566452	5.8250230	272.0913468
H	0.0433363	7.5079739	271.8258308
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15d-ma; COSMO



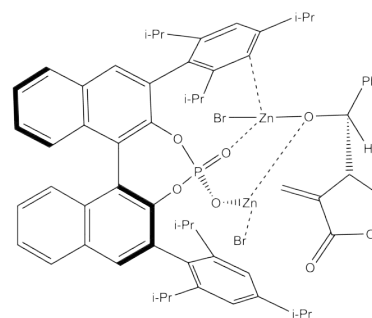
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H	1.5916735	10.2377826	328.2569133
Br	2.6322048	5.9525030	324.8149263
Zn	3.2085077	5.2187989	326.9787957
C	1.2666155	8.0877083	327.7667918
C	0.7785679	9.5352549	327.9915906
C	0.1606738	7.3003559	328.4111144
C	-0.1873679	6.0008108	328.2428992
C	-0.5922660	8.2267355	329.3287277
O	-0.1468155	9.4940155	329.1048965
O	-1.4636721	7.9593820	330.1286513
H	0.2400161	9.9287943	327.1054802
C	5.0728208	9.7000023	326.1755030
C	4.0513774	8.8347651	326.5996696
C	3.7516355	8.7013635	327.9707220
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C	5.5025360	10.3355924	328.4800600
C	5.7985281	10.4551483	327.1120228
H	5.2968027	9.7885122	325.1011818
H	3.4892002	8.2558388	325.8510743
C	2.6271008	7.8253825	328.4944815
H	4.2564483	9.3666676	329.9762240
H	6.0632258	10.9243824	329.2221517
H	6.5924568	11.1395750	326.7752760
O	2.9179925	6.4167731	328.5354938
C	0.0586674	0.9708542	329.3262438
C	0.8716239	-0.0978664	329.7325992
C	0.3732921	-0.9534366	330.7828602
C	1.1791275	-1.9471538	331.4161703
C	-0.9822824	-0.7762294	331.2462018
C	-1.4898675	-1.6386343	332.2644708
C	-1.7810919	0.2715822	330.7064292
H	-2.8196788	0.3786016	331.0534879
C	-1.2762328	1.1842568	329.7867683
C	4.3304168	0.7182931	328.2800643
C	4.7582306	-0.5210470	327.8233593
H	5.7259446	-0.6066311	327.3054060
C	3.9259846	-1.6757151	327.9227611
C	4.3484241	-2.9258480	327.3784054
C	2.6008328	-1.5647717	328.4917783
C	1.7356477	-2.6963646	328.4050154
C	2.2004965	-0.3106767	329.0889533
C	3.0849753	0.7624988	328.9774492
O	0.5326627	1.8795394	328.3730895
O	2.7516979	1.9705051	329.5788093
P	1.6683211	2.9537997	328.8453838
O	1.1956982	3.8873955	329.9746952
O	2.1853596	3.6043664	327.5600383
C	-0.6883503	-2.6142287	332.8376630
C	0.6618607	-2.7557363	332.4190339
H	-2.5298912	-1.5000874	332.5991393
H	-1.0893879	-3.2669681	333.6278884
H	2.2286805	-2.0608373	331.1109743
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C	2.1714998	-3.8924061	327.8503134
C	3.4944592	-4.0182109	327.3500104
H	0.7062027	-2.6144724	328.7791158
H	1.4818362	-4.7483613	327.7939561
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H	5.3646313	-2.9992199	326.9602566
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C	-3.7423608	4.4633273	328.3479237
H	-3.5725532	5.2428424	330.3575282
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H	-2.0078629	2.5160515	325.1168985
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C	-3.4144404	0.4873331	326.4922118
H	-1.4961512	0.5420482	327.4385066
H	-4.1322762	1.1403052	325.9531459
H	-3.9433992	0.0569646	327.3668491
H	-3.1413472	-0.3452420	325.8111751
C	-4.6222907	5.6207423	327.8841773
C	-3.7684437	6.8752037	327.6112235
H	-4.4089093	7.7314737	327.3138821
H	-3.0478457	6.6850796	326.7876753
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C	-5.5085795	5.2850953	326.6775563
H	-5.2939383	5.8622267	328.7385682
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H	-6.1043423	4.3650666	326.8463067
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H	5.5896463	6.5561148	326.2116635
H	7.7093795	3.1746650	330.5718291
H	5.1199781	0.4797055	323.7321528
C	6.3674409	6.0207058	326.8038931
H	5.1063656	3.0426357	332.4046048
H	7.0671712	7.9144912	327.6134638
H	2.7855786	1.4979005	323.8908685
C	5.7696822	4.6804413	327.2331200
C	7.1320461	2.2310055	330.6649222
C	6.7651618	6.9147936	327.9796519
H	7.6229901	6.4876756	328.5398149
C	5.8571325	4.2044791	328.5581044
C	5.4771498	1.1758686	324.5184669
H	7.2873806	5.2022792	324.9652216
C	5.2220665	3.8031885	326.2597732
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H	7.9757797	6.7613286	325.5181572
H	5.1728185	4.1394007	325.2119469
C	5.0036369	3.4357550	331.3730204
H	7.2685762	1.8516015	331.6983487
H	7.5751191	1.4934708	329.9654584
C	5.4576372	2.9060443	328.9177404
C	3.1596776	2.2208504	324.6441341
C	4.8322910	2.4787632	326.5687610
H	6.2875167	0.6713524	325.0834666
H	5.9217075	2.0579760	324.0114125
C	5.6370645	2.4600471	330.3658481

C	4.9493858	2.0312164	327.9162661
C	4.3131992	1.5901261	325.4403947
H	3.9228203	3.5750520	331.1755159
H	2.3196516	2.4956264	325.3109925
H	5.4900028	4.4328563	331.3531977
H	5.9250085	7.0608422	328.6847999
H	3.4673795	3.1378426	324.1018840
H	8.3767214	5.2431716	326.3893815
H	5.1282802	1.4817535	330.4821765
H	3.9138753	0.6655341	325.8992284
H	6.2678223	4.8624003	329.3352906
H	1.3795186	7.8340381	326.6933540
H	2.4791320	8.1420640	329.5533463
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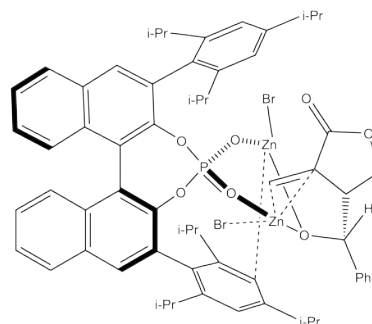
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H	1.5730836	10.2258066	328.2296797
Br	2.6965598	5.9630183	324.8016725
Zn	3.1954526	5.2270691	326.9748158
C	1.2634480	8.0727979	327.7469250
C	0.7636789	9.5186707	327.9634410
C	0.1538646	7.2827367	328.3822836
C	-0.1882265	5.9829927	328.2124853
C	-0.6136307	8.2084057	329.2898742
O	-0.1693125	9.4793703	329.0648409
O	-1.4929184	7.9390066	330.0774974
H	0.2344233	9.9060406	327.0676955
C	5.0793297	9.7192950	326.2128512
C	4.0561783	8.8477139	326.6188635
C	3.7425720	8.7027436	327.9855914
C	4.4695730	9.4567113	328.9318027
C	5.4856112	10.3348036	328.5263636
C	5.7939245	10.4678122	327.1626288
H	5.3134160	9.8174113	325.1415203
H	3.5051082	8.2711337	325.8600358
C	2.6146606	7.8204469	328.4918208
H	4.2261600	9.3481204	330.0013117
H	6.0380693	10.9180330	329.2788884
H	6.5888412	11.1576647	326.8396604
O	2.9158370	6.4141827	328.5363369
C	0.0626167	0.9775023	329.3201706
C	0.8723556	-0.0939327	329.7260382
C	0.3750063	-0.9453880	330.7798647
C	1.1783875	-1.9423724	331.4106681
C	-0.9770194	-0.7604620	331.2497416
C	-1.4830516	-1.6183799	332.2719215
C	-1.7726453	0.2899271	330.7112368
H	-2.8091105	0.4042575	331.0621627
C	-1.2690651	1.1981534	329.7867901
C	4.3334242	0.7088426	328.2718008

C	4.7556893	-0.5325846	327.8158962
H	5.7236255	-0.6212658	327.2986170
C	3.9193515	-1.6840198	327.9146464
C	4.3359031	-2.9361537	327.3715116
C	2.5951899	-1.5675604	328.4843583
C	1.7262863	-2.6962631	328.4001738
C	2.1993140	-0.3117260	329.0802640
C	3.0870141	0.7589720	328.9678526
O	0.5373224	1.8808876	328.3631716
O	2.7575717	1.9676084	329.5665425
P	1.6761398	2.9543316	328.8328021
O	1.2041465	3.8900708	329.9579764
O	2.1995261	3.5949135	327.5445128
C	-0.6845354	-2.5973495	332.8422763
C	0.6620498	-2.7468327	332.4167293
H	-2.5202770	-1.4729345	332.6122625
H	-1.0850759	-3.2463565	333.6357414
H	2.2254629	-2.0615258	331.0994656
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C	2.1572366	-3.8942530	327.8469661
C	3.4785532	-4.0252719	327.3451725
H	0.6981667	-2.6090588	328.7765222
H	1.4645427	-4.7478479	327.7929318
H	3.8121878	-4.9829394	326.9177243
H	5.3514572	-3.0136826	326.9524625
C	-2.4400471	3.4160826	330.1613363
C	-2.0823862	2.3511540	329.2824710
C	-3.2730775	4.4402940	329.6748318
C	-2.5223388	2.3720061	327.9304731
C	-3.3455054	3.4284648	327.4955589
C	-3.7509300	4.4649539	328.3515522
H	-3.5557253	5.2624604	330.3515058
C	-2.1736049	1.2654999	326.9356982
H	-3.6923379	3.4248037	326.4516143
C	-1.4064707	1.8114253	325.7175844
H	-2.0312768	2.5063607	325.1188734
H	-1.0973932	0.9829864	325.0471344
H	-0.4940051	2.3547273	326.0322590
C	-3.4299257	0.4816655	326.5124932
H	-1.5059551	0.5428196	327.4461751
H	-4.1524759	1.1306552	325.9751444
H	-3.9531431	0.0561470	327.3927105
H	-3.1616499	-0.3543595	325.8337995
C	-4.6407126	5.6154965	327.8896805
C	-3.7964411	6.8725896	327.6005640
H	-4.4438042	7.7228469	327.3009486
H	-3.0815988	6.6795245	326.7727142
H	-3.2144139	7.1830412	328.4902410
C	-5.5384272	5.2676793	326.6951179
H	-5.3050074	5.8584588	328.7494752
H	-6.2498191	6.0938501	326.4934862
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H	-4.9468217	5.1183840	325.7675696
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H	-0.9204695	4.8469735	332.9792412
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H	-0.5994460	5.1853610	331.2621323
C	-3.0703716	3.0926383	332.5943118
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C	7.1298272	2.2123319	330.6689808
C	6.7483977	6.9116326	327.9971374
H	7.6085156	6.4932360	328.5605850
C	5.8627028	4.1910226	328.5609580
C	5.5005453	1.1940660	324.4931134
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C	5.2454405	3.7916133	326.2591408
C	7.5740657	5.8046710	325.8794213
H	7.9730681	6.7822063	325.5403318
H	5.1932118	4.1331910	325.2132959
C	4.9995946	3.4167230	331.3727322
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H	7.5750009	1.4760527	329.9696764
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C	3.1697636	2.2062272	324.6499992
C	4.8543255	2.4673803	326.5629977
H	6.3235594	0.6964734	325.0459752
H	5.9289343	2.0860413	323.9895696
C	5.6362462	2.4436739	330.3651983
C	4.9604305	2.0185768	327.9111854
C	4.3393119	1.5828105	325.4290509
H	3.9189947	3.5544789	331.1746590
H	2.3292036	2.4544427	325.3261945
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H	5.9026345	7.0448994	328.6980575
H	3.4559734	3.1385646	324.1224232
H	8.3884714	5.2660397	326.4075728
H	5.1261859	1.4654590	330.4772923
H	3.9570631	0.6475935	325.8808639
H	6.2655982	4.8492503	329.3418881
H	1.3913978	7.8157621	326.6755013
H	2.4498445	8.1353108	329.5488068
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H	-1.0472892	5.5570278	328.7573663

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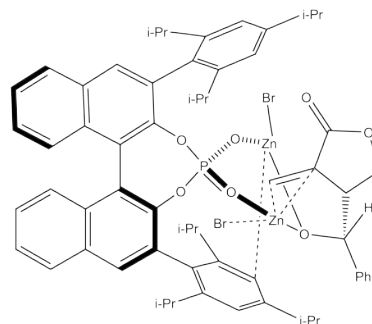


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C	0.8117744	-2.0509770	271.2459279
C	-1.3094779	-0.8676634	270.8393747
C	-1.9298009	-1.7216577	271.8004895
C	-2.0221434	0.2284527	270.2704769
H	-3.0581278	0.4134882	270.5939399
C	-1.4047584	1.1217456	269.4048468
C	4.3686634	0.5222865	268.6466866
C	4.8335907	-0.7576538	268.3620794
H	5.9017308	-0.8974101	268.1358768
C	3.9639957	-1.8801708	268.2833251
C	4.4465885	-3.1608527	267.8763213
C	2.5610184	-1.7099655	268.5703033
C	1.6917814	-2.8225529	268.3554820
C	2.0886505	-0.4219227	269.0236725
C	2.9867183	0.6575429	268.9887324
O	0.4632801	1.6156747	267.9855040

O	2.5580957	1.9343753	269.3655962	C	4.4073597	3.2350695	271.7604708
P	1.5579460	2.7776261	268.3863894	H	5.9293958	1.2428658	272.9798457
O	0.9319801	3.8787346	269.2564688	H	6.8128599	0.6777970	271.5215361
O	2.1811147	3.1620608	267.0406655	C	5.6595685	2.4344766	269.7025201
C	-1.2029618	-2.7021836	272.4589320	C	4.8137613	2.2700405	264.9041716
C	0.1839235	-2.8507111	272.1916318	C	5.7734929	2.0917447	267.2639277
H	-2.9970943	-1.5696801	272.0258620	H	7.0415022	-0.1290524	266.1787056
H	-1.6920134	-3.3492626	273.2029010	H	7.4471974	1.2683437	265.1399217
H	1.8869307	-2.1738605	271.0578993	C	5.1588771	2.0663867	271.0972200
H	0.7695135	-3.6025837	272.7423209	C	5.2752393	1.7086547	268.5424651
C	2.1875485	-4.0495281	267.9359925	C	5.4141922	1.3472325	265.9763229
C	3.5789724	-4.2297733	267.7121145	H	3.6016043	3.6127154	271.1030057
H	0.6114824	-2.6984339	268.5121246	H	3.8939986	2.7603863	265.2724251
H	1.4939025	-4.8877423	267.7690116	H	5.0890532	4.0841529	271.9761104
H	3.9612661	-5.2101905	267.3894812	H	6.3584485	6.4946246	267.5269514
H	5.5232307	-3.2759096	267.6748196	H	5.5270108	3.0566785	264.5794962
C	-1.9988572	3.4347723	270.1316018	H	8.7836076	5.2021741	270.2223805
C	-1.9451917	2.4762646	269.0783389	H	4.4386643	1.2302344	270.9903774
C	-2.3715738	4.7582418	269.8150716	H	4.6311952	0.6029593	266.2230065
C	-2.2341946	2.8675671	267.7400406	H	6.8334436	4.0770354	270.4685359
C	-2.5921759	4.2032926	267.4740941	Zn	-0.0189962	5.5665744	268.9021203
C	-2.6966091	5.1669478	268.4985991	Br	-0.2275793	7.4773146	270.2629523
C	-2.2307232	1.8638127	266.5908345	C	0.2061705	9.3747751	263.5761466
H	-2.8353054	4.4934042	266.4410954	C	0.7228140	9.0026194	264.8253961
C	-1.3726270	2.3261223	265.4024446	C	0.4445927	7.7322595	265.3755036
H	-1.7687990	3.2494559	264.9306039	C	-0.3854806	6.8582480	264.6490938
H	-1.3456343	1.5468634	264.6143085	C	-0.8982640	7.2240080	263.3947247
H	-0.3261906	2.5185861	265.7079424	C	-0.6027003	8.4821347	262.8513347
C	-3.6764710	1.5494673	266.1581169	H	0.4367236	10.3701277	263.1660184
H	-1.7915821	0.9197356	266.9717856	C	0.9491475	7.3528759	266.7667472
H	-4.1815830	2.4531248	265.7570079	H	-0.6363000	5.8773818	265.0749944
H	-4.2801257	1.1752225	267.0097052	H	-1.5292255	6.5129932	262.8400744
H	-3.6854556	0.7762382	265.3627299	H	-1.0025434	8.7708141	261.8671797
C	-3.3176145	6.5421716	268.2857844	O	0.6925182	5.9831030	267.0736606
C	-2.9644557	7.1998981	266.9501607	C	2.4744692	7.7230282	266.9911081
H	-3.4033488	8.2158954	266.8925087	C	3.3508017	6.5038608	266.9070558
H	-3.3502048	6.6278724	266.0809617	C	3.5451831	6.0094618	268.3210670
H	-1.8705715	7.2979146	266.8246107	O	3.1427972	6.9958156	269.1694131
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H	-2.9222133	7.1927387	269.0959211	O	3.9671342	4.9403635	268.6976262
H	-5.3192752	7.4310902	268.3989116	C	3.9134387	5.8863495	265.8376851
H	-5.1037993	5.9979635	269.4594235	H	3.6532583	8.8826194	268.4501616
H	-5.2914273	5.7816616	267.6899445	H	1.9249274	8.6489196	268.9459955
C	-1.6745238	3.1104575	271.5893749	Zn	1.7172232	4.7096857	265.9275717
C	-0.6153826	4.0487612	272.1940910	Br	1.6523821	4.2001970	263.6561451
H	-0.3936759	3.7422048	273.2366648	H	1.3398967	9.7257344	265.3821639
H	-0.9493546	5.1062294	272.2223316	H	-2.4624909	5.4968352	270.6259684
H	0.3273590	4.0061079	271.6145029	H	2.7724492	8.4928067	266.2564038
C	-2.9645539	3.0990499	272.4324821	H	0.3779212	7.9695925	267.5001404
H	-1.2499167	2.0890776	271.6225866	H	3.8094563	6.2800880	264.8151180
H	-2.7421766	2.8049845	273.4787136	H	4.5498043	4.9998995	266.0044621
H	-3.7126721	2.3876540	272.0269652				
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H	8.3846247	5.1043692	267.1546109				
H	7.0771773	2.3359371	272.1449314				
H	6.3500242	-0.0094482	264.5261728				
C	7.9577601	5.1349632	268.1817972				
H	3.9607245	2.9124175	272.7239628				
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H	4.5361713	1.6896060	264.0005206				
C	7.0494272	3.9187248	268.3183246				
C	6.3083955	1.5512630	271.9831520				
C	7.1460273	6.4395787	268.3046613				
H	6.6434927	6.5029825	269.2922670				
C	6.5449855	3.5163475	269.5658416				
C	6.6290200	0.5749865	265.4275100				
H	9.7178220	4.1774828	269.0883745				
C	6.6491120	3.1916400	267.1854623				
C	9.1332817	5.1159397	269.1725426				
H	9.8190100	5.9677390	268.9843795				
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15d-mi

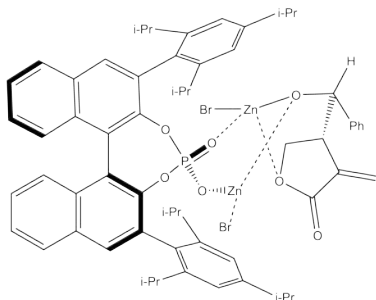


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C	0.8234773	-2.0346652	271.2744344

C	-1.3010981	-0.8601232	270.8625095	C	7.9806738	5.1138976	268.1511124
C	-1.9174810	-1.7104899	271.8287111	H	4.0051295	2.9168832	272.7255326
C	-2.0171971	0.2287932	270.2850327	H	7.8325687	7.3087834	268.1523098
H	-3.0546548	0.4118461	270.6050610	H	4.4943581	1.6960528	264.0015042
C	-1.4032603	1.1195041	269.4144882	C	7.0670176	3.9027274	268.2961125
C	4.3712448	0.5229884	268.6475837	C	6.3396175	1.5427176	271.9675751
C	4.8335785	-0.7584713	268.3667709	C	7.1747648	6.4223522	268.2709481
H	5.9007410	-0.8976546	268.1357431	H	6.6771112	6.4921330	269.2605632
C	3.9640679	-1.8811865	268.2981388	C	6.5705884	3.5040809	269.5475696
C	4.4435218	-3.1641034	267.8961777	C	6.5963670	0.5654942	265.4056199
C	2.5629188	-1.7088575	268.5914991	H	9.7381261	4.1517720	269.0562194
C	1.6927816	-2.8225169	268.3876689	C	6.6519794	3.1790907	267.1668067
C	2.0933578	-0.4182437	269.0402030	C	9.1602675	5.0943741	269.1365648
C	2.9912340	0.6609635	268.9958683	H	9.8506933	5.9406629	268.9410951
O	0.4653617	1.6162599	267.9988027	H	7.0381493	3.6789439	266.1779306
O	2.5653296	1.9392999	269.3698383	C	4.4449845	3.2359535	271.7579081
P	1.5580554	2.7807603	268.3965064	H	5.9668014	1.2367436	272.9672590
O	0.9302056	3.8770791	269.2731069	H	6.8365070	0.6670450	271.5024185
O	2.1735816	3.1754202	267.0513986	C	5.6791289	2.4285203	269.6918060
C	-1.1878080	-2.6847919	272.4920851	C	4.7855029	2.2718994	264.9035327
C	0.1987613	-2.8308529	272.2244961	C	5.7696616	2.0856800	267.2522078
H	-2.9851324	-1.5604661	272.0537788	H	7.0127764	-0.1418672	266.1513895
H	-1.6746353	-3.3288686	273.2400412	H	7.4166750	1.2532615	265.1112372
H	1.8985992	-2.1548380	271.0848678	C	5.1864947	2.0636954	271.0900733
H	0.7869576	-3.5780385	272.7786469	C	5.2806039	1.7061292	268.5349606
C	2.1860547	-4.0518551	267.9736270	C	5.3923241	1.3445454	265.9679078
C	3.5755930	-4.2337384	267.7433532	H	3.6347089	3.6163679	271.1077899
H	0.6135968	-2.6965796	268.5496014	H	3.8713864	2.7651149	265.2812913
H	1.4911555	-4.8907153	267.8156746	H	5.1303201	4.0835401	271.9671572
H	3.9562634	-5.2159729	267.4245485	H	6.3829972	6.4755681	267.4973248
H	5.5189676	-3.2800629	267.6890866	H	5.4991478	3.0552800	264.5717921
C	-2.0225547	3.4346413	270.1162827	H	8.8160982	5.1888873	270.1873665
C	-1.9532303	2.4662085	269.0729200	H	4.4614917	1.2309441	270.9883755
C	-2.4030256	4.7515642	269.7836864	H	4.6072692	0.6049429	266.2221000
C	-2.2377761	2.8416841	267.7294452	H	6.8705273	4.0622229	270.4480122
C	-2.6064912	4.1713990	267.4488765	Zn	-0.0065294	5.5681614	268.9164674
C	-2.7236970	5.1439299	268.4620585	Br	-0.2869611	7.4813359	270.2503037
C	-2.2176034	1.8275834	266.5890922	C	0.2101737	9.4779284	263.6670416
H	-2.8425717	4.4495376	266.4110446	C	0.7095688	9.0713073	264.9117974
C	-1.3530425	2.2838277	265.4029700	C	0.4523811	7.7749692	265.4091482
H	-1.7467898	3.2033950	264.9218981	C	-0.3415161	6.9101358	264.6342992
H	-1.3193250	1.5002623	264.6194948	C	-0.8352972	7.3100961	263.3828099
H	-0.3083823	2.4787851	265.7121606	C	-0.5597769	8.5935060	262.8923994
C	-3.6576066	1.4983462	266.1487363	H	0.4232523	10.4935240	263.2995540
H	-1.7748321	0.8903043	266.9825230	C	0.9440685	7.3616345	266.7950579
H	-4.1673508	2.3940016	265.7358775	H	-0.5790194	5.9087145	265.0169972
H	-4.2651989	1.1279297	266.9990742	H	-1.4337153	6.6033628	262.7884448
H	-3.6562370	0.7180417	265.3602576	H	-0.9450489	8.9083927	261.9106229
C	-3.3395006	6.5182246	268.2306193	O	0.6840840	5.9890362	267.0777607
C	-3.0071780	7.1424171	266.8738829	C	2.4690057	7.7266702	267.0361608
H	-3.4278059	8.1653656	266.8048607	C	3.3496973	6.5130369	266.9213570
H	-3.4257459	6.5615193	266.0257026	C	3.5549951	5.9890910	268.3229347
H	-1.9152800	7.2166705	266.7193469	O	3.1332828	6.9463834	269.1966363
C	-4.8636767	6.4256169	268.4497074	C	2.7739976	8.1534380	268.4890772
H	-2.9217940	7.1838431	269.0173755	O	3.9959763	4.9190583	268.6722143
H	-5.3321141	7.4273136	268.3615594	C	3.8958122	5.9117947	265.8345645
H	-5.1071211	6.0186193	269.4516638	H	3.6359840	8.8531231	268.5319222
H	-5.3313775	5.7611526	267.6931689	H	1.9066515	8.5945997	269.0155390
C	-1.7078882	3.1264017	271.5799109	Zn	1.7004782	4.7097297	265.9253311
C	-0.6593081	4.0756742	272.1855316	Br	1.6495981	4.2256242	263.6564146
H	-0.4469594	3.7819658	273.2337048	H	1.2956328	9.7878679	265.5096122
H	-0.9956363	5.1325857	272.1988453	H	-2.5003641	5.4987025	270.5859920
H	0.2904902	4.0299895	271.6181378	H	2.7655969	8.5168503	266.3221735
C	-3.0049357	3.1157333	272.4120806	H	0.3687412	7.9662550	267.5358919
H	-1.2783213	2.1075722	271.6262801	H	3.7712210	6.3159402	264.8184213
H	-2.7913675	2.8319165	273.4629433	H	4.5322470	5.0212700	265.9779526
H	-3.7469984	2.3980755	272.0064063				
H	-3.4831250	4.1175603	272.4249869				
H	8.4036698	5.0765796	267.1223859				
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H	6.3050869	-0.0157694	264.5062382				

15d-2-ma; COSMO



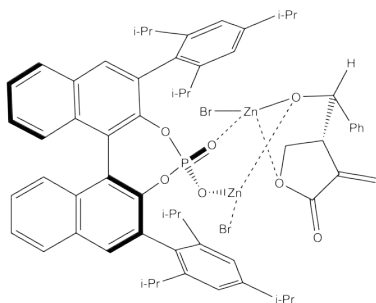
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Zn	2.3618058	1.5865726	-0.0755405
Br	4.5391680	1.7365844	-0.8271307
H	3.5651865	3.9559492	0.7405231
Br	-3.0167941	3.4249769	-0.1592142
Zn	-0.9577673	2.4739984	-0.5833715
C	1.5007853	4.8331407	0.6968965
C	2.6967296	4.1644325	1.3959699
C	0.3849407	4.3551414	1.5951120
C	-0.8088297	4.8955425	1.9100761
C	0.7893353	3.0035892	2.0704804
O	2.1763910	2.8718985	1.8512782
O	0.1258453	2.0923072	2.4998915
H	3.0303645	4.7366184	2.2849967
C	-1.2090377	6.8678917	-2.1207602
C	-0.2031509	6.2907195	-1.3294994
C	0.2496276	4.9820417	-1.5853600
C	-0.3141764	4.2781653	-2.6768120
C	-1.3172617	4.8569331	-3.4684758
C	-1.7746361	6.1527014	-3.1883066
H	-1.5597295	7.8861359	-1.8930752
H	0.2196618	6.8770950	-0.5011374
C	1.3070770	4.2688088	-0.7488175
H	0.0538477	3.2687701	-2.9228998
H	-1.7430620	4.2876915	-4.3089640
H	-2.5692964	6.6059140	-3.7998219
O	0.9710835	2.8755775	-0.6935016
C	-0.4625459	-2.4698361	1.6597810
C	-0.6106685	-3.6002017	0.8435112
C	-0.1905754	-4.8740891	1.3816653
C	-0.1164492	-0.6639543	0.5951879
C	0.2107605	-4.9506492	2.7662496
C	0.5859589	-6.2128879	3.3180588
C	0.2757006	-3.7623072	3.5474180
H	0.5854399	-3.8354306	4.6009220
C	0.0042593	-2.5099890	3.0083539
C	-0.8525055	-2.3996624	-2.8031703
C	-1.8071867	-3.2680323	-3.3194902
H	-2.0651264	-3.2173984	-4.3884220
C	-2.5098412	-4.1898751	-2.4879730
C	-3.5540708	-5.0058287	-3.0189251
C	-2.2007510	-4.2729380	-1.0786041
C	-3.0021521	-5.1225623	-0.2589488
C	-1.1185995	-3.4739215	-0.5544288
C	-0.5274599	-2.5497453	-1.4188924
O	-0.8351593	-1.2163123	1.1739769
O	0.4844383	-1.7336367	-0.9281837
P	0.0785955	-0.4817244	0.0392605
O	1.4277520	0.0213570	0.5753152
O	-0.8528063	0.5195891	-0.6557843
C	0.6108598	-7.3558806	2.5335460
C	0.2740241	-7.2723835	1.1560794
H	0.8757265	-6.2552119	4.3798040
H	0.9095104	-8.3215769	2.9691014
H	-0.3615813	-6.0173656	-0.4744736
H	0.3286197	-8.1721129	0.5242639
C	-4.0243804	-5.8877274	-0.8043151

C	-4.2944243	-5.8437474	-2.1981420
H	-2.8076485	-5.1600788	0.8220198
H	-4.6331486	-6.5295371	-0.1492912
H	-5.1013585	-6.4614982	-2.6209081
H	-3.7726531	-4.9425980	-4.0965715
C	1.5470453	-0.8107031	4.0578300
C	0.2181232	-1.2599228	3.8091656
C	1.7351831	0.2887224	4.9120401
C	-0.8837081	-0.5477703	4.3490946
C	-0.6382060	0.5514276	5.1937173
C	0.6620857	0.9784791	5.5031710
H	2.7604458	0.6382203	5.1155269
C	-2.3279641	-0.9217863	4.0253856
H	-1.4996045	1.0956423	5.6096510
C	-3.0359590	0.2139133	3.2613393
H	-3.1319166	1.1243491	3.8891943
H	-4.0586420	-0.0951171	2.9606898
H	-2.4762822	0.4956664	2.3486176
C	-3.1103044	-1.3347055	5.2847966
H	-2.3069388	-1.8058491	3.3556688
H	-3.1919469	-0.4951305	6.0065822
H	-2.6153870	-2.1790385	5.8068666
H	-4.1415388	-1.6498254	5.0219183
C	0.9418163	2.1996756	6.3740256
C	1.1268358	3.4555530	5.4977757
H	1.4010604	4.3365027	6.1150772
H	0.1879511	3.6929836	4.9557282
H	1.9220936	3.3012873	4.7406522
C	-0.1112246	2.4436117	7.4636126
H	1.9136520	2.0086728	6.8823721
H	0.2077669	3.2657299	8.1362878
H	-0.2776249	1.5377755	8.0810116
H	-1.0888442	2.7404450	7.0293545
C	2.7622347	-1.4664169	3.3992763
C	3.7712941	-0.4312240	2.8684933
H	4.5061945	-0.9146994	2.1933283
H	4.3442577	0.0468455	3.6902457
H	3.2632763	0.3715286	2.3033732
C	3.4659864	-2.4593676	4.3435926
H	2.3887902	-2.0353760	2.5222619
H	4.3412611	-2.9246114	3.8441636
H	2.7894119	-3.2733172	4.6696419
H	3.8307243	-1.9405596	5.2552117
H	0.8857934	3.0718723	-5.3067264
H	3.2080911	-2.4103841	-5.2588375
H	-4.2618999	-0.4622324	-5.2718833
C	1.6791083	2.2957898	-5.2240645
H	3.8576985	-2.8967488	-2.1516814
H	3.1411414	3.8214547	-4.6327080
H	-4.2310832	1.0012752	-3.1903970
C	1.0166540	1.0434340	-4.6644042
C	2.5878488	-3.0947519	-4.6427529
C	2.7690833	2.8368633	-4.2825129
H	3.6397001	2.1521671	-4.2245713
C	1.7821011	-0.0627372	-4.2544717
C	-3.1555089	-0.3960796	-5.3275864
H	1.4373732	1.7046050	-7.3300880
C	-0.3796258	0.9467116	-4.5525601
C	2.2332104	2.0500370	-6.6397506
H	2.6766397	2.9771792	-7.0586613
H	-0.9950053	1.7934713	-4.8987512
C	3.2825691	-1.9974912	-2.4537181
H	3.2049618	-3.9843139	-4.3987705
H	1.7338953	-3.4281874	-5.2669754
C	1.1971498	-1.2184703	-3.7116489
C	-3.1256622	1.0669546	-3.2524408
C	-1.0215147	-0.1825625	-4.0046020
H	-2.7780493	-1.3250132	-5.8019183
H	-2.8998642	0.4471350	-6.0033113
C	2.1026817	-2.3970522	-3.3564845
C	-0.2199876	-1.2736552	-3.5596891

C	-2.5482997	-0.1863972	-3.9267053
H	2.9316687	-1.4906835	-1.5342225
H	-2.7477511	1.1728385	-2.2182076
H	3.9887624	-1.3134918	-2.9680729
H	2.3906715	2.9543161	-3.2477804
H	-2.8866462	1.9995448	-3.8042690
H	3.0263314	1.2733184	-6.6239611
H	1.4962152	-3.1399739	-2.8000982
H	-2.8530950	-1.0473303	-3.2998606
H	2.8776862	-0.0231604	-4.3555300
H	2.2901675	4.3568312	-1.2720444
H	1.6264084	5.9310973	0.6714411
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H	-1.4967965	4.3467387	2.5715408

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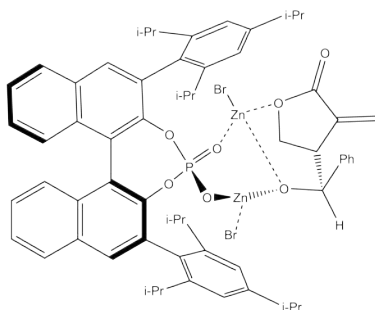
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H	3.5393654	3.9368813	0.7814922
Br	-3.0157137	3.5090096	-0.2486892
Zn	-0.9892495	2.4720475	-0.5812373
C	1.4804195	4.8269250	0.7017190
C	2.6623641	4.1545416	1.4232056
C	0.3480513	4.3576404	1.5833289
C	-0.8567469	4.8948899	1.8598160
C	0.7424844	3.0089643	2.0761413
O	2.1305023	2.8708653	1.8771448
O	0.0682166	2.1053333	2.5048339
H	2.9846709	4.7319219	2.3142137
C	-1.1099040	6.9137290	-2.1939044
C	-0.1398850	6.3151030	-1.3748231
C	0.2835517	4.9930118	-1.6094510
C	-0.2729844	4.2968273	-2.7079466
C	-1.2408415	4.8955811	-3.5266159
C	-1.6689496	6.2055886	-3.2685461
H	-1.4384042	7.9426918	-1.9820489
H	0.2773906	6.8962288	-0.5396735
C	1.3043839	4.2583347	-0.7459584
H	0.0673388	3.2730058	-2.9316335
H	-1.6645930	4.3282158	-4.3694198
H	-2.4371635	6.6746427	-3.9014000
O	0.9427669	2.8741283	-0.6876346
C	-0.4700232	-2.4780008	1.6715481
C	-0.6162460	-3.6056565	0.8512587
C	-0.1903622	-4.8800054	1.3839961
C	-0.1150482	-6.0670114	0.5937729
C	0.2157487	-4.9600203	2.7668529
C	0.5961031	-6.2228030	3.3125229
C	0.2808042	-3.7739889	3.5510275
H	0.5949906	-3.8476638	4.6031670
C	0.0039552	-2.5208834	3.0174558
C	-0.8570996	-2.3943820	-2.7915510
C	-1.8055694	-3.2665111	-3.3126826
H	-2.0591172	-3.2138718	-4.3827009

C	-2.5063951	-4.1935588	-2.4858641
C	-3.5447517	-5.0136092	-3.0207709
C	-2.2006051	-4.2786314	-1.0760354
C	-2.9993301	-5.1347430	-0.2609933
C	-1.1242018	-3.4757851	-0.5463828
C	-0.5363872	-2.5453979	-1.4065201
O	-0.8504884	-1.2240365	1.1936616
O	0.4689186	-1.7245275	-0.9119981
P	0.0567270	-0.4798823	0.0623856
O	1.4054627	0.0264978	0.5982480
O	-0.8765460	0.5219663	-0.6282504
C	0.6210271	-7.3630606	2.5250203
C	0.2796481	-7.2759277	1.1495661
H	0.8906581	-6.2672799	4.3728412
H	0.9235185	-8.3292097	2.9567591
H	-0.3638476	-6.0168860	-0.4747589
H	0.3337742	-8.1734438	0.5146604
C	-4.0154146	-5.9040026	-0.8108714
C	-4.2823361	-5.8575928	-2.2046363
H	-2.8059878	-5.1734743	0.8200442
H	-4.6218613	-6.5511635	-0.1590671
H	-5.0847413	-6.4784778	-2.6312780
H	-3.7612227	-4.9482707	-4.0987120
C	1.5469076	-0.8139273	4.0542350
C	0.2185384	-1.2716906	3.8191396
C	1.7353823	0.2868435	4.9059880
C	-0.8826416	-0.5682927	4.3706770
C	-0.6363259	0.5325220	5.2125919
C	0.6637009	0.9687661	5.5079582
H	2.7602918	0.6425715	5.0998132
C	-2.3271259	-0.9547822	4.0634560
H	-1.4974823	1.0690309	5.6387312
C	-3.0558564	0.1747678	3.3102470
H	-3.1522992	1.0840211	3.9396690
H	-4.0796556	-0.1428879	3.0233723
H	-2.5126894	0.4613898	2.3891506
C	-3.0888265	-1.3782492	5.3318568
H	-2.3056963	-1.8373602	3.3917474
H	-3.1692353	-0.5416615	6.0570930
H	-2.5786386	-2.2182117	5.8457854
H	-4.1203997	-1.7027346	5.0823584
C	0.9450636	2.1909705	6.3769534
C	1.1296441	3.4460415	5.4995207
H	1.4090346	4.3271954	6.1143331
H	0.1887500	3.6854643	4.9618856
H	1.9202402	3.2882262	4.7382720
C	-0.1053469	2.4368392	7.4682456
H	1.9174791	1.9994703	6.8842103
H	0.2150828	3.2583978	8.1408517
H	-0.2725141	1.5312552	8.0853783
H	-1.0831828	2.7352661	7.0357514
C	2.7601812	-1.4632727	3.3857505
C	3.7666770	-0.4244499	2.8572793
H	4.4961702	-0.9013419	2.1718962
H	4.3475592	0.0445702	3.6786633
H	3.2568525	0.3854662	2.3042327
C	3.4693598	-2.4612074	4.3206169
H	2.3837574	-2.0274811	2.5068885
H	4.3449147	-2.9197638	3.8157844
H	2.7968130	-3.2801904	4.6416609
H	3.8340107	-1.9487007	5.2356480
H	0.8723106	3.0725673	-5.3181246
H	3.2175731	-2.3902932	-5.2237043
H	-4.2668010	-0.4190086	-5.2843356
C	1.6641317	2.2941637	-5.2410085
H	3.8546825	-2.8637949	-2.1123181
H	3.1419387	3.8206912	-4.6949887
H	-4.2393321	0.9959233	-3.1751109
C	1.0057875	1.0488853	-4.6608444
C	2.5978495	-3.0758166	-4.6086331
C	2.7720592	2.8424092	-4.3256625

H	3.6418582	2.1564243	-4.2731273
C	1.7738827	-0.0502246	-4.2378540
C	-3.1604383	-0.3494557	-5.3349498
H	1.3830409	1.6802642	-7.3358941
C	-0.3900124	0.9473604	-4.5515333
C	2.1917654	2.0312199	-6.6638081
H	2.6315759	2.9513984	-7.1013894
H	-1.0084630	1.7889323	-4.9054173
C	3.2745736	-1.9692847	-2.4183698
H	3.2184627	-3.9614536	-4.3596405
H	1.7493172	-3.4148409	-5.2369199
C	1.1919676	-1.2050912	-3.6905994
C	-3.1318398	1.0436774	-3.2085405
C	-1.0296488	-0.1809947	-3.9993022
H	-2.7800137	-1.2614716	-5.8389248
H	-2.9060206	0.5147681	-5.9838671
C	2.1021332	-2.3775431	-3.3268089
C	-0.2257249	-1.2662353	-3.5455318
C	-2.5568833	-0.1864163	-3.9266229
H	2.9160924	-1.4657326	-1.5001800
H	-2.7781965	1.0922854	-2.1617120
H	3.9794649	-1.2802669	-2.9275678
H	2.4135840	2.9755949	-3.2859882
H	-2.8636795	1.9978310	-3.7078713
H	2.9814655	1.2511301	-6.6537224
H	1.4966980	-3.1224732	-2.7720578
H	-2.8652007	-1.0676076	-3.3306565
H	2.8696418	-0.0068512	-4.3343596
H	2.3008629	4.3215157	-1.2485085
H	1.6110061	5.9246942	0.6747521
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H	-1.5593218	4.3489054	2.5078901

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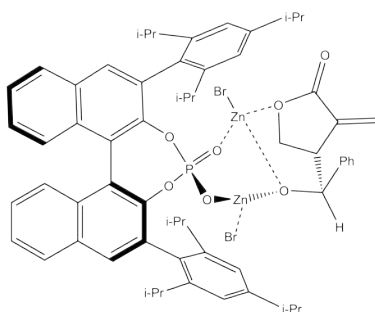
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H	1.2604830	8.4200125	269.2130332
Br	1.6563697	4.4953972	263.8445571
Zn	2.2274065	4.7350101	266.0668194
C	1.1552955	8.0881464	266.9967020
C	0.5431585	8.1746630	268.4052059
C	0.1715675	7.1404709	266.3528868
C	-0.2289321	6.9938849	265.0744645
C	-0.2820074	6.2215680	267.4326964
O	0.0398621	6.8229731	268.6673465
O	-0.7670609	5.1187830	267.3718623
H	-0.3137724	8.8769292	268.4421451
C	3.7783230	8.2823727	263.4603411
C	3.0604242	8.3504954	264.6649381
C	3.3379462	7.4575791	265.7179384
C	4.3769120	6.5123692	265.5400103
C	5.0953328	6.4469353	264.3368736
C	4.7931886	7.3276841	263.2882018
H	3.5341043	8.9795622	262.6442764
H	2.2719740	9.1096503	264.7683908

C	2.5778692	7.4394654	267.0403233
H	4.6412843	5.8310988	266.3652000
H	5.8958098	5.7001175	264.2213010
H	5.3467864	7.2721946	262.3388470
O	2.4860691	6.0798100	267.4872687
C	-0.0078971	0.8905415	269.2193009
C	0.7852074	-0.1882259	269.6355437
C	0.2721755	-1.0265667	270.6951549
C	1.0528244	-2.0380488	271.3333168
C	-1.0767219	-0.8148998	271.1638700
C	-1.6068153	-1.6659549	272.1802801
C	-1.8407128	0.2682853	270.6448077
H	-2.8668693	0.4187960	271.0129911
C	-1.3150533	1.1662248	269.7228431
C	4.4108715	0.5350567	268.5739889
C	4.8450888	-0.7275412	268.1872743
H	5.8912023	-0.8695542	267.8753760
C	3.9548522	-1.8405154	268.1263227
C	4.3973521	-3.1060602	267.6356222
C	2.5730456	-1.6833636	268.5195464
C	1.6875766	-2.7871822	268.3364428
C	2.1401901	-0.4127466	269.0509996
C	3.0548490	0.6422186	269.0144132
O	0.4568282	1.7390072	268.2137759
O	2.6500162	1.8886841	269.4757124
P	1.6643432	2.7884861	268.5344586
O	1.2372661	3.9465230	269.4496781
O	2.2945050	3.1224445	267.1762562
C	-0.8316184	-2.6631457	272.7521956
C	0.5153852	-2.8347548	272.3351811
H	-2.6425883	-1.4992632	272.5156525
H	-1.2495236	-3.3075261	273.5406317
H	2.1000274	-2.1783179	271.0330459
H	1.1425764	-3.6020838	272.8142594
C	2.1465238	-3.9986402	267.8368421
C	3.5155605	-4.1678966	267.4981337
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H	1.4415844	-4.8324982	267.6977957
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H	-1.8446130	0.5738889	267.4151031
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C	-3.6664727	6.9480679	267.7006392
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H	-3.2036170	6.6298230	266.7433712
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H	-3.2386290	3.7525861	272.8188170	H	-0.4473726	8.9172098	267.6965091
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H	4.1155868	2.6113050	272.8707845	C	5.7500804	7.0610618	264.6712945
H	6.5971403	7.8318633	268.5851503	C	5.3480485	7.0827937	263.3238265
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C	6.4375125	4.3551480	268.2369008	H	1.9732580	7.4379409	263.7579945
C	6.5019829	1.6613852	271.7483421	C	2.4561980	7.3078876	266.5489198
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C	6.0781843	3.8343253	269.4927374	H	6.0955843	6.9858282	262.5217006
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H	9.1325625	5.0084350	268.0760129	C	-0.0679073	0.9008788	269.2093062
C	6.2182952	3.5470106	267.1097822	C	0.7787930	-0.1477897	269.5892626
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H	4.7624190	0.6153116	266.1349962	C	-0.6001698	-2.6501288	272.7943503
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H	-0.9451135	6.1985872	264.8162300	H	-2.4431451	-1.5212966	272.6677262
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H	1.1983961	9.0878810	266.5270139	H	2.2116123	-2.1128348	270.9002984
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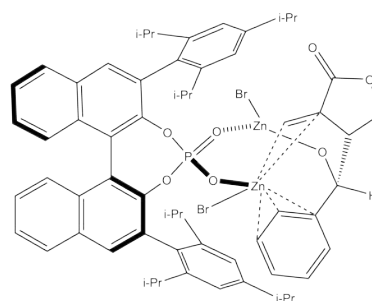


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Br	1.2585326	4.1682232	263.5393644
Zn	2.0250947	4.5025620	265.6890075
C	1.0475389	7.9716888	266.3635306

C	0.4166035	8.2231971	267.7502324
C	0.0165825	6.9995252	265.8298965
C	-0.5051716	6.7993798	264.6047228
C	-0.4290462	6.1898500	266.9985803
O	-0.0785367	6.9072381	268.1624328
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C	3.9899453	7.2264812	263.0064814
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H	3.6644560	7.2326544	261.9554735
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C	1.1828851	-1.9914981	271.2655731
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C	-1.3462781	1.1566725	269.7894881
C	4.3476907	0.7031237	268.4455884
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H	5.8540664	-0.6454580	267.7008148
C	3.9397141	-1.6667338	267.9282328
C	4.4005971	-2.9062706	267.3921974
C	2.5702497	-1.5623393	268.3765989
C	1.7143750	-2.6916848	268.2108688
C	2.1146740	-0.3165591	268.9435275
C	2.9929226	0.7695957	268.8928024
O	0.3115087	1.7373158	268.1634334
O	2.5525160	2.0080761	269.3486609
P	1.5159084	2.8139516	268.3696958
O	1.0899032	4.0340489	269.2004441
O	2.1075657	3.0338029	266.9746527
C	-0.6001698	-2.6501288	272.7943503
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H	-2.4431451	-1.5212966	272.6677262
H	-0.9581361	-3.3012127	273.6063163
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C	2.1908634	-3.8766960	267.6678162
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H	0.6604799	-2.6094966	268.5117580
H	1.5087380	-4.7313483	267.5423496
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H	5.4494589	-2.9778446	267.0637471
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H	-3.0815625	5.4369440	270.5874998
C	-2.7625132	1.2396216	267.1555577
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C	-2.1545334	1.7370017	265.8300866
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H	-1.1783943	2.2319630	265.9963907
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H	-4.0076116	-0.3119265	266.2303885
C	-4.6426753	5.8055379	268.4063446
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H	-2.5248772	2.0920002	272.6932195
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C	7.5149789	5.6369424	268.7275322
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C	6.7311367	4.3332407	268.6544498
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H	9.4936662	4.6749556	268.7650921
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H	6.5730015	4.3702015	266.5062451
C	4.4027473	2.7034695	271.9858622
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H	6.2907042	0.3880176	265.7830207
H	7.0237338	1.8510145	265.0594045
C	5.2330470	1.7695529	271.0848079
C	5.1981953	1.9377363	268.5039382
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H	3.5124539	3.0855965	271.4495109
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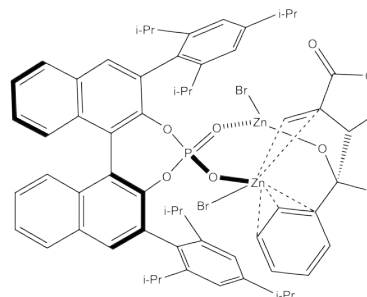
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C	0.6603906	8.5628170	266.4214608
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C	-0.9340366	6.9857004	265.4541325
H	-1.2124758	5.1256700	266.5592836
H	0.3405076	5.7993018	268.4136293
C	1.7815260	8.1066425	268.6917243
H	1.1623237	9.5430148	266.3849581
H	-0.4460576	8.9198069	264.5914166
H	-1.6466473	6.7233066	264.6590761
O	1.6308906	7.3408071	269.8060347
C	3.3091885	8.2716339	268.2355336
C	3.8751836	6.9556414	267.8302882
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O	4.5318226	7.2719588	270.0178814
C	4.1669906	8.5735224	269.4802856
O	4.2569070	5.1111479	269.4132793
C	4.1232021	6.4204830	266.6044627
H	5.0974628	9.1212371	269.2283250
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Zn	1.9209011	5.4486851	266.2756032
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C	0.8212868	0.2781904	269.5020065
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C	-1.0425656	-0.2588927	271.0556338
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C	-1.2529443	1.6672962	269.5371397
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O	0.5904021	2.2050280	268.0855948
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P	1.7940403	3.2216499	268.5470221
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C	1.7172254	-3.5892679	267.6236844

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H	0.9317443	-4.3557458	267.5390315
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H	-5.4316034	6.9468227	265.6854992
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C	-1.6320192	4.1803628	271.1330698
C	-1.1627752	5.6245269	271.3815530
H	-0.5149985	5.6664756	272.2806292
H	-2.0130459	6.3150819	271.5616176
H	-0.5934410	6.0413536	270.5254645
C	-2.5864929	3.7494774	272.2640271
H	-0.7324418	3.5317944	271.1740676
H	-2.1040606	3.8895905	273.2532522
H	-2.8818883	2.6863325	272.1792998
H	-3.5141429	4.3596499	272.2464819
H	8.5285580	5.2685339	266.8934715
H	7.7676599	1.7316263	271.4785128
H	5.8668754	0.6173170	263.8852054
C	8.2932729	5.1106325	267.9693550
H	4.8838328	2.2814102	272.6817437
H	8.4032948	7.2517127	268.4539783
H	4.1718448	2.5179635	263.7835007
C	7.2988895	3.9566670	268.0391098
C	6.9389412	1.0151589	271.2977031
C	7.6738923	6.4164477	268.5026621
H	7.3500177	6.3078150	269.5585032
C	6.9290542	3.3858553	269.2692715
C	6.2896656	1.0496000	264.8158384
H	10.0647646	3.8510600	268.3023326
C	6.7139472	3.4361799	266.8722687
C	9.6136573	4.7869747	268.6893788
H	10.3481897	5.6072307	268.5517168
H	7.0047665	3.8668449	265.8994496
C	5.1314433	2.7626937	271.7132273
H	6.7004626	0.5268900	272.2654266
H	7.3140387	0.2367869	270.6018536
C	6.0068112	2.3297024	269.3578591
C	4.6091256	2.9490731	264.7071889
C	5.7821600	2.3792227	266.9029412
H	6.6985924	0.2185033	265.4256428
H	7.1417234	1.7015699	264.5298912
C	5.6975844	1.7278915	270.7272983
C	5.4274205	1.8223381	268.1625986

C	5.2187428	1.8462529	265.5853707
H	4.2138408	3.2365063	271.3206939
H	3.7960316	3.4750716	265.2398858
H	5.8574691	3.5756330	271.9216416
H	6.7861886	6.7084689	267.9064358
H	5.3606370	3.7023821	264.3910598
H	9.4606566	4.6604447	269.7813490
H	4.9199295	0.9493268	270.5869332
H	4.3958666	1.1454148	265.8325725
H	7.3697201	3.7780774	270.1992441
H	3.9977048	7.0187263	265.6884445
H	4.6251528	5.4394410	266.5309065
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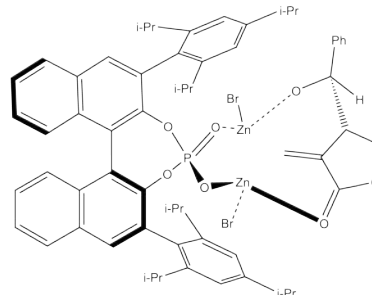
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C	0.2317262	6.4248440	267.4968964
C	0.8926907	7.6830515	267.4938697
C	0.6529456	8.5611920	266.4168065
C	-0.2465400	8.2173852	265.3968035
C	-0.9208665	6.9839980	265.4194915
H	-1.2100989	5.1190066	266.5141799
H	0.3229350	5.7872632	268.3895547
C	1.7432983	8.0948552	268.7024361
H	1.1516866	9.5437704	266.3930980
H	-0.4236811	8.9204438	264.5689557
H	-1.6186100	6.7199865	264.6120144
O	1.5647870	7.3311664	269.8074069
C	3.2831015	8.2519001	268.2817013
C	3.8571071	6.9569827	267.8223478
C	4.2514172	6.2342190	269.0761385
O	4.4799037	7.1720048	270.0364725
C	4.1133670	8.4906277	269.5603786
O	4.3431037	5.0420120	269.2828359
C	4.1018447	6.4749173	266.5740718
H	5.0436285	9.0602940	269.3565820
H	3.5354937	8.9762668	270.3693262
Zn	1.9189935	5.4311002	266.2418858
Br	1.9715236	5.6529236	263.9341782
C	0.0682797	1.3891485	269.0814464
C	0.8266609	0.2956552	269.5101181
C	0.3013829	-0.5059316	270.5888219
C	1.0600337	-1.5294727	271.2317179
C	-1.0376190	-0.2480170	271.0611766
C	-1.5763068	-1.0581558	272.1050186
C	-1.7904478	0.8198892	270.4943980
H	-2.8259478	0.9767870	270.8317895
C	-1.2503231	1.6790831	269.5446455
C	4.4321615	0.7172957	268.2294284
C	4.7113093	-0.5728176	267.7947198
H	5.7198391	-0.8030821	267.4184274

C	3.7215933	-1.5962210	267.7823675
C	4.0042419	-2.8895876	267.2495473
C	2.3998846	-1.3153883	268.2897994
C	1.4053500	-2.3334953	268.1786639
C	2.1295019	-0.0142488	268.8553402
C	3.1245265	0.9635046	268.7499860
O	0.5912015	2.2231281	268.0951823
O	2.8815916	2.2405019	269.2489912
P	1.8024511	3.2383912	268.5453687
O	1.3160061	4.2061795	269.6232196
O	2.3128207	3.8111571	267.2105250
C	-0.8204263	-2.0614252	272.6913498
C	0.5133656	-2.2860478	272.2585951
H	-2.6031253	-0.8568800	272.4487010
H	-1.2449615	-2.6728636	273.5020461
H	2.0962043	-1.7072848	270.9120530
H	1.1223736	-3.0627298	272.7456884
C	1.7082674	-3.5755111	267.6383321
C	3.0216791	-3.8651750	267.1829057
H	0.3822505	-2.1219137	268.5184221
H	0.9205844	-4.3401253	267.5579773
H	3.2521857	-4.8565059	266.7640026
H	5.0206856	-3.0918127	266.8767634
C	-2.2645393	3.9983303	269.7565967
C	-2.0388503	2.8232618	268.9809974
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C	-3.6926017	4.9027968	267.9572085
H	-3.2632994	5.9180294	269.8156148
C	-2.3099565	1.5264144	266.7637456
H	-3.8485868	3.6570713	266.1891271
C	-1.5165548	1.9564676	265.5146998
H	-2.1015063	2.6576465	264.8827767
H	-1.2645217	1.0765281	264.8877550
H	-0.5669294	2.4534057	265.7961737
C	-3.6002482	0.7760325	266.3890086
H	-1.6748322	0.8116598	267.3248400
H	-4.2883951	1.4133837	265.7953807
H	-4.1480663	0.4430760	267.2936841
H	-3.3683485	-0.1205014	265.7779298
C	-4.6288920	6.0099829	267.4830095
C	-4.8187338	6.0697222	265.9624990
H	-5.4190472	6.9583007	265.6813155
H	-5.3597315	5.1786875	265.5811010
H	-3.8494385	6.1316572	265.4283557
C	-5.9908833	5.8953852	268.1977458
H	-4.1647914	6.9710933	267.8017681
H	-6.6610066	6.7344507	267.9176452
H	-5.8728769	5.9016674	269.2996272
H	-6.4952137	4.9459018	267.9213305
C	-1.6305632	4.1938845	271.1341913
C	-1.1745740	5.6415484	271.3855182
H	-0.5196542	5.6860009	272.2795729
H	-2.0299776	6.3222179	271.5792239
H	-0.6217829	6.0720730	270.5250840
C	-2.5762925	3.7515676	272.2678616
H	-0.7248270	3.5535552	271.1720523
H	-2.0919422	3.8979654	273.2550066
H	-2.8578859	2.6847660	272.1852360
H	-3.5118325	4.3495174	272.2529110
H	8.5740362	5.2360492	266.8883594
H	7.7835258	1.7055040	271.4776695
H	5.8350319	0.6180727	263.8813104
C	8.3216311	5.0932214	267.9627058
H	4.8934343	2.2939288	272.6710247
H	8.4057896	7.2440488	268.4142340
H	4.1670381	2.5472751	263.7876747
C	7.3302909	3.9368260	268.0332178
C	6.9465131	0.9984139	271.2988797
C	7.6830232	6.4029030	268.4643735

H	7.3420576	6.3072585	269.5161058
C	6.9656007	3.3622246	269.2623119
C	6.2671954	1.0417267	264.8115385
H	10.0933221	3.8505388	268.3490779
C	6.7324194	3.4282416	266.8681038
C	9.6320087	4.7919768	268.7090425
H	10.3648321	5.6128564	268.5664989
H	7.0202076	3.8612021	265.8953666
C	5.1573117	2.7681225	271.7036367
H	6.7015337	0.5181231	272.2688597
H	7.3142720	0.2127626	270.6075305
C	6.0313577	2.3172167	269.3528884
C	4.6216207	2.9700464	264.7065718
C	5.7912120	2.3806231	266.8999507
H	6.6627834	0.2030479	265.4194089
H	7.1310335	1.6775047	264.5249451
C	5.7145268	1.7226922	270.7234851
C	5.4390068	1.8224247	268.1595037
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H	4.2500121	3.2560271	271.3044612
H	3.8237417	3.5150443	265.2427364
H	5.8944282	3.5695309	271.9174640
H	6.8016904	6.6762483	267.8498334
H	5.3860197	3.7061180	264.3810185
H	9.4639530	4.6871686	269.8009248
H	4.9286741	0.9520801	270.5843232
H	4.3787110	1.1722871	265.8349847
H	7.4140063	3.7467458	270.1916028
H	3.9504855	7.0972637	265.6785662
H	4.6168973	5.5044101	266.4601810
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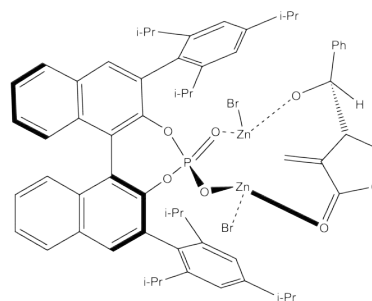


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C	1.4946957	-1.2547839	91.8332407
C	-0.7553666	-0.2535775	91.6874983
C	-1.0898983	-0.9221044	92.9034806
C	-1.6867309	0.6198974	91.0495602
H	-2.6892835	0.7354098	91.4887791
C	-1.3420275	1.3520516	89.9211215
C	4.2124864	0.7285926	88.0075765
C	4.5798656	-0.5865856	87.7486412
H	5.5565794	-0.7875197	87.2828436
C	3.7278010	-1.6833193	88.0587176
C	4.0874493	-3.0185592	87.7046549
C	2.4697182	-1.4392558	88.7213763
C	1.5963626	-2.5491266	88.9336362
C	2.1262727	-0.0878624	89.1027801
C	2.9690375	0.9476643	88.6773169
O	0.2607722	1.7717357	88.1765936
O	2.6310038	2.2769220	88.9656888
P	1.3838217	2.9513500	88.1384015
O	0.9727455	4.2195052	88.8759097

O	1.7259360	3.0669499	86.6394533	H	7.5324047	0.5189634	89.9717821
C	-0.1640334	-1.7204527	93.5593656	C	5.9387864	2.4164896	88.7095815
C	1.1428863	-1.8743265	93.0251971	C	3.8868569	2.8793737	84.2427542
H	-2.0984515	-0.7770636	93.3215741	C	5.2576566	2.3401224	86.3416884
H	-0.4349969	-2.2229622	94.5003749	H	5.3636101	-0.1740074	85.0851844
H	2.5105175	-1.3771138	91.4313248	H	6.0163772	1.0547914	83.9579683
H	1.8845464	-2.4857636	93.5614669	C	5.8416439	1.9149135	90.1490567
C	1.9655385	-3.8336392	88.5583513	C	5.1373405	1.8610920	87.6762561
C	3.2278655	-4.0774142	87.9542293	C	4.3774333	1.7921419	85.2172548
H	0.6111123	-2.3791650	89.3882384	H	4.3722647	3.4456995	90.7223092
H	1.2692575	-4.6695113	88.7256328	H	3.5509086	3.7962890	84.7758957
H	3.5124957	-5.1019204	87.6701341	H	6.0541192	3.8155109	91.2317717
H	5.0580532	-3.1879305	87.2126019	H	6.3780928	6.3757977	86.0049712
C	-2.2727041	3.6948566	89.9356882	H	4.6817825	3.2189240	83.5473064
C	-2.1338757	2.4408965	89.2734685	H	8.9384293	5.4370659	88.6603008
C	-2.6213928	4.8165657	89.1612794	H	5.1074586	1.0846342	90.1635632
C	-2.4917595	2.3113335	87.9021111	H	3.4778497	1.3549494	85.6971219
C	-2.8325829	3.4643231	87.1766244	H	7.4658855	3.8695907	89.1960304
C	-2.8319011	4.7370006	87.7733924	Zn	1.3587907	6.0087919	89.5892634
H	-2.6636361	5.8056918	89.6380896	Br	-0.3182414	7.6229419	89.8166330
C	-2.5261358	0.9472656	87.2151925	C	7.9184228	7.8756221	90.5029731
H	-3.0535116	3.3696841	86.1024122	C	3.7110134	7.6047474	89.3832898
C	-1.8373689	0.9280235	85.8415612	C	7.1788738	6.7147395	90.7795554
H	-2.3723809	1.5505860	85.0955467	C	5.9273379	8.8890721	89.5337367
H	-1.8055467	-0.1058240	85.4405340	C	5.1835403	7.7187604	89.7920119
H	-0.7981108	1.3038058	85.9063406	C	7.2841575	8.9672896	89.8830524
C	-3.9834901	0.4529880	87.1179096	C	5.8205141	6.6406936	90.4284815
H	-1.9867110	0.2282562	87.8669682	O	3.1743776	6.4086548	89.8265259
H	-4.5895773	1.1344137	86.4845578	H	8.9840556	7.9346657	90.7730047
H	-4.4621131	0.4092176	88.1173009	H	5.4414453	9.7553793	89.0538309
H	-4.0284328	-0.5604501	86.6673346	H	7.6632713	5.8577032	91.2749897
C	-2.9191306	6.0029250	86.9322707	H	7.8513904	9.8871790	89.6717649
C	-1.5490221	6.2411678	86.2623888	H	5.2209960	5.7447149	90.6352992
H	-1.5229065	7.1997370	85.7044884	H	1.5916680	8.7474781	88.1307587
H	-1.3216502	5.4277229	85.5385656	Br	-0.1047241	3.4237103	83.2952259
H	-0.7449627	6.2726497	87.0243785	Zn	1.1700571	4.0452940	85.0849997
C	-4.0543388	5.9906551	85.8980729	C	3.5774563	7.8039192	87.8014284
H	-3.0946868	6.8495180	87.6313033	C	2.3700634	8.6498167	87.3446021
H	-4.1059999	6.9615705	85.3641074	C	3.3429342	6.5051745	87.0844901
H	-5.0374494	5.8081581	86.3773286	C	3.9220454	5.3092696	87.3395394
H	-3.8996198	5.2047721	85.1295336	C	2.2419748	6.7014594	86.1361564
C	-1.9884764	3.8508056	91.4347639	O	1.7384746	7.9265237	86.2389690
C	-0.4884508	4.0146181	91.7468558	O	1.7554908	5.9168686	85.2918756
H	-0.3166353	4.0349038	92.8424723	H	2.6342765	9.6528486	86.9620015
H	-0.1238427	4.9807619	91.3369522	H	4.7122722	5.2042173	88.0924533
H	0.1270148	3.2031620	91.3141250	H	3.6075843	4.4025849	86.8103822
C	-2.7907938	4.9867134	92.0890707	H	4.5145672	8.2668002	87.4299987
H	-2.3109012	2.9083963	91.9227312	H	3.1821595	8.4914006	89.8256716
H	-2.6739013	4.9480591	93.1912547				
H	-3.8718453	4.9137938	91.8543462				
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H	8.3348663	4.8336125	85.6879737				
H	7.9737734	2.1083090	90.6712112				
H	4.4297233	0.2817422	83.6259906				
C	7.9801174	5.0400365	86.7227597				
H	5.1150739	2.5731484	92.1074014				
H	7.9297019	7.2068276	86.3641650				
H	3.0567345	2.4944788	83.6147538				
C	7.0154843	3.9116961	87.0761209				
C	7.1800070	1.3329152	90.6375220				
C	7.2464082	6.3973892	86.6943418				
H	6.8739359	6.6639811	87.7050670				
C	6.8558301	3.4370697	88.3894256				
C	5.0864873	0.6739134	84.4297928				
H	9.7288675	4.1336023	87.7087100				
C	6.2053978	3.3450850	86.0717125				
C	9.2124066	5.1120749	87.6352498				
H	9.9364165	5.8557991	87.2452558				
H	6.3157619	3.7158073	85.0396933				
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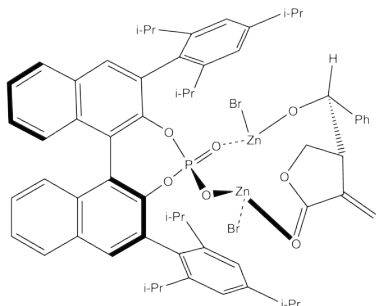


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C	1.5078743	-1.2478220	91.8305085
C	-0.7416786	-0.2457877	91.6903803
C	-1.0705356	-0.9094361	92.9100370
C	-1.6745481	0.6261244	91.0530828
H	-2.6753201	0.7444481	91.4956294

C	-1.3359479	1.3544310	89.9203121	H	3.0687030	2.5019449	83.5977238
C	4.2146558	0.7252658	87.9952077	C	7.0125820	3.9148252	87.0743098
C	4.5850033	-0.5904293	87.7445781	C	7.1822954	1.3258325	90.6264347
H	5.5639531	-0.7902240	87.2828791	C	7.2358671	6.4028994	86.7039619
C	3.7351865	-1.6873080	88.0590275	H	6.8620199	6.6633721	87.7157407
C	4.0970912	-3.0236867	87.7136706	C	6.8535877	3.4354858	88.3855684
C	2.4765786	-1.4418524	88.7197550	C	5.0839553	0.6684390	84.4279156
C	1.6060692	-2.5522626	88.9391123	H	9.7233740	4.1423178	87.7107439
C	2.1295804	-0.0893064	89.0935632	C	6.2047896	3.3495089	86.0677997
C	2.9690682	0.9461747	88.6606274	C	9.2052074	5.1198858	87.6396627
O	0.2598861	1.7599919	88.1651049	H	9.9284405	5.8659878	87.2529489
O	2.6308695	2.2761645	88.9402335	H	6.3147202	3.7240697	85.0371701
P	1.3730720	2.9482441	88.1257936	C	5.3098052	2.9862628	91.0953241
O	0.9594899	4.2066210	88.8780474	H	7.0793893	0.9085365	91.6493754
O	1.7027631	3.0819966	86.6255239	H	7.5376988	0.5151562	89.9585550
C	-0.1430225	-1.7057542	93.5649187	C	5.9394391	2.4113211	88.7012396
C	1.1608597	-1.8625482	93.0258646	C	3.8999795	2.8825463	84.2265645
H	-2.0770003	-0.7617908	93.3321972	C	5.2592107	2.3415538	86.3329450
H	-0.4104866	-2.2042194	94.5089976	H	5.3482013	-0.1807181	85.0867582
H	2.5213256	-1.3721654	91.4235724	H	6.0208997	1.0388855	83.9618745
H	1.9044591	-2.4724763	93.5610453	C	5.8424887	1.9052636	90.1391867
C	1.9781978	-3.8378981	88.5723691	C	5.1396965	1.8580513	87.6657132
C	3.2404226	-4.0826416	87.9698212	C	4.3797571	1.7956572	85.2067062
H	0.6209603	-2.3803983	89.3931068	H	4.3659044	3.4276460	90.7177942
H	1.2837574	-4.6740949	88.7452005	H	3.5602139	3.7990401	84.7548460
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H	5.0678891	-3.1939134	87.2222876	H	6.3677478	6.3815468	86.0143655
C	-2.2670365	3.6974376	89.9366390	H	4.7016399	3.2118786	83.5336329
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C	-2.6092431	4.8203347	89.1615195	H	5.1108333	1.0726711	90.1505923
C	-2.4826104	2.3159221	87.9014784	H	3.4750310	1.3669632	85.6851786
C	-2.8149540	3.4703556	87.1751901	H	7.4614407	3.8674352	89.1941002
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H	-2.6515195	5.8091287	89.6387102	Br	-0.3192322	7.6307664	89.7733701
C	-2.5256968	0.9512628	87.2162543	C	7.9002918	7.8568815	90.5252940
H	-3.0319251	3.3773585	86.0999937	C	3.6978354	7.5959544	89.3868618
C	-1.8465543	0.9257114	85.8382271	C	7.1522900	6.7036299	90.8096085
H	-2.3820357	1.5489109	85.0932820	C	5.9204801	8.8722936	89.5384138
H	-1.8226120	-0.1086534	85.4383327	C	5.1686118	7.7089421	89.8025912
H	-0.8045206	1.2948566	85.8937703	C	7.2756795	8.9464098	89.8932120
C	-3.9860116	0.4637124	87.1304745	C	5.7954951	6.6337813	90.4532894
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C	-1.9886933	3.8547047	91.4366715	O	1.7454129	7.9299531	86.2262287
C	-0.4918939	4.0362694	91.7546981	O	1.7566443	5.9134216	85.2877414
H	-0.3231297	4.0456694	92.8509819	H	2.6397241	9.6515342	86.9590944
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H	0.1358343	3.2383375	91.3144716	H	3.5936195	4.3985192	86.8080897
C	-2.8067317	4.9808763	92.0885175	H	4.5168920	8.2564622	87.4385642
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H	-2.6954462	4.9428549	93.1913102				
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H	8.3300258	4.8466179	85.6908705				
H	7.9742457	2.1028697	90.6620048				
H	4.4298189	0.2798234	83.6203083				
C	7.9736571	5.0478007	86.7263003				
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H	7.9158616	7.2168940	86.3782916				

15l-mi; COSMO



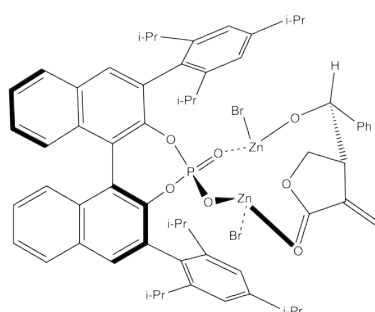
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C	-1.8012328	-1.1041790	271.8347297
C	-1.6202761	1.1160185	270.7406361
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C	4.7007461	-0.6571960	267.8112539
H	5.6796334	-0.9293598	267.3893649
C	3.5905777	-1.5172023	267.5655085
C	3.7352834	-2.6874909	266.7613405
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C	1.1731751	-1.9800957	267.6948588
C	2.1555732	-0.0062716	268.9152873
C	3.2780705	0.8086393	269.0694468
O	0.9800243	2.5976521	268.6434514
O	3.1464617	1.9695650	269.8310783
P	2.4391151	3.2326733	269.0713383
O	2.3504446	4.3492383	270.1066735
O	3.1150549	3.5431615	267.7237683
C	-1.2558530	-2.3390381	272.1511290
C	0.0287898	-2.6902155	271.6566586
H	-2.7839552	-0.8065726	272.2331416
H	-1.8063931	-3.0394845	272.7974508
H	1.7276337	-2.1058610	270.4675062
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H	0.1665051	-1.6986338	268.0335612
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H	2.7619345	-4.3633627	265.8047395
H	4.7380070	-2.9460944	266.3860901
C	-1.4056830	4.3547588	270.9222385
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H	-1.3577826	2.8384207	265.2729544
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C	0.2563753	5.0456051	272.7266061
H	0.7541379	4.7138851	273.6607731
H	-0.2173296	6.0268335	272.9382798
H	1.0445929	5.1947877	271.9652117
C	-1.8417710	3.7518189	273.3437433
H	-0.2153156	3.0443629	272.1246994
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H	-2.5479397	2.9506141	273.0458316
H	-2.4372373	4.6707179	273.5283634
H	8.2931943	5.5027633	267.6625892
H	7.8953421	1.2984796	271.7932541
H	6.1419374	0.6260469	264.2669227
C	7.9994977	5.2662633	268.7096796
H	4.9813559	1.7077545	273.1139389
H	7.5598377	7.3822403	269.1230422
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C	7.2435643	3.9453468	268.6625743
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C	7.0647237	6.3913360	269.1976348
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C	6.8893296	3.2529041	269.8338963
C	6.5355489	0.9831858	265.2411668
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C	6.8049908	3.4208103	267.4368496
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H	7.0832358	3.9529973	266.5131838
C	5.2761640	2.2976458	272.2217421
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C	5.9833140	2.2823283	267.3514184
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H	7.4552424	1.5736661	265.0451804
C	5.8039761	1.3666193	271.1173796
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H	4.3933397	2.8713437	271.8801943
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H	5.9150444	3.5737578	264.6579824
H	9.0588403	5.0028550	270.6198067
H	5.0202042	0.6072308	270.9191328
H	4.5888714	1.2066453	266.1295728
H	7.2307097	3.6349599	270.8082014
Zn	3.5797986	5.9329293	270.2264469
Br	4.4521632	6.3208722	272.3243815
C	1.5645155	10.5964142	270.2831214
C	2.5222272	10.0002301	269.4492202
C	2.4481239	8.6292628	269.1315185
C	1.3825923	7.8677498	269.6575705
C	0.4317707	8.4602118	270.5055128
C	0.5178797	9.8248319	270.8193338
H	1.6447656	11.6659112	270.5327591
H	3.3569426	10.6028346	269.0540039
C	3.5067131	7.9685637	268.2546979
H	1.2888228	6.8018199	269.3916565
H	-0.3805733	7.8428090	270.9143623
H	-0.2251225	10.2874271	271.4870205
O	3.6484774	6.6061129	268.4712652

C	3.1897697	8.1507179	266.7238404
C	1.9542634	7.3665821	266.3597135
C	2.4307305	6.0668078	265.8567364
O	3.7263360	6.1105204	265.5803872
C	4.2722016	7.4309625	265.8948120
O	1.7574076	5.0350450	265.6537075
C	0.6467806	7.6661806	266.4979711
H	4.4878791	7.9269799	264.9274960
H	5.2104655	7.2580587	266.4536454
Zn	2.3560640	3.1515216	265.9860336
Br	1.6444840	1.2287017	264.9765236
H	-0.1241052	6.9231112	266.2389244
H	0.3219441	8.6487370	266.8687578
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15l-mi



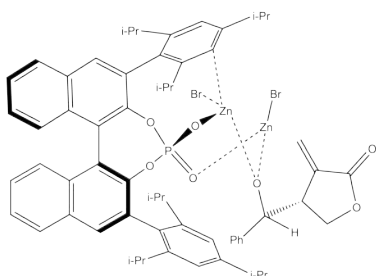
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C	-1.7983573	-1.1165142	271.8238114
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H	-2.5938090	1.3916803	271.1845777
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C	4.5623432	0.5457480	268.5011688
C	4.6883425	-0.6437352	267.7926484
H	5.6655773	-0.9162674	267.3672278
C	3.5719129	-1.4908264	267.5326141
C	3.7061431	-2.6476731	266.7083306
C	2.2699111	-1.1462011	268.0517511
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C	2.1499900	0.0087237	268.9078110
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O	0.9825649	2.6282734	268.6807968
O	3.1524381	1.9678521	269.8454304
P	2.4584164	3.2388160	269.0888931
O	2.4149173	4.3733294	270.1080976
O	3.1232097	3.5311326	267.7298047
C	-1.2559564	-2.3571813	272.1193675
C	0.0248915	-2.7046626	271.6143083
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H	-1.8061038	-3.0653611	272.7574334
H	1.7206091	-2.1071578	270.4270890
H	0.4701999	-3.6768369	271.8751691
C	1.3140847	-3.0461930	266.8381993
C	2.6026124	-3.4157260	266.3703764
H	0.1485214	-1.6566623	268.0063251
H	0.4343190	-3.6369123	266.5408118
H	2.7198677	-4.2993127	265.7247428
H	4.7060523	-2.9059029	266.3255657
C	-1.4075473	4.3546670	270.9701244
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H	-1.5226219	8.4233072	268.5529740
C	-4.7536456	7.2689407	269.2927878
H	-3.0654273	7.9378109	270.4523702
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H	-5.2079985	6.6751493	270.1110950
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C	-0.7716157	3.9846266	272.3100044
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H	-0.1531191	6.0077142	272.9515227
H	1.0785863	5.1215100	271.9867761
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H	-2.5715946	2.9938878	273.1079184
H	-2.4100334	4.7103784	273.5858355
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H	6.1887635	0.6805710	264.2804672
C	8.0945186	5.2002285	268.7868710
H	4.9670356	1.6036637	273.1366504
H	7.7122023	7.3448821	268.4646167
H	4.5182969	2.7247958	264.2571028
C	7.3002859	3.8990374	268.7463497
C	7.0425427	0.5116226	271.5877456
C	7.1432452	6.4015359	268.6004329
H	6.4959244	6.5217352	269.4940032
C	6.9188800	3.1965319	269.9003570
C	6.5780404	1.0196963	265.2628286
H	9.6154186	4.5129105	270.2222920
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H	7.1672295	3.9358937	266.5921719
C	5.2709623	2.2107245	272.2592526
H	6.8248752	-0.0817217	272.5000847
H	7.3880123	-0.1846477	270.7967811
C	6.0989985	2.0528869	269.8434690
C	5.1117235	3.0665473	265.1307948
C	6.0190473	2.2842325	267.3926352
H	6.8662797	0.1228180	265.8454645
H	7.5037274	1.6058977	265.0831936
C	5.7966761	1.3001127	271.1375711
C	5.6173639	1.6042329	268.5824767
C	5.5312705	1.8708158	266.0046607
H	4.3950609	2.7988724	271.9256252
H	4.5431498	3.8247590	265.7132044
H	6.0392484	2.9308026	272.6072641
H	6.4698475	6.2593827	267.7315970
H	5.9793706	3.6279745	264.7253411
H	8.3095473	5.5120754	270.9476235

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H	4.6270742	1.2416826	266.1392736	C	-38.1669576	-61.7416003	3561.0662926
H	7.2567347	3.5509687	270.8842555	C	-36.8016562	-61.8882767	3560.7040651
Zn	3.7617084	5.8808343	270.0943245	H	-39.9381254	-60.5066516	3560.9040314
Br	4.9333382	6.2197406	272.0416216	H	-38.6409279	-62.4775587	3561.7333364
C	1.5372222	10.5618894	270.2030249	H	-35.1333805	-61.1005621	3559.5919426
C	2.4877576	9.9745341	269.3558457	H	-36.2172289	-62.7303468	3561.1051368
C	2.4451090	8.5950054	269.0714000	C	-34.8190855	-62.4237580	3556.2251739
C	1.4213214	7.8142525	269.6468726	C	-33.4274568	-62.5498162	3555.9671054
C	0.4777341	8.3986846	270.5082416	H	-36.4028740	-61.2004219	3557.0285134
C	0.5304785	9.7723896	270.7865916	H	-35.5055710	-63.2303422	3555.9258030
H	1.5921726	11.6387606	270.4260351	H	-33.0391963	-63.4588266	3555.4830814
H	3.2927149	10.5920823	268.9232406	H	-31.4893177	-61.5908094	3556.0881826
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H	1.3616971	6.7390786	269.4133508	C	-38.8783739	-56.0959388	3558.5486278
H	-0.3021682	7.7660284	270.9550894	C	-39.2025827	-53.9713265	3559.6966423
H	-0.2070016	10.2287645	271.4645554	C	-39.1977762	-55.4707466	3557.3136486
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C	3.1226178	8.1501121	266.6463460	C	-39.5456902	-53.3197487	3558.4879137
C	1.9053576	7.3257708	266.3123271	C	-39.3260673	-56.2665823	3556.0186556
C	2.4157472	6.0450017	265.7910901	H	-39.7432663	-53.6036633	3556.3414849
O	3.7004326	6.1426966	265.4676960	C	-38.5093043	-55.6709314	3554.8628289
C	4.1989608	7.4816377	265.7687747	H	-38.8527980	-54.6532047	3554.5905184
O	1.7787429	4.9899614	265.6060358	H	-38.5920172	-56.3014110	3553.9553732
C	0.5933446	7.5752437	266.4966909	H	-37.4339662	-55.6184017	3555.1236308
H	4.3541801	7.9936503	264.7971952	C	-40.8136063	-56.4095288	3555.6381192
H	5.1671874	7.3511616	266.2870584	H	-38.9383932	-57.2868619	3556.2126101
Zn	2.3579721	3.1093355	266.0080832	H	-41.2695112	-55.4216977	3555.4172118
Br	1.6914746	1.2032623	264.9546896	H	-41.3957172	-56.8741677	3556.4592431
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H	0.2448665	8.5413139	266.8883973	C	-40.1507380	-51.9212198	3558.5442653
H	4.4489683	8.5130662	268.3174554	C	-39.8577867	-51.0501228	3557.3235051
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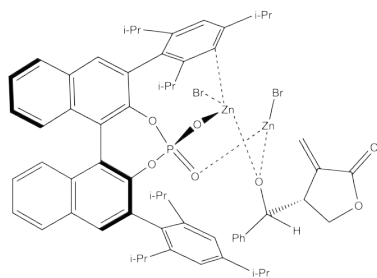
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C	-38.9848709	-58.4931291	3559.3873249	C	-30.4789414	-57.3563539	3554.6498087
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C	-32.6607792	-58.0314204	3557.7230743	C	-27.3638254	-54.5590118	3559.1222599
C	-32.1885944	-59.2380912	3557.2166955	H	-26.5296179	-53.8345830	3559.2271609
H	-31.1135581	-59.3443445	3557.0071612	H	-29.6481556	-54.7708256	3556.2182148
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C	-32.5662348	-61.5175113	3556.3065680	H	-31.4700783	-58.3668806	3562.2259556
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C	-37.7680784	-50.7887718	3554.4253274
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C	-38.4405980	-55.9051668	3561.0870750
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C	-39.6106163	-55.9695386	3562.0855639
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H	-30.2200360	-57.0297893	3561.7870320
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H	-33.3275857	-56.3874422	3562.1480248
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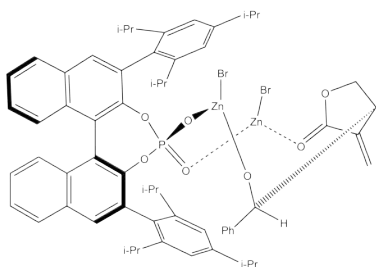


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C	-38.9846382	-58.5076266	3559.3392612
H	-39.9949203	-58.3426222	3559.7450943
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C	-30.9858203	-57.7321262	3561.3967498
C	-28.8926236	-52.7364523	3559.4525630
H	-29.0747575	-53.1049700	3560.4832953
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H	-26.4200617	-53.9261695	3559.0130343
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H	-31.4839252	-58.2004309	3562.2707485
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C	-31.3634712	-56.4276568	3559.2535301
C	-31.8771023	-55.3228291	3554.5802048
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H	-30.2215339	-58.3637834	3555.1563274
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C	-32.0143637	-57.0120439	3560.5058950
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Br	-35.3297975	-54.0213504	3552.8532498
Zn	-35.4162705	-53.9336525	3555.1540408
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C	-37.7675848	-50.6967441	3554.5006257
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H	-35.5972345	-48.8792833	3553.7409096
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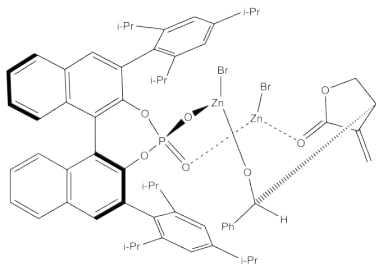
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C	5.5896841	8.5852507	807.1499697	H	-4.6349832	6.8483038	810.2568605
C	3.3772027	10.2935028	807.3631130	H	-6.5149872	7.1370269	808.6393306
C	3.2112936	8.9123260	807.5914339	H	-6.4803540	5.4537393	809.2651343
C	4.6359543	10.8160407	807.0273897	H	-5.8782968	5.8131436	807.6172008
C	4.3301140	8.0635332	807.4895576	C	-2.0173141	3.1325078	812.1382424
O	1.9223754	7.0059379	808.3146826	C	-1.1154603	4.2182909	812.7512152
H	6.7349957	10.3693189	806.6508170	H	-0.7278254	3.8839753	813.7360351
H	2.5111912	10.9705438	807.4536833	H	-1.6579165	5.1728479	812.9085916
H	6.4568556	7.9107273	807.0706702	H	-0.2537873	4.4320002	812.0902135
H	4.7535756	11.8978951	806.8579400	C	-3.1896187	2.7778967	813.0715597
H	4.1841834	6.9923104	807.6953085	H	-1.3938431	2.2221963	812.0335379
Br	1.7206376	1.3691447	804.7813116	H	-2.8165820	2.4527458	814.0649145
C	-0.1590552	1.3756503	809.2119625	H	-3.8106382	1.9592095	812.6533085
C	0.6817391	0.2680806	809.3540715	H	-3.8546659	3.6522431	813.2318789
C	0.2038217	-0.8345344	810.1544853	H	7.7315339	6.5871534	808.6107035
C	1.0258489	-1.9468098	810.5081796	H	7.2046244	1.9198361	812.1694824
C	-1.1534334	-0.8039682	810.6484969	H	5.7762742	2.4025219	804.3394276
C	-1.6419170	-1.9066114	811.4127114	C	7.5306352	6.0901230	809.5854589
C	-1.9700898	0.3374855	810.4037006	H	4.1511117	1.9144268	813.1400160
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C	-1.4851755	1.4536794	809.7317860	H	3.9767006	4.2536700	804.6219322
C	4.2586592	1.3567593	808.4446682	C	6.7130410	4.8411231	809.2828722
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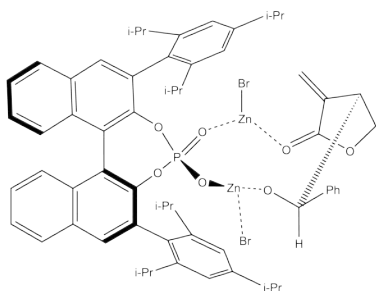
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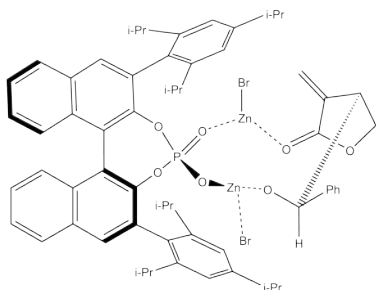
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H	-4.2634002	-6.6725341	1404.1951236
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H	-3.0410029	-10.1806922	1407.9890223
H	-4.0399836	-7.9832491	1402.9849745
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H	-9.4492919	-8.8198249	1407.3367342
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Br	-4.5768615	-1.3204457	1404.5575441
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H	-4.9112628	-4.9092243	1409.6769030
H	-1.2275984	-4.2601563	1407.7441194

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Zn	-7.6215595	-1.7731264	1407.7509173
H	-6.2475347	-3.6552933	1409.4631337
Br	-9.7174860	-1.4773678	1408.6028799
C	-9.2652861	-3.3236471	1404.6207039
C	-10.1976884	-4.2229032	1405.1454997
C	-11.4328542	-3.6914747	1405.6575035
C	-12.3518901	-4.4796005	1406.4098591
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C	-8.5621457	-7.7143025	1405.2924000
C	-9.5362690	-8.4604251	1404.6346074
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C	-12.0259201	-5.8796033	1403.5349068
C	-9.9646495	-5.6857357	1404.9934042
C	-8.8057810	-6.3170087	1405.4638257
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H	-6.9511508	-0.9869913	1400.5231345
C	-7.4194236	-3.7248571	1401.2134400
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C	-4.5555957	0.7433129	1401.0171392
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C	-8.5649793	0.5849548	1405.4617926
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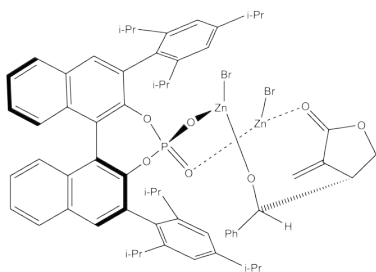


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C	-2.3390928	-6.1093495	1409.3868650
C	-2.8550420	-5.5975205	1408.1781323
C	-2.9201762	-7.2314117	1409.9968408
C	-3.9284722	-6.2650700	1407.5646418
O	-2.6824140	-4.0164732	1406.3116230
H	-4.4959704	-8.7349262	1409.8769395
H	-1.4788959	-5.6129499	1409.8672432
H	-5.3710545	-7.8735224	1407.6893898
H	-2.5109552	-7.6146268	1410.9447262
H	-4.3269784	-5.8919006	1406.6119471
C	-2.8185258	-3.1225116	1408.6178642
C	-4.3103539	-3.0332881	1408.8460776
C	-4.7385407	-1.6649419	1408.4899775
O	-3.7024520	-0.9208103	1408.1345628
C	-2.4810929	-1.7209848	1408.0685886
O	-5.8800171	-1.1667654	1408.5382593
C	-5.1840124	-3.9259206	1409.3646753
H	-4.8777934	-4.9218798	1409.7121145
H	-2.3094611	-3.2983825	1409.5877063
H	-1.7092047	-1.1762928	1408.6437744

H	-6.8109396	-0.4885303	1406.2183719
C	-9.2129636	1.9748997	1405.5263717
H	-9.2986258	-0.1319630	1405.8792761
H	-9.5107136	2.2149490	1406.5677134
H	-10.1204176	2.0219857	1404.8908543
H	-8.5228124	2.7725215	1405.1814481
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H	-8.0975975	-10.6467840	1409.4090062
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C	-4.1752529	-11.3491019	1406.5505731
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C	-5.2587408	-10.3060992	1406.3034893
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C	-6.3716428	-10.1893604	1407.1586525
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H	-5.2093358	-12.9218115	1405.4099335
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H	-3.9332325	-13.5319431	1406.5175075
H	-4.3059820	-9.5095655	1404.5389194
C	-8.2681890	-7.9227788	1408.8520345
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H	-7.7414593	-8.7559732	1402.5779282
H	-6.0981789	-9.3756589	1402.2181128
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H	-4.2439762	-6.6907944	1404.2024351
H	-7.3811903	-8.1395732	1409.4839678
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Zn	-4.2121489	-3.4190738	1405.4510321
Br	-4.5699022	-1.3250484	1404.5202157
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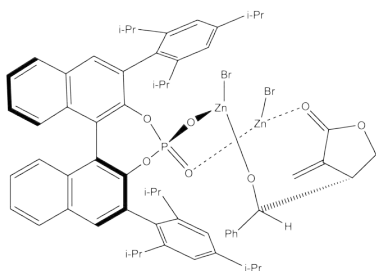
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C	-1.2499461	-0.9649187	272.5838371
C	-1.5860837	0.8433839	270.9138895
H	-2.6213248	0.9580150	271.2677915
C	-1.1011200	1.6852406	269.9221000
C	4.5745769	0.8960748	268.4145929

C	4.8411065	-0.3902996	267.9591798
H	5.8278772	-0.6070170	267.5217256
C	3.8715136	-1.4292972	268.0210552
C	4.1371571	-2.7198331	267.4717571
C	2.5886918	-1.1649332	268.6256664
C	1.6041787	-2.1994802	268.5888373
C	2.3370657	0.1361014	269.2028152
C	3.3038008	1.1350441	269.0169619
O	0.7260086	2.2954497	268.4773702
O	3.0880992	2.4235760	269.5047601
P	1.8601279	3.3676168	268.9808453
O	1.3994500	4.1890133	270.1703718
O	2.2335250	4.1117224	267.6721776
C	-0.4421188	-1.9200773	273.1833800
C	0.8897928	-2.1096577	272.7276590
H	-2.2774550	-0.7967991	272.9428321
H	-0.8262151	-2.5226038	274.0205454
H	2.4196391	-1.5121660	271.3261664
H	1.5363278	-2.8508056	273.2217978
C	1.8862394	-3.4382742	268.0296039
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H	1.1056907	-4.2140293	268.0070771
H	3.3812253	-4.7000315	267.0474918
H	5.1268235	-2.9066751	267.0261751
C	-1.9801696	4.0693928	269.8755264
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H	-2.5527692	6.1375536	269.5730791
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H	-2.9986573	3.5953807	266.1173659
C	-1.2676214	1.2404481	265.9821701
H	-1.6284453	1.9238365	265.1863949
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H	-1.7781219	0.5295008	267.9427629
H	-4.0887782	1.4365268	266.1089114
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H	-3.5751417	-0.2510205	266.4200140
C	-3.3244720	6.2265915	266.9876969
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H	-3.3389301	7.1243815	264.9981809
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C	-4.8174716	6.4703216	267.2862270
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H	-0.5264289	5.7192437	272.5971225
H	-1.9313198	6.4210613	271.7586219
H	-0.4529445	6.1126157	270.8318033
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H	-0.7412051	3.5886726	271.5422711
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H	8.4131810	1.5035980	271.4835228
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H	3.5881276	3.8162878	264.6114415
C	7.8978641	3.6242998	267.9182457

C	7.5939266	0.7875737	271.2639608
C	9.3748970	5.5795508	268.6442465
H	9.4986256	5.2078789	269.6833553
C	7.6746989	2.9745548	269.1467612
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H	7.0687329	4.0179668	265.9638393
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H	6.1578457	1.8116276	264.4253349
C	6.3399475	1.4971304	270.7272344
C	5.6349660	1.9511090	268.2960391
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H	4.8589015	2.9977254	271.3814234
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H	5.5560937	0.7208508	270.6047272
H	3.8151732	2.1909985	266.4032301
Zn	1.9640539	5.7965626	271.2187621
Br	2.8044239	5.2987824	273.3060874
H	8.4007492	3.1056210	269.9646800
C	5.3306444	5.7482726	269.6982742
C	4.1054697	6.3909547	269.4671984
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H	4.6114959	9.2465064	271.2958026
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O	1.4497959	7.2692785	270.1472299
C	1.9958944	7.8713514	267.4678773
C	0.5914166	7.4021846	267.5093873
O	-0.1836945	8.3150595	268.0723212
C	0.6349864	9.4175752	268.5824548
O	0.0893216	6.3587394	267.0475260
C	2.8991295	7.4464756	266.5645323
Zn	0.9185108	4.6849551	266.3801870
Br	0.5677630	4.1247617	264.1921661
H	3.3488773	5.9046980	268.8347212
H	5.5245455	4.7616031	269.2518110
H	7.2438428	5.8413451	270.7224789
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H	3.9229627	7.8481357	266.5407250
C	2.0957393	8.9117924	268.5521908
H	0.2641951	9.6365895	269.6006455
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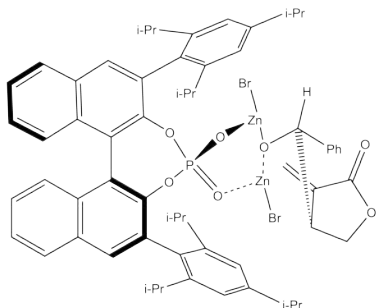
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C	0.5656566	-0.3773346	271.0241668	H	9.0457678	4.8435318	266.5806784
C	1.3709086	-1.3428799	271.6970610	H	8.4202537	1.5867410	271.5084972
C	-0.7813353	-0.1526801	271.4962550	H	4.4083413	1.3609537	264.1144013
C	-1.2724067	-0.9372667	272.5820553	C	9.1660905	4.4040885	267.5955922
C	-1.5940783	0.8507395	270.8881604	H	5.5885964	2.1044964	272.7030273
H	-2.6298937	0.9750430	271.2367262	H	10.3011597	6.1384151	268.3045716
C	-1.1024987	1.6805145	269.8896139	H	3.5620090	3.7549751	264.5987863
C	4.5819173	0.8849561	268.4338102	C	7.8946661	3.6124215	267.8815248
C	4.8605567	-0.4080598	268.0059980	C	7.6211231	0.8488904	271.2871050
H	5.8524930	-0.6238779	267.5797550	C	9.3892930	5.5672639	268.5752507
C	3.8986200	-1.4526258	268.0806919	H	9.5283307	5.2016806	269.6145910
C	4.1768840	-2.7515801	267.5594408	C	7.6823019	2.9766714	269.1189478
C	2.6093703	-1.1846552	268.6691860	C	5.1736021	1.4568045	264.9120905
C	1.6323800	-2.2264585	268.6438084	H	10.2460333	2.6518970	266.8165533
C	2.3436893	0.1253523	269.2193848	C	6.9123491	3.4593254	266.8891646
C	3.3053092	1.1281058	269.0223989	C	10.3892617	3.4684752	267.5523756
O	0.7311934	2.2596264	268.4422590	H	11.3076824	4.0268683	267.2759626
O	3.0818966	2.4249031	269.4817328	H	7.0484932	3.9841569	265.9303808
P	1.8435280	3.3520324	268.9499970	C	5.7876055	2.5634333	271.7128316
O	1.3601455	4.1704136	270.1315772	H	7.3924913	0.3256809	272.2379391
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C	-0.4696408	-1.8827824	273.2020530	C	6.5691514	2.1467371	269.3518671
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H	1.5095837	-2.8086583	273.2726988	C	6.3562984	1.5208943	270.7287295
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H	0.6272164	-2.0302584	269.0402686	H	4.8373884	2.9998019	271.3488288
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H	3.4386092	-4.7445655	267.1678246	H	6.5013814	3.3997635	271.8661973
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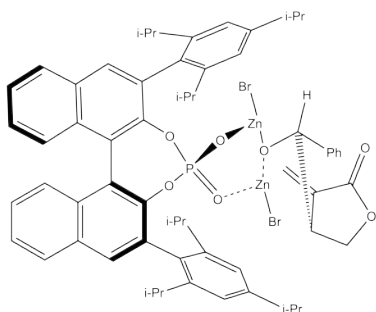
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C	5.3695668	5.9803982	283.2609538
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C	2.3532549	7.2537089	284.9113337
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O	1.0351464	7.0333205	285.4623854
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C	0.4595465	5.6669253	275.8359756
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H	3.2043339	0.9426496	286.7119197
H	5.9826142	3.8416151	280.0307916
C	3.9394900	0.1797913	283.3798256
C	1.5442541	-2.9199266	281.3198138
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C	2.8663914	-0.5583932	282.8538831
C	6.7252999	0.9952717	279.7939665
H	5.5651539	-1.4755003	284.9152386
C	4.7583492	0.8766042	282.4769029
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H	0.6797706	-3.4936565	280.9263110
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C	2.6042442	-0.6219153	281.4746863
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C	3.4596247	0.0771375	280.5756859
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H	-0.0148530	0.2326278	281.3388923

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Zn	3.6166461	4.8983808	280.7163655
Br	4.0942927	7.0048384	279.8922054
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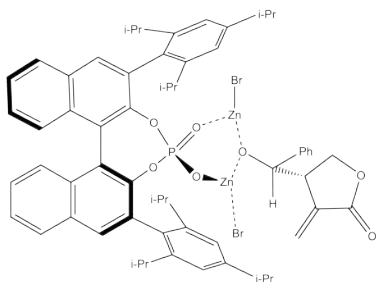
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C	4.9237882	4.0468322	284.7034009
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C	6.3008144	3.8750087	284.9063027
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O	2.6787853	4.4419665	282.3625334
H	8.2985081	4.6008703	284.4338012
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Br	-0.2185178	2.7595292	284.0199314
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C	0.2642956	6.3519006	282.0062074
C	0.1299738	6.6940535	284.4862416
O	1.0305328	7.0254070	285.4640623
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C	0.3219919	1.3101268	276.8655506
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C	-1.9565408	1.3311595	275.8668329
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C	-2.0907960	2.7030237	276.2317382
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C	-1.1012508	3.3700152	276.9426592
C	3.1731548	0.0186820	279.0994006
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P	1.4963313	3.0906545	279.3714132
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C	4.1399052	-1.4850289	274.5294371
H	1.3479768	0.5158431	274.5168866
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H	4.7851766	-2.0381610	273.8301966
H	5.2906493	-2.0375911	276.2776388
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C	-0.0767164	9.3267598	279.6488321
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H	2.1416321	0.0269151	285.6123581

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H	1.3439844	-1.3366159	279.8944586
H	4.8388559	1.9135576	279.2407337
Zn	3.5795378	4.9352570	280.6964480
Br	4.0695583	7.0487795	279.9157332
H	2.2035989	-1.0821245	283.5405215
H	-2.6061095	2.8585644	278.8053051
H	2.9176399	7.1647947	282.7614152
H	2.4188370	4.5932849	284.3945349
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15q-mi; COSMO



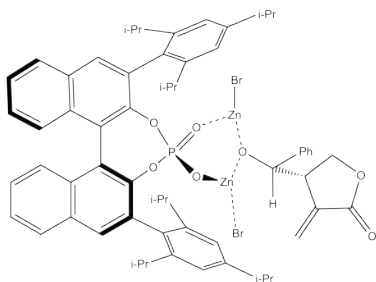
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C	-7.5376689	-3.0178637	508.4994132
C	-2.0453618	-4.6031655	507.1544191
C	-1.9187597	-5.8947204	506.6602705
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C	-3.0095741	-6.8151009	506.6842043
C	-2.8835948	-8.1108475	506.0988064
C	-4.2789700	-6.4224354	507.2546016
C	-5.3791886	-7.3237821	507.1403005
C	-4.3874024	-5.1262710	507.8835671
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O	-5.5678925	-2.6357075	507.1917963
O	-3.3650959	-3.0251373	508.4042184
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C	-6.3798283	-7.1869731	511.2358767
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H	-8.0318901	-0.0608609	511.7951565
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H	-9.3588202	0.4544924	510.6993902
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H	-0.1105915	2.4793618	507.5195469
H	-3.2026904	-3.7641039	503.2093373
C	0.1309049	-0.9168270	506.8171235
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H	2.3447315	1.7851778	507.1108070
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H	0.7883671	-4.7285267	510.7984792

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C	-0.5610017	-3.5568101	509.5197925
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H	-3.5467730	-3.4992001	504.9496044
H	-0.2879765	-1.8278583	510.8643706
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H	-6.4110004	5.8110262	509.5793184
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Zn	-4.3875666	0.2667572	505.5380837
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C	-2.3951725	2.6545034	504.7074528
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15q-mi



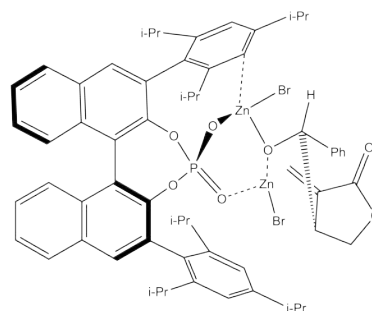
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C	-4.2732920	-6.4297597	507.2597530
C	-5.3682282	-7.3374458	507.1478750
C	-4.3905753	-5.1302293	507.8800452
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O	-4.5284411	-0.8360478	508.8104309
O	-3.6153359	-1.2801221	506.4015647
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C	-6.3813904	-7.1900032	511.2334551
H	-9.2571016	-5.3213964	511.4073234
H	-8.1877436	-7.3196670	512.4610875
H	-4.7188327	-6.8403107	509.9026886
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H	-6.3544802	-7.0354163	507.5260542
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C	-8.9242233	0.4401695	507.6447729
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C	-10.2836478	1.3289937	505.6790136
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H	2.3592904	1.7741686	507.0844248
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H	-3.5397776	-3.5112102	504.9320903
H	-0.3318447	-1.7955917	510.8606711
H	-1.4113560	1.2996628	507.2604975
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Br	-3.0138578	2.2827004	510.4573172
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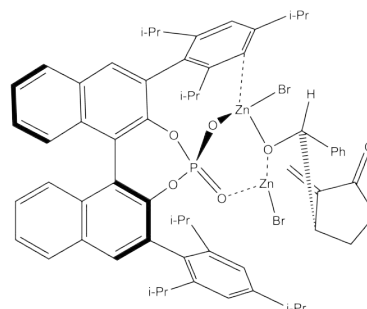


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H	-31.4668610	-59.9414252	3567.0189505
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C	-33.0995434	-62.0755211	3566.8239008
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C	-35.1751294	-59.2278892	3568.2194117
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O	-36.5563484	-56.9028648	3567.3219282
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O	-35.7002434	-54.8017106	3568.7239208
O	-34.5811121	-55.5939529	3566.4976219
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C	-37.2915940	-61.5115266	3571.3368485
H	-40.3215984	-59.8979686	3571.2512792
H	-39.1937351	-61.8286657	3572.3721443
H	-35.5425685	-60.9913755	3570.1905298
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C	-35.4159561	-62.7930734	3566.9632453
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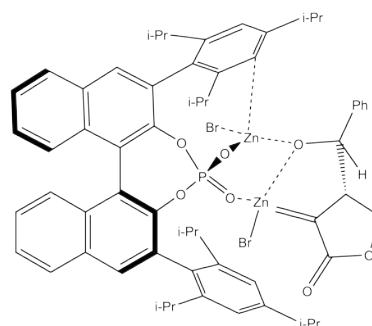


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C	-32.8484977	-58.4513270	3567.7186618
C	-32.4971236	-59.7425351	3567.3497871
H	-31.4686502	-59.9585501	3567.0227884
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C	-35.7998710	-61.5568129	3567.4616265
C	-35.1756389	-59.2326623	3568.2166596
C	-34.1776199	-58.2572711	3568.2165497
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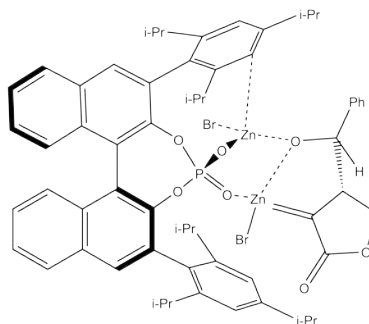


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C	0.6023625	8.6270135	237.0980932
C	-1.0141043	10.4618469	237.0536271
C	0.5539619	8.5743424	235.6903605
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H	-1.7115537	11.0805824	235.0859966
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H	1.1576843	7.8391067	235.1365393
Br	0.3568120	5.1347157	234.2972128
Zn	1.0041785	5.1387019	236.4959876
H	4.3395353	9.0804684	236.5411294
C	2.9491506	7.6169446	237.4345532
C	3.5985428	9.0190652	237.3654828
C	3.8306619	6.9417551	238.4580354
C	4.0370731	5.6374861	238.7175178

C	4.5210994	8.0174128	239.2364105	H	0.4705878	4.1284322	242.2744037
O	4.2868465	9.2166642	238.6189220	C	-2.9100151	3.3732489	242.8534741
O	5.2044769	7.9243595	240.2353593	H	-1.1914787	2.2763169	242.1708068
H	2.8653804	9.8392751	237.2466503	H	-2.7804457	3.0753116	243.9141338
C	0.0053966	0.9715006	239.3104583	H	-3.6595507	2.6973912	242.3932865
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C	2.4613027	-1.5253624	238.2450740	C	5.2593853	1.3649031	234.6981635
C	1.5502605	-2.6202047	238.1424020	H	9.1757528	4.2945633	236.3757134
C	2.1148776	-0.2781483	238.8878333	C	6.2084084	3.7359492	236.8809701
C	3.0163849	0.7890573	238.7524506	C	9.2949354	4.8044674	237.3531400
O	0.4101790	1.8293473	238.2962887	H	9.9890039	5.6594920	237.2152143
O	2.7189408	2.0377897	239.3057617	H	6.2957871	4.3475140	235.9692407
P	1.5362391	2.9585398	238.6619934	C	5.1840781	2.3739328	241.6380876
O	1.1265079	3.9098042	239.7920091	H	7.0138889	0.2866023	241.9526264
O	1.8787424	3.5572628	237.2845306	H	7.5847256	0.2059765	240.2519096
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H	-2.3867381	-1.4961554	242.7085630	C	5.3251485	2.6415008	236.8892557
H	-0.9451140	-3.3576038	243.5468692	H	5.5199770	0.4103849	235.1948775
H	2.2176620	-2.1635970	240.8317674	H	6.2042432	1.8322391	234.3496419
H	1.3785126	-3.6520373	242.6276907	C	5.8150408	1.4762407	240.5562957
C	1.9219202	-3.8078799	237.5271769	C	5.2147395	1.8678021	238.0798229
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H	1.1966873	-4.6327458	237.4550627	H	3.6106467	4.3279697	235.5493316
H	3.5111694	-4.9141776	236.5070711	H	5.8396496	3.2366494	241.8794587
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C	-2.1545175	2.9587478	238.2932933	H	3.5817677	1.7986113	235.9870641
C	-2.3544573	4.3074513	237.9478366	Zn	0.3436389	5.7203089	239.7910148
C	-2.2782558	5.3453065	238.8958555	Br	0.4636293	7.4743005	241.3385080
H	-2.0527780	5.7595769	241.0218740	H	7.3971716	3.6094759	240.0716597
C	-2.3747834	1.8824289	237.2347516	H	3.5867353	4.8413399	238.1125380
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C	-1.6880489	2.1817363	235.8940422	H	2.9880634	7.1133014	236.4422774
H	-2.1168301	3.0708075	235.3880723	H	1.4889943	8.0798165	238.9529140
H	-1.8112840	1.3239138	235.2025361				
H	-0.6028551	2.3566148	236.0261760				
C	-3.8904343	1.6563665	237.0543343				
H	-1.9515715	0.9345650	237.6249236				
H	-4.3856025	2.5713172	236.6671144				
H	-4.3772424	1.3885284	238.0139092				
H	-4.0769993	0.8361632	236.3311095				
C	-2.5811013	6.7975791	238.5353500				
C	-2.5802925	7.0700763	237.0287095				
H	-2.6746732	8.1561442	236.8378848				
H	-3.4286935	6.5658216	236.5210203				
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C	-3.9121879	7.2410353	239.1756712				
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H	-4.1045107	8.3111855	238.9578359				
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H	-4.7587375	6.6496602	238.7684396				
C	-1.5602990	3.3182611	242.1091749				
C	-0.5053982	4.1972426	242.7950412				
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15r-mi

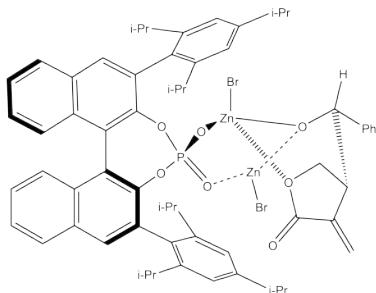


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C	-0.2026382	9.5853160	237.8624546
C	0.5544962	8.6407685	237.1391270

C	-1.0578367	10.4783784	237.1975824	H	-4.0481148	0.8369746	236.2714871
C	0.4382934	8.6081605	235.7346426	C	-2.5985155	6.7907707	238.5416991
O	0.9222951	6.3632831	237.9731481	C	-2.6143852	7.0664853	237.0359988
H	-1.8394198	11.1334295	235.2741861	H	-2.7008607	8.1536848	236.8480056
H	-0.1166655	9.6103472	238.9609641	H	-3.4741622	6.5716051	236.5379364
H	-0.5065626	9.4486289	233.9729985	H	-1.6852923	6.7239092	236.5400720
H	-1.6399420	11.2118278	237.7765769	C	-3.9157619	7.2479316	239.1997265
H	1.0061322	7.8737208	235.1429843	H	-1.7834471	7.4039655	238.9905650
Br	0.4178073	5.1662287	234.2793818	H	-4.1001288	8.3199299	238.9842451
Zn	1.0267953	5.1382909	236.4847187	H	-3.8959587	7.1228288	240.3004459
H	4.2178667	9.1216631	236.3436911	H	-4.7745988	6.6655907	238.8053680
C	2.9205346	7.6428979	237.3471201	C	-1.5844493	3.2989042	242.1002214
C	3.5525465	9.0523280	237.2309527	C	-0.4999350	4.1536904	242.7717257
C	3.8633732	6.9812821	238.3239361	H	-0.3511842	3.8184853	243.8183075
C	4.0642529	5.6816644	238.6092081	H	-0.7576182	5.2312499	242.8049552
C	4.6214290	8.0645221	239.0302185	H	0.4692723	4.0523395	242.2443215
O	4.3401883	9.2587669	238.4163489	C	-2.9247436	3.3895289	242.8571106
O	5.3806920	7.9778652	239.9698432	H	-1.2414697	2.2482754	242.1628090
H	2.8016475	9.8634210	237.1707204	H	-2.7938100	3.0924095	243.9178624
C	-0.0018420	0.9669009	239.3044284	H	-3.6953565	2.7313362	242.4059936
C	0.8231278	-0.1085076	239.6292644	H	-3.3228507	4.4256631	242.8439504
C	0.3756186	-0.9851290	240.6866146	H	7.6030638	5.9287309	237.1651143
C	1.1870735	-2.0273337	241.2245695	H	7.8769213	1.6677308	241.2972644
C	-0.9414539	-0.7827358	241.2494574	H	4.6646880	1.1293613	233.8226875
C	-1.4068613	-1.6746280	242.2615189	C	8.0176330	5.2221342	237.9192043
C	-1.7314892	0.3360223	240.8452562	H	4.9884385	1.8618594	242.6041135
H	-2.7119400	0.4911612	241.3213866	H	8.8856171	6.8709777	239.0522888
C	-1.2589622	1.2591284	239.9217899	H	3.3015180	3.3183479	234.1520096
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C	4.6714666	-0.5538938	237.6624376	C	7.1188023	0.8864367	241.0812097
H	5.6772635	-0.6806414	237.2339647	C	8.2155821	6.0044467	239.2249550
C	3.7784791	-1.6628474	237.6673491	H	8.6959462	5.3804257	240.0076051
C	4.1445986	-2.9041800	237.0660823	C	6.8498076	3.3240831	239.1963696
C	2.4695067	-1.5228108	238.2595813	C	5.2777476	1.3578609	234.7189676
C	1.5625819	-2.6201822	238.1503378	H	9.2342639	4.1792261	236.4033694
C	2.1148945	-0.2760643	238.8986527	C	6.2558998	3.7089752	236.8979205
C	3.0140103	0.7943432	238.7697763	C	9.3629402	4.7012986	237.3730468
O	0.4070173	1.8260870	238.2945939	H	10.0817675	5.5339234	237.2257722
O	2.7080408	2.0423229	239.3188906	H	6.3611550	4.3077486	235.9795251
P	1.5291545	2.9592320	238.6616815	C	5.1646992	2.4182301	241.6602002
O	1.1078940	3.9156607	239.7827303	H	6.9633292	0.3085758	242.0155561
O	1.8802933	3.5497163	237.2834282	H	7.5491814	0.2029681	240.3213601
C	-0.6038784	-2.7003879	242.7365714	C	5.9592752	2.2354145	239.2668549
C	0.7097044	-2.8638884	242.2242624	C	4.0818967	3.5706965	234.8970108
H	-2.4160773	-1.5188250	242.6741442	C	5.3515731	2.6323100	236.9123405
H	-0.9752665	-3.3753979	243.5224102	H	5.5268751	0.3985912	235.2123022
H	2.2079460	-2.1603459	240.8409453	H	6.2286479	1.8162889	234.3753969
H	1.3584278	-3.6572344	242.6256250	C	5.7938696	1.4998956	240.5950579
C	1.9424324	-3.8072297	237.5399114	C	5.2212347	1.8725693	238.1093995
C	3.2496062	-3.9608936	237.0074335	C	4.5260300	2.3142365	235.6650527
H	0.5432385	-2.5147444	238.5459192	H	4.1941670	2.8228595	241.3117522
H	1.2199464	-4.6339978	237.4629270	H	3.6549632	4.3323234	235.5783966
H	3.5424013	-4.9101157	236.5337127	H	5.8276883	3.2765078	241.8963841
H	5.1520687	-2.9984728	236.6313976	H	7.2611919	6.3976289	239.6289759
C	-1.8105867	3.6180882	240.6249713	H	4.9224743	4.0438149	234.3483192
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C	-2.0299926	4.9651261	240.2394841	H	5.0910351	0.6575403	240.4295080
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C	-2.3673313	4.3035440	237.9408316	Zn	0.3532549	5.7355309	239.7804892
C	-2.3016915	5.3356193	238.8960772	Br	0.3891616	7.4856448	241.3223198
H	-2.0744943	5.7395605	241.0222987	H	7.4157455	3.6013147	240.0984178
C	-2.3631699	1.8853421	237.2071621	H	3.5588145	4.8746466	238.0655208
H	-2.6067051	4.5537142	236.8984141	H	4.7844962	5.4040930	239.3942352
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H	-1.7708920	1.3498981	235.1755926				
H	-0.5776400	2.3771738	236.0246499				
C	-3.8745291	1.6510968	237.0047829				
H	-1.9388129	0.9367779	237.5947071				
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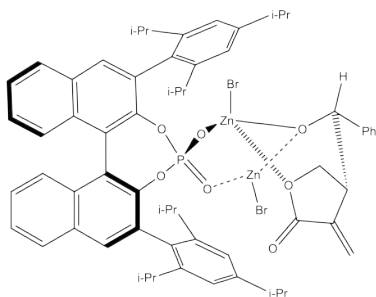
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C	4.7063763	3.7745765	1.6076661
C	2.5403874	4.8388148	2.0753916
C	3.2184991	6.0880378	2.2080801
C	1.1200174	4.7697382	2.1083629
H	0.5485434	5.7001079	2.2458794
C	0.4330991	3.5838690	1.8800511
C	3.7551553	-0.9267463	0.1601885
C	4.9338510	-1.1594800	0.8599166
H	5.5787649	-2.0018898	0.5673206
C	5.2960815	-0.3849257	1.9988700
C	6.4376425	-0.7204658	2.7880862
C	4.4652875	0.7247605	2.3986515
C	4.7751523	1.3976551	3.6181574
C	3.3513118	1.1002889	1.5600732
C	3.0036558	0.2387595	0.5147346
O	0.5030703	1.1723094	1.7271854
O	1.9044556	0.5486345	-0.2861408
P	0.3927189	0.3548436	0.3138418
O	-0.5227194	1.0509733	-0.7089019
O	0.0834772	-1.1100437	0.6523886
C	4.5925034	6.1733952	2.0442483
C	5.3353038	5.0073341	1.7187211
H	2.6213061	6.9887974	2.4203590
H	5.1043788	7.1429595	2.1410739
H	5.2989522	2.8892016	1.3424958
H	6.4198777	5.0804693	1.5455162
C	5.8768418	1.0291853	4.3785435
C	6.7280211	-0.0257756	3.9529054
H	4.1223178	2.2133645	3.9592553
H	6.0893325	1.5566943	5.3209533
H	7.6048846	-0.3017429	4.5582461
H	7.0716671	-1.5607529	2.4640614
C	-1.5086058	3.9330682	0.3312589
C	-1.0421362	3.5731640	1.6297768
C	-2.8893515	3.8640654	0.0789119
C	-1.9541670	3.1993260	2.6468462
C	-3.3302939	3.1830480	2.3506878
C	-3.8182355	3.4944859	1.0714788
H	-3.2603214	4.1046948	-0.9298042
C	-1.4491871	2.8946033	4.0556836
H	-4.0337146	2.8905933	3.1416861
C	-2.2825718	1.8523076	4.8141748
H	-3.2971002	2.2314751	5.0593968
H	-1.7924324	1.6011497	5.7770569
H	-2.3909419	0.9242049	4.2217999
C	-1.3311534	4.1997950	4.8687664
H	-0.4257300	2.4759840	3.9478746
H	-2.3274982	4.6748187	4.9893614
H	-0.6665299	4.9332396	4.3700752
H	-0.9217801	4.0001443	5.8810053
C	-5.3018265	3.4570037	0.7155266
C	-6.1781497	2.7304764	1.7425589
H	-7.2149967	2.6259651	1.3636632

H	-6.2343316	3.2917430	2.6988188
H	-5.7907567	1.7183000	1.9749895
C	-5.8405652	4.8789849	0.4592487
H	-5.3689862	2.9001753	-0.2476490
H	-6.8992987	4.8496419	0.1275491
H	-5.2536452	5.4046746	-0.3198808
H	-5.7883984	5.4870897	1.3868394
C	-0.5575163	4.4632177	-0.7453171
C	-0.8608413	3.9811023	-2.1707413
H	-0.0849505	4.3581554	-2.8682651
H	-1.8397574	4.3470362	-2.5421912
H	-0.8666785	2.8782536	-2.2348094
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H	0.4629841	4.1073070	-0.4943019
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H	4.4660934	-0.9852997	-4.5226361
H	3.3284957	-5.5372069	2.1293652
C	1.1645737	-4.5715859	-3.6172236
H	2.8452022	1.6794282	-3.7433135
H	0.0790579	-4.6703881	-5.5113048
H	2.4632528	-3.3949468	3.0891215
C	1.8554094	-3.5947864	-2.6717080
C	4.7398540	-0.3846425	-3.6297989
C	0.6463209	-3.9311440	-4.9098576
H	1.4790055	-3.5704516	-5.5490841
C	2.3193127	-2.3356067	-3.0765784
C	2.9750132	-5.2243308	1.1259673
H	2.4382388	-6.2691613	-3.0152853
C	2.0967566	-3.9881435	-1.3391535
C	2.0900269	-5.7630258	-3.9375293
H	1.5653135	-6.5150875	-4.5627717
H	1.7352505	-4.9744646	-1.0174413
C	2.4392854	0.6886902	-3.4523822
H	5.1657493	0.5763166	-3.9862177
H	5.5355739	-0.9341418	-3.0868465
C	2.9820514	-1.4654368	-2.1882091
C	2.1588615	-3.0408387	2.0825992
C	2.7723950	-3.1753415	-0.4142277
H	3.6060848	-5.7320674	0.3683564
H	1.9350516	-5.5948447	1.0161693
C	3.5149577	-1.0385691	-2.7268350
C	3.1932421	-1.8764712	-0.8462388
C	3.0469305	-3.6942258	1.0056595
H	1.5582284	0.8583470	-2.8033402
H	2.2258167	-1.9371764	2.0746818
H	2.0948627	0.1910530	-4.3830371
H	-0.0201042	-3.0675204	-4.7096487
H	1.0959793	-3.3099699	1.9277119
H	2.9881749	-5.4207776	-4.4936024
H	3.8689548	0.4625448	-1.8652038
H	4.0930250	-3.4121673	1.2431024
H	2.1714199	-2.0097494	-4.1162043
Zn	-2.2847431	0.5687616	-1.3398646
Br	-3.5737337	1.4840507	-3.0418956
C	-3.2713087	-6.1024989	-2.8517663
C	-3.6550944	-2.0015526	-1.4527447
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C	-4.3087826	-4.5045862	-1.3386681
O	-2.3484480	-1.4389268	-1.2120467
H	-3.1632013	-7.1317887	-3.2263728
H	-2.0447138	-2.9395564	-3.3674524
H	-4.7656821	-6.6257537	-1.3609747
H	-1.8221992	-5.2709804	-4.2441106
H	-5.0263748	-4.3137233	-0.5281946
Br	-1.0037018	-4.7161120	0.4377641

Zn	-1.0863679	-2.4741713	-0.1196792
H	-5.1326472	0.2367439	-1.1540210
C	-4.5942385	-1.7300215	-0.2344789
C	-4.9784854	-0.2455010	-0.1705968
C	-3.8390881	-1.8591319	1.0690486
C	-3.5795708	-2.9235166	1.8566996
C	-3.2576701	-0.5147615	1.3563091
O	-3.8176778	0.3957835	0.4498665
O	-2.4083836	-0.1819567	2.1467326
H	-5.8578982	-0.0643034	0.4792861
H	-3.9520734	-3.9310301	1.6256056
H	-2.9709596	-2.7909738	2.7657769
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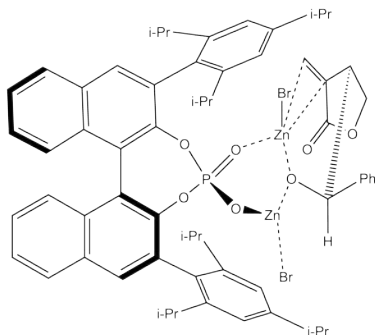
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C	4.7090756	3.7786770	1.5890870
C	2.5444014	4.8471795	2.0513690
C	3.2236608	6.0962939	2.1735324
C	1.1243825	4.7782863	2.0879921
H	0.5521495	5.7090846	2.2194026
C	0.4362731	3.5912698	1.8707502
C	3.7464580	-0.9322648	0.1704693
C	4.9247825	-1.1645054	0.8706148
H	5.5652661	-2.0113853	0.5810472
C	5.2925289	-0.3839375	2.0032408
C	6.4345332	-0.7166163	2.7921775
C	4.4664911	0.7313298	2.3966905
C	4.7819268	1.4122037	3.6100278
C	3.3519400	1.1047071	1.5582884
C	2.9998777	0.2381944	0.5185751
O	0.5054353	1.1796936	1.7315126
O	1.9012682	0.5473678	-0.2832067
P	0.3900968	0.3608977	0.3208433
O	-0.5252790	1.0594211	-0.7009860
O	0.0753273	-1.1025658	0.6586023
C	4.5970102	6.1798990	2.0079397
C	5.3385618	5.0114411	1.6909014
H	2.6270604	6.9989409	2.3793024
H	5.1092037	7.1499842	2.0969054
H	5.3000382	2.8904304	1.3303537
H	6.4230399	5.0823980	1.5165572
C	5.8844931	1.0465254	4.3696416
C	6.7306741	-0.0141323	3.9501871
H	4.1322395	2.2326243	3.9453714
H	6.1013794	1.5810226	5.3070192
H	7.6083967	-0.2883770	4.5549571
H	7.0648105	-1.5615985	2.4730800
C	-1.5149792	3.9336854	0.3316581
C	-1.0399768	3.5770702	1.6278055
C	-2.8968085	3.8586717	0.0873776

C	-1.9444974	3.2003600	2.6505254
C	-3.3220001	3.1793882	2.3625408
C	-3.8182519	3.4882177	1.0862158
H	-3.2746108	4.0963007	-0.9194881
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H	-4.0193196	2.8862519	3.1586056
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H	-3.2698935	2.2300492	5.0721222
H	-1.7590556	1.6085944	5.7826895
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H	-2.3081111	4.6807012	4.9893678
H	-0.6506259	4.9403119	4.3629014
H	-0.8977685	4.0111296	5.8770943
C	-5.3038804	3.4495407	0.7393480
C	-6.1728820	2.7206885	1.7709736
H	-7.2121911	2.6140782	1.3992390
H	-6.2252223	3.2813557	2.7276895
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C	-5.8456246	4.8713881	0.4899512
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H	-6.9065177	4.8430987	0.1651515
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H	-0.1117625	4.3637580	-2.8768762
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H	0.4514624	4.1225626	-0.5036787
H	0.1537655	6.4186727	-1.4551621
H	-0.3018529	6.4073926	0.2788959
H	-1.5760313	6.4057568	-0.9739168
H	0.2944546	-4.9867023	-3.0586069
H	4.4760655	-1.0081550	-4.5070835
H	3.2980919	-5.5348286	2.1563201
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H	2.8533810	1.6611703	-3.7443438
H	0.1350484	-4.7089711	-5.5238191
H	2.4280784	-3.3881166	3.1041539
C	1.8601594	-3.6106766	-2.6604748
C	4.7458676	-0.4044235	-3.6152636
C	0.6881990	-3.9647155	-4.9153216
H	1.5331522	-3.6079631	-5.5404092
C	2.3250774	-2.3526642	-3.0668109
C	2.9504604	-5.2245238	1.1501785
H	2.4385827	-6.2898137	-2.9686146
C	2.0906062	-3.9975793	-1.3243776
C	2.1069332	-5.7918762	-3.9010760
H	1.5909065	-6.5489108	-4.5275641
H	1.7264626	-4.9821164	-1.0005909
C	2.4455699	0.6722671	-3.4502426
H	5.1747827	0.5544044	-3.9736113
H	5.5382635	-0.9534307	-3.0673704
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H	3.5848577	-5.7356556	0.3977184
H	1.9105738	-5.5940819	1.0374773
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C	3.1841321	-1.8845947	-0.8330828
C	3.0242282	-3.6949069	1.0254532
H	1.5630088	0.8467837	-2.8047717
H	2.1954774	-1.9344863	2.0845925
H	2.1021225	0.1722410	-4.3799281
H	0.0166314	-3.1005429	-4.7362175
H	1.0679458	-3.3094751	1.9360964
H	3.0158017	-5.4583542	-4.4445711
H	3.8686511	0.4494533	-1.8574019

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Zn	-2.2975390	0.5969932	-1.3124842
Br	-3.6176144	1.4912288	-2.9949112
C	-3.2645625	-6.0495962	-2.9354971
C	-3.6563516	-1.9789993	-1.4531568
C	-4.1606023	-5.7901765	-1.8897450
C	-2.6456774	-3.6982066	-2.9688856
C	-3.5438269	-3.4243953	-1.9146772
C	-2.5122067	-4.9956895	-3.4788158
C	-4.3034971	-4.4866617	-1.3894016
O	-2.3545771	-1.4170121	-1.1992024
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H	-2.0468521	-2.8739777	-3.3865191
H	-4.7535006	-6.6082102	-1.4531597
H	-1.8192223	-5.1845923	-4.3112565
H	-5.0186769	-4.3147553	-0.5723976
Br	-1.0218025	-4.7133723	0.4026552
Zn	-1.0812907	-2.4664798	-0.1262050
H	-5.1431647	0.2474533	-1.1177286
C	-4.5991634	-1.7336779	-0.2398951
C	-4.9911203	-0.2514105	-0.1416552
C	-3.8456334	-1.8818096	1.0713953
C	-3.5723558	-2.9591850	1.8361426
C	-3.2729250	-0.5387699	1.3841229
O	-3.8390421	0.3843726	0.4926061
O	-2.4289494	-0.2159834	2.1827289
H	-5.8751473	-0.0860149	0.5076764
H	-3.9285420	-3.9674295	1.5844249
H	-2.9602025	-2.8365531	2.7441396
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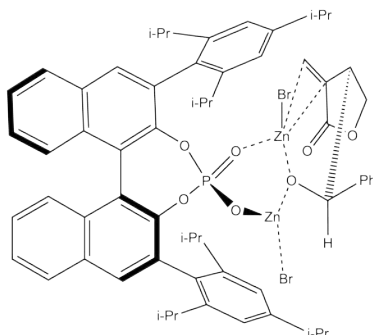
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Br	-0.3909645	4.7137045	295.8459728
C	0.0978351	1.0579585	299.5702111
C	0.8695168	-0.0642266	299.8913064
C	0.3639943	-0.9558987	300.9060101
C	1.1424968	-2.0240208	301.4442970
C	-0.9660583	-0.7447283	301.4261455
C	-1.4715845	-1.6319243	302.4233001
C	-1.7528325	0.3344672	300.9280178
H	-2.7952261	0.4346028	301.2675781
C	-1.2431121	1.2550260	300.0200717
C	4.3481591	0.5184226	298.3493978
C	4.5870305	-0.7108291	297.7459182
H	5.5314006	-0.8663641	297.2018840
C	3.6171017	-1.7542505	297.7546514
C	3.8516989	-2.9793933	297.0601305
C	2.3528122	-1.5534130	298.4243471
C	1.3561757	-2.5681235	298.2997523

C	2.1388491	-0.3245353	299.1533987
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O	0.6229583	2.0214457	298.7033106
O	2.9478475	1.8534757	299.7703793
P	1.8458011	2.9463396	299.2915354
O	1.4339854	3.6647239	300.5955025
O	2.3337462	3.8288607	298.1346209
C	-0.6941552	-2.6705536	302.9140304
C	0.6272474	-2.8582703	302.4269064
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H	-1.0939287	-3.3432001	303.6880812
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C	1.6099738	-3.7406491	297.6008393
C	2.8731354	-3.9593475	296.9892238
H	0.3695172	-2.4118996	298.7564591
H	0.8215968	-4.5040628	297.5157344
H	3.0654609	-4.8964849	296.4449859
H	4.8247470	-3.1227366	296.5645645
C	-2.2847560	3.5778436	300.0787380
C	-2.0838819	2.3395600	299.4147582
C	-3.0825559	4.5586232	299.4584800
C	-2.6771623	2.1073271	298.1428257
C	-3.4636824	3.1206324	297.5666364
C	-3.6804323	4.3541240	298.2032608
H	-3.2499182	5.5227618	299.9652902
C	-2.4590400	0.8022114	297.3780643
H	-3.9124845	2.9411077	296.5774595
C	-1.5266521	1.0144217	296.1701385
H	-1.9884963	1.6941921	295.4240819
H	-1.3140058	0.0475451	295.6680928
H	-0.5663456	1.4716917	296.4779873
C	-3.7852375	0.1430713	296.9610994
H	-1.9514395	0.0931951	298.0636782
H	-4.3428839	0.7644889	296.2297678
H	-4.4468359	-0.0248332	297.8353535
H	-3.5950027	-0.8385110	296.4800852
C	-4.5640730	5.4291111	297.5826900
C	-4.2102993	5.7218713	296.1153311
H	-4.7965385	6.5850699	295.7376341
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H	-3.1313105	5.9448050	295.9950280
C	-6.0534154	5.0662359	297.7376912
H	-4.3865739	6.3604698	298.1660995
H	-6.7031254	5.8707520	297.3343337
H	-6.3219442	4.9053003	298.8013673
H	-6.2890218	4.1316091	297.1863755
C	-1.6695811	3.8482785	301.4486684
C	-1.1669527	5.2940106	301.5928077
H	-0.4821945	5.3970616	302.4620746
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H	-2.1808078	3.6974171	303.5790572
H	-2.9509345	2.4448626	302.5541703
H	-3.5664436	4.1261926	302.5177378
H	7.3692852	5.7928180	296.9135855
H	8.1102087	1.5947650	301.0856204
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C	7.8900537	5.1346138	297.6428985
H	5.4119617	1.9816003	302.7485631
H	8.7574404	6.8710804	298.6411994
H	3.1017639	2.6438488	294.2421954
C	6.9573525	3.9515139	297.8756067
C	7.2909722	0.8485684	301.0181824
C	8.1710052	5.9659489	298.9004106
H	8.7640744	5.3991013	299.6488013
C	6.8397229	3.3035489	299.1161393
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H	9.0091869	4.0988804	296.0523453

C	6.1996891	3.4510343	296.8016031
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C	5.5127667	2.5055423	301.7756036
H	7.2313555	0.3243095	301.9947009
H	7.5766266	0.1060800	300.2454515
C	6.0051770	2.1848124	299.2994568
C	3.6748079	3.0174180	295.1159229
C	5.3456736	2.3426127	296.9290172
H	6.0563905	0.4320623	295.0489840
H	6.1857924	2.0309539	294.2563220
C	5.9489449	1.5219211	300.6744707
C	5.2631229	1.6907462	298.1938067
C	4.5408739	1.8902735	295.7086382
H	4.5355775	2.9684929	301.5342224
H	2.9477838	3.3858337	295.8641179
H	6.2534955	3.3205417	301.9136401
H	7.2287167	6.2939263	299.3819097
H	4.2835188	3.8814426	294.7799333
H	9.7579433	3.9804259	297.6747658
H	5.1872614	0.7166344	300.6322203
H	3.8443699	1.0928005	296.0370928
H	7.4147646	3.6768489	299.9768458
C	-1.8409925	9.9683079	297.1748403
C	1.4643046	7.7659354	298.9680965
C	-1.9808549	8.6061054	297.4778865
C	0.4358922	9.9073420	298.0325152
C	0.3087517	8.5332209	298.3291255
C	-0.6280976	10.6191824	297.4603637
C	-0.9165460	7.8939277	298.0565509
O	1.1804873	6.3781306	299.0843097
H	-2.6748301	10.5243583	296.7199089
H	1.3753642	10.4376577	298.2560257
H	-2.9245615	8.0845338	297.2599768
H	-0.5084818	11.6900492	297.2348405
H	-1.0409641	6.8270894	298.2929193
C	2.8185747	7.9531942	298.2343623
C	2.9481856	7.2378728	296.9142051
C	4.3583173	6.7139463	296.8224273
O	4.9620151	6.8991587	298.0261807
C	4.0281495	7.3853737	299.0127033
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C	2.0646781	7.0884243	295.8924658
H	4.5462625	8.1336839	299.6399230
H	3.7321240	6.5306809	299.6560512
H	1.6085632	8.1766444	299.9968900
H	2.9856767	9.0370789	298.0570078
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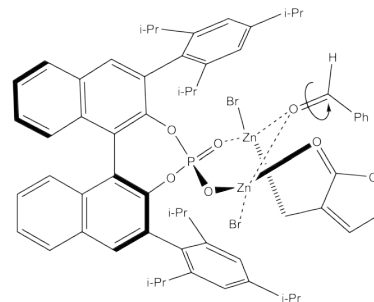


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Br	-0.3818514	4.7265054	295.8172897

C	0.0973201	1.0516029	299.5746358
C	0.8684402	-0.0707384	299.8963148
C	0.3600237	-0.9632768	300.9086454
C	1.1368175	-2.0321385	301.4472262
C	-0.9715024	-0.7534450	301.4251064
C	-1.4792162	-1.6431117	302.4182729
C	-1.7561653	0.3270731	300.9271598
H	-2.7997226	0.4276534	301.2630665
C	-1.2439801	1.2495835	300.0229767
C	4.3461345	0.5207120	298.3555898
C	4.5871270	-0.7077028	297.7516509
H	5.5312197	-0.8582895	297.2058338
C	3.6210924	-1.7542433	297.7610967
C	3.8583446	-2.9783775	297.0667095
C	2.3568473	-1.5574521	298.4316848
C	1.3636887	-2.5753391	298.3076423
C	2.1396881	-0.3292896	299.1609823
C	3.1249527	0.6567511	299.0793982
O	0.6223988	2.0148272	298.7084257
O	2.9441983	1.8498869	299.7798566
P	1.8431490	2.9411389	299.2988769
O	1.4244293	3.6631827	300.5984047
O	2.3319144	3.8237658	298.1418176
C	-0.7037188	-2.6824989	302.9089397
C	0.6187143	-2.8686761	302.4257263
H	-2.5004077	-1.4796951	302.7970557
H	-1.1059749	-3.3567695	303.6802078
H	2.1638640	-2.1794743	301.0843737
H	1.2404878	-3.6800026	302.8338298
C	1.6209289	-3.7468963	297.6091985
C	2.8836697	-3.9614704	296.9967095
H	0.3772985	-2.4217178	298.7655830
H	0.8349848	-4.5128632	297.5251293
H	3.0788487	-4.8978766	296.4523491
H	4.8312693	-3.1180246	296.5699183
C	-2.2808527	3.5745778	300.0861764
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C	-3.6640880	4.3611199	298.2056953
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C	-2.4480021	0.8100954	297.3733483
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C	-1.5159106	1.0257319	296.1659568
H	-1.9757204	1.7083820	295.4215148
H	-1.3036729	0.0608120	295.6603063
H	-0.5547579	1.4805316	296.4741888
C	-3.7747870	0.1528871	296.9553587
H	-1.9408967	0.0986533	298.0568194
H	-4.3328103	0.7762927	296.2261277
H	-4.4365616	-0.0167602	297.8289437
H	-3.5860678	-0.8272015	296.4708957
C	-4.5443149	5.4399846	297.5869769
C	-4.2066169	5.7202888	296.1136206
H	-4.7880385	6.5875848	295.7377807
H	-4.4598622	4.8552225	295.4662324
H	-3.1268988	5.9288080	295.9755772
C	-6.0346862	5.0917255	297.7637914
H	-4.3507762	6.3737175	298.1619079
H	-6.6835553	5.8980741	297.3627973
H	-6.2907776	4.9399342	298.8316592
H	-6.2848669	4.1547053	297.2234201
C	-1.6713350	3.8395250	301.4600437
C	-1.1750850	5.2863045	301.6160114
H	-0.4937249	5.3881095	302.4875908
H	-1.9956451	6.0135998	301.7865473
H	-0.6873433	5.6404216	300.6760847
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H	-0.7862593	3.1790473	301.5573941
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H	-3.5752537	4.0993714	302.5217462
H	7.3613876	5.7960487	296.9066203
H	8.1135813	1.6048195	301.0795642
H	4.8614005	0.8962337	293.7860340
C	7.8822018	5.1380796	297.6360509
H	5.4221714	1.9848252	302.7528260
H	8.7551264	6.8752269	298.6286383
H	3.0877231	2.6451959	294.2471928
C	6.9484054	3.9568657	297.8734507
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H	8.7631238	5.4058618	299.6388769
C	6.8342047	3.3099796	299.1146017
C	5.4501403	1.2738502	294.6477191
H	8.9948946	4.0953662	296.0460912
C	6.1875340	3.4559755	296.8021487
C	9.1925693	4.6557971	296.9818856
H	9.8548161	5.5122572	296.7363321
H	6.2433053	3.9775158	295.8342981
C	5.5148364	2.5082371	301.7788630
H	7.2417686	0.3315148	301.9905848
H	7.5814480	0.1168429	300.2397332
C	6.0015579	2.1906767	299.3009102
C	3.6654957	3.0207876	295.1167452
C	5.3350561	2.3470158	296.9323938
H	6.0387284	0.4282503	295.0587474
H	6.1723258	2.0230605	294.2613584
C	5.9510218	1.5270499	300.6758019
C	5.2573576	1.6954650	298.1975337
C	4.5274407	1.8931610	295.7143812
H	4.5333039	2.9647520	301.5437412
H	2.9413460	3.3966956	295.8638931
H	6.2509441	3.3279190	301.9132251
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H	4.2767975	3.8800829	294.7736097
H	9.7472527	3.9791144	297.6658185
H	5.1914320	0.7196048	300.6351741
H	3.8281106	1.0993281	296.0459077
H	7.4119883	3.6838923	299.9732014
C	-1.8347877	9.9735095	297.1618720
C	1.4580522	7.7581259	298.9602090
C	-1.9720496	8.6062558	297.4401270
C	0.4279755	9.9094138	298.0519570
C	0.3048436	8.5298060	298.3224555
C	-0.6306865	10.6258602	297.4769542
C	-0.9133973	7.8898265	298.0232544
O	1.1742160	6.3719112	299.0748725
H	-2.6643139	10.5327973	296.7032172
H	1.3608121	10.4409387	298.3002420
H	-2.9082368	8.0822388	297.1978738
H	-0.5140284	11.7012421	297.2726909
H	-1.0364141	6.8189384	298.2410101
C	2.8133490	7.9475198	298.2266729
C	2.9456786	7.2352884	296.9044888
C	4.3559934	6.7109720	296.8123632
O	4.9610891	6.9029956	298.0177135
C	4.0239657	7.3775643	299.0033101
O	4.9188574	6.2409359	295.8491970
C	2.0636089	7.0864449	295.8822769
H	4.5368250	8.1211338	299.6412750
H	3.7271397	6.5191595	299.6413846
H	1.6030926	8.1664407	299.9905569
H	2.9777266	9.0327373	298.0520854
H	2.3822185	6.5391072	294.9799125
H	1.0668341	7.5527462	295.8874417



Energy(Hartree)= -11970.04020619

C	0.9292203	2.2366900	1.5999716
C	2.3187298	2.2376999	1.7749717
C	2.9852441	3.5155389	1.8885394
C	4.4061574	3.6587754	1.8819838
C	2.1848884	4.7134545	1.9794536
C	2.8292750	5.9764291	2.1479674
C	0.7728360	4.6278472	1.8223481
H	0.1805760	5.5554082	1.8417450
C	0.1330145	3.4222405	1.5567327
C	3.6722179	-1.1626284	0.5946274
C	4.6870972	-1.3793145	1.5213003
H	5.3331273	-2.2643335	1.4115080
C	4.8733627	-0.5299454	2.6484414
C	5.8479080	-0.8326965	3.6470724
C	4.0295078	0.6291384	2.8131880
C	4.1550083	1.3884621	4.0155761
C	3.0792762	0.9563663	1.7762405
C	2.8950792	0.0291706	0.7418089
O	0.2610577	1.0219137	1.4947267
O	1.9549153	0.2906470	-0.2486664
P	0.3548382	0.1668103	0.0945831
O	-0.3298171	0.9225802	-1.0621393
O	-0.0823694	-1.2472214	0.4323552
C	4.2120878	6.0733323	2.1796577
C	5.0035333	4.9040269	2.0240561
H	2.2019617	6.8780986	2.2295546
H	4.6971610	7.0537540	2.3020866
H	5.0352370	2.7679085	1.7523658
H	6.1012680	4.9846442	2.0093641
C	5.0973181	1.0549175	4.9789489
C	5.9654241	-0.0535465	4.7881833
H	3.4849772	2.2436131	4.1806171
H	5.1673113	1.6517538	5.9011911
H	6.7151632	-0.3024723	5.5546600
H	6.4932681	-1.7131860	3.5006975
C	-1.6297866	3.9307056	-0.1596416
C	-1.2978989	3.3842325	1.1182306
C	-2.9759236	3.9426985	-0.5556578
C	-2.3150304	2.8235983	1.9319278
C	-3.6540479	2.8749128	1.4885592
C	-4.0131321	3.4475391	0.2579001
C	-2.0171310	2.2002526	3.2932350
H	-4.4339612	2.4621919	2.1457112
C	-2.4485433	0.7243020	3.3473082
H	-3.5468275	0.6105897	3.2279168
H	-2.1772303	0.2685342	4.3216969
H	-1.9591587	0.1243782	2.5566206
C	-2.6483427	3.0197814	4.4342338
H	-0.9189380	2.2288378	3.4443339
H	-3.7564716	3.0263773	4.3650698
H	-2.3040716	4.0739131	4.4117329
H	-2.3779436	2.5899317	5.4209627
C	-5.4552097	3.5773233	-0.2253846
C	-6.4768378	2.8096293	0.6190600
H	-7.4865598	2.8781011	0.1671982
H	-6.5450489	3.2154294	1.6500940

7.2 Pathways from Complexes 14 to 15

7.2.1 Pathways starting from 14d-mi

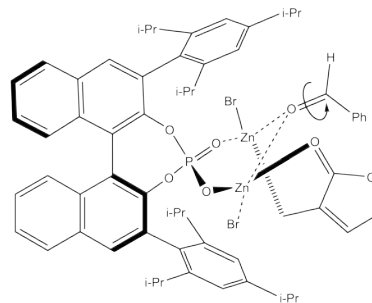
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TS1-8-d; COSMO

H	-6.2188298	1.7351233	0.7036114
C	-5.8633492	5.0611317	-0.3295210
H	-5.4723356	3.1498828	-1.2545060
H	-6.8849837	5.1615769	-0.7509093
H	-5.1708974	5.6339325	-0.9775384
H	-5.8571061	5.5382256	0.6731901
C	-0.5827409	4.5202091	-1.1082564
C	-0.6543992	3.9300738	-2.5270374
H	0.1522142	4.3567498	-3.1583371
H	-1.6203687	4.1455300	-3.0274028
H	-0.5219415	2.8322799	-2.5019489
C	-0.6890443	6.0570360	-1.1522416
H	0.4186154	4.2647191	-0.7080948
H	0.1017182	6.4885033	-1.8004997
H	-0.5871447	6.5062843	-0.1438708
H	-1.6718866	6.3747550	-1.5595367
H	1.7707661	-5.9339967	-3.0042776
H	5.3461918	-1.3044312	-3.8646653
H	3.6001689	-5.3554844	2.7618073
C	2.2557947	-5.0840979	-3.5334952
H	3.4348921	1.2551365	-3.5257374
H	0.9489404	-5.3274085	-5.2761542
H	1.1902818	-4.5647588	2.7786144
C	2.6248143	-4.0580359	-2.4690123
C	5.3980775	-0.6669312	-2.9571158
C	1.2450905	-4.5368963	-4.5560255
H	1.6721803	-3.6977052	-5.1434524
C	3.0881106	-2.7769493	-2.8148762
C	3.6658149	-5.0872666	1.6871050
H	4.2274176	-6.0611508	-3.4991867
C	2.5407491	-4.3734952	-1.1036405
C	3.5167887	-5.6279019	-4.2316908
H	3.2558652	-6.4159357	-4.9686276
H	2.1753804	-5.3735968	-0.8173855
C	3.0424663	0.2478971	-3.2752459
H	5.8270908	0.3119281	-3.2565962
H	6.1022195	-1.1487336	-2.2484238
C	3.4500320	-1.8232551	-1.8482009
C	1.2726620	-4.2202686	1.7274690
C	2.8851505	-3.4576846	-0.0903083
H	4.7235546	-4.8432487	1.4575855
H	3.3986155	-5.9909373	1.1002148
C	4.0061898	-0.4815718	-2.3224312
C	3.3426749	-2.1612685	-0.4684070
C	2.7334378	-3.9048506	1.3654527
H	2.0436509	0.3728967	-2.8141456
H	0.6473962	-3.3115229	1.6350165
H	2.9153856	-0.3032089	-4.2304467
H	0.3286617	-4.1667553	-4.0555992
H	0.8397620	-5.0125724	1.0817791
H	4.0475870	-4.8184200	-4.7757431
H	4.1445830	0.1657529	-1.4340384
H	3.0390523	-3.0634291	2.0164379
H	3.1790063	-2.5085396	-3.8792608
Zn	-1.9001929	0.3800409	-2.0351117
Br	-3.6602997	1.4046798	-3.1441972
C	-5.8191114	-4.0428196	0.1466883
C	-4.8506956	-3.0981753	-0.1964464
C	-5.0909725	-1.7208174	0.0454430
C	-6.3113038	-1.3120662	0.6376051
C	-7.2695234	-2.2645758	0.9965433
C	-7.0225406	-3.6278462	0.7492217
H	-5.6362176	-5.1107958	-0.0427475
C	-4.1105059	-0.7158829	-0.3131933
H	-6.4958854	-0.2423117	0.8193073
H	-8.2124733	-1.9493713	1.4668259
H	-7.7793788	-4.3775747	1.0272709
O	-2.9493601	-0.9817301	-0.7090841
C	-2.8982290	-4.3242712	-3.1235106
C	-1.8991835	-3.6246488	-2.4995939
C	-1.8771819	-2.3031288	-3.1645413

O	-2.7909827	-2.2335321	-4.1462175
C	-3.5123328	-3.4822486	-4.1916452
O	-1.1574247	-1.3300658	-2.8788516
C	-1.0266654	-3.8969588	-1.3599094
H	-3.4130430	-3.9009213	-5.2175447
H	-4.5886081	-3.2518241	-4.0262630
Zn	-1.4353413	-2.7332003	0.2439011
Br	-2.5083719	-3.0219878	2.3213708
H	0.0139297	-3.5718504	-1.5666090
H	-1.0354484	-4.9632698	-1.0636847
H	-3.9095658	-3.4062825	-0.6732470
H	-3.2296368	-5.3467722	-2.8970793
H	-4.4197260	0.3553864	-0.2477949
H	-3.2330642	4.3519077	-1.5449358

TS1-8-d

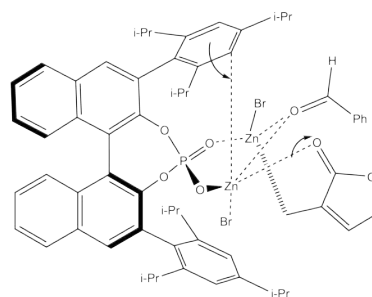


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C	2.3134215	2.2323606	1.7757514
C	2.9751356	3.5120752	1.8944780
C	4.3952735	3.6604619	1.8910551
C	2.1705538	4.7066921	1.9881785
C	2.8105460	5.9706968	2.1615258
C	0.7594689	4.6160204	1.8284342
H	0.1628128	5.5407346	1.8488733
C	0.1239105	3.4093832	1.5582205
C	3.6772934	-1.1615115	0.5900120
C	4.6920491	-1.3766259	1.5167907
H	5.3393578	-2.2605153	1.4054694
C	4.8754688	-0.5291996	2.6454253
C	5.8499470	-0.8299987	3.6440240
C	4.0283335	0.6270096	2.8112992
C	4.1516790	1.3850677	4.0143940
C	3.0778437	0.9535455	1.7745448
C	2.8966439	0.0277920	0.7382988
O	0.2598263	1.0107151	1.4919633
O	1.9562715	0.2874218	-0.2521508
P	0.3562672	0.1585271	0.0912343
O	-0.3309181	0.9193683	-1.0611732
O	-0.0779400	-1.2573271	0.4227585
C	4.1923658	6.0725674	2.1961383
C	4.9877329	4.9069261	2.0385465
H	2.1797723	6.8698034	2.2445432
H	4.6735796	7.0543383	2.3224572
H	5.0269312	2.7717763	1.7598481
H	6.0851722	4.9911708	2.0264041
C	5.0942518	1.0529964	4.9773373
C	5.9649869	-0.0525084	4.7858346
H	3.4790310	2.2380366	4.1791742
H	5.1622584	1.6491327	5.9001049
H	6.7150884	-0.3005318	5.5521737
H	6.4974460	-1.7087489	3.4967387
C	-1.6298125	3.9271053	-0.1634707

C	-1.3044801	3.3707887	1.1119242	H	4.1495030	0.1639870	-1.4387659
C	-2.9738537	3.9448407	-0.5648599	H	3.0389809	-3.0566292	2.0136330
C	-2.3256070	2.8033634	1.9156021	H	3.1884718	-2.5137624	-3.8817416
C	-3.6624900	2.8619554	1.4668642	Zn	-1.9086236	0.3904521	-2.0279886
C	-4.0154972	3.4468334	0.2405263	Br	-3.6739426	1.4111517	-3.1221876
C	-2.0350663	2.1654309	3.2717803	C	-5.8265215	-4.0198021	0.1923442
H	-4.4456001	2.4466063	2.1185595	C	-4.8561123	-3.0818987	-0.1654672
C	-2.4715587	0.6905099	3.3108853	C	-5.0836875	-1.7036311	0.0792570
H	-3.5698630	0.5802024	3.1873416	C	-6.2913915	-1.2872795	0.6899284
H	-2.2055172	0.2236342	4.2811057	C	-7.2508094	-2.2327548	1.0630041
H	-1.9794090	0.0947227	2.5188496	C	-7.0172299	-3.5974430	0.8119894
C	-2.6661396	2.9777921	4.4178223	H	-5.6512356	-5.0891326	0.0035440
H	-0.9373985	2.1878851	3.4266399	C	-4.0976042	-0.7055543	-0.2891848
H	-3.7739852	2.9906908	4.3456861	H	-6.4629498	-0.2159518	0.8751732
H	-2.3175945	4.0305006	4.4054155	H	-8.1841854	-1.9112481	1.5480557
H	-2.4013732	2.5383442	5.4017491	H	-7.7745741	-4.3420357	1.1024931
C	-5.4547136	3.5862604	-0.2486024	O	-2.9460516	-0.9828944	-0.7003420
C	-6.4859256	2.8309417	0.5950268	C	-2.9076155	-4.3093064	-3.1231220
H	-7.4930434	2.9033045	0.1378640	C	-1.8971476	-3.6134136	-2.5127783
H	-6.5566358	3.2429332	1.6234577	C	-1.8890511	-2.2852886	-3.1706215
H	-6.2358274	1.7549710	0.6852219	O	-2.8222484	-2.2117622	-4.1349630
C	-5.8512019	5.0723997	-0.3604277	C	-3.5425356	-3.4581877	-4.1736513
H	-5.4709832	3.1534755	-1.2755433	O	-1.1657250	-1.3153939	-2.8930058
H	-6.8699737	5.1798594	-0.7870403	C	-1.0080731	-3.8877728	-1.3894778
H	-5.1516258	5.6375024	-1.0070829	H	-3.4642715	-3.8689994	-5.2052066
H	-5.8450919	5.5540116	0.6399391	H	-4.6156042	-3.2275507	-3.9853156
C	-0.5784223	4.5196538	-1.1056582	Zn	-1.4198085	-2.7507561	0.2372393
C	-0.6418127	3.9319884	-2.5260301	Br	-2.5133091	-3.0795085	2.2881489
H	0.1621388	4.3671124	-3.1547910	H	0.0246707	-3.5418479	-1.6005685
H	-1.6082783	4.1381578	-3.0290854	H	-0.9979821	-4.9567359	-1.1034448
H	-0.4981355	2.8356604	-2.5038236	H	-3.9237110	-3.3957432	-0.6551520
C	-0.6870016	6.0562768	-1.1474880	H	-3.2322711	-5.3340364	-2.8973852
H	0.4213539	4.2655722	-0.7008330	H	-4.3940157	0.3688661	-0.2144349
H	0.1082388	6.4907807	-1.7880338	H	-3.2252610	4.3592344	-1.5533449
H	-0.5946940	6.5039200	-0.1375975				
H	-1.6667354	6.3740121	-1.5618929				
H	1.7864227	-5.9411435	-3.0025049				
H	5.3545643	-1.3065627	-3.8676979				
H	3.6132790	-5.3465823	2.7632055				
C	2.2678840	-5.0898008	-3.5330130				
H	3.4407446	1.2519035	-3.5319379				
H	0.9618576	-5.3406941	-5.2758976				
H	1.1980160	-4.5621665	2.7801067				
C	2.6330080	-4.0610611	-2.4696697				
C	5.4048135	-0.6688749	-2.9602945				
C	1.2537064	-4.5488829	-4.5554027				
H	1.6753589	-3.7071985	-5.1430301				
C	3.0966984	-2.7808253	-2.8170931				
C	3.6798811	-5.0769460	1.6889711				
H	4.2433512	-6.0578931	-3.4979872				
C	2.5476723	-4.3740066	-1.1041467				
C	3.5306481	-5.6293132	-4.2308788				
H	3.2738538	-6.4191448	-4.9673256				
H	2.1825731	-5.3737807	-0.8163456				
C	3.0488421	0.2448162	-3.2806392				
H	5.8342324	0.3097079	-3.2597956				
H	6.1082614	-1.1509004	-2.2513767				
C	3.4572563	-1.8254001	-1.8519565				
C	1.2808811	-4.2253735	1.7267396				
C	2.8911301	-3.4569278	-0.0920333				
H	4.7364420	-4.8259425	1.4620410				
H	3.4220560	-5.9825483	1.1010252				
C	4.0123664	-0.4837296	-2.3271008				
C	3.3486428	-2.1613242	-0.4720585				
C	2.7395363	-3.9017099	1.3644914				
H	2.0497347	0.3706809	-2.8207744				
H	0.6489532	-3.3218979	1.6292041				
H	2.9217645	-0.3062267	-4.2358414				
H	0.3354928	-4.1836994	-4.0548883				
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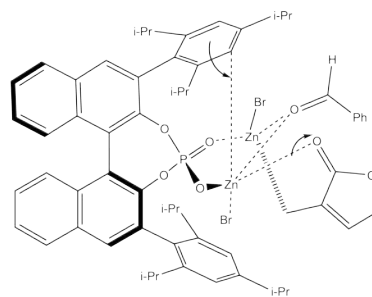


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C	1.1053135	2.4113599	1.8333274
C	2.5020696	2.4209790	1.8296278
C	3.1635764	3.7054685	1.8330170
C	4.5735884	3.8538645	1.6704118
C	2.3646482	4.9018574	1.9733091
C	3.0147582	6.1713945	2.0295212
C	0.9407358	4.8109987	1.9719452
H	0.3517257	5.7399247	2.0210555
C	0.2910543	3.5915381	1.8335729
C	3.5773156	-1.0756356	0.6300164
C	4.6652310	-1.3227457	1.4598529
H	5.2382383	-2.2536955	1.3305024
C	5.0257177	-0.4362022	2.5140870
C	6.0842304	-0.7582578	3.4165641
C	4.2790462	0.7843622	2.7067463
C	4.5848266	1.5861907	3.8482428
C	3.2344069	1.1229054	1.7688176
C	2.8917272	0.1672756	0.7994768
O	0.4501284	1.1883979	1.8429648
O	1.8654292	0.4309084	-0.1015486

P	0.3069032	0.3922479	0.4054535	H	5.6342121	0.1534573	-3.3296451
O	-0.4373782	1.2729709	-0.6130849	H	5.8775565	-1.2811337	-2.2765598
O	-0.2259122	-0.9852920	0.7536263	C	3.2041579	-1.8127973	-1.7678470
C	4.3926849	6.2751888	1.9087433	C	0.9219575	-4.0442635	1.9133878
C	5.1731064	5.1058994	1.7079799	C	2.5349054	-3.3070252	0.0748759
H	2.3944990	7.0735682	2.1504958	H	4.4095585	-4.4432372	1.7837764
H	4.8796996	7.2614766	1.9472228	H	3.1717674	-5.6899062	1.4498976
H	5.1900476	2.9596158	1.5059532	C	3.8120057	-0.5204540	-2.3085781
H	6.2625074	5.1914088	1.5755729	C	3.1001379	-2.0792785	-0.3736722
C	5.6067768	1.2345889	4.7198036	C	2.3645809	-3.6470386	1.5568511
C	6.3774884	0.0623852	4.4953086	H	1.8645434	0.3843690	-2.7713158
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H	5.8160356	1.8671829	5.5959866	H	2.6714381	-0.3528419	-4.1860345
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H	-2.8551137	0.6045275	4.2744357	C	-6.1250530	-2.1425381	-2.3824935
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H	-1.2986328	0.1692205	3.5180291	C	-7.1916380	-3.8509477	-1.0305275
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H	-6.6155604	0.5407880	0.4142852	C	-1.9193763	-2.8406286	-2.4555358
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H	3.8224870	-6.0443682	-3.2863380				
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TS2-8-d

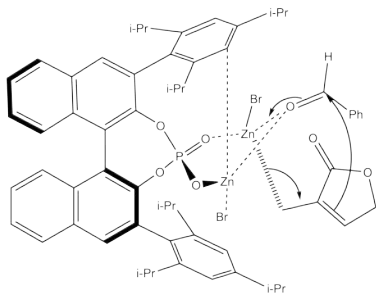


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C	3.2351988	1.1234700	1.7685039	C	3.0798446	-5.6130757	-4.0438899
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H	2.3940179	7.0728382	2.1499657	H	4.4068851	-4.4362359	1.7871075
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C	-1.5636124	2.3288009	3.8016007	C	-6.2651682	-3.6430998	-0.0164268
H	-3.8382336	1.5388776	2.5590669	C	-5.2423409	-2.7022260	-0.1759735
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C	-5.1009160	2.0857279	0.1378783	O	-3.2190625	-0.5974427	-0.8297663
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H	-5.9947836	1.2008287	1.9385836	C	-1.2040471	-1.6487870	-3.0235192
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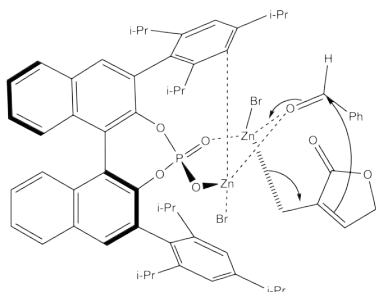
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C	-6.4821087	-3.3311089	0.2176424
C	-5.3413768	-2.5572622	-0.0317527
C	-5.2127272	-1.8569569	-1.2527548
C	-6.2601332	-1.9367259	-2.2081292
C	-7.4000899	-2.7017926	-1.9491688
C	-7.5116467	-3.4079465	-0.7352424
H	-6.5681963	-3.8708921	1.1726371
C	-4.0597668	-1.0255037	-1.5946234
H	-6.1684335	-1.3845300	-3.1571191
H	-8.2100405	-2.7499357	-2.6923563
H	-8.4083820	-4.0131654	-0.5319120
O	-3.1808336	-0.6023450	-0.7285856
C	-3.0481948	-2.6455280	-3.0400341
C	-1.9137576	-2.7435203	-2.2403492
C	-0.8986301	-1.8023154	-2.8383371

O	-1.3757840	-1.3485467	-4.0377013
C	-2.6783103	-1.8977048	-4.2929944
O	0.1744545	-1.4626002	-2.3889253
C	-1.6599701	-3.3930310	-1.0048998
H	-2.6152433	-2.5744821	-5.1752712
H	-3.3545923	-1.0559842	-4.5568608
Zn	-1.9816678	-1.9439440	0.4800912
Br	-2.8415643	-2.3591089	2.6395166
H	-0.5849623	-3.5295195	-0.7766409
H	-2.3115224	-4.2431245	-0.7385819
H	-4.5607487	-2.4865618	0.7400763
H	-3.9086224	-3.3250840	-3.0023563
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TS3-8-d



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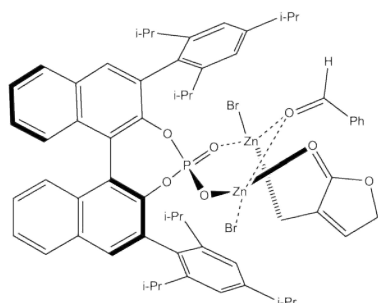
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C	3.0533589	6.1665692	1.7614623
C	0.9759797	4.8091484	1.7872242
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C	0.3235922	3.5892128	1.6718191
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H	5.2560793	-2.2751543	1.2968219
C	5.0518859	-0.4055954	2.3977492
C	6.1142514	-0.6851991	3.3088301
C	4.3068830	0.8223723	2.5339943
C	4.6172018	1.6752885	3.6365117
C	3.2588247	1.1166055	1.5835464
C	2.9061829	0.1161470	0.6640620
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O	1.8768020	0.3401075	-0.2496277
P	0.3210312	0.3399749	0.2568821
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O	-0.2304335	-1.0080706	0.6958805
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H	2.4394147	7.0712524	1.8952968
H	4.9165305	7.2513322	1.6137716
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H	0.0838927	4.8573261	-0.3957706
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H	-2.6493261	6.1168428	-1.0919320
H	1.4932211	-6.1578882	-2.5596531
H	5.2812603	-1.8317522	-3.8173410
H	3.1840534	-4.7846270	3.2178091
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H	0.7404268	-4.1530075	3.0376849
C	2.2945197	-4.2138613	-2.2078900
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H	1.6259816	-5.2727433	-0.4474191
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H	5.8794434	-0.2089016	-3.3496621
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C	3.3215426	-2.0173275	-1.7999882
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H	4.3465050	-4.3385357	1.9252344
H	3.1475557	-5.6314656	1.6369840
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H	2.1013090	0.1645302	-2.9712859
H	0.1289980	-3.2452731	1.6340401
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H	-0.2314681	-4.5640511	-3.3586399
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H	4.1710845	-0.0665922	-1.5445681

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C	-5.2145101	-1.8571992	-1.2651121
C	-6.2599628	-1.9355010	-2.2227982
C	-7.3956066	-2.7097014	-1.9733277
C	-7.5055211	-3.4263361	-0.7655964
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C	-4.0651176	-1.0160953	-1.5999282
H	-6.1693691	-1.3724766	-3.1659153
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C	-3.0365522	-2.6212903	-3.0485161
C	-1.9123874	-2.7336767	-2.2357770
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O	-1.3426344	-1.3278535	-4.0160650
C	-2.6461516	-1.8597640	-4.2884951
O	0.1910386	-1.4768985	-2.3542370
C	-1.6757131	-3.3885256	-1.0008845
H	-2.5814269	-2.5248124	-5.1803591
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Br	-2.8803656	-2.3289985	2.6326417
H	-0.6041903	-3.5348663	-0.7624132
H	-2.3381090	-4.2313778	-0.7390144
H	-4.5654338	-2.4973700	0.7271759
H	-3.9028825	-3.2939747	-3.0257661
H	-4.1620269	-0.4146971	-2.5256215
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H	2.5875292	7.0084359	2.2707727
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H	6.3761838	4.9822356	1.6567670
C	5.5559080	1.0826885	4.7480062
C	6.3381412	-0.0750813	4.4901400
H	3.9336919	2.3463544	4.1008948
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H	7.1506037	-0.3539546	5.1783598
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C	-1.1144823	3.5378619	1.5520602
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C	-1.9985439	2.8301133	2.4093053
C	-3.2972856	2.5329748	1.9583972
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H	-6.7116452	1.0631695	0.3391019
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H	-6.2152322	4.1185245	1.2932460
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H	0.0831305	4.8990573	-2.6980856
H	-1.6046210	4.3154479	-2.6051897
H	-0.2653618	3.2414634	-2.1064346
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H	0.3482383	4.7965202	-0.2631731
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H	-1.1335913	6.7131815	0.3952203
H	-2.1731952	6.4034914	-1.0270851
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H	4.8016073	-1.3597373	-4.0240063
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C	1.6371795	-5.0598680	-3.3169248
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H	0.7322478	-5.2905112	-5.2907378
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H	2.9650312	-6.6293621	-2.5219982
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H	2.2951790	-6.9878338	-4.1488218
H	1.7565931	-5.2670019	-0.6211576
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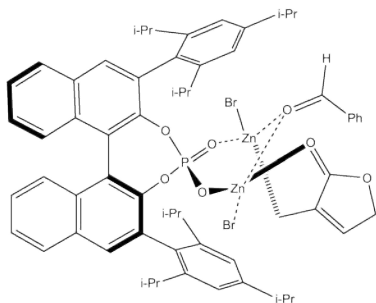


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C	3.1714897	6.0849430	2.1315824
C	1.0447130	4.8100801	2.0456153
H	0.4914292	5.7592738	2.1164274
C	0.3432942	3.6241707	1.8709667
C	3.5575931	-1.1151188	0.5844314
C	4.6514605	-1.3752314	1.4032513
H	5.2340958	-2.2957918	1.2435395
C	5.0004588	-0.5214745	2.4874768
C	6.0580343	-0.8631278	3.3839757
C	4.2420530	0.6852813	2.7152756
C	4.5359996	1.4538790	3.8822832
C	3.2013263	1.0479541	1.7812753
C	2.8564239	0.1139734	0.7927122
O	0.3907510	1.2199200	1.8108417
O	1.8262726	0.3952928	-0.0954076
P	0.2585015	0.3901342	0.4035566

H	5.7196850	-1.2296828	-2.4913103
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C	1.0294063	-4.0586117	1.9038656
C	2.5868023	-3.3694046	0.0074199
H	4.4729262	-4.6886116	1.5714483
H	3.1413796	-5.8452886	1.2729580
C	3.6539754	-0.4814847	-2.3613428
C	3.0810364	-2.1045119	-0.4313841
C	2.4795847	-3.7552620	1.4846585
H	1.6909891	0.4547164	-2.6586361
H	0.3794022	-3.1813287	1.7193929
H	2.3698207	-0.2821171	-4.1441764
H	0.4815064	-3.6659002	-4.5720816
H	0.6082126	-4.9255062	1.3534201
H	3.6076936	-5.7763430	-3.9585832
H	3.9038237	0.1662870	-1.4977189
H	2.8033488	-2.8841577	2.0868448
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Zn	-1.7317556	0.6715440	-2.0130263
Br	-2.9854537	1.7726181	-3.6312756
C	-6.0371075	-3.9401542	-0.7768372
C	-5.0316104	-2.9765876	-0.8829712
C	-5.3479991	-1.6826040	-1.3689860
C	-6.6796751	-1.3767369	-1.7507740
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H	-5.7957525	-4.9437355	-0.3966424
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H	-8.7169006	-2.1060712	-1.9221661
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O	-3.1572332	-0.7076151	-1.1499191
C	-2.4505660	-4.0482520	-3.2171146
C	-1.6867565	-3.3392433	-2.3294977
C	-1.3747217	-2.0656049	-3.0166375
O	-1.8810718	-2.0482748	-4.2640236
C	-2.6056301	-3.2764715	-4.4834185
O	-0.7763941	-1.0773498	-2.5576632
C	-1.2596032	-3.5863419	-0.9518741
H	-2.1716820	-3.7807502	-5.3754163
H	-3.6564580	-3.0043938	-4.7284636
Zn	-1.8576753	-2.1983274	0.3884874
Br	-3.4311168	-1.9598646	2.1246417
H	-0.1641952	-3.4315274	-0.8675551
H	-1.5081249	-4.6126793	-0.6192805
H	-3.9983985	-3.2094535	-0.5939270
H	-2.8956143	-5.0397723	-3.0582188
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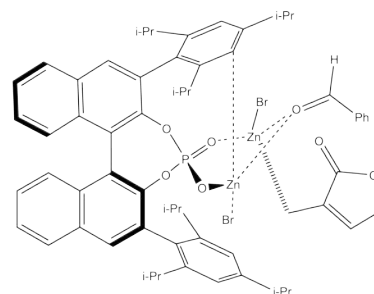
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C	4.6410445	3.7060938	1.7124172
C	2.4753684	4.8353098	2.0222770
C	3.1762413	6.0751415	2.1119950
C	1.0504297	4.7985617	2.0165914

H	0.4944269	5.7458970	2.0912187
C	0.3507153	3.6127425	1.8357475
C	3.5656800	-1.1422696	0.6095381
C	4.6437892	-1.3989522	1.4498892
H	5.2191300	-2.3274867	1.3120577
C	4.9843758	-0.5328364	2.5260355
C	6.0255138	-0.8689189	3.4428814
C	4.2318153	0.6821992	2.7245326
C	4.5133489	1.4643122	3.8854294
C	3.2090434	1.0392614	1.7688997
C	2.8740446	0.0965888	0.7853040
O	0.4004643	1.2102762	1.7567572
O	1.8634839	0.3764451	-0.1264876
P	0.2891019	0.3779357	0.3499504
O	-0.4290756	1.2005106	-0.7371148
O	-0.2433078	-1.0002333	0.7104107
C	4.5576004	6.1260057	2.0043255
C	5.2908359	4.9308784	1.7829829
H	2.5911017	6.9982724	2.2484747
H	5.0836907	7.0906329	2.0687563
H	5.2222365	2.7918484	1.5312269
H	6.3838087	4.9740807	1.6599830
C	5.5175760	1.0985631	4.7707768
C	6.2952266	-0.0675111	4.5412109
H	3.9138274	2.3634609	4.0821922
H	5.7072818	1.7156054	5.6622685
H	7.0953767	-0.3422738	5.2452527
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C	-1.5679442	3.9884105	0.2559161
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C	-1.9836573	2.8096449	2.3838823
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C	-3.7438311	2.9049011	0.6723727
C	-1.5580365	2.4026833	3.7924990
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C	1.9557652	-5.2083897	-3.2991270
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H	1.8451427	-5.3374193	-0.5723577
C	2.7240758	0.1618637	-3.2433005
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C	3.1902629	-1.8741911	-1.7945132
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C	-1.8494279	-3.2924186	-2.3306593
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H	-2.7829914	-3.6338578	-5.2900114
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H	-1.4423784	-4.5998368	-0.6840254
H	-4.1019605	-3.1114533	-0.4397785
H	-3.2045079	-4.9378370	-2.9139487
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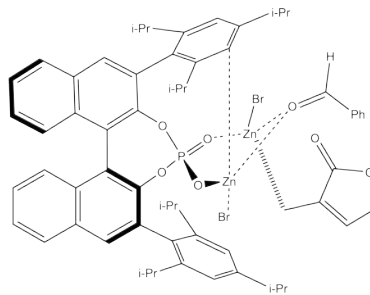


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C	3.2607176	6.1592158	1.3627385
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H	0.5915879	5.8146418	1.5699444
C	0.4607238	3.6609441	1.5093910
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C	5.1080519	-0.4351503	2.2447962
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O	0.5431735	1.2639124	1.6378538
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P	0.3134756	0.3399054	0.2853727
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H	-2.9720688	3.5041705	4.7102143
H	-1.6747955	4.6679176	4.2882044
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H	0.6017152	-4.0510524	-4.5087561				
C	2.7055784	-3.1462492	-2.6703381				
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C	2.6942151	-5.9372626	-4.0147795				
H	2.3196241	-6.7848602	-4.6255176				
H	1.5014790	-5.3229673	-0.3480742				
C	2.9004498	-0.1874751	-3.4737156				
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H	5.8681697	-1.7274451	-2.3736185				
C	3.1728109	-2.1155037	-1.8387582				
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C	3.8330486	-0.8940857	-2.4742413				
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H	1.9239140	0.0424000	-3.0073610				
H	0.1167742	-3.2464434	1.7220712				
H	2.7031727	-0.8223015	-4.3629872				
H	-0.4683773	-4.6490473	-3.2069364				
H	0.5296066	-4.9909137	1.6046683				
H	3.0442322	-5.1523047	-4.7172586				
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C	-6.3535626	-3.4331090	0.6346628				
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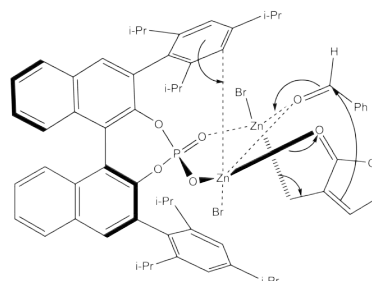


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C	6.2041137	-0.6982872	3.1120944
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O	1.8470084	0.2975520	-0.3047313
P	0.3157716	0.3418428	0.2745584
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O	-0.2310190	-0.9727399	0.8019924
C	4.6247996	6.2168213	1.1478926
C	5.3571509	5.0138846	0.9689991
H	2.6710698	7.0911531	1.4714032
H	5.1403852	7.1877162	1.0948882
H	5.2996305	2.8589197	0.8993185
H	6.4372829	5.0568253	0.7618979
C	5.8344875	1.4099565	4.2557717
C	6.5668543	0.2033551	4.1004750
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C	-1.4189901	1.1404079	4.2275631	C	-5.2997650	-1.8452644	-0.9127803
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H	-0.9947360	0.3944497	3.5300010	C	-7.4003771	-3.6314161	-0.3491292
C	-1.8670670	3.6118186	4.6504399	H	-6.4029420	-3.9467248	1.5629930
H	-0.1453280	2.7801733	3.6763384	C	-4.2544236	-0.9062480	-1.2809581
H	-2.9656921	3.4687975	4.7218074	H	-6.3100740	-1.5166166	-2.8193295
H	-1.6832456	4.6477406	4.2996260	H	-8.1844674	-3.0997540	-2.3130708
H	-1.4457622	3.5133556	5.6719168	H	-8.2201934	-4.3325117	-0.1285215
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C	-5.6543744	1.1049030	1.2959976	C	-3.1147873	-2.7884332	-3.0040501
H	-6.6197593	0.7344541	0.8976087	C	-2.0612718	-2.7677668	-2.1235505
H	-5.8425887	1.4601958	2.3302847	C	-1.0279373	-1.8567501	-2.7286800
H	-4.9555692	0.2483888	1.3604818	O	-1.4504195	-1.4707781	-3.9749055
C	-6.0183929	3.4746598	0.4711495	C	-2.7444213	-2.0203543	-4.2392054
H	-5.1144202	1.8818920	-0.6500270	O	0.0230554	-1.4832449	-2.2529070
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H	0.1728135	4.8020652	-0.6239289	H	-4.3711048	-0.4001600	-2.2645618
H	-0.9236819	6.8076333	-1.6110410	H	-3.4126076	3.7271865	-1.1297388
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H	3.2056330	-4.7594274	3.2542103				
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C	0.3523112	-4.9486762	-3.8621977				
H	0.5879455	-4.0631560	-4.4890270				
C	2.7069459	-3.1573800	-2.6655969				
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H	3.5695160	-6.2946891	-3.4295755				
C	1.9694373	-4.4156819	-0.7526726				
C	2.6857071	-5.9486808	-4.0024643				
H	2.3107502	-6.7999719	-4.6077667				
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C	2.9192451	-0.2081149	-3.4940171				
H	5.7001606	-0.3985560	-3.5316359				
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C	3.1752981	-2.1231476	-1.8395604				
C	0.8370354	-3.9967931	2.0486317				
C	2.4229775	-3.4106525	0.1237292				
H	4.3236239	-4.3648774	1.9068976				
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C	2.2661915	-3.6131936	1.6323266				
H	1.9387259	0.0287221	-3.0399557				
H	0.1147235	-3.2211874	1.7366890				
H	2.7281052	-0.8484315	-4.3805443				
H	-0.4754624	-4.6646640	-3.1833637				
H	0.5173214	-4.9680206	1.6172564				
H	3.0307015	-5.1666232	-4.7104022				
H	4.0563763	-0.1760431	-1.6750950				
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7.2.1.2 to 15r-mi TS1-8-r; COSMO

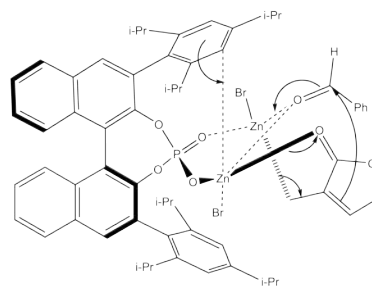


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C	-4.8875702	3.0418374	-3.8311214
O	-2.5211770	1.6397135	-1.4049465
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Zn	-2.5522268	-0.5088996	-1.0973315
H	-0.8099121	1.9156412	-5.9877298
H	-1.4257023	-1.8334642	-2.8344280
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C	3.9496209	1.8919081	5.5867659	C	1.0224370	-3.3056511	-5.4318863
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C	2.3075924	-3.0234776	0.2807266	C	1.3618390	-3.2353829	-3.9474037
C	2.7667180	-4.1415241	0.9673415	C	5.3334068	-2.3755945	-2.1810700
H	2.9466413	-5.0739916	0.4108972	C	0.5530858	-1.9383029	-5.9643936
C	2.9573041	-4.1361317	2.3776201	H	1.3383622	-1.1647663	-5.8322173
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C	2.7204603	-2.9230729	3.1223811	C	0.1287731	-6.0569433	-0.7149077
C	2.7945044	-2.9859830	4.5473274	H	2.5199072	-4.8491958	-5.8927523
C	2.3800969	-1.7148897	2.4062151	C	0.5462707	-3.8588088	-2.9884751
C	2.1379212	-1.8158998	1.0271789	C	2.1888673	-3.8598108	-6.2682322
O	0.0782069	-0.1685700	2.0962174	H	1.8919679	-3.9754307	-7.3312777
O	1.7720309	-0.6838795	0.2986465	H	-0.3391426	-4.4179697	-3.3338641
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O	-0.8613345	-0.9074250	-0.1059901	H	5.3813356	-3.4104255	-1.7841663
C	5.1875955	1.2822059	5.7269809	C	2.8074712	-2.4308287	-2.1277796
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H	5.9385571	1.7041706	6.4120884	H	1.1878858	-6.3255641	-0.5271091
H	4.8067524	-1.3185983	3.5163908	H	-0.1378076	-6.4435371	-1.7211520
H	6.4897198	-0.3385094	5.0491754	C	4.0553039	-1.6549147	-1.7131844
C	3.1408885	-4.1628010	5.1974179	C	1.9740321	-3.0807129	-1.1778074
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H	2.5599461	-2.0897632	5.1375714	H	3.0779752	0.3012007	-1.8719618
H	3.1827445	-4.1840269	6.2971791	H	-1.7634601	-3.1119057	-0.6871752
H	3.7149561	-6.2643356	4.9830701	H	4.0582970	-0.1294822	-3.3019176
H	3.5233156	-6.2373017	2.4882258	H	-0.3517983	-1.5909958	-5.4280506
C	-0.0836836	3.5273061	2.1853924	H	-1.9581130	-4.4869705	-1.8281503
C	-0.3376415	2.3851973	2.9940839	H	3.0656722	-3.1796166	-6.2417880
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H	-0.9869436	4.9983379	0.8579753	H	3.1345102	-2.0186634	-4.2225398
C	-1.9905340	0.7587363	4.0940263	H	-2.4714772	3.0956212	-2.8459606
H	-3.6934968	1.9845617	2.3813359				
C	-2.8489118	-0.3686616	3.5055431				
H	-3.8687713	-0.0257011	3.2362313				
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H	-2.3907733	-0.7918454	2.5919958				
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H	-1.0316920	0.3127845	4.4278186				
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H	-4.5691790	2.2985735	0.1286609				
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TS1-8-r



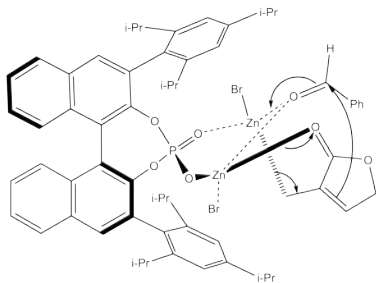
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C	-6.6310672	1.0877427	-2.8449397	H	-1.0193586	0.3123905	4.4317087
C	-4.8829990	3.0409808	-3.8447089	H	-3.6123353	1.8516385	5.0860886
O	-2.5237699	1.6468637	-1.4072004	H	-1.9976912	2.1589773	5.8007772
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H	-4.9836721	0.4087233	-1.6194386	C	-3.6005152	4.1785200	0.6891276
H	-6.5621814	3.7410977	-5.0229989	C	-4.8348693	3.2869262	0.5104466
H	-7.3139046	0.3238167	-2.4431760	H	-5.5385970	3.7424965	-0.2140100
H	-4.1918010	3.8086605	-4.2289042	H	-5.3843712	3.1585331	1.4660534
Br	-4.3722273	-1.2555123	0.2125739	H	-4.5665980	2.2796597	0.1382655
Zn	-2.5604403	-0.5075254	-1.0895421	C	-3.9762962	5.5190773	1.3532897
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H	-1.4428583	-1.8345599	-2.8289035	H	-4.7639030	6.0351228	0.7674006
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C	-2.1680366	-1.0383707	-3.0865164	H	2.8431599	4.8693105	0.7806930
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C	3.3273379	-5.3205434	3.0733671	C	2.4830068	-2.5293701	-3.4926895
C	2.7207832	-2.9186701	3.1197514	C	0.1192347	-6.0512930	-0.7130884
C	2.7973271	-2.9806042	4.5443417	H	2.5157716	-4.8502400	-5.8906516
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C	5.1939160	1.2810016	5.7229928	C	2.8041049	-2.4309964	-2.1294158
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H	3.7200715	2.8090827	6.1458784	C	0.8171049	-3.7948431	-1.6083859
H	5.9455924	1.7015696	6.4080973	H	1.1779434	-6.3219399	-0.5265743
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7.2.1.3 to 15s-mi

TS1-8-s; woelfling data



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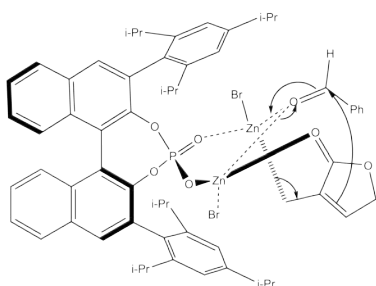
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O	0.013896	1.827835	-3.909744
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H	-3.970660	1.426977	-3.363770
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C	0.354946	-0.901517	3.519097
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C	3.203193	-3.639697	-1.792312
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TS1-8-l; COSMO



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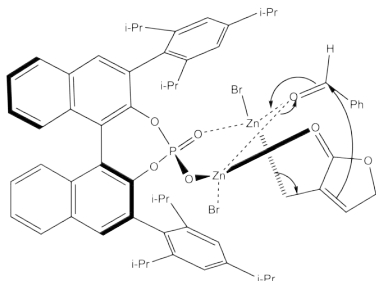
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TS1-8-1



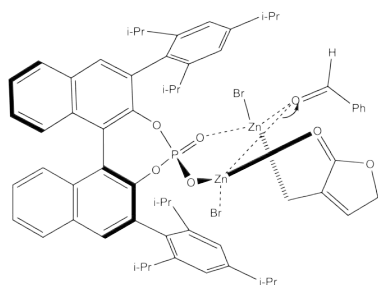
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C	0.1790086	-4.4265037	0.9434825	C	-0.110355	7.498099	-0.928037
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H	3.5915739	-4.7905554	1.6807467	H	0.922540	4.514280	-2.265027
H	2.5122962	-6.0052865	0.9348343	C	0.997992	3.552897	0.281300
C	3.9512664	-0.5331268	-2.0973768	H	0.268872	5.580282	1.888241
C	2.8737288	-2.2976143	-0.5347726	H	-0.399856	7.899584	1.192704
C	1.6548851	-3.9856974	0.9962888	H	-0.411415	8.511125	-1.237228
H	2.1890219	0.6306582	-2.7143033	O	1.211892	2.602557	-0.487934
H	-0.4295959	-3.6872916	0.3833552	C	3.347368	3.712541	-3.304200
H	3.1150942	-0.0469293	-4.0843582	C	2.647921	2.529749	-3.317992
H	-0.3581301	-4.1179167	-3.7940090	C	3.335799	1.676820	-2.333738
H	0.0552790	-5.4115404	0.4468590	O	4.372440	2.299839	-1.761946
H	3.7879041	-5.1372328	-4.7069729	C	4.456346	3.632960	-2.306379
H	4.0393267	0.0094640	-1.1353371	O	3.010709	0.517722	-2.009694
H	1.7076027	-3.1132906	1.6796540	C	1.399195	2.069208	-3.906174
H	3.0725694	-2.2548982	-3.9584196	H	5.479573	3.759866	-2.724808
Zn	-1.5492593	0.2501453	-2.2618345	H	4.351498	4.341609	-1.453416
Br	-0.8533461	1.3244595	-4.2075496	Zn	0.022569	2.012409	-2.387118
C	-3.8046124	-4.5214574	-5.3905857	Br	-2.013240	3.171403	-2.145661
C	-3.3593707	-4.2047935	-4.1019475	C	-1.366094	-0.874031	1.944581
C	-2.8525815	-2.9151883	-3.8154864	C	-2.075095	-2.062096	1.705716
C	-2.7912675	-1.9486370	-4.8449637	C	-2.420219	-2.887330	2.842402
C	-3.2478390	-2.2679350	-6.1292507	C	-2.935171	-4.213283	2.712869
C	-3.7557919	-3.5499656	-6.4067324	C	-2.205801	-2.376395	4.173378
H	-4.1900928	-5.5294322	-5.6073572	C	-2.586590	-3.162459	5.301491
H	-3.3952828	-4.9625227	-3.3017702	C	-1.562328	-1.120585	4.339137
C	-2.4009093	-2.6216730	-2.4427052	H	-1.394746	-0.736028	5.356764
H	-2.3728999	-0.9491607	-4.6436550	C	-1.079941	-0.392069	3.259150
H	-3.1988582	-1.5083845	-6.9243427	C	-1.656775	-3.062194	-1.983383
H	-4.1097283	-3.7957463	-7.4197247	C	-2.923968	-3.559359	-2.268591
O	-1.5595570	-1.7301633	-2.1298463	H	-3.117840	-4.001488	-3.257820
C	-4.6452182	-1.8288211	-1.7382539	C	-4.003062	-3.451064	-1.344174
C	-4.0932327	-0.7143816	-1.0892322	C	-5.322794	-3.862731	-1.699371
C	-3.6847828	-1.2387444	0.2366754	C	-3.775606	-2.863695	-0.045364
O	-4.1237153	-2.4929470	0.4249820	C	-4.899615	-2.651925	0.807274
C	-4.9296530	-2.8851856	-0.7180178	C	-2.430723	-2.489213	0.323155
C	-3.0087180	-0.6694221	1.1108098	C	-1.443426	-2.553363	-0.663083
O	-3.7017494	0.5627757	-1.5390286	O	-0.973732	-0.064884	0.884486
H	-5.9900771	-2.9148879	-0.3768828	O	-0.154395	-2.153491	-0.335025
H	-4.6364759	-3.9194583	-0.9972531	P	0.164446	-0.548949	-0.203318
Zn	-1.6776669	-1.7086286	2.2463609	O	1.561913	-0.534666	0.464080
Br	-2.1452948	-3.1144799	3.9709838	O	-0.087543	0.193155	-1.499281
H	-3.3985170	1.3001921	-0.7761196	C	-3.112190	-4.433999	5.137579
H	-4.1531510	0.9550060	-2.4640757	C	-3.264473	-4.967871	3.830371
H	-2.5564335	-3.4457969	-1.7035016	H	-2.430800	-2.743003	6.307960
H	-5.1347534	-1.8098960	-2.7200581	H	-3.388848	-5.037315	6.015444
				H	-3.053647	-4.646911	1.710689
				H	-3.642989	-5.993237	3.700778
				C	-6.175150	-3.038257	0.419951
				C	-6.389244	-3.667102	-0.835008
				H	-4.747664	-2.160412	1.778173
				H	-7.027822	-2.849854	1.090014
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				H	-5.481007	-4.322416	-2.687691
				C	1.107682	0.662409	3.893480
				C	-0.252214	0.830087	3.516313
				C	1.844017	1.797488	4.280110
				C	-0.839571	2.122484	3.501118
				C	-0.063530	3.223811	3.914171
				C	1.274820	3.081193	4.327897
				H	2.895184	1.675706	4.587142
				C	-2.286578	2.324929	3.060853
				H	-0.536818	4.218280	3.947286
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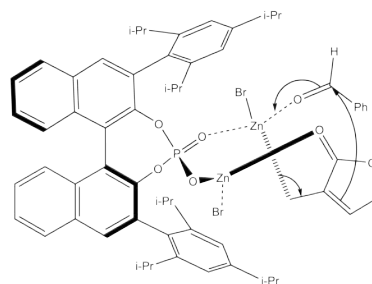
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H	-2.748865	1.317772	2.996525
H	-2.756557	4.181433	4.157999
H	-3.045681	2.682469	5.096353
H	-4.173346	3.163774	3.784140
C	2.068330	4.241792	4.918585
C	2.054185	5.509564	4.053330
H	2.701312	6.294852	4.494608
H	1.033067	5.939499	3.978780
H	2.417663	5.307828	3.025685
C	1.577739	4.542036	6.348544
H	3.124560	3.900830	4.991602
H	2.186850	5.339506	6.822657
H	1.630828	3.638552	6.988282
H	0.520578	4.881222	6.338350
C	1.764900	-0.716102	3.943447
C	3.162983	-0.719486	3.318869
H	3.540519	-1.752798	3.184350
H	3.911156	-0.171550	3.926882
H	3.148244	-0.239933	2.326809
C	1.825137	-1.257371	5.383614
H	1.136051	-1.404602	3.342341
H	2.291166	-2.264170	5.400791
H	0.820394	-1.337974	5.841687
H	2.437928	-0.589095	6.024329
H	2.398194	-1.402827	-6.444291
H	1.809151	-6.169214	-2.961967
H	-3.741725	-1.546134	-5.833479
C	2.761179	-2.166987	-5.721669
H	2.199369	-5.039337	0.019971
H	4.751801	-1.242087	-5.662583
H	-2.873179	0.636610	-4.763968
C	1.597118	-2.469490	-4.787801
C	0.946038	-6.047787	-2.274414
C	3.951167	-1.555107	-4.960849
H	4.396528	-2.285470	-4.253143
C	1.735317	-3.349862	-3.699912
C	-2.759299	-2.024339	-5.639468
H	2.328363	-3.824214	-7.100827
C	0.345325	-1.869321	-4.985579
C	3.182557	-3.406452	-6.530793
H	3.988755	-3.155762	-7.251239
H	0.219025	-1.191325	-5.845274
C	2.131514	-4.322721	-0.824287
H	1.045412	-6.804698	-1.468738
H	0.026409	-6.276802	-2.850056
C	0.682916	-3.601320	-2.804096
C	-1.890957	0.138045	-4.642512
C	-0.744252	-2.081115	-4.119451
H	-2.928436	-3.109148	-5.482358
H	-2.144453	-1.917674	-6.557868
C	0.894346	-4.623575	-1.687952
C	-0.566359	-2.944006	-2.999489
C	-2.062414	-1.372036	-4.430126
H	2.076144	-3.302355	-0.397130
H	-1.409720	0.599101	-3.760921
H	3.073645	-4.409946	-1.404534
H	3.636909	-0.673443	-4.367778
H	-1.277855	0.378560	-5.535398
H	3.565551	-4.208531	-5.865569
H	0.010766	-4.586159	-1.019690
H	-2.728973	-1.491191	-3.553647
H	2.699642	-3.858173	-3.539377
H	1.031634	2.697999	-4.737191
H	1.444977	0.999632	-4.196587
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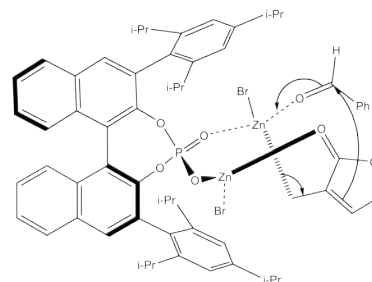
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C	-5.9612214	4.1742756	0.9212372
C	-5.0388647	3.4412955	0.1638310
C	-3.7621593	3.1484947	0.6891936
C	-3.4345327	3.5801024	1.9901476
C	-4.3591766	4.3167815	2.7463761
C	-5.6223484	4.6205212	2.2127412
H	-6.9563994	4.3968579	0.5061767
H	-5.2920944	3.0720947	-0.8416008
C	-2.7821584	2.3617155	-0.1179464
H	-2.4661729	3.2943976	2.4299037
H	-4.0959198	4.6460283	3.7635074
H	-6.3487135	5.1957332	2.8070704
O	-3.2451835	1.5947149	-1.0443594
C	-1.8231419	3.9661412	-1.0523331
C	-1.1398328	3.3328612	-2.1265637
O	0.2676705	3.1939850	-1.6799316
C	0.4605617	3.8352159	-0.5247774
C	-0.7703381	4.4839317	-0.1066832
O	1.1917511	2.5887623	-2.2484701
C	-1.6250455	2.7230332	-3.2888261
H	-0.6105693	5.5805696	-0.1802958
H	-0.9238986	4.2307496	0.9626350
Zn	-2.1669794	0.7371065	-2.4400134
Br	-3.0635147	-1.0315880	-3.6670904
C	-0.5094016	-1.9030502	1.4034066
C	-0.3230061	-3.1287905	0.7386857
C	-0.1442168	-4.3096849	1.5600594
C	0.2376990	-5.5783561	1.0234748
C	-0.3073011	-4.2127506	2.9911922
C	-0.1749782	-5.3822433	3.7990721
C	-0.5332398	-2.9403147	3.5849337
H	-0.6278282	-2.8698232	4.6796688
C	-0.5857095	-1.7806261	2.8244321
C	1.1387068	-2.4673830	-2.7565554
C	0.5573762	-3.4965050	-3.4931778
H	0.8498084	-3.6640694	-4.5381590
C	-0.4688618	-4.3257605	-2.9490715
C	-1.1369340	-5.2842326	-3.7689218
C	-0.8858672	-4.1706289	-1.5750077
C	-1.9928314	-4.9357209	-1.1066558
C	-0.1751269	-3.2299986	-0.7463905
C	0.7524406	-2.4054538	-1.3787282
O	-0.6892671	-0.7023295	0.7137460
O	1.3419637	-1.4133240	-0.6128235
P	0.3802532	-0.1085814	-0.3759724
O	1.3556923	0.9502256	0.1727059
O	-0.4089300	0.2785774	-1.6170076
C	0.1526295	-6.6056578	3.2359284
C	0.3805934	-6.6939669	1.8371659
H	-0.3198138	-5.2856203	4.8865546
H	0.2582370	-7.4993962	3.8694090
H	0.4355407	-5.6716396	-0.0519770
H	0.6810917	-7.6544467	1.3912074
C	-2.6368806	-5.8410798	-1.9392684

TS2-8-a; COSMO

C	-2.1976693	-6.0300994	-3.2766936
H	-2.3404719	-4.7922748	-0.0736029
H	-3.4980645	-6.4128120	-1.5610764
H	-2.7116353	-6.7556697	-3.9253247
H	-0.8081087	-5.4027526	-4.8133987
C	0.5210333	0.3005272	3.7088521
C	-0.6779564	-0.4277268	3.4611855
C	0.4227222	1.5528619	4.3359593
C	-1.9378356	0.1114207	3.8265399
C	-1.9785755	1.3755421	4.4527212
C	-0.8111658	2.1095807	4.7245318
H	1.3441929	2.1167391	4.5496976
C	-3.2305496	-0.6479759	3.5267307
H	-2.9560385	1.7849597	4.7444995
C	-3.8377912	-0.2079705	2.1801041
H	-4.1572459	0.8531818	2.2205622
H	-4.7303394	-0.8199062	1.9341315
H	-3.1143425	-0.3083546	1.3477975
C	-4.2690104	-0.5498586	4.6553923
H	-2.9588429	-1.7194303	3.4265069
H	-4.6768001	0.4778650	4.7551054
H	-3.8382904	-0.8407230	5.6351140
H	-5.1289421	-1.2177871	4.4444068
C	-0.8160154	3.4727665	5.4157347
C	-0.5305091	4.6105392	4.4136683
H	-0.4023136	5.5791833	4.9393856
H	-1.3691849	4.7299352	3.6965768
H	0.3894749	4.4147280	3.8267880
C	-2.0828481	3.7602383	6.2304195
H	0.0388746	3.4544762	6.1289705
H	-1.9771295	4.7115554	6.7898717
H	-2.2931311	2.9531681	6.9608669
H	-2.9763426	3.8622472	5.5795733
C	1.8937206	-0.2866219	3.3750456
C	2.9481585	0.7689522	3.0097960
H	3.8573357	0.2762829	2.6097409
H	3.2653274	1.3610709	3.8936109
H	2.5766837	1.4621697	2.2328232
C	2.3996710	-1.1737904	4.5307180
H	1.7660377	-0.9428491	2.4872441
H	3.3836114	-1.6211830	4.2785936
H	1.6979248	-2.0003296	4.7561452
H	2.5241238	-0.5719653	5.4553413
H	4.1363855	2.2192057	-5.6116548
H	5.8186303	-1.7937174	-2.7065853
H	0.2063298	-2.2716487	-7.1199332
C	4.1650193	2.2856832	-4.5007520
H	4.8499803	-1.9660989	0.3476845
H	3.9779270	4.4622611	-4.6036157
H	-1.2542853	-0.2609741	-6.4669191
C	3.3985905	1.0572666	-4.0170621
C	5.0684504	-2.5471276	-2.3882755
C	3.4675911	3.6064944	-4.1164849
H	3.5087844	3.7682575	-3.0198249
C	3.7991680	0.2844007	-2.8948756
C	1.0244204	-1.8529480	-6.4983979
H	6.1586061	1.3609231	-4.3447990
C	2.2963933	0.5923956	-4.7466512
C	5.6384320	2.3010542	-4.0701739
H	6.1694380	3.1405539	-4.5621932
H	1.9890088	1.1618066	-5.6368733
C	4.4015345	-1.2120965	-0.3301438
H	5.5834353	-3.2891313	-1.7442114
H	4.7062408	-3.0706242	-3.2961348
C	3.1670905	-0.9487792	-2.5733265
C	-0.3889791	0.1468004	-5.9084778
C	1.5807248	-0.5752540	-4.4143974
H	1.6523235	-2.6926981	-6.1389487
H	1.6664177	-1.2280004	-7.1540844
C	3.9045009	-1.8863992	-1.6176438
C	1.9941042	-1.3531890	-3.2841422

C	0.4483304	-1.0071535	-5.3419180
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H	-0.8016400	0.7699902	-5.0952208
H	5.1794124	-0.4453243	-0.5244330
H	2.4029106	3.6119073	-4.4208031
H	0.1839193	0.7956275	-6.6026203
H	5.7361848	2.4479016	-2.9745232
H	3.2136090	-2.7016298	-1.3286361
H	-0.2516435	-1.6342860	-4.7526556
H	4.7584249	0.5156812	-2.4072885
H	-2.6063122	3.0295496	-3.6847199
H	-0.8751147	2.3855277	-4.0230392
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TS2-8-a

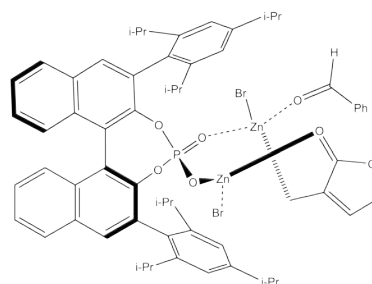


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C	-5.0355369	3.4239332	0.1710501
C	-3.7569353	3.1366461	0.6940462
C	-3.4287829	3.5698669	1.9940260
C	-4.3542665	4.3057436	2.7499238
C	-5.6184045	4.6060554	2.2176030
H	-6.9553130	4.3738953	0.5153295
H	-5.2881373	3.0460392	-0.8312064
C	-2.7757070	2.3541325	-0.1176688
H	-2.4601876	3.2847010	2.4339186
H	-4.0895683	4.6361771	3.7662316
H	-6.3454249	5.1805059	2.8118368
O	-3.2401650	1.5920675	-1.0460403
C	-1.8243918	3.9585602	-1.0435282
C	-1.1398443	3.3324578	-2.1230012
C	0.2684790	3.1963203	-1.6790327
O	0.4603511	3.8350930	-0.5205582
C	-0.7710229	4.4742967	-0.0966815
O	1.1968725	2.5994811	-2.2481299
C	-1.6260140	2.7253827	-3.2842406
H	-0.6150556	5.5727887	-0.1606834
H	-0.9233279	4.2125883	0.9709136
Zn	-2.1810758	0.7225956	-2.4474689
Br	-3.0580791	-1.0042742	-3.7255851
C	-0.5077438	-1.8932584	1.4009888
C	-0.3203428	-3.1194079	0.7376217
C	-0.1395407	-4.2994456	1.5594915
C	0.2409027	-5.5683176	1.0231312
C	-0.3004866	-4.2016430	2.9906002
C	-0.1666592	-5.3705662	3.7982722
C	-0.5268770	-2.9288763	3.5827170
H	-0.6200621	-2.8556491	4.6774512
C	-0.5825384	-1.7696319	2.8219065
C	1.1341943	-2.4624722	-2.7615573
C	0.5477307	-3.4905804	-3.4951892

H	0.8361970	-3.6577244	-4.5411940	C	3.4932611	3.5912669	-4.1207745
C	-0.4780941	-4.3179192	-2.9484292	H	3.5379714	3.7488518	-3.0237847
C	-1.1505739	-5.2755320	-3.7649000	C	3.8129207	0.2688123	-2.9082703
C	-0.8896151	-4.1619896	-1.5731010	C	1.0170398	-1.8571218	-6.5052449
C	-1.9952463	-4.9258661	-1.1002797	H	6.1778530	1.3397827	-4.3574156
C	-0.1752801	-3.2215140	-0.7476015	C	2.3120034	0.5840696	-4.7584177
C	0.7509979	-2.3976416	-1.3829459	C	5.6605752	2.2809545	-4.0808771
O	-0.6903533	-0.6943276	0.7102835	H	6.1945135	3.1192800	-4.5716584
O	1.3410779	-1.4032585	-0.6196747	H	2.0079176	1.1545423	-5.6491046
P	0.3760876	-0.1007512	-0.3827156	C	4.3999138	-1.2215235	-0.3356931
O	1.3460148	0.9609525	0.1708401	H	5.5709238	-3.3133221	-1.7397904
O	-0.4138382	0.2847566	-1.6230905	H	4.6980161	-3.0938294	-3.2937138
C	0.1592175	-6.5940756	3.2357007	C	3.1726353	-0.9576138	-2.5835904
C	0.3842583	-6.6831914	1.8370948	C	-0.3745809	0.1579225	-5.9218705
H	-0.3093843	-5.2732779	4.8859876	C	1.5881376	-0.5777506	-4.4251027
H	0.2656421	-7.4873450	3.8697399	H	1.6383586	-2.7013775	-6.1448283
H	0.4355521	-5.6614128	-0.0528773	H	1.6648427	-1.2415001	-7.1640036
H	0.6829130	-7.6441071	1.3909960	C	3.9013251	-1.8968297	-1.6220573
C	-2.6427962	-5.8307236	-1.9298802	C	1.9961098	-1.3553202	-3.2928468
C	-2.2094083	-6.0202656	-3.2685004	C	0.4512955	-1.0019823	-5.3509276
H	-2.3381964	-4.7806043	-0.0660764	H	3.5710532	-0.7253190	0.2059005
H	-3.5034991	-6.4007832	-1.5483742	H	-0.7819947	0.7868697	-5.1106121
H	-2.7273518	-6.7443891	-3.9154063	H	5.1829438	-0.4597327	-0.5284505
H	-0.8271186	-5.3930242	-4.8111152	H	2.4280698	3.6002351	-4.4233100
C	0.5153919	0.3168441	3.7054562	H	0.2043504	0.7986562	-6.6188480
C	-0.6799744	-0.4176454	3.4596500	H	5.7589279	2.4270311	-2.9852909
C	0.4111859	1.5652538	4.3388774	H	3.2036191	-2.7058314	-1.3315624
C	-1.9418609	0.1118746	3.8317208	H	-0.2566485	-1.6185014	-4.7597573
C	-1.9881445	1.3731063	4.4626995	H	4.7665375	0.5031147	-2.4119185
C	-0.8244362	2.1124669	4.7339699	H	-2.6094854	3.0275675	-3.6772264
H	1.3303256	2.1331948	4.5515210	H	-0.8800871	2.3811833	-4.0189630
C	-3.2310950	-0.6534768	3.5321347	H	-2.7442866	4.5360051	-1.2062118
H	-2.9672439	1.7749553	4.7590989	H	-1.8642856	2.0294245	0.4460856
C	-3.8430188	-0.2137634	2.1875894				
H	-4.1709144	0.8446386	2.2307853				
H	-4.7313450	-0.8307839	1.9399809				
H	-3.1208566	-0.3074317	1.3535283				
C	-4.2679116	-0.5640155	4.6629474				
H	-2.9536940	-1.7232745	3.4290972				
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H	-3.8343922	-0.8543470	5.6415079				
H	-5.1247479	-1.2358594	4.4522691				
C	-0.8348938	3.4716250	5.4331415				
C	-0.5558554	4.6171902	4.4384351				
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H	-1.3958068	4.7365712	3.7229929				
H	0.3641007	4.4289150	3.8491918				
C	-2.1018437	3.7481578	6.2511774				
H	0.0203419	3.4525767	6.1460194				
H	-2.0010251	4.6959263	6.8175232				
H	-2.3080048	2.9351511	6.9758517				
H	-2.9962378	3.8500094	5.6016349				
C	1.8906450	-0.2591693	3.3631295				
C	2.9376407	0.8053071	3.0028340				
H	3.8497580	0.3228033	2.5975664				
H	3.2539331	1.3931583	3.8896841				
H	2.5619382	1.5030841	2.2321484				
C	2.4058332	-1.1521750	4.5100558				
H	1.7642693	-0.9096183	2.4709520				
H	3.3916437	-1.5911442	4.2511588				
H	1.7107994	-1.9853365	4.7310242				
H	2.5294862	-0.5573292	5.4391175				
H	4.1574065	2.2066635	-5.6221887				
H	5.8183654	-1.8236561	-2.7071660				
H	0.1945349	-2.2699332	-7.1247840				
C	4.1869677	2.2701441	-4.5108318				
H	4.8405994	-1.9760978	0.3466659				
H	4.0041383	4.4485483	-4.6047885				
H	-1.2452211	-0.2425791	-6.4768107				
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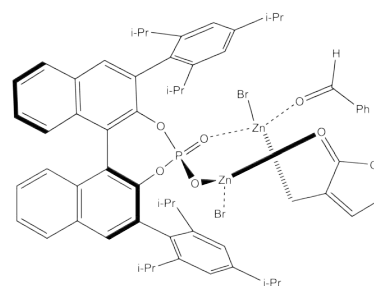


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C	-3.3843101	5.7074621	1.2482548
C	-2.4268814	4.7024901	1.0799633
C	-2.3378810	3.6481160	2.0195887
C	-3.2261613	3.6144886	3.1194864
C	-4.1888557	4.6172516	3.2812720
C	-4.2656644	5.6646091	2.3454920
H	-3.4551348	6.5253438	0.5157719
H	-1.7452125	4.7222676	0.2184796
C	-1.3495291	2.5729379	1.8837967
H	-3.1528884	2.7844244	3.8366406
H	-4.8820711	4.5855048	4.1352482
H	-5.0216562	6.4553523	2.4698561
O	-0.5863610	2.4237319	0.9205384
C	1.1682662	5.1119769	1.1188587
C	1.3408334	4.4617720	-0.0783158
C	2.3641483	3.4386591	0.1931575
O	2.7471839	3.4379051	1.4776947
C	2.0144471	4.4774480	2.1698077
O	2.8575857	2.6329761	-0.6217656
C	0.6374533	4.4816187	-1.3571717

H	2.7576664	5.1510386	2.6495153	H	2.2929094	0.8207793	2.8770473
H	1.4288692	3.9866750	2.9804967	C	1.8449616	-2.4141406	4.1520471
Zn	-0.6427303	2.8764940	-1.2632703	H	1.3933019	-1.4821433	2.2633235
Br	-2.9195647	2.5857423	-1.8254199	H	2.8243515	-2.8226725	3.8274521
C	-0.9104678	-1.8866169	0.6665659	H	1.0885234	-3.2163602	4.0413916
C	-1.0386175	-2.8960777	-0.3018288	H	1.9186055	-2.1630541	5.2311691
C	-1.1506021	-4.2642407	0.1485919	H	4.9357002	2.3249880	-5.3156277
C	-1.0971429	-5.3794150	-0.7433399	H	4.7598759	-3.2455747	-4.5211041
C	-1.2742096	-4.5337970	1.5597867	H	-1.1785139	1.1467921	-6.7497574
C	-1.4002716	-5.8821348	2.0115447	C	5.0698339	1.7348124	-4.3808384
C	-1.2534182	-3.4484261	2.4774572	H	3.9303266	-3.9358486	-1.5021380
H	-1.3925701	-3.6551861	3.5501058	H	5.8340978	3.4897646	-3.2965331
C	-1.0552564	-2.1341780	2.0666020	H	-1.1056255	2.8255597	-4.7324971
C	0.3640550	-1.6703520	-3.6558846	C	3.8829820	0.7798029	-4.3000486
C	-0.5697921	-2.1792352	-4.5502397	C	3.7493003	-3.6362848	-4.2787360
H	-0.4052498	-2.0669591	-5.6318112	C	5.0321889	2.7283421	-3.2011174
C	-1.7671928	-2.8170475	-4.1065455	H	5.1871706	2.1926274	-2.2411266
C	-2.7557708	-3.2527445	-5.0394841	C	3.9896488	-0.5259882	-3.7926373
C	-2.0057305	-3.0078824	-2.6944319	C	-0.1728648	0.7726694	-6.4662707
C	-3.2464537	-3.5790251	-2.2839845	H	6.4719736	0.2911071	-5.2750626
C	-0.9896731	-2.5902182	-1.7610445	C	2.6082760	1.2236739	-4.6960723
C	0.1079811	-1.8998414	-2.2686967	C	6.4339783	1.0368244	-4.4552527
O	-0.7148653	-0.5613057	0.2859975	H	7.2389331	1.7795188	-4.6286102
O	1.0474249	-1.4271420	-1.3620247	H	2.5142795	2.2415434	-5.1063563
P	0.6288460	-0.0748412	-0.5326144	C	3.8748883	-2.8845020	-1.8522533
O	1.8247238	0.1007253	0.4352473	H	3.8617830	-4.6940583	-3.9618144
O	0.2565145	1.0640899	-1.4637502	H	3.1490015	-3.6171634	-5.2110306
C	-1.3727371	-6.9387219	1.1144943	C	2.8680268	-1.3658070	-3.6513800
C	-1.2039673	-6.6807622	-0.2724913	C	-0.0461784	2.5119627	-4.6491129
H	-1.5063570	-6.0658762	3.0923127	C	1.4510536	0.4379619	-4.5538194
H	-1.4645065	-7.9749927	1.4739399	H	-0.1184613	-0.3005356	-6.7347052
H	-0.9534823	-5.2022822	-1.8177003	H	0.5774835	1.3053008	-7.0879200
H	-1.1501802	-7.5207452	-0.9818594	C	3.0835812	-2.7998815	-3.1679617
C	-4.1942161	-3.9755378	-3.2180859	C	1.5812623	-0.8745528	-4.0108649
C	-3.9440943	-3.8243386	-4.6081904	C	0.0987349	1.0161999	-4.9682186
H	-3.4515803	-3.6937576	-1.2100255	H	3.3913804	-2.2847012	-1.0570164
H	-5.1488482	-4.4052835	-2.8779881	H	0.2903142	2.7288030	-3.6174114
H	-4.6998834	-4.1478832	-5.3400325	H	4.9158594	-2.5181851	-1.9654762
H	-2.5618020	-3.1108905	-6.1143958	H	4.0577524	3.2516281	-3.1355242
C	0.1103223	-0.6282229	3.7445206	H	0.5495974	3.1495322	-5.3353062
C	-1.0849275	-1.0491241	3.1046043	H	6.6727404	0.5145185	-3.5052414
C	0.0149857	0.2465795	4.8459950	H	2.0876364	-3.2513813	-2.9830098
C	-2.3483771	-0.5543577	3.5448795	H	-0.6795967	0.4865480	-4.3810014
C	-2.3873648	0.2938346	4.6691201	H	4.9754664	-0.9118165	-3.4955255
C	-1.2184429	0.6926577	5.3479297	H	0.0662654	5.4120698	-1.5344463
H	0.9360555	0.5605327	5.3619705	H	1.3161871	4.2744580	-2.2079092
C	-3.6300763	-0.9092240	2.7897516	H	0.4702948	5.9329576	1.3294009
H	-3.3653560	0.6348612	5.0418986	H	-1.2883050	1.8470093	2.7336043
C	-3.8514816	0.0554412	1.6043378				
H	-4.0637801	1.0830396	1.9661730				
H	-4.7202648	-0.2671089	0.9946099				
H	-2.9730623	0.1134047	0.9329723				
C	-4.8800563	-0.9742140	3.6789821				
H	-3.4813159	-1.9220834	2.3604577				
H	-5.1779796	0.0282590	4.0520210				
H	-4.7276107	-1.6334827	4.5576811				
H	-5.7393947	-1.3673805	3.0990825				
C	-1.2744066	1.5186255	6.6290049				
C	-2.0085428	2.8588244	6.4631653				
H	-1.9614015	3.4487479	7.4015094				
H	-3.0834519	2.7090748	6.2276257				
H	-1.5648551	3.4712821	5.6526209				
C	-1.8818306	0.6929668	7.7792332				
H	-0.2214686	1.7493698	6.9029934				
H	-1.8621986	1.2636094	8.7308782				
H	-1.3255450	-0.2536186	7.9322044				
H	-2.9391244	0.4304701	7.5646677				
C	1.4744900	-1.1688186	3.3229698				
C	2.5917478	-0.1143505	3.3906150				
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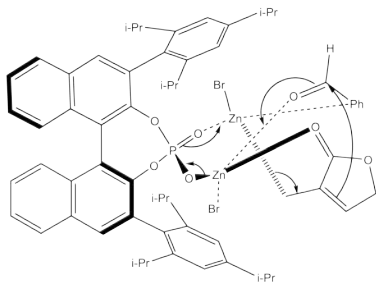


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C	-2.3502926	4.7382302	1.0966055
C	-2.2641070	3.6925601	2.0455388
C	-3.1404038	3.6803124	3.1546464
C	-4.0849753	4.6992947	3.3199991
C	-4.1590369	5.7384670	2.3753636

H	-3.3651960	6.5648982	0.5231183	C	-1.3927763	1.4639017	6.6738291
H	-1.6829390	4.7355039	0.2241399	C	-2.1515280	2.7946500	6.5523155
C	-1.2928954	2.6008475	1.9069798	H	-2.1413581	3.3403535	7.5180857
H	-3.0725873	2.8526551	3.8750237	H	-3.2168709	2.6351340	6.2820761
H	-4.7672723	4.6851567	4.1832731	H	-1.7014689	3.4548740	5.7842085
H	-4.9030696	6.5404065	2.5008131	C	-1.9938105	0.5837023	7.7866917
O	-0.5299360	2.4463734	0.9455852	H	-0.3473715	1.7051263	6.9678443
C	1.2131725	5.1338417	1.0885286	H	-1.9962579	1.1172764	8.7597953
C	1.4047520	4.4452516	-0.0848835	H	-1.4198877	-0.3564954	7.9087230
C	2.4005324	3.4096130	0.2454397	H	-3.0424225	0.3064969	7.5499013
O	2.7396613	3.4350682	1.5441856	C	1.4295167	-1.1581705	3.3815847
C	2.0065621	4.5045270	2.1836079	C	2.5359948	-0.0926034	3.4578643
O	2.9106574	2.5771046	-0.5283811	H	3.4648436	-0.4710839	2.9827654
C	0.7399130	4.4431528	-1.3809034	H	2.7950598	0.1699188	4.5050517
H	2.7482872	5.1712088	2.6766646	H	2.2356313	0.8359131	2.9329517
H	1.3796096	4.0447323	2.9822773	C	1.7990051	-2.3946211	4.2234176
Zn	-0.6060182	2.8885082	-1.2710353	H	1.3661029	-1.4779984	2.3228282
Br	-2.8908479	2.6668499	-1.7683407	H	2.7874723	-2.7947819	3.9170122
C	-0.9233351	-1.8821568	0.6669830	H	1.0531424	-3.2052412	4.1039043
C	-1.0285457	-2.9045977	-0.2907295	H	1.8524364	-2.1385810	5.3025168
C	-1.1288374	-4.2687667	0.1733979	H	4.6792521	2.6512199	-5.0885658
C	-1.0543579	-5.3925296	-0.7056963	H	4.8103035	-3.1554057	-4.4985136
C	-1.2641960	-4.5243711	1.5858230	H	-1.2552419	1.0922577	-6.7457117
C	-1.3803981	-5.8687640	2.0502225	C	5.0084411	1.8066765	-4.4430034
C	-1.2642958	-3.4287217	2.4908934	H	4.0207238	-3.8170713	-1.4640938
H	-1.4114591	-3.6238362	3.5646667	H	6.1625677	3.1347582	-3.1226081
C	-1.0761601	-2.1166739	2.0682709	H	-1.2069225	2.7675548	-4.7161053
C	0.3784464	-1.6809627	-3.6444963	C	3.8293929	0.8470709	-4.3446973
C	-0.5415621	-2.2132374	-4.5395606	C	3.8116819	-3.5677286	-4.2434693
H	-0.3723240	-2.1020643	-5.6204793	C	5.3447070	2.3872412	-3.0554247
C	-1.7297089	-2.8693180	-4.0999716	H	5.6760099	1.5893278	-2.3573185
C	-2.7046328	-3.3287581	-5.0351578	C	3.9725863	-0.4457595	-3.8100457
C	-1.9740832	-3.0522471	-2.6882442	C	-0.2411037	0.7364234	-6.4694495
C	-3.2084754	-3.6390868	-2.2815079	H	6.0053900	0.7540698	-6.0979316
C	-0.9701107	-2.6119660	-1.7521858	C	2.5441888	1.2531128	-4.7363496
C	0.1215570	-1.9091598	-2.2571801	C	6.2457902	1.1745816	-5.1006620
O	-0.7396204	-0.5607068	0.2698238	H	7.0495662	1.9285403	-5.2280956
O	1.0527959	-1.4248449	-1.3484622	H	2.4231978	2.2619417	-5.1611200
P	0.6260860	-0.0773482	-0.5160088	C	3.9307979	-2.7736477	-1.8299203
O	1.7934673	0.0761514	0.4885907	H	3.9530309	-4.6173792	-3.9116290
O	0.2828428	1.0705912	-1.4456003	H	3.2065827	-3.5776857	-5.1726021
C	-1.3323505	-6.9341669	1.1654517	C	2.8765057	-1.3110172	-3.6472611
C	-1.1523824	-6.6892741	-0.2219213	C	-0.1388645	2.4798576	-4.6565562
H	-1.4952037	-6.0420123	3.1318281	C	1.4065031	0.4410688	-4.5693028
H	-1.4159901	-7.9673674	1.5353900	H	-0.1695668	-0.3357751	-6.7374877
H	-0.9027198	-5.2239033	-1.7802266	H	0.4948932	1.2805445	-7.0980241
H	-1.0829390	-7.5360368	-0.9216988	C	3.1309489	-2.7311789	-3.1421048
C	-4.1424922	-4.0594488	-3.2182597	C	1.5742929	-0.8577354	-4.0083366
C	-3.8856636	-3.9163187	-4.6073808	C	0.0375516	0.9867560	-4.9739492
H	-3.4187703	-3.7468769	-1.2079974	H	3.4330908	-2.1803897	-1.0385986
H	-5.0921981	-4.5017454	-2.8806651	H	0.2133587	2.7090854	-3.6326833
H	-4.6310514	-4.2581556	-5.3414766	H	4.9599537	-2.3778183	-1.9505226
H	-2.5061251	-3.1911339	-6.1097616	H	4.4611995	2.8782801	-2.6004483
C	0.0559156	-0.6231090	3.7787270	H	0.4271717	3.1301536	-5.3558866
C	-1.1245718	-1.0275244	3.1018041	H	6.6636246	0.3549508	-4.4799362
C	-0.0639024	0.2336843	4.8916780	H	2.1479302	-3.2048807	-2.9442293
C	-2.3945306	-0.5237358	3.5103579	H	-0.7247678	0.4415173	-4.3803048
C	-2.4584951	0.3079944	4.6456864	H	4.9717570	-0.7959073	-3.5078686
C	-1.3072014	0.6804208	5.3675546	H	0.2042766	5.3830590	-1.6101551
H	0.8454505	0.5297827	5.4384885	H	1.4291455	4.1726644	-2.2044991
C	-3.6566386	-0.8522263	2.7125339	H	0.5254693	5.9733527	1.2540196
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C	-3.8532649	0.1584467	1.5619883				
H	-4.0633829	1.1738965	1.9579573				
H	-4.7142340	-0.1323602	0.9261348				
H	-2.9653332	0.2324986	0.9049233				
C	-4.9253327	-0.9568648	3.5712241				
H	-3.4936478	-1.8471857	2.2478866				
H	-5.2377933	0.0296000	3.9739071				
H	-4.7885960	-1.6472128	4.4283349				
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TS1-8-j; COSMO



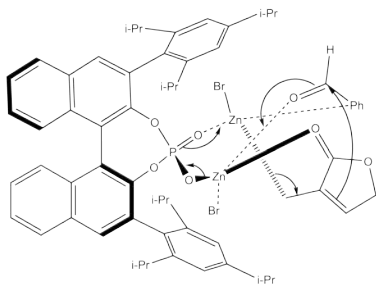
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C	-1.0548399	2.1833893	-2.6228805
C	-0.7303308	2.1381556	-4.0055946
C	-1.7232236	2.4774347	-4.9481207
C	-2.9978815	2.8832859	-4.5262444
C	-3.3067056	2.9542697	-3.1574796
H	-2.5517293	2.6881477	-1.1266341
H	-0.2586919	2.0161983	-1.8821700
C	0.6641593	1.8322181	-4.4399195
H	-1.4863935	2.4491503	-6.0239672
H	-3.7603222	3.1498251	-5.2734667
H	-4.3100084	3.2648953	-2.8332776
O	1.6348734	1.7666052	-3.5851473
C	0.4747730	0.0472282	-5.4418974
C	0.1058877	-0.8254523	-4.3837864
C	1.3962710	-1.0518526	-3.6633593
O	2.4259283	-0.8287676	-4.5041210
C	1.9336603	-0.2357068	-5.7296688
O	1.5792572	-1.2545988	-2.4652696
C	-1.1283390	-1.2933900	-3.9226763
H	2.0713907	-0.9612387	-6.5599615
H	2.5600038	0.6581369	-5.9228033
Zn	-2.0234028	-0.0640013	-2.3875336
Br	-4.3541751	-0.3085241	-2.4461159
C	0.1500013	0.9835083	2.4657110
C	0.7287165	0.0071370	3.2815267
C	1.6233128	0.4503791	4.3235092
C	2.4095781	-0.4501438	5.1031538
C	1.7547700	1.8664969	4.5730569
C	2.6116060	2.3116213	5.6245164
C	1.0516312	2.7977929	3.7548362
H	1.1364076	3.8710165	3.9818865
C	0.2863444	2.3896196	2.6685845
C	0.3770369	-3.3973433	1.5151911
C	-0.0077838	-4.2102690	2.5747488
H	-0.1403059	-5.2894894	2.4028403
C	-0.2778298	-3.6823808	3.8696977
C	-0.7563205	-4.5212059	4.9211107
C	-0.0981385	-2.2713741	4.1178761
C	-0.4710379	-1.7598493	5.3977099
C	0.4131453	-1.4336022	3.0581128
C	0.5761354	-2.0098207	1.7931356
O	-0.6640837	0.5792141	1.4110716
O	1.0266473	-1.2212036	0.7374301
P	0.0767737	-0.0565832	0.0952884
O	1.0387680	0.9712242	-0.5228047
O	-1.0705654	-0.6038191	-0.7549726
C	3.3424325	1.4074244	6.3806655
C	3.2496823	0.0169096	6.1048230
H	2.6939424	3.3938189	5.8120653
H	4.0060808	1.7649041	7.1826660
H	2.3535969	-1.5277324	4.8949304
H	3.8531471	-0.6969659	6.6860392
C	-0.9513280	-2.5996481	6.3935096

C	-1.0816486	-3.9951731	6.1623029
H	-0.3863422	-0.6814427	5.5898464
H	-1.2388837	-2.1778017	7.3687031
H	-1.4555114	-4.6522222	6.9622862
H	-0.8769789	-5.5972922	4.7197190
C	0.3542848	4.1426982	0.8351884
C	-0.4020581	3.3644409	1.7605647
C	-0.3180790	5.0967643	0.0511936
C	-1.8139942	3.5149427	1.8212415
C	-2.4346823	4.4933758	1.0180021
C	-1.7065035	5.3086930	0.1373613
H	0.2601549	5.7005447	-0.6662058
C	-2.6927927	2.6511174	2.7244407
H	-3.5264496	4.6113084	1.0873458
C	-3.6920012	1.8152151	1.9012558
H	-4.4111310	2.4606905	1.3545587
H	-4.2826845	1.1495063	2.5638891
H	-3.1700297	1.1783034	1.1597768
C	-3.4047417	3.4950989	3.7974425
H	-2.0346942	1.9394594	3.2624449
H	-4.1047625	4.2270326	3.3427640
H	-2.6755559	4.0631895	4.4102582
H	-3.9948160	2.8467450	4.4775704
C	-2.3478418	6.4191967	-0.6885090
C	-3.8432310	6.2191192	-0.9642100
H	-4.2184320	7.0052392	-1.6501260
H	-4.4451144	6.2853994	-0.0338754
H	-4.0470418	5.2345567	-1.4301073
C	-2.0946351	7.7869988	-0.0215785
H	-1.8217547	6.4250314	-1.6699507
H	-2.4936349	8.6142333	-0.6447153
H	-1.0123388	7.9663235	0.1376070
H	-2.5919343	7.8332155	0.9700083
C	1.8613944	3.9564437	0.6554461
C	2.3006913	4.0436424	-0.8169640
H	3.3297029	3.6485113	-0.9354655
H	2.3053860	5.0889808	-1.1905038
H	1.6319030	3.4654333	-1.4856497
C	2.6667063	4.9672577	1.4950582
H	2.1099399	2.9349168	1.0109962
H	3.7559998	4.8153700	1.3478731
H	2.4552527	4.8743914	2.5774607
H	2.4229767	6.0075490	1.1926663
H	0.1341046	-5.7573980	-4.2946172
H	4.3232360	-5.3720256	-0.2505152
H	-3.4832124	-5.7223250	0.6607127
C	1.1243989	-5.3844178	-3.9517110
H	4.8404763	-2.2868326	0.3515031
H	1.7054463	-4.6473871	-5.9391005
H	-3.9780636	-3.5249688	-0.5328389
C	0.9332466	-4.8676235	-2.5297393
C	3.9419204	-4.9072544	0.6829570
C	1.5494061	-4.2575366	-4.9116052
H	2.4967021	-3.7820101	-4.5822610
C	2.0282925	-4.4608075	-1.7470681
C	-2.4715843	-5.7370968	0.2046525
H	1.7997270	-7.3812470	-3.3259905
C	-0.3469422	-4.7893400	-1.9563245
C	2.1091448	-6.5653829	-4.0099374
H	2.1672422	-6.9795176	-5.0377890
H	-1.2136643	-5.1150764	-2.5551036
C	3.9737259	-2.5520913	-0.2879958
H	4.8178830	-4.6639564	1.3195196
C	3.3318207	-5.6679122	1.2118549
H	1.8747101	-3.9916130	-0.4315109
C	-2.9678158	-3.5526533	-0.9896183
C	-0.5590520	-4.3222925	-0.6434269
H	-1.7901614	-6.2713262	0.8976890
H	-2.5301435	-6.3346323	-0.7293785
C	3.1195257	-3.6397448	0.3805243
C	0.5676411	-3.9185163	0.1249045

C	-1.9816477	-4.3050740	-0.0844592
H	3.3885132	-1.6314303	-0.4624459
H	-2.6495097	-2.5048444	-1.1366904
H	4.3737045	-2.8810287	-1.2694872
H	0.7729472	-3.4680232	-4.9649048
H	-3.0733962	-4.0261980	-1.9878789
H	3.1341328	-6.2537702	-3.7197143
H	2.7836862	-3.2370576	1.3578788
H	-1.9561599	-3.7603386	0.8809068
H	3.0434659	-4.5138408	-2.1714245
H	-1.9727138	-1.2956181	-4.6316720
H	-1.0863568	-2.1327595	-3.2016777
H	-0.2121085	0.2887683	-6.2667566
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TS1-8-j



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Zn	2.3861418	0.8995115	-1.9599505
Br	4.6628603	0.9871767	-1.6801145
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C	-1.0983933	2.1850805	-2.5942003
C	-0.7779058	2.1503973	-3.9773966
C	-1.7771347	2.4800853	-4.9162461
C	-3.0580957	2.8591554	-4.4902892
C	-3.3652190	2.9132212	-3.1206924
H	-2.6015499	2.6498081	-1.0930757
H	-0.2970671	2.0198461	-1.8585059
C	0.6201604	1.8644097	-4.4099577
H	-1.5402184	2.4624014	-5.9926000
H	-3.8282134	3.1134489	-5.2338956
H	-4.3749307	3.1960465	-2.7913455
O	1.5827250	1.7894087	-3.5588074
C	0.4323258	0.0431026	-5.4435556
C	0.0792305	-0.8296513	-4.3836286
C	1.3765707	-1.0447084	-3.6699844
O	2.4002442	-0.8071516	-4.5179782
C	1.8957128	-0.2127117	-5.7332283
O	1.5698305	-1.2559177	-2.4768429
C	-1.1441189	-1.3183645	-3.9134358
H	2.0475689	-0.9273781	-6.5717203
H	2.5067768	0.6945164	-5.9183592
Zn	-2.0625502	-0.1105525	-2.3672117
Br	-4.3811284	-0.3497325	-2.4724302
C	0.1452865	0.9841058	2.4639589
C	0.7164327	0.0056284	3.2827921
C	1.6099038	0.4449111	4.3274100
C	2.3883638	-0.4590517	5.1104874
C	1.7491053	1.8601689	4.5760358
C	2.6048798	2.3007224	5.6296012
C	1.0547499	2.7938494	3.7538363
H	1.1441149	3.8671715	3.9785142
C	0.2912536	2.3895689	2.6652044
C	0.3754017	-3.3979880	1.5144426
C	-0.0151319	-4.2105645	2.5719634

H	-0.1448575	-5.2897984	2.3981287
C	-0.2940932	-3.6834601	3.8650010
C	-0.7771819	-4.5219893	4.9138668
C	-0.1161989	-2.2727006	4.1145070
C	-0.4923177	-1.7624224	5.3935906
C	0.3987102	-1.4342682	3.0573488
C	0.5689807	-2.0097976	1.7931294
O	-0.6665934	0.5841466	1.4062938
O	1.0230946	-1.2204023	0.7404108
P	0.0740872	-0.0582410	0.0931171
O	1.0359613	0.9650227	-0.5311946
O	-1.0728863	-0.6150936	-0.7516360
C	3.3276948	1.3936251	6.3889029
C	3.2274987	0.0040329	6.1141574
H	2.6937299	3.3826935	5.8154233
H	3.9911997	1.7482297	7.1922133
H	2.3264535	-1.5361375	4.9021692
H	3.8249957	-0.7129135	6.6976355
C	-0.9761875	-2.6026078	6.3866960
C	-1.1071402	-3.9971773	6.1537480
H	-0.4062833	-0.6842435	5.5859746
H	-1.2658607	-2.1814988	7.3615235
H	-1.4841942	-4.6548416	6.9516493
H	-0.8971480	-5.5978746	4.7111140
C	0.3772019	4.1393534	0.8303700
C	-0.3874697	3.3680674	1.7543926
C	-0.2873482	5.0944016	0.0412497
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C	-1.6745392	5.3141145	0.1212528
H	0.2971616	5.6923320	-0.6759389
C	-2.6848400	2.6717730	2.7143003
H	-3.5018813	4.6303346	1.0667130
C	-3.6906308	1.8398873	1.8955976
H	-4.4046456	2.4871935	1.3443439
H	-4.2880285	1.1831883	2.5609332
H	-3.1743824	1.1921087	1.1597552
C	-3.3886129	3.5261069	3.7843750
H	-2.0322835	1.9570027	3.2548270
H	-4.0821700	4.2629732	3.3279296
H	-2.6543024	4.0905034	4.3941459
H	-3.9844313	2.8864278	4.4676267
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C	-3.7978729	6.2319795	-1.0006003
H	-4.1662139	7.0235997	-1.6839102
H	-4.4101287	6.2915646	-0.0766803
H	-3.9959874	5.2513586	-1.4769067
C	-2.0577328	7.7931215	-0.0310323
H	-1.7692924	6.4382146	-1.6828522
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H	-0.9772583	7.9689816	0.1423711
H	-2.5651759	7.8351876	0.9553781
C	1.8831027	3.9402597	0.6536158
C	2.3287231	4.0342995	-0.8163250
H	3.3494652	3.6189565	-0.9374291
H	2.3568949	5.0833826	-1.1785907
H	1.6498796	3.4783070	-1.4937507
C	2.6972596	4.9353092	1.5033243
H	2.1203965	2.9136977	1.0022865
H	3.7848057	4.7731431	1.3556326
H	2.4848054	4.8351381	2.5846181
H	2.4646186	5.9807893	1.2104151
H	0.1660286	-5.7618976	-4.2939966
H	4.3357073	-5.3446590	-0.2396983
H	-3.4646909	-5.7617607	0.6442150
C	1.1517261	-5.3772946	-3.9501202
H	4.8341448	-2.2506408	0.3612939
H	1.7331041	-4.6358570	-5.9364068
H	-3.9744106	-3.5610789	-0.5417084
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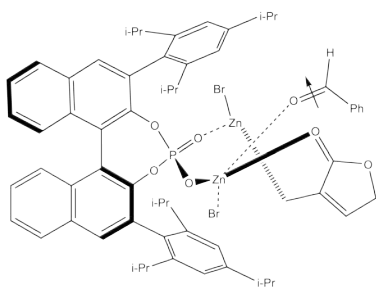
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C	2.0420333	-4.4437337	-1.7446182
C	-2.4517480	-5.7658605	0.1911098
H	1.8479433	-7.3653100	-3.3214325
C	-0.3286343	-4.7974287	-1.9573266
C	2.1489753	-6.5475969	-4.0064864
H	2.2136464	-6.9627801	-5.0335099
H	-1.1911338	-5.1328673	-2.5569031
C	3.9732694	-2.5253623	-0.2816256
H	4.8239878	-4.6313820	1.3292297
H	3.3429112	-5.6428129	1.2202193
C	1.8821564	-3.9775763	-0.4290400
C	-2.9623032	-3.5802311	-0.9941369
C	-0.5480412	-4.3323941	-0.6452128
H	-1.7678812	-6.2983504	0.8829406
H	-2.5027001	-6.3605020	-0.7450444
C	3.1227583	-3.6165423	0.3853337
C	0.5735175	-3.9185447	0.1252313
C	-1.9723840	-4.3288746	-0.0901830
H	3.3846024	-1.6082960	-0.4620849
H	-2.6530643	-2.5289289	-1.1347469
H	4.3827435	-2.8523002	-1.2596948
H	0.7766497	-3.4689943	-4.9692779
H	-3.0622091	-4.0481094	-1.9955802
H	3.1701036	-6.2252861	-3.7149000
H	2.7818793	-3.2148392	1.3613484
H	-1.9541578	-3.7882445	0.8775545
H	3.0584361	-4.4846136	-2.1671718
H	-1.9977771	-1.3303349	-4.6107858
H	-1.0833689	-2.1575569	-3.1938799
H	-0.2629658	0.2833791	-6.2618746
H	0.8671074	2.3438243	-5.3909277

C	0.1674038	2.6618247	-4.0352757
C	1.3964185	2.0819571	-3.4566844
O	2.4140473	2.9613032	-3.4808913
C	1.9366320	4.1968782	-4.0602570
O	1.5251341	0.9416898	-2.9828218
C	-1.0866953	1.9040994	-4.0262865
H	2.5783410	4.4310230	-4.9379297
H	2.0853717	5.0010069	-3.3044431
Zn	-1.7375449	1.8519037	-2.1213873
Br	-2.9554679	3.4032477	-0.8340302
H	-0.9207711	0.8379293	-4.2751844
H	-1.8613525	2.3451035	-4.6810266
H	-0.1531164	4.6962814	-4.8393139
C	-0.2192030	-1.1624294	2.4074954
C	-0.7532218	-2.4573146	2.3947144
C	-0.2832479	-3.3873616	3.3970788
C	-0.5924366	-4.7810959	3.3700544
C	0.5672507	-2.9018271	4.4573876
C	1.0030679	-3.8040028	5.4744269
C	0.9916416	-1.5426763	4.4533056
H	1.6283537	-1.1854956	5.2764540
C	0.6638240	-0.6723375	3.4206198
C	-2.3143880	-3.1493518	-1.0573546
C	-3.4339254	-3.8916416	-0.6989363
H	-4.0636862	-4.3351469	-1.4859680
C	-3.8214706	-4.0540316	0.6628460
C	-5.0332697	-4.7255896	1.0076426
C	-3.0000590	-3.4972026	1.7120029
C	-3.4754475	-3.5805227	3.0553369
C	-1.7493501	-2.8643969	1.3617563
C	-1.4868839	-2.6567068	0.0026605
O	-0.6043919	-0.2570657	1.4265130
O	-0.3134422	-2.0307672	-0.3747607
P	-0.0263665	-0.4361213	-0.1004164
O	1.5032585	-0.3493195	-0.1436616
O	-0.8661750	0.4911410	-0.9611494
C	0.6555695	-5.1458991	5.4351400
C	-0.1337374	-5.6379880	4.3615975
H	1.6399879	-3.4134685	6.2837433
H	1.0049069	-5.8328786	6.2209617
H	-1.1926312	-5.1816562	2.5418308
H	-0.3799132	-6.7096611	4.3102981
C	-4.6709868	-4.2196220	3.3554260
C	-5.4504866	-4.8140772	2.3274269
H	-2.8864919	-3.1195462	3.8604585
H	-5.0189546	-4.2609630	4.3989078
H	-6.3913593	-5.3273467	2.5781222
H	-5.6423822	-5.1573258	0.1978265
C	2.5995487	0.9302162	3.1064920
C	1.2095170	0.7208948	3.3489332
C	3.0850893	2.2490895	3.0670115
C	0.3462139	1.8366798	3.5192401
C	0.8868002	3.1363888	3.4660239
C	2.2540658	3.3698884	3.2523229
H	4.1600053	2.4139660	2.8851493
C	-1.1448605	1.6799579	3.8105447
H	0.2071068	3.9894120	3.6066563
C	-2.0159753	2.3875987	2.7594013
H	-1.8574736	3.4862330	2.7630047
H	-3.0927069	2.2104005	2.9608814
H	-1.7995392	2.0218215	1.7379862
C	-1.4766384	2.1519544	5.2392090
H	-1.3889283	0.5994835	3.7675979
H	-1.2743643	3.2364779	5.3649921
H	-0.8735072	1.6077156	5.9945204
H	-2.5493836	1.9827116	5.4677910
C	2.8678636	4.7673815	3.2690111
C	1.8580576	5.8994676	3.0491571
H	2.3816420	6.8710942	2.9443314
H	1.1608946	5.9939298	3.9077951
H	1.2514840	5.7391089	2.1362359

7.2.2 Pathways starting from 14j-mi

7.2.2.1 to 15d-mi

TS1-8-d; COSMO



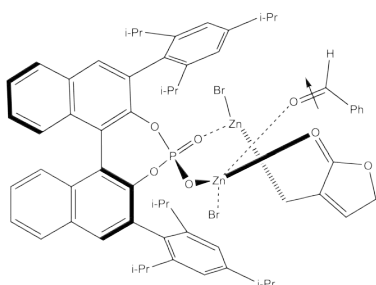
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Br	4.6941242	-0.8029248	-2.1814407
C	0.1935162	5.4582050	-0.6248182
C	0.9908539	4.3151769	-0.5290339
C	2.3988629	4.4443572	-0.4417406
C	2.9965166	5.7259572	-0.4299310
C	2.1933406	6.8689674	-0.5336591
C	0.7964540	6.7326407	-0.6345893
H	-0.9000339	5.3446639	-0.6926267
H	0.5409372	3.3101168	-0.5144967
C	3.2448262	3.2519254	-0.4307960
H	4.0919546	5.8153920	-0.3529236
H	2.6524364	7.8688142	-0.5323578
H	0.1654905	7.6314830	-0.7130087
O	2.7917713	2.1173045	-0.6107594
C	0.5055688	3.9396046	-4.3927203

C	3.6603625	4.9883717	4.5736913
H	3.5995363	4.8018154	2.4292533
H	4.1670497	5.9759622	4.5696610
H	4.4322158	4.2064010	4.7204427
H	2.9795573	4.9559184	5.4500851
C	3.5806033	-0.2270863	2.9142457
C	4.5231636	-0.0271560	1.7180861
H	5.1332408	-0.9361847	1.5444842
H	5.2274463	0.8170229	1.8721708
H	3.9579816	0.1712190	0.7907640
C	4.3975503	-0.4768786	4.1974599
H	2.9831564	-1.1376225	2.7050523
H	5.0724142	-1.3487261	4.0710221
H	3.7484047	-0.6715899	5.0739355
H	5.0253055	0.4063782	4.4404993
H	-1.3561533	-0.3877630	-6.5767516
H	0.4609750	-5.5163300	-4.1193890
H	-6.2769911	-1.2696518	-3.2265992
C	-0.7227841	-1.2804357	-6.3751988
H	2.2390644	-4.5029045	-1.6758284
H	0.9878287	-0.2940568	-7.3247679
H	-5.0126826	0.3637924	-1.6905051
C	-1.1608286	-1.8288043	-5.0226524
C	0.0884985	-5.5944612	-3.0763178
C	0.7453164	-0.8209476	-6.3792966
H	1.4425226	-1.6801584	-6.2946567
C	-0.3602946	-2.7288836	-4.2999556
C	-5.3065758	-1.5299853	-3.6966879
H	-2.0604949	-2.5949593	-7.5277438
C	-2.3988312	-1.4653227	-4.4667972
C	-0.9914499	-2.3027155	-7.4961088
H	-0.7163519	-1.8882230	-8.4884347
H	-3.0425488	-0.7708033	-5.0308608
C	1.6319774	-3.7573137	-2.2290989
H	0.7020014	-6.3582502	-2.5548330
H	-0.9569027	-5.9625598	-3.1196238
C	-0.7344519	-3.2179513	-3.0371462
C	-4.0508341	-0.0017411	-2.1043185
C	-2.8297284	-1.9285958	-3.2084823
H	-5.3874726	-2.5563596	-4.1086013
H	-5.1606784	-0.8351346	-4.5496517
C	0.1749619	-4.2367659	-2.3508381
C	-1.9687961	-2.7908848	-2.4676445
C	-4.1709170	-1.4283267	-2.6653138
H	1.6973396	-2.7980938	-1.6813424
H	-3.3069661	0.0381798	-1.2828728
H	2.1112432	-3.6167423	-3.2198992
H	0.9600441	-0.1397913	-5.5317795
H	-3.7621401	0.7122974	-2.9098028
H	-0.3950430	-3.2255328	-7.3359325
H	-0.2069165	-4.3988916	-1.3226889
H	-4.4533612	-2.0718464	-1.8107290
H	0.5997953	-3.0564401	-4.7274060
H	4.3454716	3.4045609	-0.2784511

C	0.1885055	5.4428636	-0.6044813
C	0.9861714	4.2995589	-0.5079991
C	2.3933668	4.4274637	-0.4177236
C	2.9908874	5.7084704	-0.4036269
C	2.1888827	6.8520148	-0.5086923
C	0.7921534	6.7163061	-0.6123710
H	-0.9048583	5.3246175	-0.6752190
H	0.5342856	3.2953796	-0.4952134
C	3.2380871	3.2314900	-0.4066696
H	4.0863179	5.7972756	-0.3227719
H	2.6485091	7.8517122	-0.5048129
H	0.1619151	7.6157771	-0.6905578
O	2.7887602	2.1009189	-0.6017697
C	0.4899854	3.9452331	-4.3720543
C	0.1628932	2.6609505	-4.0269368
C	1.3962043	2.0880068	-3.4453506
O	2.4044662	2.9820226	-3.4554101
C	1.9163517	4.2153939	-4.0254042
O	1.5349400	0.9474855	-2.9820598
C	-1.0802193	1.8906151	-4.0261309
H	2.5633337	4.4657162	-4.8956337
H	2.0495325	5.0135254	-3.2596679
Zn	-1.7396592	1.8572309	-2.1189397
Br	-2.9380151	3.4210850	-0.8492508
H	-0.9022001	0.8231244	-4.2589271
H	-1.8561934	2.3182139	-4.6878567
H	-0.1762371	4.6972851	-4.8147892
C	-0.2202299	-1.1568934	2.3963769
C	-0.7548114	-2.4518501	2.3916292
C	-0.2871098	-3.3756184	3.4007024
C	-0.5976041	-4.7689657	3.3826070
C	0.5618253	-2.8843055	4.4591936
C	0.9941499	-3.7800971	5.4826295
C	0.9876150	-1.5261549	4.4458521
H	1.6240072	-1.1628876	5.2665502
C	0.6627002	-0.6621407	3.4072408
C	-2.3091085	-3.1582355	-1.0599703
C	-3.4291907	-3.8990725	-0.7011973
H	-4.0585796	-4.3412278	-1.4893903
C	-3.8185139	-4.0589643	0.6601104
C	-5.0298585	-4.7299365	1.0055749
C	-2.9993922	-3.4981066	1.7087560
C	-3.4773664	-3.5771023	3.0511417
C	-1.7482596	-2.8660696	1.3589936
C	-1.4822173	-2.6646070	-0.0002105
O	-0.6039337	-0.2565149	1.4106093
O	-0.3079683	-2.0416106	-0.3776870
P	-0.0263684	-0.4440698	-0.1158978
O	1.5017238	-0.3492140	-0.1601981
O	-0.8715310	0.4703981	-0.9856820
C	0.6449600	-5.1211776	5.4522569
C	-0.1425814	-5.6191511	4.3809343
H	1.6305377	-3.3847462	6.2900038
H	0.9919122	-5.8030599	6.2434728
H	-1.1966818	-5.1735323	2.5556923
H	-0.3903584	-6.6906909	4.3363508
C	-4.6722449	-4.2164501	3.3511690
C	-5.4491982	-4.8147655	2.3243342
H	-2.8892977	-3.1129113	3.8548854
H	-5.0216709	-4.2547010	4.3942085
H	-6.3899898	-5.3281338	2.5748610
H	-5.6373376	-5.1646578	0.1961245
C	2.6035395	0.9342341	3.0949687
C	1.2119291	0.7294136	3.3311449
C	3.0934520	2.2515688	3.0618921
C	0.3512352	1.8474680	3.4987268
C	0.8964922	3.1452490	3.4512466
C	2.2657129	3.3744652	3.2477089
H	4.1705888	2.4122733	2.8885697
C	-1.1412802	1.6953679	3.7843444
H	0.2184947	3.9996073	3.5913092

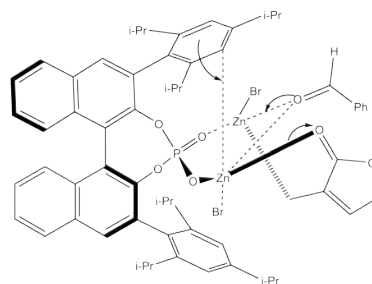
TS1-8-d



Energy(Hartree) = -11970.02600673
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Br	4.7196507	-0.7925964	-2.1919626

C	-2.0067989	2.4060144	2.7309770
H	-1.8454794	3.5042141	2.7334064
H	-3.0847461	2.2333373	2.9281339
H	-1.7910341	2.0386546	1.7101337
C	-1.4754877	2.1667804	5.2125346
H	-1.3882939	0.6157139	3.7398733
H	-1.2706833	3.2504378	5.3407563
H	-0.8760526	1.6205528	5.9690993
H	-2.5493222	2.0008940	5.4378361
C	2.8850819	4.7693409	3.2808576
C	1.8806780	5.9078726	3.0697068
H	2.4075083	6.8789767	2.9763375
H	1.1828367	5.9965659	3.9282167
H	1.2736935	5.7595219	2.1552105
C	3.6732602	4.9738301	4.5906589
H	3.6201857	4.8105160	2.4438521
H	4.1843434	5.9591356	4.6002957
H	4.4401852	4.1865954	4.7335279
H	2.9886277	4.9341040	5.4634239
C	3.5820331	-0.2258714	2.9057277
C	4.5256421	-0.0321119	1.7096646
H	5.1381846	-0.9401350	1.5411329
H	5.2289861	0.8139925	1.8584076
H	3.9626097	0.1570102	0.7794005
C	4.3976068	-0.4739891	4.1900191
H	2.9826076	-1.1354020	2.6982592
H	5.0695513	-1.3484265	4.0670911
H	3.7479949	-0.6631575	5.0672339
H	5.0283869	0.4074904	4.4313308
H	-1.3646593	-0.3843845	-6.5762203
H	0.4623563	-5.5143656	-4.1341507
H	-6.2824875	-1.3221301	-3.2060735
C	-0.7310624	-1.2777187	-6.3773944
H	2.2462136	-4.5063919	-1.6913389
H	0.9764675	-0.2938968	-7.3359401
H	-5.0321091	0.3825734	-1.7433456
C	-1.1640496	-1.8260373	-5.0231710
C	0.0924991	-5.5953002	-3.0904825
C	0.7368750	-0.8182051	-6.3883182
H	1.4351706	-1.6764306	-6.3044317
C	-0.3614566	-2.7272576	-4.3045020
C	-5.3125204	-1.5912612	-3.6722730
H	-2.0740032	-2.5929238	-7.5226793
C	-2.3992345	-1.4626942	-4.4620610
C	-1.0051495	-2.3001454	-7.4966588
H	-0.7344717	-1.8873316	-8.4908667
H	-3.0445411	-0.7660820	-5.0221288
C	1.6367508	-3.7596745	-2.2400019
H	0.7076140	-6.3605503	-2.5732537
H	-0.9526280	-5.9637151	-3.1333811
C	-0.7320122	-3.2203184	-3.0425607
C	-4.0669915	0.0159561	-2.1482787
C	-2.8266649	-1.9292186	-3.2040197
H	-5.3838861	-2.6353601	-4.0386651
H	-5.1827641	-0.9345117	-4.5574096
C	0.1800017	-4.2399102	-2.3610352
C	-1.9654633	-2.7958988	-2.4694797
C	-4.1676085	-1.4309851	-2.6584798
H	1.7036567	-2.8039861	-1.6865824
H	-3.3252486	0.0907777	-1.3270667
H	2.1159087	-3.6137278	-3.2299783
H	0.9557502	-0.1350260	-5.5436891
H	-3.7869490	0.7088491	-2.9741512
H	-0.4091059	-3.2233150	-7.3384201
H	-0.2002891	-4.4052569	-1.3327802
H	-4.4277690	-2.0489535	-1.7783348
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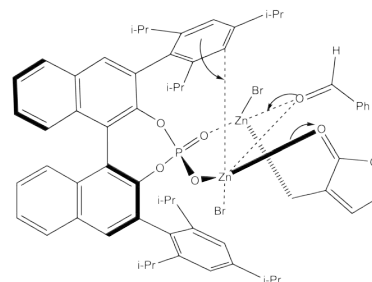
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Br	4.6791105	0.3025645	1.7168258
C	1.7550944	6.7969876	1.7568540
C	1.6793626	5.4057917	1.6358826
C	2.8698241	4.6418650	1.5622856
C	4.1303148	5.2940853	1.6399083
C	4.1966696	6.6826513	1.7688026
C	3.0068244	7.4363671	1.8205340
H	0.8274941	7.3866065	1.8093224
H	0.6955984	4.9111087	1.6103365
C	2.8872503	3.2005408	1.4195908
H	5.0531306	4.6940365	1.5930576
H	5.1730286	7.1860379	1.8295632
H	3.0583432	8.5317615	1.9190951
O	1.8769293	2.4322772	1.3908910
C	3.5513791	3.8416201	-1.5313586
C	2.4221780	3.0702130	-1.5685790
C	2.8961489	1.6503577	-1.5056075
O	4.2617591	1.6239565	-1.5965557
C	4.7621747	2.9659655	-1.6089567
O	2.2415242	0.6350855	-1.3421707
C	1.0029009	3.3920203	-1.5867351
H	5.3460007	3.1270300	-2.5441443
H	5.4703692	3.0809764	-0.7568750
Zn	-0.0484595	2.8569843	0.0623712
Br	-1.6385543	3.9327776	1.4571578
H	0.4671788	2.7310122	-2.3024670
H	0.8068848	4.4559196	-1.8185409
H	3.5996994	4.9392759	-1.5287239
C	-1.6440374	-2.2876310	1.5699131
C	-2.1854336	-3.2011464	0.6624643
C	-2.2076575	-4.5939298	1.0462058
C	-2.5857817	-5.6405095	0.1526747
C	-1.7972449	-4.9561027	2.3840475
C	-1.8650856	-6.3235470	2.7878161
C	-1.2542736	-3.9647942	3.2548226
H	-0.8925585	-4.2740243	4.2476824
C	-1.1032833	-2.6454788	2.8487362
C	-2.1680274	-1.4318126	-2.7568403
C	-3.3866916	-1.8468857	-3.2819149
H	-3.6646796	-1.5386126	-4.3014402
C	-4.3151514	-2.6100288	-2.5185018
C	-5.6016000	-2.9410237	-3.0420116
C	-3.9727070	-3.0152823	-1.1757670
C	-4.9737456	-3.6693943	-0.3951984
C	-2.6569176	-2.7099605	-0.6648974
C	-1.8253766	-1.8944443	-1.4484005
O	-1.6255497	-0.9435453	1.2263330
O	-0.5644430	-1.5382525	-0.9823610
P	-0.4214472	-0.4342437	0.2209201
O	0.9508726	-0.7415416	0.8447884
O	-0.7833793	0.9894344	-0.1596703
C	-2.2767458	-7.3104619	1.9043153
C	-2.6203777	-6.9643607	0.5706292
H	-1.5621364	-6.5829721	3.8145085
H	-2.3176637	-8.3617911	2.2275554

TS2-8-d; COSMO

H	-2.8464043	-5.3901790	-0.8847396
H	-2.9119855	-7.7518551	-0.1410150
C	-6.2234243	-3.9584295	-0.9264565
C	-6.5377207	-3.6089531	-2.2670857
H	-4.7511864	-3.9356563	0.6472543
H	-6.9787749	-4.4568383	-0.2997748
H	-7.5286360	-3.8512669	-2.6804667
H	-5.8423196	-2.6361744	-4.0726434
C	1.1410725	-1.7695108	3.5868653
C	-0.2735050	-1.6111318	3.5420908
C	1.9354628	-0.6502904	3.9391918
C	-0.8636860	-0.3780839	3.9401512
C	-0.0367340	0.7085774	4.2755944
C	1.3666919	0.6075972	4.2728907
H	3.0256740	-0.7811013	4.0367611
C	-2.3765277	-0.2435114	4.0777344
H	-0.5087316	1.6610942	4.5515995
C	-2.9416648	1.0458760	3.4681529
H	-2.6135035	1.9507829	4.0195964
H	-4.0501645	1.0285787	3.5002970
H	-2.6252184	1.1693241	2.4153506
C	-2.7630004	-0.3882080	5.5643012
H	-2.8366899	-1.0979683	3.5409767
H	-2.3257548	0.4335291	6.1695613
H	-2.4021904	-1.3481574	5.9867571
H	-3.8653145	-0.3500440	5.6850633
C	2.2689902	1.7557799	4.7202301
C	1.5837946	3.1278951	4.6898143
C	2.3284199	3.9344222	4.8431991
H	0.8295867	3.2207142	5.4985760
H	1.0654133	3.3136086	3.7287121
C	2.8503858	1.4626639	6.1185395
H	3.1321218	1.7764899	4.0143391
H	3.5477070	2.2681617	6.4272815
H	3.4051775	0.5036102	6.1404000
H	2.0379597	1.4034786	6.8726096
C	1.8285924	-3.0987046	3.2840984
C	2.9754794	-2.9985111	2.2675001
H	3.3794030	-4.0094713	2.0555263
H	3.8187624	-2.3779721	2.6321407
H	2.6203737	-2.5691833	1.3094110
C	2.2989626	-3.7496249	4.6002603
H	1.0701945	-3.7695960	2.8373042
H	2.7386523	-4.7494102	4.4051477
H	1.4612290	-3.8746258	5.3165091
H	3.0743353	-3.1301435	5.0981428
H	0.8179852	3.1931994	-5.7780877
H	1.2385988	-2.6920567	-5.8076428
H	-4.9601095	1.9882875	-4.0331183
C	1.3084619	2.1947073	-5.7859000
H	2.1348359	-3.4785173	-2.8107031
H	3.3231644	3.0591819	-5.8162255
H	-3.8192537	3.0311924	-2.0202437
C	0.4327683	1.2660542	-4.9527132
C	0.5223204	-3.1492727	-5.0929501
C	2.7184320	2.3663123	-5.1949407
H	3.2620116	1.3997426	-5.1480925
C	0.8240347	-0.0564093	-4.6821965
C	-3.9747477	1.6366659	-4.4034670
H	0.3579987	1.6290420	-7.6885642
C	-0.8116316	1.6923290	-4.4604865
C	1.3723305	1.7196544	-7.2500129
H	1.9566039	2.4286320	-7.8729898
H	-1.1266154	2.7309189	-4.6549370
C	1.8593988	-2.4291826	-3.0447091
H	0.8321788	-4.2032906	-4.9341363
H	-0.4766852	-3.1535681	-5.5752322
C	0.0088317	-0.9484365	-3.9652840
C	-2.8348138	2.6767225	-2.3884876
C	-1.6677082	0.8434540	-3.7307069
H	-4.1397659	0.7108729	-4.9913059

H	-3.5817676	2.4064065	-5.1005378
C	0.4965235	-2.3807089	-3.7581111
C	-1.2589063	-0.5007722	-3.4978756
C	-3.0022539	1.4012408	-3.2318826
H	1.8402100	-1.8470878	-2.1038011
H	-2.2024963	2.4814351	-1.5028103
H	2.6668340	-2.0092201	-3.6805801
H	2.6756285	2.7769663	-4.1674865
H	-2.3789612	3.5071352	-2.9667995
H	1.8600497	0.7249491	-7.3239552
H	-0.2345462	-2.8988576	-3.1060652
H	-3.4582431	0.6400361	-2.5676949
H	1.7991746	-0.4138313	-5.0491144
H	3.8938523	2.7203962	1.4004034

TS2-8-d

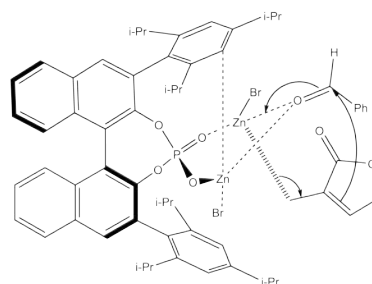


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C	1.7061467	6.7915856	1.7976355
C	1.6436366	5.4010532	1.6588849
C	2.8412030	4.6500095	1.5833649
C	4.0941530	5.3128753	1.6784153
C	4.1471370	6.7002353	1.8248412
C	2.9502184	7.4421938	1.8777865
H	0.7710072	7.3691410	1.8509414
H	0.6633927	4.8985412	1.6203824
C	2.8718729	3.2080448	1.4240003
H	5.0219186	4.7202454	1.6314532
H	5.1183382	7.2119132	1.8994261
H	2.9911392	8.5367486	1.9905208
O	1.8698327	2.4345914	1.3794804
C	3.5281917	3.8864547	-1.5227034
C	2.4081505	3.1014204	-1.5615398
C	2.9021928	1.6872444	-1.4947446
O	4.2667688	1.6780192	-1.5895311
C	4.7493614	3.0236299	-1.6011769
O	2.2607652	0.6658048	-1.3200216
C	0.9867575	3.4061992	-1.5855940
H	5.3309932	3.1914330	-2.5371838
H	5.4569315	3.1448919	-0.7487731
Zn	-0.0902900	2.8613327	0.0477741
Br	-1.6511207	3.9172726	1.4676257
H	0.4620269	2.7375823	-2.3029131
H	0.7789323	4.4671541	-1.8202217
H	3.5611035	4.9846861	-1.5189472
C	-1.6344889	-2.2897991	1.5655849
C	-2.1907145	-3.2004822	0.6638641
C	-2.2244634	-4.5915455	1.0530019
C	-2.6178769	-5.6370092	0.1650672
C	-1.8103714	-4.9539227	2.3895261
C	-1.8894358	-6.3192393	2.7967559
C	-1.2553029	-3.9648079	3.2547158
H	-0.8905209	-4.2733317	4.2466979

C	-1.0938593	-2.6486309	2.8437595	H	-3.8292212	3.0120164	-2.0524947
C	-2.1746486	-1.4388287	-2.7591865	C	0.4366070	1.2420425	-4.9635335
C	-3.4008624	-1.8421662	-3.2759055	C	0.5107657	-3.1693820	-5.0703562
H	-3.6813203	-1.5292493	-4.2935055	C	2.6977397	2.3958703	-5.1569437
C	-4.3319151	-2.5964629	-2.5074383	H	3.2642278	1.4473132	-5.0502967
C	-5.6237036	-2.9166852	-3.0231905	C	0.8307998	-0.0746359	-4.6708920
C	-3.9862003	-3.0038764	-1.1662760	C	-3.9484625	1.6871303	-4.4687742
C	-4.9887582	-3.6485598	-0.3804293	H	0.4639365	1.4974149	-7.7138834
C	-2.6651709	-2.7100994	-0.6628288	C	-0.8146693	1.6681172	-4.4908860
C	-1.8299931	-1.9047382	-1.4524769	C	1.4563599	1.6361391	-7.2398240
O	-1.6001313	-0.9471253	1.2211336	H	2.0441945	2.3391351	-7.8661346
O	-0.5637778	-1.5621671	-0.9921628	H	-1.1333866	2.7021543	-4.7032360
P	-0.4031011	-0.4518217	0.2020553	C	1.8672444	-2.4424253	-3.0369707
O	0.9764364	-0.7657830	0.8085304	H	0.8210168	-4.2228736	-4.9093222
O	-0.7539858	0.9719059	-0.1849834	H	-0.4925950	-3.1745645	-5.5430325
C	-2.3157059	-7.3044134	1.9191390	C	0.0115779	-0.9622817	-3.9540607
C	-2.6634957	-6.9587430	0.5870505	C	-2.8426609	2.6283879	-2.3835154
H	-1.5832172	-6.5785832	3.8225105	C	-1.6754279	0.8248649	-3.7600456
H	-2.3649829	-8.3542484	2.2458895	H	-4.1058683	0.7881254	-5.0991414
H	-2.8819070	-5.3859287	-0.8711911	H	-3.5302903	2.4800367	-5.1237073
H	-2.9671168	-7.7451110	-0.1207242	C	0.4989787	-2.3936708	-3.7393446
C	-6.2430399	-3.9274257	-0.9050619	C	-1.2628636	-0.5141323	-3.5040259
C	-6.5612098	-3.5760800	-2.2436445	C	-3.0140940	1.3902309	-3.2807475
H	-4.7620651	-3.9157820	0.6607647	H	1.8601660	-1.8526350	-2.1006836
H	-6.9991526	-4.4191385	-0.2741246	H	-2.2665223	2.3759677	-1.4741236
H	-7.5561788	-3.8099901	-2.6519499	H	2.6734301	-2.0345251	-3.6819669
H	-5.8671536	-2.6098973	-4.0525873	H	2.5993224	2.8421305	-4.1485746
C	1.1560695	-1.7718477	3.5634990	H	-2.3232135	3.4578776	-2.9069856
C	-0.2594129	-1.6155832	3.5336860	H	1.9756532	0.6552347	-7.2584734
C	1.9510947	-0.6560642	3.9193898	H	-0.2277844	-2.9069751	-3.0792390
C	-0.8477404	-0.3872369	3.9458295	H	-3.5057351	0.6163063	-2.6586526
C	-0.0183925	0.6972224	4.2837517	H	1.8108339	-0.4329099	-5.0236524
C	1.3843202	0.5977487	4.2677030	H	3.8833906	2.7363536	1.4031792
H	3.0430699	-0.7835468	3.9965233				
C	-2.3598832	-0.2493892	4.0913840				
H	-0.4903682	1.6476103	4.5675491				
C	-2.9319668	1.0133086	3.4328182				
H	-2.5843941	1.9418691	3.9298497				
H	-4.0394386	1.0065770	3.4919668				
H	-2.6422756	1.0841696	2.3681711				
C	-2.7352836	-0.3292244	5.5853786				
H	-2.8220834	-1.1270603	3.5945180				
H	-2.2993204	0.5209089	6.1508581				
H	-2.3664463	-1.2666942	6.0491829				
H	-3.8367650	-0.2905475	5.7128369				
C	2.2916901	1.7471804	4.7013941				
C	1.5960543	3.1138465	4.7108771				
H	2.3356679	3.9236267	4.8722660				
H	0.8523272	3.1832614	5.5315735				
H	1.0622684	3.3170662	3.7616525				
C	2.9251398	1.4428138	6.0741793				
H	3.1303888	1.7823920	3.9671758				
H	3.6278790	2.2491736	6.3682748				
H	3.4873946	0.4881223	6.0651773				
H	2.1417757	1.3678834	6.8570235				
C	1.8406058	-3.0997917	3.2466827				
C	2.9953456	-2.9937505	2.2396304				
H	3.4068399	-4.0023421	2.0310521				
H	3.8335276	-2.3688906	2.6086700				
H	2.6463315	-2.5684057	1.2778812				
C	2.3000365	-3.7679788	4.5581528				
H	1.0816834	-3.7620053	2.7873778				
H	2.7339478	-4.7689958	4.3563443				
H	1.4590245	-3.8932313	5.2704284				
H	3.0771032	-3.1589570	5.0660485				
H	0.8025605	3.1463948	-5.8483855				
H	1.2200185	-2.7168253	-5.7947843				
H	-4.9401562	2.0347539	-4.1122675				
C	1.3191536	2.1622271	-5.7989327				
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TS3-8-d; COSMO



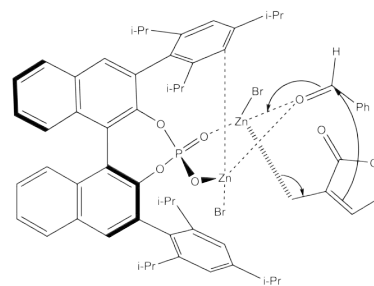
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Br	4.8078551	0.7990579	1.1706692
C	1.8693754	7.0472218	-0.1497168
C	1.7679950	5.6527710	-0.0616437
C	2.9350493	4.8551084	-0.0686317
C	4.2038425	5.4882023	-0.1472595
C	4.2988500	6.8800213	-0.2239703
C	3.1287503	7.6649153	-0.2317990
H	0.9518696	7.6550921	-0.1435613
H	0.7734680	5.1917108	0.0329271
C	2.9219106	3.3958898	0.0211081
H	5.1167925	4.8709591	-0.1427508
H	5.2873115	7.3611109	-0.2752667
H	3.2029270	8.7614653	-0.2949070
O	1.8904305	2.6968933	0.4071756
C	3.3119849	3.0320469	-2.3128674
C	2.0924707	2.3829766	-2.4797465
C	2.3841204	0.9084194	-2.3582735
O	3.7407103	0.7320618	-2.3240324
C	4.4078627	2.0027757	-2.3866428
O	1.6016698	-0.0150078	-2.2961806
C	0.7573770	2.8534296	-2.5706855

H	4.9703522	2.0652834	-3.3459239
H	5.1454723	2.0387776	-1.5560046
Zn	-0.0190904	2.7553617	-0.6200250
Br	-1.6014316	4.2500425	0.2942739
H	0.0448996	2.1188849	-2.9938724
H	0.6108507	3.8973164	-2.8975981
H	3.4971338	4.0934430	-2.5194979
C	-1.3243989	-1.7243637	2.2424583
C	-1.9208293	-2.8657245	1.7041210
C	-1.8738234	-4.0779695	2.4886804
C	-2.2919457	-5.3449883	1.9827697
C	-1.3550689	-4.0191841	3.8364771
C	-1.3539323	-5.2024890	4.6348188
C	-0.7847123	-2.8069286	4.3274502
H	-0.3540090	-2.7964222	5.3406054
C	-0.6977058	-1.6741833	3.5293453
C	-2.3654459	-2.1713496	-2.0580189
C	-3.6215718	-2.7228488	-2.2820164
H	-4.0284107	-2.7278721	-3.3047062
C	-4.4241146	-3.2291012	-1.2214738
C	-5.7513541	-3.6972557	-1.4614670
C	-3.9073066	-3.2240960	0.1257834
C	-4.7847074	-3.6171997	1.1819303
C	-2.5494989	-2.7856507	0.3551325
C	-1.8473748	-2.2312169	-0.7266987
O	-1.3529707	-0.5471963	1.5132754
O	-0.5464466	-1.7609071	-0.5465144
P	-0.2873034	-0.3642319	0.2659583
O	1.1686340	-0.4544696	0.7614985
O	-0.7491840	0.9028118	-0.4384386
C	-1.8028627	-6.4106645	4.1222608
C	-2.2571325	-6.4823305	2.7786176
H	-0.9680788	-5.1406690	5.6646026
H	-1.7893994	-7.3167174	4.7469850
H	-2.6395311	-5.4166862	0.9430025
H	-2.5801715	-7.4482950	2.3613828
C	-6.0782500	-4.0472344	0.9186483
C	-6.5634781	-4.1073855	-0.4151088
H	-4.4320482	-3.5647243	2.2209042
H	-6.7350379	-4.3369283	1.7531416
H	-7.5876500	-4.4589777	-0.6124112
H	-6.1242341	-3.7069220	-2.4977564
C	1.5497103	-0.5769651	3.8080768
C	0.1320202	-0.4629370	3.8126599
C	2.3235197	0.6129140	3.7519820
C	-0.4803561	0.8228133	3.8592673
C	0.3223872	1.9756262	3.7952695
C	1.7267863	1.9060499	3.7342336
H	3.4199307	0.5378366	3.8376930
C	-1.9859440	0.9675348	4.0492637
H	-0.1673557	2.9586246	3.8008327
C	-2.6330802	1.9872879	3.1029329
H	-2.3019145	3.0251697	3.3111140
H	-3.7357233	1.9672206	3.2193346
H	-2.3918114	1.7692122	2.0456113
C	-2.2764080	1.2975353	5.5283886
H	-2.4441488	-0.0210580	3.8435033
H	-1.8370598	2.2771893	5.8110739
H	-1.8549339	0.5287083	6.2076131
H	-3.3702742	1.3522408	5.7047521
C	2.6110479	3.1504306	3.7691681
C	1.8794140	4.4354895	3.3650079
H	2.6030665	5.2623311	3.2231086
H	1.1612220	4.7563583	4.1477882
H	1.3167418	4.3089512	2.4202924
C	3.2606991	3.2962149	5.1607965
H	3.4399007	2.9751533	3.0442395
H	3.9425707	4.1706207	5.1795333
H	3.8487917	2.3988018	5.4381219
H	2.4839089	3.4494364	5.9387925
C	2.2626429	-1.9230937	3.8960498

C	3.3327088	-2.1442867	2.8178717
H	3.7432892	-3.1708679	2.9037557
H	4.1837870	-1.4401169	2.9084945
H	2.9035649	-2.0347949	1.8018391
C	2.8413357	-2.1075606	5.3133546
H	1.4989335	-2.7097067	3.7471792
H	3.3002766	-3.1121891	5.4159925
H	2.0580264	-2.0044651	6.0919736
H	3.6279214	-1.3536818	5.5274242
H	0.0318578	1.2849972	-6.7140464
H	0.4879736	-4.3712903	-5.1370987
H	-5.3690492	0.7759557	-3.7765986
C	0.6228959	0.3966865	-6.3986140
H	1.8364857	-4.3576430	-2.2094122
H	2.5541151	1.3908890	-6.7315141
H	-3.9788686	2.3733028	-2.3923609
C	-0.1556902	-0.2759111	-5.2737232
C	-0.1096405	-4.5828053	-4.2254866
C	1.9918305	0.9044114	-5.9072314
H	2.6127236	0.0713567	-5.5161106
C	0.2586485	-1.5067843	-4.7377729
C	-4.4410135	0.3130238	-4.1719453
H	-0.2113802	-0.8735464	-7.9887209
C	-1.3001536	0.3263158	-4.7251926
C	0.7745232	-0.5184451	-7.6262533
H	1.2759446	0.0178267	-8.4584723
H	-1.6362859	1.2919878	-5.1379372
C	1.5315059	-3.3970984	-2.6746239
H	0.2173483	-5.5671711	-3.8300120
H	-1.1716306	-4.6713398	-4.5337906
C	-0.4294140	-2.1347783	-3.6868183
C	-3.0491639	1.9178743	-2.7903778
C	-2.0316955	-0.2609369	-3.6740859
H	-4.6611638	-0.7474116	-4.4091798
H	-4.1889128	0.8207781	-5.1267387
C	0.0762496	-3.4787673	-3.1679056
C	-1.5913992	-1.5116271	-3.1568556
C	-3.2876934	0.4444242	-3.1580392
H	1.6524047	-2.5821870	-1.9362115
H	-2.2781763	2.0096831	-2.0042438
H	2.2332039	-3.1949074	-3.5108444
H	1.8727992	1.6441254	-5.0912724
H	-2.7344230	2.5251189	-3.6645491
H	1.3884507	-1.4130055	-7.3915802
H	-0.5489995	-3.7617791	-2.2968564
H	-3.6006666	-0.0684504	-2.2261021
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H	3.9106888	2.9119641	0.1436322

TS3-8-d

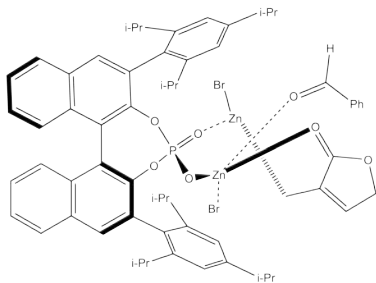


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number of imaginary frequencies: 1

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Br	4.8172766	0.8215198	1.2060154
C	1.8884399	7.0476574	-0.1792853
C	1.7822955	5.6545488	-0.0769200
C	2.9470426	4.8538862	-0.0753871
C	4.2171858	5.4834109	-0.1586883
C	4.3163809	6.8737479	-0.2499774

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H	5.1277439	4.8626055	-0.1445905	C	2.5947605	3.1568547	3.7675717
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C	3.3204264	3.0084166	-2.3074732	H	1.2937643	4.3053809	2.4146564
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C	2.3645862	0.8966650	-2.3535846	H	3.4236495	2.9798163	3.0430872
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C	0.7617840	2.8590247	-2.5603932	C	2.2649967	-1.9178140	3.9024473
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H	5.1320318	1.9861916	-1.5344293	H	3.7487198	-3.1608673	2.9076772
Zn	-0.0216838	2.7619781	-0.6112938	H	4.1847357	-1.4295689	2.9112802
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O	-1.3463311	-0.5507309	1.5167674	H	1.2662410	0.0297631	-8.4598317
O	-0.5424773	-1.7588827	-0.5460830	H	-1.6382431	1.3005622	-5.1310242
P	-0.2829353	-0.3634756	0.2677103	C	1.5323912	-3.3985034	-2.6848946
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C	-1.7989384	-6.4160536	4.1184669	C	-0.4294079	-2.1286740	-3.6881342
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H	-6.1189984	-3.7052366	-2.4963206	H	1.8706521	1.6520738	-5.0906868
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int1-8-d; COSMO



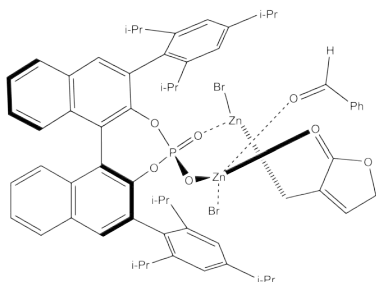
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C	3.1088313	6.0438261	0.2294861
C	2.6839708	7.3631213	0.0351872
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H	-0.6596483	6.7772516	-0.5702006
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H	4.1645972	5.8206472	0.4512315
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C	0.0992726	2.1149927	-3.9639210
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H	1.3984522	4.7857504	-4.6771934
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O	-1.0716587	-0.1164029	1.3284826
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H	0.3866519	-5.5415432	-3.9350867
H	-5.4707110	-0.3384512	-4.8083364
C	0.7203134	-1.1196714	-6.1991784
H	1.6144997	-4.8431303	-1.0386549
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C	-0.1772184	-1.5950324	-5.0635991
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C	0.2208731	-2.6259791	-4.1950811
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C	-1.4458190	-1.0271834	-4.8627630
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H	-1.7802566	-0.2342802	-5.5518577
C	1.3481076	-4.0236045	-1.7374647
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H	-4.5769208	-1.8079006	-5.3251093

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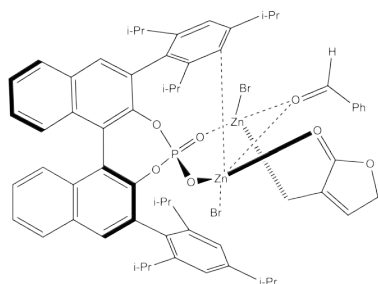
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H	3.3956897	8.1701968	0.1230962
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H	3.0972402	5.1361540	-2.5749525
Zn	-1.0134165	2.1656848	-2.2866669
Br	-2.3470979	3.8348990	-1.3143318
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H	-0.4349812	2.5008925	-4.8191852
H	1.3775481	4.7713541	-4.6623456
C	-1.1217432	-1.0897698	2.3040667
C	-1.9510620	-2.2050279	2.1259222
C	-2.0065123	-3.1824294	3.1919200
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C	-1.3504133	-2.8891500	4.4437091
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H	-0.6638806	3.9338832	2.4661717
H	-2.3498040	3.3404971	2.4332062
H	-1.1034106	2.5132141	1.4625594
C	-1.3173801	2.7542957	4.9648972
H	-1.6714808	1.2076000	3.5217818
H	-0.6876566	3.6534798	5.1307142
H	-1.1419479	2.0618168	5.8132012
H	-2.3778797	3.0791953	4.9985877
C	4.0224603	3.0436789	3.7308699
C	3.6237729	4.5238733	3.7472439
H	4.5258587	5.1689721	3.7423075
H	3.0449942	4.7748369	4.6608341
H	3.0016603	4.8101253	2.8766136
C	4.8817706	2.7187241	4.9696761
H	4.6598383	2.8610341	2.8333120
H	5.7732023	3.3779259	5.0167625
H	5.2374257	1.6700159	4.9631568
H	4.2946479	2.8684244	5.8999547
C	2.4667108	-1.7455435	3.3487354
C	3.4497165	-2.0710866	2.2127389
H	3.6547789	-3.1612469	2.1897906
H	4.4222470	-1.5509852	2.3261194
H	3.0283082	-1.7857676	1.2306317
C	3.0213821	-2.2285832	4.7033490
H	1.5422619	-2.3206619	3.1428022
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H	2.3054601	-2.0480408	5.5301727
H	3.9622836	-1.6969245	4.9578268
H	0.2820880	-0.1530577	-6.5689540
H	0.3705533	-5.5440330	-3.9567640
H	-5.4789311	-0.3265719	-4.7924070
C	0.7011324	-1.1232501	-6.2200964
H	1.6153459	-4.8511208	-1.0636117
H	2.7373026	-0.3979747	-6.5844573
H	-4.4707677	1.2458218	-3.0436635
C	-0.1893608	-1.5959294	-5.0777963

C	-0.2592286	-5.5330538	-3.0423839
C	2.1496932	-0.8672066	-5.7689272
H	2.6649438	-1.8115107	-5.4962064
C	0.2115219	-2.6273047	-4.2117005
C	-4.4680776	-0.7525539	-4.9580993
H	-0.3898245	-2.2512214	-7.7628429
C	-1.4557728	-1.0263605	-4.8699652
C	0.6491945	-2.1063141	-7.4046984
H	1.2612292	-1.7405289	-8.2553978
H	-1.7921758	-0.2323579	-5.5568731
C	1.3475405	-4.0308334	-1.7607743
H	0.0408447	-6.3974209	-2.4142525
H	-1.3109710	-5.6855639	-3.3590580
C	-0.5764982	-3.0410326	-3.1253732
C	-3.4915324	0.7347222	-3.1420423
C	-2.2945247	-1.4082141	-3.8052911
H	-4.5877190	-1.7934801	-5.3213047
H	-3.9957146	-0.1669903	-5.7739819
C	-0.0933548	-4.2101538	-2.2686624
C	-1.8265882	-2.3989601	-2.8925703
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H	1.4653647	-3.0710007	-1.2218539
H	-3.0287697	0.7370032	-2.1344573
H	2.0841988	-4.0559431	-2.5907639
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H	1.0422078	-3.1012215	-7.1074580
H	-0.7513093	-4.2752183	-1.3789534
H	-4.2301432	-1.2425486	-2.8896998
H	1.1811866	-3.1215432	-4.3771531
H	3.7099269	3.4277250	0.5513519

H	5.2166420	1.9289113	-1.6948602
Zn	-0.0680335	2.7873197	-0.7002654
Br	-1.5948359	4.2053046	0.4375859
H	0.1590009	2.2087829	-3.0543783
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C	-1.9532151	-2.8445034	1.7119517
C	-1.9090863	-4.0690749	2.4771726
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C	-1.3687512	-4.0378178	3.8173951
C	-1.3688292	-5.2333714	4.5972372
C	-0.7767066	-2.8400471	4.3176945
H	-0.3287708	-2.8507672	5.3233338
C	-0.6925316	-1.6949007	3.5373734
C	-2.3930803	-2.1146742	-2.0422079
C	-3.6571592	-2.6464388	-2.2696366
H	-4.0633417	-2.6417205	-3.2925548
C	-4.4672761	-3.1481280	-1.2123433
C	-5.8008862	-3.5962051	-1.4552401
C	-3.9500854	-3.1625124	0.1347755
C	-4.8307455	-3.5562148	1.1878696
C	-2.5877423	-2.7420056	0.3671514
C	-1.8786380	-2.1872556	-0.7098498
O	-1.3714124	-0.5271632	1.5508692
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P	-0.3180288	-0.3305454	0.2908671
O	1.1379701	-0.4302188	0.7847813
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C	-1.8399248	-6.4281641	4.0733713
C	-2.3156467	-6.4734460	2.7359959
H	-0.9662544	-5.1919395	5.6216464
H	-1.8274582	-7.3439758	4.6837353
H	-2.7131095	-5.3754480	0.9230676
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C	-6.1300920	-3.9666271	0.9217566
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H	-4.4752588	-3.5196540	2.2266912
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C	1.5646222	-0.6105652	3.8032565
C	0.1474655	-0.4938267	3.8338761
C	2.3411127	0.5793169	3.7632409
C	-0.4607691	0.7907767	3.9266113
C	0.3433124	1.9440146	3.8802733
C	1.7452476	1.8737726	3.7923076
H	3.4384535	0.5007563	3.8390664
C	-1.9621158	0.9305845	4.1486046
H	-0.1449944	2.9268756	3.9204769
C	-2.6267355	1.9756432	3.2433682
H	-2.2949085	3.0078612	3.4774492
H	-3.7272845	1.9482784	3.3770537
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C	-2.2236243	1.2184023	5.6419191
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H	-1.7784650	2.1897024	5.9437886
H	-1.7899274	0.4304925	6.2909345
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H	2.6224216	5.2402425	3.3477643
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C	3.3027412	3.2291784	5.2272834
H	3.4508639	2.9534139	3.1027786
H	3.9877210	4.1009068	5.2552722
H	3.8915917	2.3240239	5.4761354
H	2.5377558	3.3674868	6.0195177
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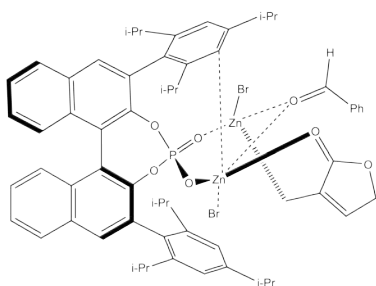


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Br	4.7966370	0.7866971	1.1084397
C	1.7581194	7.0215740	-0.3803883
C	1.6961901	5.6531292	-0.0944908
C	2.8861857	4.8862069	-0.0602605
C	4.1360743	5.5233185	-0.2901904
C	4.1901568	6.8908102	-0.5654210
C	2.9978614	7.6411252	-0.6181035
H	0.8287141	7.6100481	-0.4093433
H	0.7225997	5.1848199	0.1184330
C	2.9151346	3.4636721	0.2190899
H	5.0610849	4.9258557	-0.2539186
H	5.1595036	7.3806336	-0.7413654
H	3.0396484	8.7188475	-0.8393738
O	1.9120334	2.7403716	0.5320342
C	3.4417488	2.9313273	-2.5374590
C	2.1994640	2.3520152	-2.4991146
C	2.4299456	0.8753199	-2.3430546
O	3.7779595	0.6261273	-2.4085813
C	4.4918696	1.8614070	-2.5376330
O	1.6140825	-0.0084293	-2.1817059
C	0.8536031	2.8895829	-2.5180111
H	5.0777231	1.8424941	-3.4850781

H	3.7549329	-3.1836247	2.8306430	H	0.7598344	5.1961203	0.0845610
H	4.2019924	-1.4562030	2.8895663	C	2.9368815	3.4495431	0.1951777
H	2.9261458	-2.0145664	1.7574474	H	5.0985591	4.8976121	-0.2451211
C	2.8419134	-2.1920536	5.2645788	H	5.2260983	7.3558343	-0.7118822
H	1.5054345	-2.7391403	3.6719409	H	3.1203585	8.7151312	-0.8218546
H	3.2960879	-3.2013265	5.3387985	O	1.9271645	2.7396702	0.5186179
H	2.0550473	-2.1093466	6.0419379	C	3.4372076	2.8997850	-2.5017526
H	3.6300886	-1.4479747	5.5053992	C	2.1862373	2.3338454	-2.4852979
H	0.0757557	1.2824649	-6.7052635	C	2.3992307	0.8521962	-2.3332648
H	0.4693535	-4.3555226	-5.0764276	O	3.7442117	0.5889455	-2.3810073
H	-5.3527600	0.8555682	-3.7963634	C	4.4733165	1.8138763	-2.5004831
C	0.6573384	0.3928513	-6.3762248	O	1.5698357	-0.0204871	-2.1880645
H	1.7952295	-4.3342444	-2.1333304	C	0.8494430	2.8819193	-2.5095377
H	2.5978399	1.3684768	-6.7084400	H	5.0629066	1.7906640	-3.4461938
H	-3.9441227	2.4503496	-2.4161073	H	5.1946003	1.8657090	-1.6533240
C	-0.1343253	-0.2605630	-5.2492306	Zn	-0.0637604	2.7934776	-0.6762448
C	-0.1364166	-4.5560572	-4.1677199	Br	-1.5344398	4.2330827	0.4833378
C	2.0272586	0.8947531	-5.8823231	H	0.1419390	2.2021999	-3.0292506
H	2.6401388	0.0612501	-5.4794500	H	0.7864804	3.9188835	-2.8868449
C	0.2673533	-1.4875256	-4.6950552	H	3.6747175	3.9600919	-2.6576517
C	-4.4292885	0.3763199	-4.1829447	C	-1.3348854	-1.7202961	2.2589205
H	-0.1787699	-0.8877297	-7.9574813	C	-1.9414744	-2.8522578	1.7109186
C	-1.2799957	0.3545117	-4.7181747	C	-1.8949712	-4.0752943	2.4782806
C	0.8080296	-0.5377142	-7.5924417	C	-2.3266164	-5.3321670	1.9589230
H	1.3199986	-0.0156963	-8.4273393	C	-1.3625803	-4.0399017	3.8213569
H	-1.6043960	1.3190677	-5.1426185	C	-1.3623786	-5.2343273	4.6020831
C	1.5051151	-3.3760351	-2.6127528	C	-0.7795412	-2.8384702	4.3227152
H	0.1787840	-5.5409568	-3.7639490	H	-0.3375946	-2.8443093	5.3311732
H	-1.1970655	-4.6368495	-4.4828169	C	-0.6949341	-1.6946086	3.5408198
C	-0.4373031	-2.1021907	-3.6472101	C	-2.3853945	-2.1179590	-2.0418226
C	-3.0233044	1.9822057	-2.8198134	C	-3.6458805	-2.6572925	-2.2694702
C	-2.0262819	-0.2176085	-3.6691362	H	-4.0510304	-2.6514348	-3.2927581
H	-4.6619530	-0.6840921	-4.4076361	C	-4.4524061	-3.1671205	-1.2138580
H	-4.1679555	0.8688677	-5.1432146	C	-5.7825358	-3.6237489	-1.4568538
C	0.0525923	-3.4472075	-3.1156227	C	-3.9346816	-3.1809578	0.1327723
C	-1.6024410	-1.4676673	-3.1368127	C	-4.8128345	-3.5821324	1.1848033
C	-3.2772434	0.5065552	-3.1675063	C	-2.5746702	-2.7529486	0.3655068
H	1.6304686	-2.5523287	-1.8849686	C	-1.8689632	-2.1917553	-0.7104056
H	-2.2424537	2.0740714	-2.0434557	O	-1.3661839	-0.5332570	1.5500129
H	2.2149054	-3.1937877	-3.4468411	O	-0.5684772	-1.7292024	-0.5230532
H	1.9109292	1.6427755	-5.0739138	P	-0.3117279	-0.3320748	0.2917886
H	-2.7107545	2.5763635	-3.7035145	O	1.1440882	-0.4306996	0.7889876
H	1.4119218	-1.4352437	-7.3434131	O	-0.7836641	0.9348518	-0.3992423
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H	1.1708982	-1.9831985	-5.0838931	H	-0.9658135	-5.1898346	5.6287400
H	3.9213601	2.9916244	0.2685765	H	-1.8122967	-7.3462187	4.6894798
				H	-2.6844213	-5.3854102	0.9216738
				H	-2.6269193	-7.4378651	2.3101730
				C	-6.1087451	-4.0014023	0.9180255
				C	-6.5958847	-4.0416002	-0.4151385
				H	-4.4571489	-3.5445573	2.2233746
				H	-6.7659335	-4.2979973	1.7497280
				H	-7.6223971	-4.3842649	-0.6157163
				H	-6.1567165	-3.6182083	-2.4927044
				C	1.5559120	-0.6007344	3.8184145
				C	0.1382216	-0.4892330	3.8382155
				C	2.3274998	0.5914608	3.7759195
				C	-0.4758370	0.7938409	3.9155018
				C	0.3240838	1.9494184	3.8623852
				C	1.7269740	1.8832104	3.7866333
				H	3.4249469	0.5177527	3.8532665
				C	-1.9791954	0.9296836	4.1280286
				H	-0.1688883	2.9305518	3.8834073
				C	-2.6459337	1.9620920	3.2100427
				H	-2.3186919	2.9985686	3.4304761
				H	-3.7464825	1.9328108	3.3423867
				H	-2.4197737	1.7652075	2.1455421
				C	-2.2482810	1.2306723	5.6173704
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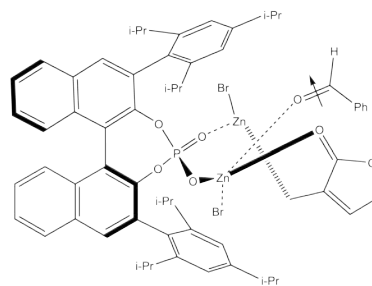
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C	1.8196415	7.0252648	-0.3904254
C	1.7412236	5.6548097	-0.1162589
C	2.9228301	4.8765160	-0.0760247
C	4.1799720	5.5047781	-0.2879635
C	4.2501329	6.8737354	-0.5511427
C	3.0660031	7.6359936	-0.6101992
H	0.8945150	7.6203107	-0.4229412

H	-1.8134636	0.4519578	6.2765858
H	-3.3394094	1.2778741	5.8116471
C	2.6090448	3.1287360	3.8288865
C	1.8725129	4.4185926	3.4461676
H	2.5940996	5.2479959	3.3066006
H	1.1653458	4.7313969	4.2420196
H	1.2914992	4.3049901	2.5103735
C	3.2710636	3.2607966	5.2159538
H	3.4326171	2.9605888	3.0959238
H	3.9525675	4.1354573	5.2399591
H	3.8620945	2.3611232	5.4789545
H	2.5014110	3.4042636	6.0026935
C	2.2695315	-1.9484728	3.8745576
C	3.3337912	-2.1492503	2.7867736
H	3.7459976	-3.1767260	2.8510959
H	4.1861427	-1.4473332	2.8830541
H	2.8990204	-2.0252639	1.7748081
C	2.8551942	-2.1617601	5.2848510
H	1.5036560	-2.7307844	3.7137940
H	3.3139147	-3.1684146	5.3665208
H	2.0767918	-2.0722595	6.0700230
H	3.6439013	-1.4134844	5.5103147
H	0.0586149	1.3116994	-6.6921932
H	0.4296017	-4.3454994	-5.1116872
H	-5.3568615	0.8560513	-3.7535092
C	0.6405757	0.4183226	-6.3737401
H	1.7983172	-4.3490623	-2.1846337
H	2.5828483	1.3903396	-6.7098755
H	-3.9433374	2.4497936	-2.3762439
C	-0.1456926	-0.2427712	-5.2474678
C	-0.1627877	-4.5478035	-4.1947216
C	2.0142288	0.9139793	-5.8838604
H	2.6264613	0.0767903	-5.4877484
C	0.2573885	-1.4745404	-4.7060628
C	-4.4349636	0.3800332	-4.1475264
H	-0.2079764	-0.8487345	-7.9584444
C	-1.2866941	0.3700057	-4.7044991
C	0.7816230	-0.5022490	-7.5984248
H	1.2885229	0.0248412	-8.4332120
H	-1.6129525	1.3377154	-5.1201721
C	1.5083170	-3.3871228	-2.6561324
H	0.1530742	-5.5368344	-3.8019265
H	-1.2282730	-4.6204578	-4.4945111
C	-0.4409008	-2.0961080	-3.6584533
C	-3.0250355	1.9862862	-2.7902310
C	-2.0270373	-0.2087368	-3.6553396
H	-4.6666745	-0.6801622	-4.3734638
H	-4.1820975	0.8744084	-5.1089667
C	0.0489194	-3.4460065	-3.1396964
C	-1.6009354	-1.4631448	-3.1359965
C	-3.2755191	0.5108208	-3.1407357
H	1.6507188	-2.5684748	-1.9259187
H	-2.2386511	2.0798802	-2.0198794
H	2.2096635	-3.2064719	-3.4975379
H	1.9035744	1.6583464	-5.0712977
H	-2.7234202	2.5855979	-3.6742322
H	1.3855251	-1.4027385	-7.3610289
H	-0.5744688	-3.7182941	-2.2640445
H	-3.5871725	0.0100943	-2.2016901
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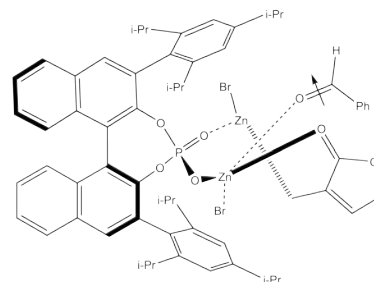
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H	-2.1601704	-2.7037082	-0.6924523
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H	-3.1071378	-5.2361816	3.6849357
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O	-0.7706740	-2.0135149	2.5537280
H	-3.2646733	-5.2112383	1.8932144
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C	2.1903421	0.3499895	-2.8842173
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C	1.2806734	3.3664743	-0.6612897
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O	0.3217165	0.8055517	-1.4474898
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O	0.2099255	0.3255725	0.1191408
P	1.0951081	-0.8921740	0.4027261
O	-1.2781709	0.2782863	0.4194299
C	5.8785693	3.5693163	-3.1943113
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H	6.8531816	3.8573570	-3.6170292
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7.2.2.2 to 15r-mi TS1-8-r; COSMO

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C	1.6379162	-1.0165659	-3.1419910
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C	-0.4066483	0.0038232	-4.3414353
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H	0.6583866	0.0097102	-6.2687850
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H	-1.7426334	-6.1906231	-4.2382925
H	-1.5961594	-4.6931546	-5.2006631
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H	0.1935596	-5.5994540	-2.8488164
H	0.6270200	-6.8027423	-5.0042701
H	2.0131626	-5.7472648	-4.5720912
H	0.8609956	-5.2307115	-5.8406313
C	3.7402696	-2.0735258	-2.0400742
C	3.7960083	-2.7651623	-0.6700845
H	4.8188099	-2.7129423	-0.2441956
H	3.5121867	-3.8366270	-0.7185018
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C	4.8290500	-2.6166677	-2.9860672
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H	4.8176094	-2.0943658	-3.9646861
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C	-2.2924267	2.3396050	4.1123389
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C	-3.4981483	2.7849971	1.1678282
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H	-4.0843716	2.0484205	1.7613815
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Zn	1.0188129	-2.3974104	1.6383688
Br	2.6588509	-3.3197017	2.9738538
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TS1-8-r

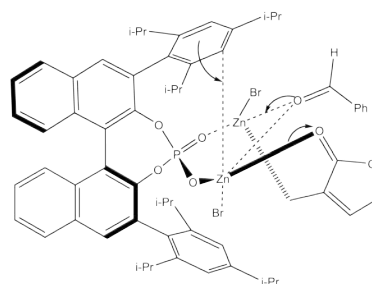


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C	-1.7762276	-4.8300195	-0.5584604
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C	-2.5856030	-3.7038555	-0.8453127
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H	-5.4237551	-5.3312030	-1.8479517
H	-1.6418554	-7.0055168	-0.5288040
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H	-3.9893453	-7.3279294	-1.3717348
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C	-1.7802187	-2.7148282	2.6637418
O	-1.7320846	-4.0636348	2.6517233
O	-0.7624306	-2.0215143	2.5432733
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O	0.3247140	0.7999338	-1.4423584	H	-2.2328126	1.0628583	8.3710682
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H	1.6401670	4.6637270	-3.0617297	H	2.2285495	0.3629818	2.7408984
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C	-0.1211454	-2.4857310	-3.9756761	Zn	1.0421217	-2.4058389	1.6348620
C	0.5732947	-3.6282712	-3.5485459	Br	2.6517856	-3.3839757	2.9489091
H	2.3693761	-4.3204088	-2.5585124	H	0.5783217	1.1354526	5.4851147
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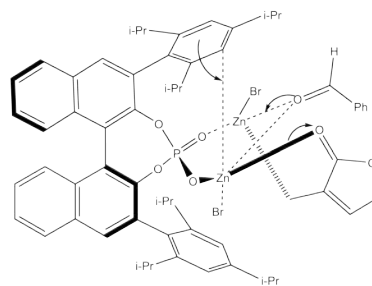


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C	-4.9074348	-2.6570504	-1.0483552
C	-7.0175088	-3.8883410	-1.0663285
C	-5.6196249	-1.4328494	-1.0601078
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H	-7.5665338	-0.4904197	-1.0618312
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H	-5.0803702	-0.4728867	-1.0846467
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Zn	-2.8404687	0.1915335	0.2210086
H	-3.1201165	-5.1612497	2.9057512
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C	-3.8305652	-3.3388035	1.9414096
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H	-4.9242847	-3.3266079	2.0447591
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C	-3.2406811	-0.8194504	1.9362930

C	-1.6191490	-2.8047291	1.7027742	H	1.9045915	-3.9465242	-2.7959890
O	-1.6584309	-4.1691454	1.8045776	H	2.3038285	-2.7416336	-1.5265983
O	-0.5912253	-2.2079905	1.4323002	C	3.1318981	-2.5314296	-4.9320302
H	-3.2516540	-5.3035618	1.1241080	H	3.4065902	-1.2805001	-3.2068400
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TS2-8-r

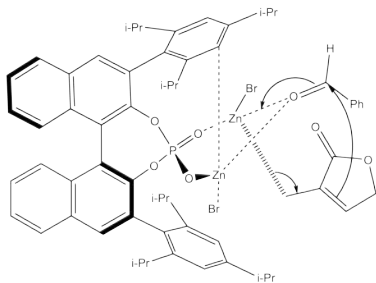


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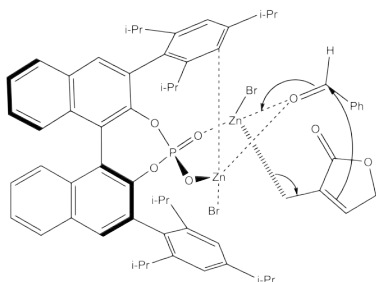
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Zn	-1.1574382	-2.6875143	0.2155550
Br	-1.0154822	-4.6817298	1.4807351
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TS3-8-r



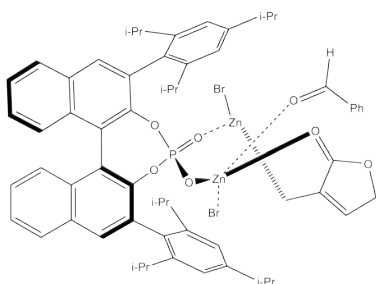
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C	-4.6398624	-2.0156036	2.5880100
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H	-4.6006532	-3.8983734	3.6896937
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C	-1.6443507	-0.4210243	3.6389417
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O	-0.0431336	-2.1061624	3.8981734
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C	2.9006354	-1.0475814	-4.8186962
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H	3.5262594	-2.3599795	-6.4411549
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C	3.6289417	4.4470903	-4.6071146
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H	2.8466689	2.4513085	-4.8142447
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C	-1.7802757	-1.2736421	-3.3210593
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H	-1.4687263	-4.7226740	-1.5040876
C	-1.9797653	-0.0217450	-4.1682188
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H	-3.7830025	0.8409465	-3.2257188
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C	-2.6778562	-0.4146558	-5.4869163
H	-0.9743458	0.3608387	-4.4375849
H	-3.6938497	-0.8185789	-5.2944031
H	-2.1051319	-1.1889379	-6.0368010
H	-2.7846700	0.4701696	-6.1473869
C	-3.9811477	-3.6769954	-1.2320093
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H	-5.8837695	-3.1720992	-0.2909178
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H	-4.7663479	-1.7797184	-0.4406646
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H	-3.6159989	-4.0863352	-0.2611367
H	-5.3187038	-5.3847335	-1.5491793
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H	-4.8319426	-4.5445092	-3.0589254
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H	0.6964989	-5.1770692	-0.7890514
H	1.5388526	-3.6039205	-0.6138855
C	0.7095072	-5.2114887	-3.6253639
H	1.6770532	-3.3691617	-3.0913625
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H	1.3612332	0.2880416	5.9474934	O	-0.2819750	-2.6158760	1.3608571
C	2.6573079	1.8151965	3.7987587	H	-2.7929718	-5.8277147	1.7063070
C	0.6924047	5.8669796	1.4653027	H	-3.8098235	-1.1508239	2.8169918
H	2.8561321	3.8204652	6.4680432	C	1.6741814	1.9992688	-1.8745999
C	0.8590546	3.3761149	3.4555428	C	2.5070436	2.7837781	-1.0724478
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C	3.9837630	-0.4742113	2.2285994	C	5.3762580	3.2012891	-3.5159940
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H	1.7747968	6.0523499	1.3138726	H	1.1920947	4.0547223	4.0439128
H	0.4519316	6.1529948	2.5107902	C	1.8228585	4.8576056	2.1189364
C	4.1679892	1.0246910	1.9337492	C	1.9089154	6.2081847	2.5743128
C	2.2383019	2.6963636	1.5706469	C	2.1086498	4.5570280	0.7366997
C	0.3207900	4.3953315	1.1986543	C	2.3935902	5.6455599	-0.1426042
H	3.0130012	-0.8376430	1.8427217	C	2.0614121	3.1832403	0.2924293
H	-1.4755007	3.1461321	1.0796409	C	1.5665210	2.2223958	1.1872227
H	4.0054633	-0.6805516	3.3191083	O	0.4192806	1.6425946	-1.3935047
H	-0.2781029	0.9087960	5.5895522	O	1.4551569	0.8961256	0.7866931
H	-1.5552415	4.3938619	2.3709530	P	0.2915009	0.4425210	-0.2841094
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H	4.2162459	1.1377200	0.8315603	O	-1.1231887	0.5263382	0.2678375
H	0.5733420	4.1713692	0.1423599	C	6.3178169	3.8592483	-2.7385417
Zn	-1.1510187	-2.6943220	0.2220907	C	6.0376179	4.1324486	-1.3734432
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H	3.2418644	1.1596535	4.4633775	H	7.2875799	4.1505694	-3.1701153
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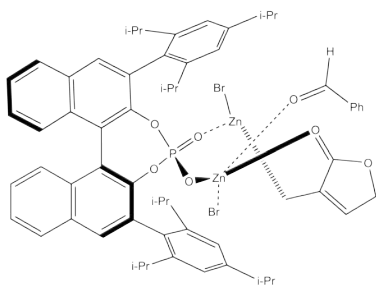


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C	-6.1984072	-3.7788392	-0.2119072	C	-1.5246324	-2.8022283	-4.7929466
C	-4.4598230	-5.1026088	-1.9886951	C	-3.0123813	-2.5088898	-4.5550113
C	-3.9932993	-4.0084364	-1.2152871	H	-3.6126568	-3.4383014	-4.6359804
C	-5.7878635	-5.5242050	-1.8776806	H	-3.4111438	-1.8012696	-5.3115881
C	-4.8738603	-3.3491107	-0.3207828	H	-3.2017944	-2.0543873	-3.5602274
O	-2.0396959	-2.6580865	-0.8100716	C	-1.2874529	-3.3058458	-6.2304867
H	-7.7018086	-5.1909072	-0.9014608	H	-1.2162953	-3.6249834	-4.1066784
H	-3.7676473	-5.6108189	-2.6785277	H	-1.9050165	-4.2027864	-6.4458731
H	-6.8853293	-3.2653585	0.4769406	H	-0.2244579	-3.5724327	-6.3966820
H	-6.1529899	-6.3684821	-2.4808124	H	-1.5568220	-2.5192433	-6.9663745
H	-4.5087035	-2.5007104	0.2720300	C	3.1249531	-1.1784093	-3.6423845
Br	-4.2939866	0.0405543	-1.2695061	C	3.3346633	-2.2920384	-2.6051849
Zn	-2.8104248	-0.5780139	0.4508651	H	4.4186907	-2.4499814	-2.4283386
H	-2.1579281	-5.7130860	3.3820049				
H	-2.0424499	-0.7681944	2.7802616				
C	-3.2140694	-3.9147790	2.6969496				
C	-2.3759370	-5.1256049	2.4626600				
H	-4.2397610	-3.9592904	3.0870408				
C	-2.5130288	-2.7902326	2.3526615				
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H	2.9051706	-3.2614685	-2.9285298
H	2.8647236	-2.0224234	-1.6393675
C	3.8199628	-1.5190027	-4.9750172
H	3.6204490	-0.2751472	-3.2368932
H	4.9014084	-1.7139122	-4.8179758
H	3.7214945	-0.6923108	-5.7084005
H	3.3754970	-2.4263355	-5.4357394
H	-2.2379135	-1.3020823	6.1345202
H	3.5821110	-0.5587365	5.3598834
H	-2.5493198	4.5777583	4.3100103
C	-1.1367523	-1.4592723	6.1652447
H	4.0509777	-1.3351031	2.2951103
H	-1.3981860	-3.6048559	6.5072631
H	-3.4963911	3.1796398	2.4113658
C	-0.5273877	-0.4709085	5.1779245
C	3.7795774	0.2272008	4.6009258
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H	0.2118305	-3.1768619	5.8656230
C	0.7825955	-0.6177556	4.6925930
C	-1.9495523	3.7060187	4.6443461
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H	4.8350708	0.1212183	4.2746871
H	3.6713345	1.2114711	5.1005353
C	1.3744375	0.3228718	3.8301864
C	-2.8870235	2.3117310	2.7370388
C	-0.7192608	1.6222578	3.8864318
H	-1.0322360	4.0895738	5.1360090
H	-2.5396295	3.1681485	5.4158347
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C	0.6220500	1.4628179	3.4302017
C	-1.6115862	2.7882274	3.4549795
H	2.3266975	-1.3118031	1.7953214
H	-2.6271346	1.7253986	1.8347609
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H	-1.2136229	-3.1624977	4.7788549
H	-3.5248686	1.6813077	3.3906527
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C	-4.3028452	-5.4701218	-1.6283892
C	-3.9306001	-4.1705860	-1.2017260
C	-5.6219510	-5.9078915	-1.4700694
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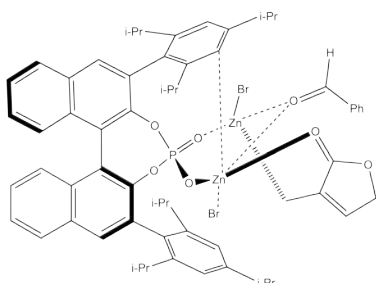
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H	-6.9657957	-3.0787824	-0.0410415
H	-5.9144344	-6.9160246	-1.7994073
H	-4.6065143	-2.2922040	-0.3264449
Br	-4.3548896	0.2467808	-1.1992157
Zn	-2.8549011	-0.4042165	0.4760624
H	-2.4503443	-5.7434714	3.0466774
H	-2.0474900	-0.7748962	2.7744251
C	-3.4070405	-3.8421929	2.4995384
C	-2.6391673	-5.0794525	2.1734892
H	-4.4369406	-3.8532381	2.8803048
C	-2.6428126	-2.7383928	2.2334272
C	-2.8935928	-1.3005706	2.2854356
C	-1.3623343	-3.2656382	1.7064102
O	-1.3667236	-4.6142798	1.6826692
O	-0.3997467	-2.6177586	1.2685552
H	-3.1017128	-5.6989287	1.3714829
H	-3.8372532	-1.0579092	2.8105676
C	1.6758713	2.0428727	-1.8747120
C	2.5169466	-2.8189765	-1.0727363
C	3.8106597	3.1794306	-1.6095033
C	4.8275175	3.8104254	-0.8320122
C	4.1088405	2.8607293	-2.9864218
C	5.3621202	3.2609105	-3.5391944
C	3.1865581	2.0861130	-3.7489792
H	3.4534233	1.8048889	-4.7796417
C	2.0055793	1.6061534	-3.1982225
C	1.2548192	2.5158702	2.5509733
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H	1.2529101	4.0430592	4.0673929
C	1.8770242	4.8624045	2.1470086
C	1.9797130	6.2066815	2.6159298
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C	2.4293652	5.6708598	-0.1110783
C	2.0850867	3.2064079	0.3000216
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P	0.2854482	0.4875141	-0.2848691
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H	6.8131525	4.6476842	-0.7686846
C	2.4992679	6.9702542	0.3712016
C	2.2919922	7.2425375	1.7495650
H	2.5821139	5.4776391	-1.1816280
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C	1.6660403	-0.7888275	-3.8735382
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C	-1.0634417	-0.2880708	-4.3882118
C	-0.6004020	-1.6146808	-4.3908858
H	1.1497770	-2.8704194	-4.1722597
C	-0.7563510	2.2195515	-4.1674878
H	-2.1239741	-0.0814011	-4.5897214
C	-2.0724896	2.4094752	-3.3993537
H	-2.9104238	1.8452533	-3.8576925
H	-2.3646080	3.4797568	-3.3938674
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H	-0.0002513	2.8855832	-3.7021611
H	-1.6281871	2.0242782	-6.1758624
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C	-1.5153044	-2.8051438	-4.6619817
C	-3.0056254	-2.5075475	-4.4457064
H	-3.6007032	-3.4432638	-4.4854364
H	-3.4038075	-1.8400005	-5.2380839
H	-3.2011361	-2.0093951	-3.4744551
C	-1.2692654	-3.3751622	-6.0727535
H	-1.2062728	-3.5938571	-3.9370121
H	-1.8822823	-4.2837298	-6.2489168
H	-0.2049560	-3.6451681	-6.2222530
H	-1.5376800	-2.6254275	-6.8462430
C	3.1420654	-1.1188796	-3.6459620
C	3.3807438	-2.1583426	-2.5399769
H	4.4691395	-2.3049470	-2.3812105
H	2.9440668	-3.1471420	-2.7850866
H	2.9368904	-1.8225449	-1.5823391
C	3.7996288	-1.5482111	-4.9714865
H	3.6489455	-0.1912584	-3.3176950
H	4.8855135	-1.7311156	-4.8321395
H	3.6777534	-0.7726846	-5.7554832
H	3.3468926	-2.4849075	-5.3589718
H	-2.2296634	-1.1997079	6.2176921
H	3.5725621	-0.6247869	5.3188428
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C	-1.1479657	-1.4500749	6.1447308
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H	-1.5492388	-3.5904342	6.3839973
H	-3.4498907	3.2799795	2.4609482
C	-0.5333542	-0.4578481	5.1648675
C	3.7804547	0.1621701	4.5638299
C	-1.0423038	-2.9087558	5.6699781
H	0.0142074	-3.2399794	5.5945448
C	0.7688269	-0.6269006	4.6657416
C	-1.8812756	3.7455311	4.6922161
H	-0.6484549	-0.2341883	7.9094862
C	-1.2410673	0.6861889	4.7625735
C	-0.5339574	-1.2754821	7.5471596
H	-1.0154943	-1.9534347	8.2824511
H	-2.2709583	0.8236899	5.1316763
C	2.9700584	-1.2712760	2.6193735
H	4.8318109	0.0379466	4.2310631
H	3.6941214	1.1442635	5.0714858
C	1.3736055	0.3098710	3.8093822
C	-2.8511329	2.3983012	2.7680382
C	-0.6921286	1.6513461	3.8965890
H	-0.9554388	4.1029140	5.1872740
H	-2.4790107	3.2083213	5.4580867
C	2.8151460	0.0653556	3.3672362
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C	-1.5646656	2.8403450	3.4876182
H	2.2788043	-1.3284642	1.7570714
H	-2.6030325	1.8287844	1.8517872
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H	-1.5121087	-3.0432549	4.6758428
H	-3.4954430	1.7636199	3.4110645
H	0.5518747	-1.5063625	7.5330500
H	3.0985806	0.8717375	2.6625894
H	-0.9916895	3.4472604	2.7597956
Zn	0.1269447	-2.6635584	-0.7538163
Br	0.7947465	-4.7307750	-1.5806850
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C	-5.1779576	-4.2083053	1.7886788
C	-4.6551908	-2.9732764	1.3171885
C	-6.4577340	-4.2661434	2.3432028
C	-5.4497169	-1.8038471	1.3972945
O	-2.7169716	-2.0135129	0.2100911
H	-8.2402173	-3.1365274	2.8787562
H	-4.5608229	-5.1182207	1.7167143
H	-7.3378858	-0.9546980	2.0258080
H	-6.8596070	-5.2240006	2.7058487
H	-5.0764121	-0.8458405	1.0028411
Br	-4.2835082	1.4515023	0.2822171
Zn	-2.5985903	0.0804198	1.2417140
H	-0.8838849	-4.7434584	4.2303324
H	-1.5593637	0.0964346	3.4432909
C	-2.2164727	-3.2383072	3.3825351
C	-1.1209520	-4.2540272	3.2579881
H	-3.2162389	-3.4762219	3.7688061
C	-1.7157480	-1.9909107	3.1121939
C	-2.3002962	-0.6643238	3.1174484
C	-0.2918574	-2.1953788	2.6785695
O	0.0283489	-3.5230115	2.8137988
O	0.5018238	-1.3752967	2.2659407
H	-1.3235357	-5.0594086	2.5160674
H	-3.2425077	-0.5902378	3.6912610
C	1.1742099	1.1508832	-2.6749687
C	2.3658067	1.8337779	-2.4235276
C	3.4153818	1.7368133	-3.4116923
C	4.7312764	2.2457824	-3.1975214
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C	1.8877291	0.4109313	-4.8569367
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C	0.9243436	0.3814555	-3.8576542
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C	3.6010906	5.9802720	0.1608369
C	2.9203734	3.9788410	-1.1325264
C	3.0661410	4.7595332	-2.3194795
C	2.5086807	2.5941989	-1.1496147
C	2.2034321	1.9847354	0.0775619
O	0.1490209	1.2306444	-1.7485973
O	1.7629809	0.6636072	0.1070856
P	0.2423962	0.3011740	-0.3837414
O	0.2988217	-1.1939408	-0.7504482
O	-0.8795048	0.8181471	0.4997816
C	5.4118290	1.5554047	-5.4365668
C	5.7045333	2.1574417	-4.1840343
H	3.9250879	0.5164494	-6.6193509
H	6.1880766	1.5004875	-6.2149108
H	4.9748003	2.7077601	-2.2309521
H	6.7130288	2.5535315	-3.9900920
C	3.4780079	6.0841269	-2.2618405
C	3.7669038	6.6982150	-1.0138691
H	2.8349563	4.3052629	-3.2926747
H	3.5745238	6.6644428	-3.1922562
H	4.1019082	7.7461786	-0.9811772
H	3.7910377	6.4521723	1.1377456
C	-0.0999693	-1.9124887	-3.6927841
C	-0.2774956	-0.5077582	-3.8274127
C	-1.2256806	-2.7065052	-3.3423906
C	-1.5782125	0.0612603	-3.7116732
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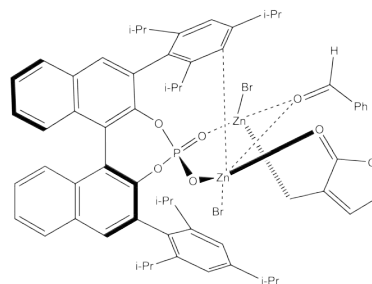
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C	-2.6925674	2.2556310	-3.0014121
H	-3.7367715	1.8814055	-2.9948934
H	-2.7354904	3.3389603	-3.2345235
H	-2.2925242	2.1349006	-1.9771503
C	-2.4070603	1.6420927	-5.4573295
H	-0.8323091	2.0343452	-4.0530909
H	-3.3996194	1.1483126	-5.5177040
H	-1.7453697	1.1661439	-6.2094819
H	-2.5396733	2.7070219	-5.7384242
C	-3.7122878	-3.0580239	-2.8783820
C	-4.9380892	-2.3200429	-2.3256078
H	-5.6928270	-3.0459348	-1.9635241
H	-5.4255931	-1.7035815	-3.1089923
H	-4.6748445	-1.6474931	-1.4860658
C	-4.0750301	-3.8606592	-4.1450216
H	-3.3725128	-3.7984303	-2.1167246
H	-4.9064556	-4.5633815	-3.9332479
H	-3.2154808	-4.4515491	-4.5193445
H	-4.4000653	-3.1782929	-4.9578126
C	1.2418032	-2.5928970	-3.9461314
C	1.6882128	-3.5514076	-2.8335032
H	2.7025959	-3.9386712	-3.0587998
H	1.0176236	-4.4273755	-2.7267101
H	1.7355169	-3.0327083	-1.8549073
C	1.2091796	-3.2964977	-5.3178951
H	2.0076355	-1.7962199	-4.0016564
H	2.2011325	-3.7345487	-5.5516540
H	0.9415085	-2.5932852	-6.1327960
H	0.4648606	-4.1203068	-5.3283389
H	0.0760404	0.5573063	6.8018242
H	5.2899987	0.1165231	4.1134489
H	-0.2937684	5.6825780	3.3745173
C	0.9062941	-0.0344241	6.3565365
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H	0.0982742	-1.9538853	7.0573429
H	-2.0766944	4.1130056	2.4838299
C	1.2905171	0.6552785	5.0525842
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C	0.3741287	-1.4575219	6.1033963
H	1.1360447	-2.0883980	5.5992864
C	2.3979777	0.2257949	4.3024404
C	0.2890943	4.8117118	3.7402858
H	2.4388327	0.9832621	7.5627442
C	0.5371807	1.7301579	4.5527532
C	2.0646020	-0.0424850	7.3694630
H	1.7400721	-0.4797951	8.3364891
H	-0.3359887	2.0749402	5.1310011
C	3.8801885	-1.1726198	2.0035773
H	6.1780496	0.3011154	2.5675418
H	5.3831791	1.7225296	3.3256562
C	2.7638210	0.8361138	3.0917877
C	-1.5022735	3.2467051	2.8707020
C	0.8597891	2.3808265	3.3456094
H	1.3631616	5.0858145	3.7209418
H	0.0104980	4.6383228	4.8011127
C	3.9938914	0.3231235	2.3468368
C	1.9951661	1.9322522	2.6144791
C	0.0022359	3.5615116	2.8858072
H	2.9336093	-1.3839635	1.4713709
H	-1.7174527	2.3891544	2.2080666
H	3.8949949	-1.8013884	2.9186348
H	-0.5239598	-1.4389055	5.4554111
H	-1.8950643	3.0151943	3.8825249
H	2.9192252	-0.6483695	7.0023220
H	4.0627607	0.8742273	1.3872251
H	0.2884115	3.7957026	1.8402674
Zn	-1.0070902	-2.5893935	-0.9728507
Br	-0.7994641	-4.8941870	-0.4868519
H	2.9962865	-0.6248229	4.6654788

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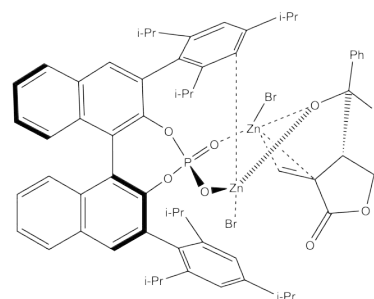


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C	-5.1606069	-4.2489661	1.7838740
C	-4.6410554	-3.0055145	1.3324034
C	-6.4441410	-4.3227166	2.3272364
C	-5.4436799	-1.8430905	1.4216627
O	-2.7108119	-2.0265674	0.2250107
H	-8.2384912	-3.2123682	2.8635340
H	-4.5366700	-5.1536962	1.7030799
H	-7.3404143	-1.0134983	2.0448347
H	-6.8428673	-5.2882445	2.6729744
H	-5.0762205	-0.8765156	1.0411757
Br	-4.3108867	1.3886766	0.2476775
Zn	-2.6065645	0.0730092	1.2197808
H	-0.8507834	-4.7344094	4.1822511
H	-1.5524794	0.1099132	3.4140864
C	-2.1972625	-3.2363958	3.3409452
C	-1.0897793	-4.2410883	3.2116708
H	-3.1931360	-3.4832183	3.7312231
C	-1.7016227	-1.9799297	3.0945200
C	-2.2910414	-0.6604696	3.1076835
C	-0.2732135	-2.1707838	2.6628219
O	0.0530149	-3.4977591	2.7780003
O	0.5149826	-1.3384700	2.2671131
H	-1.2797208	-5.0430850	2.4623875
H	-3.2338102	-0.5859368	3.6798154
C	1.1792858	1.1456794	-2.6745060
C	2.3742138	1.8229242	-2.4233821
C	3.4212141	1.7244071	-3.4139492
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C	3.1389123	1.0649009	-4.6685438
C	4.1530198	1.0115842	-5.6710327
C	1.8844013	0.4140386	-4.8620588
H	1.7060948	-0.1229390	-5.8067057
C	0.9232681	0.3836132	-3.8608392
C	2.3853583	2.6160660	1.3436875
C	2.9148778	3.9009460	1.3418008
H	3.0997222	4.4025664	2.3038553
C	3.1754271	4.6097529	0.1357875
C	3.6250661	5.9640115	0.1590633
C	2.9382512	3.9647840	-1.1328178
C	3.0902840	4.7437422	-2.3198280
C	2.5208410	2.5818216	-1.1492392
C	2.2103538	1.9746153	0.0777406
O	0.1562885	1.2247829	-1.7473160
O	1.7671772	0.6543689	0.1082014
P	0.2471853	0.2935216	-0.3836535
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C	5.4127940	1.5438809	-5.4427887	C	2.7601917	0.8392726	3.1030508
C	5.7103019	2.1382321	-4.1883582	C	-1.5107231	3.2455451	2.8427054
H	3.9195271	0.5179163	-6.6276208	C	0.8496349	2.3798018	3.3341108
H	6.1871852	1.4890214	-6.2229146	H	1.3535721	5.0863762	3.6909578
H	4.9854039	2.6823840	-2.2313184	H	-0.0017776	4.6477183	4.7693523
H	6.7208372	2.5287872	-3.9941681	C	3.9977376	0.3276556	2.3698958
C	3.5090444	6.0657296	-2.2627017	C	1.9914181	1.9297575	2.6144628
C	3.7978962	6.6796459	-1.0153678	C	-0.0056989	3.5572592	2.8616944
H	2.8586511	4.2891575	-3.2926204	H	2.9595824	-1.4022135	1.5104151
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C	-0.1124099	-1.9057586	-3.7056700	H	-1.9091464	3.0233166	3.8544118
C	-0.2829142	-0.4993773	-3.8309771	H	2.8907241	-0.6228751	7.0226249
C	-1.2399201	-2.6947515	-3.3525062	H	4.0656136	0.8673970	1.4037241
C	-1.5794017	0.0767113	-3.7014386	H	0.2847582	3.7834355	1.8155218
C	-2.6677293	-0.7387875	-3.3427262	Zn	-1.0001010	-2.5999796	-0.9648772
C	-2.5308720	-2.1260400	-3.1551600	Br	-0.8287146	-4.9146248	-0.5352228
H	-1.1386059	-3.7927860	-3.3430266	H	2.9850856	-0.6120376	4.6857287
C	-1.8157107	1.5492115	-4.0171064	H	-2.7975471	-4.0061109	0.7170361
H	-3.6524703	-0.2714059	-3.2090114				
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H	-2.2623703	2.1589420	-1.9552051				
C	-2.4148847	1.6667811	-5.4342428				
H	-0.8245588	2.0457354	-4.0442686				
H	-3.4111069	1.1796681	-5.4867128				
H	-1.7640886	1.1878837	-6.1939228				
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C	-3.7226719	-3.0347767	-2.8626912				
C	-4.9385437	-2.2922207	-2.2943520				
H	-5.6928843	-3.0144373	-1.9238234				
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H	-4.6636898	-1.6202452	-1.4581291				
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C	1.2248293	-2.5930305	-3.9668905				
C	1.6832682	-3.5354348	-2.8450757				
H	2.6939960	-3.9289565	-3.0760019				
H	1.0129234	-4.4084053	-2.7149323				
H	1.7448477	-3.0017961	-1.8754978				
C	1.1754712	-3.3156406	-5.3278562				
H	1.9910872	-1.7985517	-4.0430810				
H	2.1635588	-3.7589270	-5.5681277				
H	0.8984266	-2.6239283	-6.1495236				
H	0.4306963	-4.1390139	-5.3195662				
H	0.0454512	0.5719468	6.7937471				
H	5.2857886	0.1592659	4.1461872				
H	-0.3013891	5.6822475	3.3348256				
C	0.8809837	-0.0193667	6.3575310				
H	4.7603871	-1.4887035	1.4174772				
H	0.0764957	-1.9397254	7.0617085				
H	-2.0825082	4.1089591	2.4462929				
C	1.2729042	0.6651924	5.0531823				
C	5.2784348	0.6630424	3.1568269				
C	0.3550384	-1.4453367	6.1074697				
H	1.1213435	-2.0751891	5.6088374				
C	2.3870610	0.2349867	4.3141347				
C	0.2793661	4.8132649	3.7080843				
H	2.4014320	1.0098842	7.5681124				
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H	1.7016700	-0.4502104	8.3468820				
H	-0.3572108	2.0813501	5.1127782				
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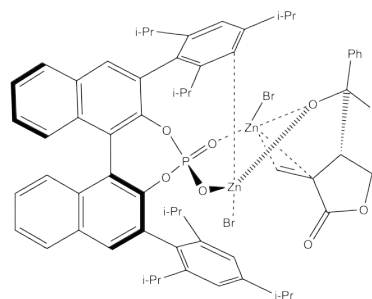


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C	-5.1977972	-3.2757485	2.7046949
C	-4.4927525	-2.0552625	2.7323096
C	-6.5987119	-3.2999347	2.8012834
C	-5.2204345	-0.8565874	2.8693536
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H	-7.1714162	0.0734178	3.0423077
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H	4.5625065	5.8144922	-1.7323142	H	0.2981075	0.7996047	5.7078892
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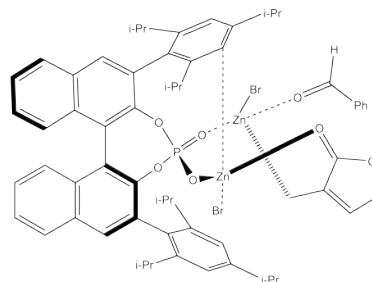
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C	0.3011805	-1.0724348	-3.7396171	H	-1.2867289	4.8773980	0.9179575
C	2.8603851	2.5676124	0.0761148	C	2.1706008	2.3774153	4.3510039
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C	3.6131853	3.8565600	-1.8801348	H	1.9175983	0.1037167	5.9639843
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C	2.4249939	1.5404631	-0.8182420	C	3.1842182	2.5636520	6.6751090
O	0.0423453	0.4845617	-1.9359770	H	2.9571569	2.5745753	7.7612394
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H	5.1216708	-1.6201052	-7.0519998	H	2.3339210	5.8710087	1.3488795
H	4.8110652	0.9492291	-3.5725084	H	1.1004144	6.0342246	2.6317132
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H	2.6672701	2.3924307	-4.8651467	H	3.1382693	-1.0768702	1.6857489
H	3.6269957	4.4897245	-5.7525843	H	-1.0820373	3.1491841	1.2994393
H	4.6349401	6.1945979	-4.1986766	H	4.2039026	-1.0344168	3.1190488
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C	-0.9049790	-3.0120785	-2.6849409	H	-1.0101770	4.3818458	2.6081450
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C	-2.0091198	-3.4727756	-1.9208684	H	4.4331803	0.8228398	0.6610515
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C	-3.1788380	-2.6867043	-1.7295178	Br	-1.2357660	-4.8297223	1.3290646
H	-2.0034835	-4.5129278	-1.5564505	H	3.7333206	0.8752217	4.3593895
C	-2.2912459	0.4342454	-3.7819921	H	-2.7022600	-3.1604538	2.5834368
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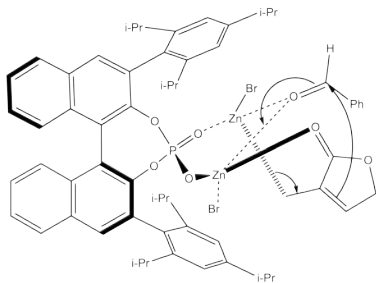


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O	-0.3369286	-1.1513022	1.4238420	H	-1.2907241	7.2842466	-5.0950070
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C	-1.5843555	-1.9423543	-1.1074239	H	-3.6388153	6.6721220	-0.7031060
C	-2.0474185	-2.8318868	-0.1293702	H	-4.4128779	8.4496189	-2.3054465
C	-3.4417443	-3.2069658	-0.1568445	H	-3.2367446	8.7446135	-4.4964139
C	-4.2451633	-2.8199397	-1.2900475	H	2.5299718	4.8400650	4.6950288
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C	-2.3946278	-1.4655709	-2.1865761	H	2.6130695	2.6711540	-0.0114279
C	-5.6094228	-3.2344620	-1.3532171	H	2.0412727	4.3694634	-0.2587355
C	-6.1815498	-3.9643456	-0.3226853	H	1.8321434	5.8585326	2.2227911
C	-5.4082977	-4.2947574	0.8217438	H	-4.3141456	-1.6701140	-3.1381107
C	-4.0723149	-3.9268883	0.9017378	H	1.4035523	-4.7390777	3.6070154
C	-1.0991228	-3.3802215	0.8756776	H	-6.2064482	-2.9410116	-2.2310424
C	-0.9858842	-4.8051911	1.1000978	H	-7.2374317	-4.2698222	-0.3794412
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C	0.7322519	-3.0119115	2.5126890	H	-2.2641328	-5.4442301	-0.5540456
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C	-1.9655303	1.9802988	-3.7133957	H	1.6446563	-1.5150060	-2.8096851
C	-0.8138943	1.8328422	-4.5023585	H	-0.5574301	-2.6145448	-3.3506909
C	-0.2322506	0.5563463	-4.5856275	H	-0.0042547	-1.8105240	-6.2769592
C	-0.7468121	-0.5458575	-3.8833139	H	-1.5244899	-2.5162759	-5.6487443
C	1.8408612	-2.1330161	3.0023891	H	-0.0083462	-3.4794262	-5.6210709
C	1.6979092	-1.3157996	4.1504275	H	1.5105522	4.4057682	-4.8570883
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C	4.1517624	-1.3736526	2.7690534	H	-0.9236161	3.8638015	-5.1228505
C	3.0827410	-2.1786605	2.2959099	H	0.5019500	3.7230592	-7.1543760
Zn	-0.0255019	2.8179302	0.2660505	H	-0.8016414	2.4892484	-7.2270828
O	2.1054901	1.3524349	2.4911786	H	0.8759324	2.0093136	-6.8240227
C	2.0360098	2.5713643	2.7349144	H	-4.6054364	2.4322284	-0.5902341
C	2.0352460	3.7025377	1.7872947	H	-3.6097127	3.3220914	-1.7707457
C	1.9198381	4.8208270	2.5701105	H	-2.8284438	2.2691970	-0.5320635
C	1.7702292	4.4225340	3.9981066	H	-3.9648272	0.2766872	-1.5296139
O	1.9118262	2.9861731	4.0040574	H	-5.9482299	1.4221082	-2.5145394
C	1.9194581	3.4556244	0.3524428	H	-5.1308915	0.4242477	-3.7643935
Zn	3.1540628	0.2382745	1.1839247	H	-4.9106394	2.1959950	-3.7564767
Br	5.1485986	1.1310453	0.3771960	H	6.1021571	-0.0767273	3.8019479
C	-3.7939976	1.1636845	-2.1695813	H	1.0946412	-0.7676860	6.8998576
C	-5.0132967	1.3052992	-3.1012530	H	4.1263811	-5.2174434	0.9721442
C	-0.1008559	-1.9161390	-4.0806791	H	-1.2601673	0.2623833	5.1146280
C	-0.4291674	-2.4614517	-5.4842370	H	5.9206188	2.2569358	4.7054480
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C	5.6109943	-0.2099360	5.8980964	H	6.5348727	0.3102693	6.2240632
C	0.3571864	-1.1917474	4.8642657	H	5.1296187	-1.4305863	2.2660826
C	-0.2695151	0.1953189	4.6202044	H	-0.5348892	-1.4931994	6.8374214
C	3.3371626	-3.1811587	1.1647732	H	0.9114657	-2.5136000	6.5377554
C	4.1682464	-2.6449995	-0.0113327	H	3.4169495	-4.8787512	2.5818192
Br	-1.5058635	3.4001857	2.0869104	H	5.0149140	-4.1973762	2.1514091
O	-0.7628442	4.0856776	-1.3195865	H	-0.4147380	0.3933323	3.5413609
C	-1.6322020	4.9340279	-1.0668306	H	3.6600658	-1.8095217	-0.5295333
C	-2.0407578	5.9804688	-2.0089522	H	0.3703525	1.0061887	5.0241633
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C	-1.8059251	7.1456925	-4.1324062	H	5.1771066	-2.3008889	0.2944071
C	-2.8993341	7.9669413	-3.7938096	H	4.8068130	0.0654388	6.6119970
C	-3.5609048	7.8032257	-2.5642473	H	-0.3211513	-1.9476665	4.4156003
C	-3.1303627	6.8148388	-1.6700949	H	2.3497209	-3.4773315	0.7568485
C	1.4150258	-1.9074244	-3.8190753	H	2.6941519	0.0379484	5.5137077
C	1.0824521	3.4762965	-4.4250496	H	-2.1432769	4.9094754	-0.0680638
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7.2.2.4 to 15s-mi

TS1-8-s; COSMO



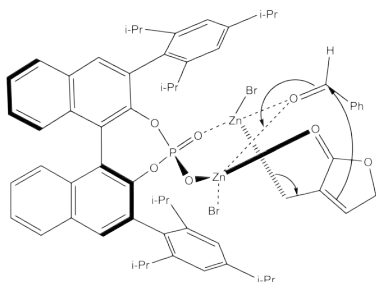
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O	-1.3488746	-2.8791398	-0.8316654
H	-7.1334331	-4.8377876	-1.7870692
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H	-6.2428611	-2.5179025	-1.4054192
H	-5.5588118	-6.7927616	-1.8012432
H	-3.8120456	-2.1561616	-1.0354615
Br	-3.7432208	-0.3881120	1.1181438
Zn	-1.7866558	-1.6122492	0.7993314
H	-0.3743902	-7.0779918	1.3003794
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O	0.7449974	-5.5102470	0.4867026
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H	-0.6332210	-6.7259614	-0.4452952
H	-2.2006627	-3.1463420	2.8632424
C	0.7696705	2.3065697	-1.5414365
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C	2.6999128	3.6270000	-2.1835009
C	4.0230011	4.1205935	-1.9787589
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C	2.7979949	4.5458988	-4.4796673
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H	0.3029197	3.5117309	-4.6970782
C	0.1234885	2.5067117	-2.7994310
C	2.7702646	1.4920401	2.3286007
C	3.1468687	2.6397035	3.0150960
H	3.4243866	2.5647473	4.0776951
C	3.1104688	3.9257988	2.4025110
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C	2.5050419	5.3734660	0.5047691
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C	2.4629452	1.6370501	0.9418595
O	0.0843251	1.5094415	-0.6277583
O	2.2354186	0.4625737	0.2318346
P	0.7283464	0.0575850	-0.2391336
O	0.9504691	-0.8442908	-1.4736925
O	-0.1370756	-0.5041481	0.8839261
C	4.0757630	5.0302140	-4.2410063
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H	2.3153835	4.6992316	-5.4577486
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C	2.7996209	6.4959561	1.2670227
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H	2.1217119	5.4982329	-0.5166143
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H	3.7623537	4.9813647	4.1930479
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H	-2.8520226	5.8924388	-1.4294548
C	-5.2308937	0.1721507	-3.3610215
C	-6.1354373	0.3528738	-2.1337535
H	-7.0743421	-0.2258599	-2.2559380
H	-6.4310887	1.4137799	-1.9943732
H	-5.6322313	0.0212524	-1.2026202
C	-5.9122160	0.7045390	-4.6373672
H	-5.0703986	-0.9208967	-3.5013279
H	-6.8956934	0.2158387	-4.7998737
H	-5.2856559	0.5268628	-5.5346577
H	-6.0827455	1.7990155	-4.5594939
C	-0.2747192	0.0182310	-4.4178397
C	-0.4249275	-1.5108408	-4.4049011
H	0.5360988	-2.0070256	-4.6447094
H	-1.1697950	-1.8663627	-5.1471366
H	-0.7623481	-1.8745028	-3.4132966
C	-0.0676952	0.5182640	-5.8606032
H	0.6378614	0.2626050	-3.8352765
H	0.7885009	-0.0020639	-6.3380651
H	0.1338787	1.6064011	-5.8965741
H	-0.9720501	0.3239407	-6.4748433
H	0.6662556	-3.7421580	5.0417119
H	6.0164486	-1.9591919	3.0970256
H	-0.0128407	2.5670143	5.7631502
C	1.7735166	-3.6598535	4.9536466
H	5.4425282	-1.6760018	-0.0166573
H	1.9397437	-5.8272460	4.7373663
H	-1.6882281	1.6171647	4.0925898
C	2.0508273	-2.3462430	4.2288395
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C	2.2721164	-4.9080367	4.2136476
H	3.3804576	-4.9440585	4.1683467
C	3.1404262	-2.1691508	3.3618969
C	0.6651606	1.7102551	5.5689015
H	1.9510266	-2.7383703	6.9466353
C	1.2132928	-1.2394897	4.4606044
C	2.3467585	-3.6078561	6.3843343
H	2.0961142	-4.5290754	6.9505439
H	0.3472591	-1.3653393	5.1316451
C	4.5729928	-1.8193862	0.6575340
H	6.8163271	-0.8159433	1.9733129
H	5.9854650	-0.2025789	3.4429140
C	3.4093132	-0.9346880	2.7404014
C	-1.0207251	0.7455526	3.9339658
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H	0.4608342	0.9354669	6.3377844
C	4.6262808	-0.8187313	1.8255975

C	2.5568112	0.1702324	3.0006955
C	0.4475173	1.1500599	4.1502697
H	3.6498429	-1.6851263	0.0624407
H	-1.1889886	0.3809989	2.9035635
H	4.5949933	-2.8702096	1.0127622
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H	-1.3474986	-0.0461724	4.6403921
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H	0.6599386	1.9685760	3.4334576
Zn	0.7072353	-2.7495407	-1.4021837
Br	1.2835818	-4.5212443	-2.7649682
H	3.8061462	-3.0185910	3.1489201
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TS1-8-s



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C	-3.3198177	-4.2662894	-1.1539986
C	-5.1892454	-5.7688201	-1.6200452
C	-4.2085230	-3.1688026	-1.1759875
O	-1.3625966	-2.8736049	-0.8228517
H	-7.1460090	-4.8287121	-1.7946396
H	-3.1337344	-6.4266517	-1.4026317
H	-6.2554148	-2.5092145	-1.4083291
H	-5.5720601	-6.7837436	-1.8061121
H	-3.8270586	-2.1482490	-1.0307260
Br	-3.7592108	-0.3761808	1.1093375
Zn	-1.8031728	-1.5994931	0.8019468
H	-0.3957983	-7.0629222	1.3249706
H	-0.4933755	-2.4093203	2.7573667
C	-1.5472569	-5.2275956	0.9706237
C	-0.5078171	-6.2465329	0.5769757
H	-2.5735312	-5.5237007	1.2297605
C	-0.8579869	-4.1578140	1.5777174
C	-1.2800292	-3.0533420	2.3232200
C	0.5035775	-4.2410280	0.9551006
O	0.7281026	-5.4960705	0.5208468
O	1.2825706	-3.3184413	0.7043279
H	-0.6397165	-6.7098665	-0.4235865
H	-2.2354221	-3.1230655	2.8686198
C	0.7670533	2.3065837	-1.5409182
C	1.9671969	2.9160763	-1.1582317
C	2.6989487	3.6258857	-2.1795393
C	4.0210947	4.1201364	-1.9719067
C	2.0880716	3.8208198	-3.4738301
C	2.8031472	4.5426793	-4.4755011
C	0.7890021	3.2909614	-3.7324133
H	0.3083549	3.5071800	-4.6985496
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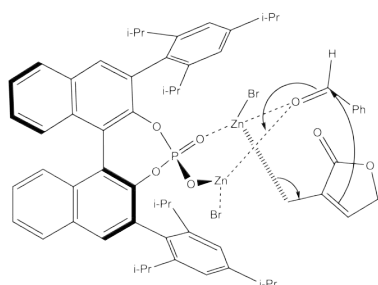
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C	2.4553650	1.6366122	0.9452979
O	0.0790215	1.5112059	-0.6284955
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P	0.7193367	0.0588721	-0.2357706
O	0.9414293	-0.8474442	-1.4666493
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C	4.0796614	5.0276512	-4.2341105
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H	2.3232293	4.6947840	-5.4550859
H	4.6213612	5.5755341	-5.0200734
H	4.5087119	3.9435725	-1.0027088
H	5.7195117	5.1637814	-2.7942227
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H	2.1183533	5.4970276	-0.5132518
H	2.6474335	7.4969768	0.8405943
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C	-2.7329699	0.1943288	-3.8350957
C	-2.3523739	2.5479125	-2.3556067
C	-3.6286276	1.9687613	-2.4824168
C	-3.8441466	0.7905613	-3.2129591
H	-2.8885993	-0.7397529	-4.3973789
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H	-2.3411539	4.4058720	0.6086340
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H	-5.2732904	0.5237986	-5.5507916
H	-6.0729137	1.7968081	-4.5801051
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C	-0.4181466	-1.5154887	-4.4013041
H	0.5432027	-2.0130703	-4.6364712
H	-1.1602100	-1.8722725	-5.1457513
H	-0.7591874	-1.8775930	-3.4105599
C	-0.0550740	0.5108099	-5.8589986
H	0.6428752	0.2583677	-3.8306164
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H	0.1468218	1.5987291	-5.8963006
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H	0.6976674	-3.7618783	5.0387547
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H	-0.0105001	2.5428730	5.7814257
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H	1.9853308	-5.8378312	4.7275992
H	-1.6898320	1.5924128	4.1148094
C	2.0702130	-2.3548871	4.2238633

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C	2.3088625	-4.9154525	4.2037908
H	3.4171825	-4.9436470	4.1551958
C	3.1557146	-2.1693342	3.3540827
C	0.6699705	1.6895999	5.5810391
H	1.9829840	-2.7519372	6.9407809
C	1.2271392	-1.2538095	4.4611511
C	2.3820271	-3.6180761	6.3759858
H	2.1400238	-4.5416658	6.9421491
H	0.3639788	-1.3863702	5.1346878
C	4.5771498	-1.8042801	0.6457931
H	6.8193963	-0.7925603	1.9581431
H	5.9895155	-0.1880362	3.4318272
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C	1.4337755	0.0017816	3.8633174
H	1.7117294	2.0401182	5.7263834
H	0.4726088	0.9116149	6.3483814
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H	-1.1916790	0.3625529	2.9200490
H	4.6059886	-2.8562448	0.9970518
H	1.9322095	-4.9629625	3.1627381
H	-1.3408057	-0.0705637	4.6563672
H	3.4867481	-3.5145869	6.3433747
H	4.6180639	0.2135386	1.3820253
H	0.6541228	1.9549916	3.4465684
Zn	0.6954522	-2.7517908	-1.3899474
Br	1.2674928	-4.5320150	-2.7393732
H	3.8255078	-3.0143002	3.1363439
H	-1.2132918	-4.8151385	-1.4630699

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O	2.4402851	0.0892251	-0.8442960
P	0.8395451	0.0669876	-0.5541520
O	0.2630713	0.9661820	-1.6811480
O	0.2442984	-1.3314338	-0.4625932
C	4.7476922	5.8017559	1.3336037
C	5.5209909	4.6256297	1.1406952
H	2.7571333	6.6160797	1.5883484
H	5.2432467	6.7836701	1.3747279
H	5.5200104	2.4780278	0.9348119
H	6.6123701	4.7027835	1.0202237
C	5.6681899	0.7485146	4.3290259
C	6.4165615	-0.4495772	4.1832439
H	4.1638509	2.0491574	3.4952264
H	5.8197633	1.3839994	5.2148665
H	7.1555924	-0.7320487	4.9484381
H	6.7496667	-2.2186414	2.9798972
C	-1.8073314	3.2490875	0.6371872
C	-0.8403945	3.0107944	1.6459402
C	-3.1724045	3.2018922	0.9813236
C	-1.2524103	2.6883291	2.9700672
C	-2.6270102	2.6372583	3.2562437
C	-3.6055676	2.9012450	2.2824839
H	-3.9309116	3.4041367	0.2078574
C	-0.2425938	2.3521223	4.0670653
H	-2.9444311	2.3746678	4.2774224
C	-0.1697244	0.8284978	4.2900633
H	-1.1365608	0.4381805	4.6705707
H	0.6196726	0.5791666	5.0297348
H	0.0455813	0.2919383	3.3456783
C	-0.5163876	3.1017716	5.3815354
H	0.7566028	2.6806187	3.7145924
H	-1.4717347	2.7850110	5.8494425
H	-0.5657024	4.1981833	5.2211721
H	0.2892450	2.8975471	6.1164476
C	-5.0893451	2.8494028	2.6244076
C	-5.5252930	1.4366560	3.0539032
H	-6.6224719	1.3939009	3.2164735
H	-5.0333324	1.1398405	4.0035351
H	-5.2473127	0.6763665	2.2967073
C	-5.4688450	3.8997941	3.6834755
H	-5.6411423	3.1080060	1.6924049
H	-6.5611556	3.8874930	3.8795730
H	-5.1872978	4.9218100	3.3584202
H	-4.9547877	3.6997593	4.6467705
C	-1.3952991	3.5726582	-0.7960618
C	-2.2487988	2.8246638	-1.8336801
H	-1.8076057	2.9110403	-2.8488472
H	-3.2850006	3.2134282	-1.9096091
H	-2.3619577	1.7544050	-1.5414084
C	-1.4188844	5.0884380	-1.0645218
H	-0.3515260	3.2226304	-0.9260935
H	-1.0963476	5.3137163	-2.1022605
H	-0.7405827	5.6256679	-0.3721236
H	-2.4401061	5.5005774	-0.9241109
H	0.0328306	-5.0164627	-3.2468447
H	5.4054024	-2.3742461	-4.3371894
C	0.6283277	-4.2432195	-3.7761217
H	4.5667815	0.7353945	-4.0371927
H	-1.1901569	-3.4237447	-4.7009056
H	1.3882192	-3.6191660	2.7836778
C	1.7084711	-3.7530505	-2.8246193
C	5.6990479	-1.7727675	-3.4512771
C	-0.3318668	-3.0779344	-4.0909703
H	0.1821323	-2.2675091	-4.6493068
C	2.6407866	-2.7840598	-3.2359096
C	2.3565465	-5.5405981	1.0763515
H	1.8637891	-5.7203085	-4.8344300
C	1.7409545	-4.1677322	-1.4835324
C	1.1851824	-4.8733989	-5.0621234
H	0.3593288	-5.2554391	-5.6965932

7.2.2.5 to 15q-mi

TS1-8-q; COSMO

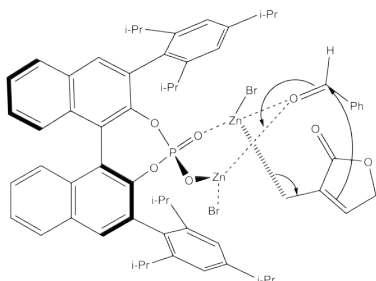


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C	4.9116491	3.3791338	1.0953997
C	2.7095468	4.4458325	1.3949890
C	3.3690216	5.7101731	1.4543057
C	1.2929302	4.3439006	1.5074793
H	0.7075472	5.2518605	1.7203519
C	0.6309259	3.1286486	1.3756131
C	3.9597435	-1.5406447	0.0785405
C	4.9455766	-1.8225649	1.0156088
H	5.4939746	-2.7753579	0.9570777
C	5.2367500	-0.9282982	2.0893171
C	6.1967891	-1.2722700	3.0880841
C	4.5155000	0.3188295	2.2087226
C	4.7408718	1.1231062	3.3655560
C	3.5788603	0.6806154	1.1708324
C	3.3319725	-0.2567354	0.1707144

H	1.0479557	-4.9623975	-1.1661895	C	4.9132697	3.3750327	1.1134838
C	3.8419829	-0.0688946	-3.7955393	C	2.7121811	4.4414526	1.4162987
H	6.4493401	-1.0241239	-3.7808032	C	3.3726638	5.7046271	1.4778717
H	6.1880427	-2.4571879	-2.7286077	C	1.2953823	4.3406654	1.5251887
C	3.4841234	-2.1343017	-2.3226438	H	0.7091053	5.2486423	1.7354171
C	1.3905172	-3.2919986	1.7235175	C	0.6325141	3.1265894	1.3914561
C	2.5748301	-3.5602718	-0.5247023	C	3.9603926	-1.5374146	0.0719175
C	4.4710360	-1.0826568	-2.8252158	C	4.9557845	-1.8199143	0.9984885
C	3.4044780	-2.4799352	-0.9439140	H	5.5085896	-2.7692954	0.9267381
C	2.4992582	-4.0159007	0.9364276	C	5.2519162	-0.9327496	2.0763105
H	2.9413861	0.4002916	-3.3528901	C	6.2211454	-1.2787192	3.0647810
H	1.5132123	-2.1924087	1.7016645	C	4.5280558	0.3113124	2.2091040
H	3.5489593	-0.5417822	-4.7558962	C	4.7624738	1.1103654	3.3674296
H	-0.7362122	-2.6407921	-3.1538817	C	3.5810974	0.6761643	1.1818727
H	0.3908775	-3.5187030	1.2964095	C	3.3272137	-0.2571693	0.1793574
H	1.7550062	-4.1364472	-5.6664961	O	0.7389921	0.7651981	0.9630653
H	4.8355722	-0.5146260	-1.9439175	O	2.4221696	0.0891106	-0.8224777
H	3.4587805	-3.7410362	1.4177526	P	0.8253050	0.0567996	-0.5130309
H	2.6738125	-2.4864885	-4.2955832	O	0.2267831	0.9457229	-1.6362284
Zn	-1.1112662	0.3553164	-2.8497784	O	0.2432036	-1.3463487	-0.4043783
Br	-1.6638749	0.5353465	-5.0650362	C	4.7507829	5.7963048	1.3573056
C	-7.0583860	1.0513401	-1.8262757	C	5.5230224	4.6207302	1.1616066
C	-3.4908000	-1.1675932	-2.4952240	H	2.7609792	6.6104607	1.6132489
C	-6.0303797	1.0873362	-0.8620730	H	5.2464522	6.7780092	1.4004497
C	-5.7452760	-0.4622985	-3.1954854	H	5.5203436	2.4736167	0.9508359
C	-4.7067426	-0.4303572	-2.2263477	H	6.6143555	4.6973811	1.0408781
C	-6.9128028	0.2821513	-2.9950973	C	5.6988623	0.7331678	4.3204318
C	-4.8527853	0.3625102	-1.0565697	C	6.4481558	-0.4620615	4.1622809
O	-2.3833199	-0.9463963	-1.8769500	H	4.1842514	2.0343623	3.5054914
H	-7.9790724	1.6328411	-1.6652106	H	5.8569019	1.3647171	5.2078790
H	-5.6072985	-1.0448319	-4.1199893	H	7.1944610	-0.7469896	4.9193672
H	-6.1551979	1.6885635	0.0503826	H	6.7758141	-2.2228500	2.9466096
H	-7.7107524	0.2692761	-3.7523580	C	-1.7962800	3.2687425	0.6278470
H	-4.0508685	0.3677821	-0.2999866	C	-0.8417748	3.0093676	1.6437977
Br	-2.6042107	-0.8626116	1.7006735	C	-3.1645976	3.2248384	0.9582482
Zn	-1.5913385	-2.0199943	-0.0999200	C	-1.2697219	2.6596043	2.9549919
H	-6.2800689	-4.4830148	-1.9114800	C	-2.6472015	2.6120328	3.2262820
H	-1.3378213	-4.5410701	-0.9363776	C	-3.6133860	2.9047457	2.2493644
C	-4.5781702	-3.3535907	-1.1699562	H	-3.9135488	3.4447277	0.1802488
C	-5.4870926	-3.7872367	-2.2709342	C	-0.2772928	2.2972431	4.0590302
H	-4.9097604	-2.7804416	-0.2921852	H	-2.9758992	2.3297754	4.2387883
C	-3.3403640	-3.9306596	-1.3454339	C	-0.2953011	0.7814300	4.3349260
C	-2.1588558	-3.9362347	-0.5109986	H	-1.2807811	0.4581030	4.7297629
C	-3.3874824	-4.6256478	-2.6791982	H	0.4797618	0.5110088	5.0820976
O	-4.6501439	-4.4829247	-3.2065760	H	-0.1128170	0.2023787	3.4088803
O	-2.5149531	-5.2441449	-3.2524087	C	-0.5031554	3.1132260	5.3432169
H	-6.0045340	-2.9523168	-2.7937997	H	0.7390083	2.5522739	3.6952849
H	3.1290010	-6.0798634	0.4915562	H	-1.4847793	2.8880967	5.8097116
H	1.3629981	-5.8987206	0.7350665	H	-0.4685445	4.2033014	5.1419353
H	2.4584349	-5.8374333	2.1401679	H	0.2777656	2.8771023	6.0951299
H	-2.3756517	-4.2139157	0.5408769	C	-5.1004680	2.8682079	2.5786194
H	-3.4670757	-1.8134862	-3.4017226	C	-5.5562776	1.4668307	3.0232653
				H	-6.6564423	1.4355346	3.1673246
				H	-5.0858945	1.1809554	3.9868481
				H	-5.2709633	0.6902308	2.2857138
				C	-5.4768925	3.9383307	3.6189869
				H	-5.6412425	3.1210320	1.6381157
				H	-6.5696947	3.9377264	3.8128914
				H	-5.1856629	4.9525930	3.2792776
				H	-4.9660672	3.7500413	4.5862149
				C	-1.3689957	3.6045294	-0.7985932
				C	-2.2258591	2.8822279	-1.8521909
				H	-1.7665222	2.9552020	-2.8597848
				H	-3.2493088	3.3016842	-1.9403003
				H	-2.3653436	1.8132544	-1.5742201
				C	-1.3670271	5.1238027	-1.0472820
				H	-0.3297931	3.2393265	-0.9249061
				H	-1.0402060	5.3576677	-2.0817941
				H	-0.6809632	5.6423268	-0.3485785
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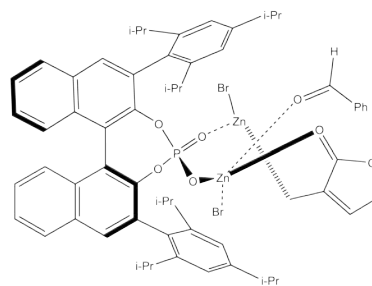
TS1-8-q



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number of imaginary frequencies: 1

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C	3.4990858	3.2424556	1.2539609

H	5.3627391	-2.3142526	-4.3663486
C	0.6229079	-4.2437582	-3.7782270
H	4.5012742	0.7842691	-4.0310006
H	-1.2027742	-3.4388178	-4.7000388
H	1.4509131	-3.6623788	2.7868983
C	1.7021818	-3.7458145	-2.8299784
C	5.6607534	-1.7178807	-3.4786579
C	-0.3408343	-3.0840972	-4.1008806
H	0.1659395	-2.2782849	-4.6721944
C	2.6175512	-2.7605750	-3.2398944
C	2.3925899	-5.5642887	1.0449906
H	1.8626115	-5.7235313	-4.8267200
C	1.7542509	-4.1735426	-1.4939788
C	1.1825359	-4.8796609	-5.0601352
H	0.3584103	-5.2667218	-5.6934176
H	1.0756025	-4.9811459	-1.1787810
C	3.7853384	-0.0266485	-3.7854743
H	6.4013164	-0.9603942	-3.8098743
H	6.1630545	-2.4052187	-2.7683132
C	3.4628108	-2.1104383	-2.3292561
C	1.4402311	-3.3217251	1.7311111
C	2.5908028	-3.5665189	-0.5375290
C	4.4339627	-1.0444547	-2.8325744
C	3.4026577	-2.4717191	-0.9535686
C	2.5356310	-4.0384869	0.9193747
H	2.8888002	0.4344651	-3.3267306
H	1.5665567	-2.2224618	1.7228551
H	3.4820129	-0.4923014	-4.7461192
H	-0.7406931	-2.6394025	-3.1647775
H	0.4344435	-3.5388131	1.3141247
H	1.7526426	-4.1452587	-5.6672833
H	4.8035251	-0.4815589	-1.9500497
H	3.5028103	-3.7705914	1.3894077
H	2.6371043	-2.4531255	-4.2970690
Zn	-1.0675471	0.2801448	-2.8609397
Br	-1.6455275	0.5057521	-5.0567043
C	-7.0396544	1.0336711	-1.8501477
C	-3.4721292	-1.1985513	-2.4768373
C	-6.0113882	1.0882145	-0.8878959
C	-5.7267426	-0.5050782	-3.1904231
C	-4.6882061	-0.4554764	-2.2224305
C	-6.8942164	0.2429375	-3.0041391
C	-4.8332818	0.3605187	-1.0691655
O	-2.3676594	-0.9719663	-1.8579532
H	-7.9603911	1.6182675	-1.7004168
H	-5.5866514	-1.1045733	-4.1038632
H	-6.1334819	1.7053684	0.0141956
H	-7.6919218	0.2168508	-3.7614423
H	-4.0309346	0.3802875	-0.3133273
Br	-2.6850097	-0.9127076	1.7115163
Zn	-1.5973993	-2.0283760	-0.0637673
H	-6.2811364	-4.4913621	-1.8159481
H	-1.3209913	-4.5449680	-0.9407173
C	-4.5687743	-3.3632273	-1.0924413
C	-5.4981469	-3.7859983	-2.1814303
H	-4.8765188	-2.7947574	-0.2026226
C	-3.3351688	-3.9395490	-1.2994510
C	-2.1381917	-3.9534886	-0.4908051
C	-3.4038849	-4.6081012	-2.6478969
O	-4.6812483	-4.4594571	-3.1464002
O	-2.5382867	-5.2033161	-3.2502965
H	-6.0318350	-2.9430026	-2.6758454
H	3.1494210	-6.0991431	0.4365197
H	1.3907059	-5.9164171	0.7225586
H	2.5168148	-5.8742753	2.1026071
H	-2.3302422	-4.2374106	0.5639641
H	-3.4463994	-1.8549230	-3.3761436



Energy(Hartree)=-11970.03578386

Zn	2.1370786	2.3123032	-1.3312866
Br	4.4138856	2.1796183	-1.6198545
C	-2.5055911	2.6752869	-0.4995100
C	-1.2222243	3.2207025	-0.5657748
C	-0.9759017	4.3511971	-1.3783923
C	-2.0426740	4.9554338	-2.0863432
C	-3.3263792	4.3967693	-2.0269926
C	-3.5550583	3.2525690	-1.2413818
H	-2.6887987	1.7926116	0.1280881
H	-0.4034586	2.7806404	0.0165349
C	0.3742073	4.8876830	-1.5238434
H	-1.8507162	5.8475875	-2.7040883
H	-4.1518827	4.8501282	-2.5954559
H	-4.5536903	2.7912542	-1.2043323
O	1.4291318	4.3170866	-1.2049768
C	-0.1284311	0.6255103	-5.8199713
C	-0.5341088	1.2481608	-4.6722908
C	0.7129030	1.5765071	-3.9493050
O	1.7955837	1.1634352	-4.6235694
C	1.3591552	0.5219126	-5.8390273
O	0.7984158	2.1642682	-2.8616227
C	-1.8446892	1.5114675	-4.0731547
H	1.7317469	-0.5249228	-5.8105862
H	1.8511443	1.0381589	-6.6927640
Zn	-2.1474529	0.3516827	-2.4451362
Br	-3.9544419	-0.6488966	-1.3597768
H	-2.6753209	1.3640557	-4.7893439
H	-1.8921208	2.5407431	-3.6606232
H	-0.7727569	0.2174161	-6.6100131
C	-0.5924742	-0.4271106	2.3110164
C	-0.2621907	-1.7635228	2.5751588
C	0.0833297	-2.1295786	3.9299416
C	0.6208487	-3.4071907	4.2747345
C	-0.0858383	-1.1612200	4.9841151
C	0.2177283	-1.5256626	6.3298188
C	-0.5248842	0.1506464	4.6557690
H	-0.6760173	0.8800203	5.4664258
C	-0.7380596	0.5518786	3.3424868
C	0.8005730	-3.5273046	-0.6579026
C	0.2080134	-4.7736841	-0.4889345
H	0.4078822	-5.5665928	-1.2250414
C	-0.6894204	-5.0442018	0.5830810
C	-1.3683242	-6.2955633	0.6814032
C	-0.9410842	-4.0276387	1.5753845
C	-1.9083973	-4.2948675	2.5892688
C	-0.2239591	-2.7790674	1.4882182
C	0.5557647	-2.5500342	0.3534903
O	-0.8812435	-0.0229546	1.0103928
O	1.1925613	-1.3196570	0.2201640
P	0.2712402	-0.0236381	-0.1739717
O	1.2052242	1.1873397	-0.0022259
O	-0.4493424	-0.2111026	-1.5047536
C	0.7083124	-2.7859689	6.6328115
C	0.9262138	-3.7255051	5.5904910
H	0.0694169	-0.7755166	7.1225188
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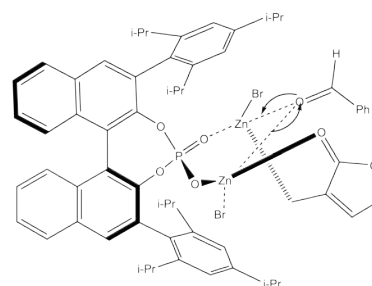
7.2.2.6 to 15l-mi
int1-8-l

H	0.8068872	-4.1431852	3.4810318
H	1.3476436	-4.7147365	5.8256958
C	-2.5661463	-5.5155783	2.6451241
C	-2.2855453	-6.5318901	1.6936859
H	-2.1394712	-3.5128134	3.3259739
H	-3.3165269	-5.6942224	3.4302819
H	-2.8086399	-7.4984727	1.7524548
H	-1.1604247	-7.0664446	-0.0773197
C	-0.1657286	2.9741120	2.8947930
C	-1.1510918	1.9606902	3.0458252
C	-0.5968973	4.3014472	2.7040609
C	-2.5344671	2.2816732	2.9899186
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C	-1.9575654	4.6510491	2.6649388
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C	-3.6041430	1.2133201	3.2206899
H	-3.9802101	3.8769625	2.7740687
C	-4.7580898	1.2517762	2.2062196
H	-5.2930212	2.2243376	2.2137238
H	-5.5039928	0.4677589	2.4489427
H	-4.4083706	1.0504780	1.1741251
C	-4.1286165	1.3063140	4.6673641
H	-3.1152207	0.2231711	3.1127359
H	-4.6263983	2.2823988	4.8470491
H	-3.3042054	1.2113971	5.4025483
H	-4.8664622	0.5035247	4.8735836
C	-2.3828873	6.1062108	2.5094210
C	-3.3130695	6.3201271	1.3041028
H	-3.5608603	7.3949009	1.1819208
H	-4.2702928	5.7717823	1.4266337
H	-2.8463066	5.9628319	0.3655722
C	-3.0181550	6.6373265	3.8079788
H	-1.4558135	6.6934702	2.3258538
H	-3.2747229	7.7131356	3.7152322
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H	-3.9527564	6.0877540	4.0468285
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H	2.9125084	2.4956896	4.4871069
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H	5.5214605	-4.0000892	-1.0463773
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C	3.7752262	-2.5114369	-2.8069039
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H	4.5278879	-4.1651552	-5.8580560
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H	5.1884463	-4.2231920	0.6997519
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C	3.7260825	-2.9482298	-0.3253465
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H	-0.8689065	-1.3268982	-3.8573212
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H	4.1256965	0.0589169	-4.7616231
H	-0.8145287	-2.3902860	-5.2876091
H	5.7723725	-3.3956162	-4.8275780
H	2.9607937	-3.1551156	0.4493818
H	-0.9342317	-3.3851340	-2.3724826
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TS1-8-a; woelfling data



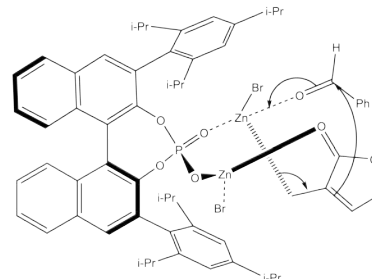
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C	-2.582802	5.655387	-0.195708
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H	-4.988127	2.745141	-1.236823
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C	0.665455	5.259343	-2.291843
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C	-1.149233	2.302770	-3.822584
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Br	-4.094149	0.118363	-1.986721
H	-0.514303	1.584154	-4.381970
H	-1.933735	2.711700	-4.486612
H	-1.360702	5.296516	-3.354326
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C	0.111454	-3.533637	3.025054
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C	0.178658	-2.894507	4.318199
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C	-0.070671	-1.497369	4.426979
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H	-0.209752	-5.286627	-2.946344
C	-1.154478	-5.249445	-0.979094
C	-1.936314	-6.420961	-1.206441
C	-1.257007	-4.572531	0.294649
C	-2.179338	-5.079281	1.257005
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C	0.279726	-2.904551	-0.555075
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O	1.015408	-1.749646	-0.380048
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O	-0.565693	0.062226	-1.469913
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H	1.165679	-5.582965	6.238813
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H	1.171645	-6.675112	3.970579
C	-2.938820	-6.211546	0.995181
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C	-3.836619	0.716240	2.116889
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H	-2.718809	-0.564907	3.426066
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C	-0.891677	5.089132	4.009588
C	-2.060385	5.785582	3.302092
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H	-3.042104	5.454160	3.698116
H	-2.066612	5.582456	2.218189
C	-0.963975	5.351898	5.526355
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H	-1.898768	4.924013	5.945266
C	2.076830	1.024569	3.454974
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H	3.999606	1.300945	2.445771
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H	2.621813	2.114612	1.637189
C	2.618667	0.828482	4.884988
H	2.007696	0.026282	2.975062
H	3.628417	0.368774	4.867700
H	1.958692	0.178065	5.491689
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H	2.997427	-0.347498	-6.580898
H	5.028375	-3.999217	-2.695047
H	-2.079355	-3.643996	-5.890538
C	3.502486	-0.292861	-5.590549

H	4.623021	-2.822803	0.251260
H	3.914228	1.853772	-5.810569
H	-2.720530	-1.458805	-4.551478
C	2.735307	-1.228884	-4.662204
C	4.242582	-4.402067	-2.022429
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H	5.062238	-1.758587	-6.108937
C	1.395115	-1.554529	-4.926386
C	4.970203	-0.700114	-5.792434
H	5.446003	-0.065129	-6.567365
H	0.926487	-1.149773	-5.839111
C	4.160919	-2.290867	-0.605514
H	4.747269	-4.946551	-1.197533
H	3.646556	-5.133535	-2.605022
C	2.603533	-2.602054	-2.622503
C	-1.627326	-1.288969	-4.500760
C	0.621684	-2.355825	-4.062883
H	-0.462933	-4.392372	-5.647376
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H	3.513041	-1.492588	-0.193646
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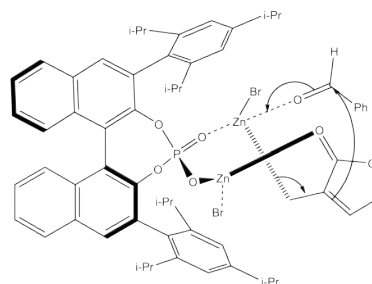


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C	-6.2007055	4.6753708	1.3478055
H	-6.6247020	3.4679960	-0.4143136
H	-4.3679636	2.4174578	-0.4693826
C	-2.2708526	2.8679603	1.2384404
H	-3.2146330	4.7129809	3.0318660
H	-5.4868310	5.7391810	3.1105897
H	-7.2020480	5.1318252	1.3788072
O	-2.0383813	1.8927216	0.4215506
C	-1.0539545	4.4593915	0.7845362
C	-0.5658449	4.1315465	-0.5199215
C	0.8159962	3.6465307	-0.3265659
O	1.2057780	3.8052666	0.9391603
C	0.1426620	4.4360235	1.7100360

O	1.5826250	3.1356888	-1.1662891	H	-3.1232633	1.5037350	6.9527598
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Br	-3.6845599	1.3176533	-2.9845759	H	2.3107447	1.4283162	2.6084978
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C	-0.5062261	-2.1514491	2.3427864	H	-1.5902426	1.5947090	-5.2228951
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C	0.3982316	-2.9307949	-4.1806220	C	4.9049671	-2.8571935	-3.3739345
H	0.6214913	-2.9062024	-5.2573299	C	4.0027775	3.7228891	-3.4876567
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O	1.3559270	-1.2734759	-1.0765409	H	2.0436301	2.1063141	-5.2881841
P	0.4152424	-0.0556202	-0.5151959	C	4.5168846	-1.7882402	-1.0997089
O	1.3973399	0.7344523	0.3826693	H	5.3031976	-3.7687338	-2.8818444
O	-0.2970376	0.6889008	-1.6407591	H	4.4377707	-3.1588506	-4.3333457
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H	-2.8054803	-6.2160965	-4.8793803	H	5.4001557	-1.1256741	-1.2040741
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C	0.1462187	0.8773857	4.5540517	H	3.0720747	-2.8635309	-2.2669758
C	-2.0506129	-0.4972792	3.4664616	H	-0.5304691	-0.4496959	-4.4888365
C	-2.2366490	0.5902187	4.3413205	H	5.1267908	0.1944214	-2.9584888
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TS2-8-a

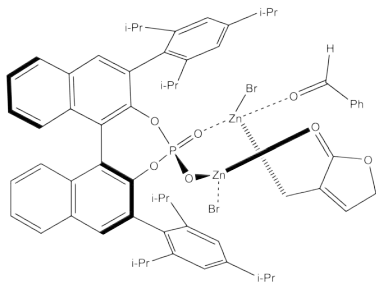


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Br	5.1079801	1.9511109	0.0216564
C	-5.8727250	3.7364721	0.3465044
C	-4.5993925	3.1491661	0.3071274
C	-3.6264254	3.4901845	1.2689704

C	-3.9616970	4.4217456	2.2774185	H	-3.5146458	0.1305308	1.1803466
C	-5.2349227	5.0026889	2.3204160	C	-4.1061259	-1.8729567	4.0075879
C	-6.1956612	4.6632666	1.3502117	H	-2.8925614	-2.0353547	2.2469490
H	-6.6179040	3.4587952	-0.4145823	H	-4.5406539	-1.1139127	4.6913912
H	-4.3655794	2.4086114	-0.4728643	H	-3.4924572	-2.5640586	4.6208894
C	-2.2673235	2.8555357	1.2385754	H	-4.9478584	-2.4523064	3.5751870
H	-3.2121658	4.6928532	3.0367754	C	-1.3577705	2.3669211	5.9661308
H	-5.4827886	5.7232131	3.1151151	C	-2.0778674	3.5967441	5.3905676
H	-7.1966557	5.1204194	1.3815375	H	-2.1898184	4.3911829	6.1572741
O	-2.0287791	1.8857629	0.4202007	H	-3.0928934	3.3357396	5.0262334
C	-1.0508662	4.4623663	0.7768708	H	-1.5142008	4.0274334	4.5373712
C	-0.5639779	4.1304966	-0.5270162	C	-2.0908053	1.8280340	7.2081266
C	0.8177840	3.6449281	-0.3334564	H	-0.3457570	2.6948236	6.2915782
O	1.2090474	3.8097005	0.9337796	H	-2.1701867	2.6086523	7.9929344
C	0.1466181	4.4402798	1.7015216	H	-1.5595621	0.9564993	7.6398671
O	1.5840939	3.1318570	-1.1699699	H	-3.1209007	1.5006989	6.9558860
C	-1.2231494	3.9600504	-1.7436430	C	1.8235532	-0.5846900	3.3245769
H	0.5072238	5.4499002	1.9941721	C	2.7668598	0.6247653	3.2074698
H	0.0203079	3.8297531	2.6203735	H	3.7164900	0.3311041	2.7162323
Zn	-1.9403804	1.8234764	-1.5322628	H	3.0318596	1.0429969	4.2010918
Br	-3.6885695	1.3521150	-2.9925357	H	2.3095354	1.4341703	2.6062605
H	-0.6100493	3.7648329	-2.6394656	C	2.3871443	-1.6061396	4.3316472
H	-2.2101792	4.4223752	-1.9027728	H	1.7955065	-1.0738685	2.3285174
H	-1.8033008	5.2516442	0.9094588	H	3.4264443	-1.8871654	4.0630136
C	-0.4505431	-2.1016887	0.9169280	H	1.7824885	-2.5331692	4.3606095
C	-0.2170682	-3.2250451	0.1088241	H	2.4024388	-1.1782985	5.3559860
C	0.0499107	-4.4827322	0.7706195	H	4.3934851	2.8439463	-5.4133008
C	0.4714426	-5.6538732	0.0697091	H	5.7689414	-2.1844192	-3.6062752
C	-0.0701587	-4.5630327	2.2069511	H	-0.9192566	-0.2527084	-6.9568718
C	0.1545999	-5.8110504	2.8615364	C	4.5297071	2.5593940	-4.3448910
C	-0.3627428	-3.3871932	2.9530925	H	4.8547214	-2.7034738	-0.5738699
H	-0.4483813	-3.4567799	4.0486056	H	4.5426352	4.6688881	-3.7259776
C	-0.5088328	-2.1483495	2.3419913	H	-1.5926561	1.5889171	-5.2232038
C	1.0364167	-2.0408217	-3.3218399	C	3.6799773	1.3095657	-4.1312320
C	0.4021361	-2.9315406	-4.1785335	C	4.9110676	-2.8480431	-3.3700844
H	0.6257996	-2.9047357	-5.2550684	C	4.0004023	3.7297731	-3.4904315
C	-0.5698498	-3.8642952	-3.7058246	H	4.1498617	3.5180602	-2.4114239
C	-1.2768525	-4.7077846	-4.6139061	C	4.1128685	0.2023549	-3.3803892
C	-0.8711304	-3.9490307	-2.2946677	C	0.1112683	-0.2513534	-6.5455691
C	-1.9041613	-4.8360192	-1.8713057	H	6.4286202	1.5019929	-4.6963717
C	-0.1375451	-3.1109754	-1.3784559	C	2.3905303	1.2503081	-4.6875304
C	0.7257187	-2.1670416	-1.9330543	C	6.0291337	2.3482713	-4.1017079
O	-0.7119373	-0.8589521	0.3446853	H	6.5969654	3.2590479	-4.3795942
O	1.3589088	-1.2764057	-1.0741782	H	2.0415568	2.1052006	-5.2876557
P	0.4194456	-0.0557426	-0.5172209	C	4.5179313	-1.7836198	-1.0944304
O	1.4029888	0.7352356	0.3784095	H	5.3122795	-3.7591194	-2.8796136
O	-0.2922329	0.6859663	-1.6448114	H	4.4457646	-3.1491003	-4.3304049
C	0.5255725	-6.9371544	2.1440504	C	3.2983593	-0.9302805	-3.1812558
C	0.7021112	-6.8479565	0.7381345	C	-0.5126714	1.6287329	-4.9822666
H	0.0439706	-5.8552229	3.9564728	C	1.5190805	0.1658559	-4.4849166
H	0.7022919	-7.8921836	2.6617067	H	0.5249721	-1.2737225	-6.6519593
H	0.6258591	-5.6032906	-1.0162029	H	0.7304695	0.4192290	-7.1778877
H	1.0315325	-7.7319771	0.1711141	C	3.8947600	-2.1363340	-2.4548797
C	-2.5841860	-5.6291946	-2.7851582	C	1.9777844	-0.9443411	-3.7164457
C	-2.2608982	-5.5764535	-4.1665618	C	0.1143940	0.2293559	-5.0811570
H	-2.1652985	-4.8777253	-0.8043510	H	3.7850216	-1.2730878	-0.4396211
H	-3.3843510	-6.2993969	-2.4359427	H	-0.4173627	2.0221699	-3.9522631
H	-2.8025644	-6.2139298	-4.8817527	H	5.3994808	-1.1183544	-1.1949543
H	-1.0351732	-4.6422479	-5.6863965	H	2.9179858	3.9021850	-3.6522225
C	0.3871464	-0.1927744	3.6719132	H	-0.0364161	2.3533740	-5.6751966
C	-0.7287566	-0.9094784	3.1593479	H	6.2380623	2.1473223	-3.0304422
C	0.1470156	0.8792007	4.5526652	H	3.0771500	-2.8609322	-2.2649772
C	-2.0511655	-0.4944380	3.4673899	H	-0.5299996	-0.4530361	-4.4895433
C	-2.2357442	0.5921692	4.3433698	H	5.1242786	0.2032523	-2.9504369
C	-1.1501921	1.2709316	4.9258890	H	-1.7880459	2.7545570	2.2405284
H	1.0036696	1.4188040	4.9866694				
C	-3.2687270	-1.2171695	2.8950069				
H	-3.2641134	0.8989787	4.5948336				
C	-4.1183044	-0.2920503	2.0062384				
H	-4.5388821	0.5591298	2.5826013				
H	-4.9717171	-0.8487569	1.5673149				

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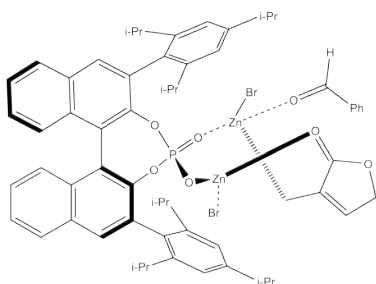
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C	-4.5465774	2.9655436	1.3124124
C	-4.0266389	2.2082653	2.3895179
C	-4.6542879	2.2686554	3.6567873
C	-5.7724186	3.0876904	3.8512758
C	-6.2789621	3.8438364	2.7779386
H	-6.0723990	4.3617008	0.6708610
H	-4.0793897	2.8994840	0.3157874
C	-2.8331628	1.3697280	2.2190083
H	-4.2503440	1.6747534	4.4898325
H	-6.2546321	3.1378883	4.8391377
H	-7.1607028	4.4857375	2.9288942
O	-2.1212690	1.3409158	1.2046465
C	-0.9675820	3.1963150	3.6739897
C	-0.3634723	3.5114036	2.4770885
C	0.9265951	2.7968109	2.5059950
O	1.0749715	2.0858799	3.6358772
C	-0.0958999	2.2765758	4.4635983
O	1.8215741	2.7792395	1.6366218
C	-0.8140574	4.2139566	1.2863309
H	0.2442202	2.6851021	5.4403934
H	-0.5338116	1.2702799	4.6513124
Zn	-1.3799490	2.8256520	-0.1412060
Br	-2.7946740	3.0087582	-2.0358081
H	0.0100294	4.7550296	0.7810559
H	-1.6753640	4.8828526	1.4686027
H	-1.9391049	3.5599654	4.0324602
C	-0.5933628	-2.1158400	-0.8261643
C	-0.1576210	-2.4226662	-2.1241879
C	-0.0300445	-3.8182611	-2.4790149
C	0.5652607	-4.2554885	-3.7020688
C	-0.4803364	-4.8266359	-1.5493232
C	-0.3870848	-6.2053075	-1.9078981
C	-0.9736971	-4.4333072	-0.2737147
H	-1.3237327	-5.2088790	0.4250480
C	-1.0023285	-3.1017899	0.1217744
C	1.8250587	0.5549055	-3.5139032
C	1.4067174	0.5792446	-4.8383423
H	1.8686610	1.2857477	-5.5433999
C	0.3594319	-0.2684127	-5.3101554
C	-0.1203094	-0.1629761	-6.6502961
C	-0.2485697	-1.2338743	-4.4234082
C	-1.3431612	-2.0088452	-4.9082519
C	0.2559583	-1.3512103	-3.0778367
C	1.2132915	-0.4230256	-2.6708611
O	-0.7189661	-0.7926342	-0.4149624
O	1.6312603	-0.4549178	-1.3457537
P	0.5779593	0.1973082	-0.2689592
O	1.3117542	-0.0088919	1.0804969
O	0.1545560	1.6031683	-0.6553391
C	0.1646926	-6.5915549	-3.1197146
C	0.6598749	-5.6049131	-4.0136406
H	-0.7490523	-6.9589662	-1.1908813
H	0.2370503	-7.6579900	-3.3823018

H	0.9655013	-3.5096109	-4.4016670
H	1.1294116	-5.9115957	-4.9608419
C	-1.7969155	-1.8674617	-6.2128749
C	-1.1738333	-0.9471626	-7.0973225
H	-1.8362974	-2.7184853	-4.2287065
H	-2.6498882	-2.4693587	-6.5619164
H	-1.5377868	-0.8474093	-8.1312710
H	0.3547744	0.5697731	-7.3214945
C	-0.5584703	-2.6675224	2.5751489
C	-1.4772015	-2.7151765	1.4911566
C	-1.0589015	-2.4175348	3.8672858
C	-2.8570437	-2.4501481	1.7059592
C	-3.3023968	-2.1890571	3.0169406
C	-2.4246022	-2.2000060	4.1172109
H	-0.3629924	-2.4136806	4.7209565
C	-3.8570887	-2.4538991	0.5495199
H	-4.3754606	-2.0008803	3.1839271
C	-4.2958559	-1.0269565	0.1702931
H	-4.8050330	-0.5251707	1.0208731
H	-5.0109470	-1.0522409	-0.6777723
H	-3.4338078	-0.3994709	-0.1269679
C	-5.0683523	-3.3602242	0.8298272
H	-3.3344379	-2.8765607	-0.3330995
H	-5.6910973	-2.9730946	1.6633896
H	-4.7513907	-4.3893283	1.0955745
H	-5.7210393	-3.4212802	-0.0651069
C	-2.9270950	-2.0361359	5.5480354
C	-3.5476481	-0.6532543	5.8020432
H	-3.8648633	-0.5456436	6.8598573
H	-4.4446916	-0.4954525	5.1675718
H	-2.8227217	0.1585651	5.5832517
C	-3.9069520	-3.1606078	5.9302186
H	-2.0382877	-2.1276373	6.2102319
H	-4.2100587	-3.0775213	6.9945327
H	-3.4498382	-4.1589174	5.7782495
H	-4.8294227	-3.1163001	5.3141789
C	0.9340253	-2.9308266	2.3758889
C	1.8255435	-2.1082552	3.3217719
H	2.8808040	-2.1410229	2.9827544
H	1.8039636	-2.5015675	4.3597455
H	1.5106544	-1.0469710	3.3488573
C	1.2581252	-4.4321463	2.5066056
H	1.1837700	-2.6195871	1.3405201
H	2.3412957	-4.6129377	2.3466839
H	0.7001248	-5.0397795	1.7679164
H	0.9952635	-4.8027637	3.5197603
H	5.5671285	4.9917969	-1.0852666
H	6.5130354	-0.0838067	-3.0943715
H	0.6092671	4.5599098	-5.0933166
C	5.4664477	4.0394658	-0.5162420
H	4.9508259	-2.3492982	-1.4472220
H	5.3342638	5.1243310	1.3916393
H	-0.3481879	4.8201546	-2.6590342
C	4.5939748	3.1242601	-1.3713195
C	5.6202483	-0.5891976	-3.5187888
C	4.7561101	4.3751730	0.8118568
H	4.6601058	3.4641614	1.4385600
C	4.8604101	1.7563718	-1.5541545
C	1.5430546	4.1310807	-4.6741980
H	7.4023627	3.2375766	-1.1934104
C	3.4439280	3.6493054	-1.9872733
C	6.8765473	3.4974160	-0.2523077
H	7.4862726	4.2533780	0.2826182
H	3.2266958	4.7210778	-1.8586822
C	4.7396434	-1.2809301	-1.2353758
H	5.8978163	-1.6416921	-3.7359989
H	5.3766744	-0.0912811	-4.4793126
C	4.0130935	0.9249989	-2.3136957
C	0.6826811	4.5638676	-2.3445432
C	2.5431565	2.8592772	-2.7227304
H	1.9354754	3.3921392	-5.4000324

H	2.2909592	4.9485819	-4.5989532
C	4.4307277	-0.5281290	-2.5401446
C	2.8303494	1.4721573	-2.8882395
C	1.2816853	3.5088455	-3.2884783
H	3.8824759	-1.2344756	-0.5357712
H	0.6389078	4.1780408	-1.3077662
H	5.6246920	-0.8650030	-0.7118133
H	3.7361712	4.7743138	0.6444166
H	1.2769849	5.5015213	-2.3307801
H	6.8453409	2.5901228	0.3864049
H	3.5873950	-1.0540167	-3.0317279
H	0.5197170	2.7100085	-3.4022676
H	5.7608036	1.3154501	-1.1036450
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Energy(Hartree)= -11970.0195831

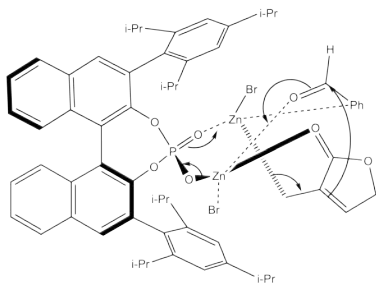
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C	-4.5747788	3.0360048	1.2347139
C	-4.1044033	2.2155016	2.2875736
C	-4.7796932	2.2130922	3.5311315
C	-5.8958229	3.0337663	3.7288777
C	-6.3520360	3.8549101	2.6814872
H	-6.0586327	4.4834934	0.6147892
H	-4.0730220	3.0184047	0.2521637
C	-2.9145245	1.3696280	2.1166860
H	-4.4156287	1.5640650	4.3413422
H	-6.4162679	3.0340406	4.6985428
H	-7.2318782	4.4989544	2.8349158
O	-2.1777673	1.3695280	1.1216145
C	-1.0117999	3.0800279	3.6450126
C	-0.3849489	3.4532319	2.4756353
C	0.9147008	2.7534121	2.5035736
O	1.0464909	1.9989586	3.6092145
C	-0.1510018	2.1258258	4.4068745
O	1.8289827	2.7795397	1.6571597
C	-0.8152666	4.1991868	1.3078118
H	0.1530480	2.4768102	5.4180293
H	-0.5801701	1.1032825	4.5153504
Zn	-1.3775473	2.8653425	-0.1829406
Br	-2.7708097	3.1429272	-2.0639768
H	0.0156119	4.7517409	0.8276742
H	-1.6810193	4.8604408	1.4952112
H	-1.9954267	3.4185115	3.9946971
C	-0.5988876	-2.1017320	-0.8156875
C	-0.1707460	-2.4066653	-2.1169171
C	-0.0476794	-3.8016673	-2.4754186
C	0.5379393	-4.2367604	-3.7036174
C	-0.4929053	-4.8118129	-1.5454434
C	-0.4046816	-6.1890314	-1.9087846
C	-0.9749109	-4.4206931	-0.2652436
H	-1.3195679	-5.1966476	0.4358789
C	-0.9993005	-3.0903044	0.1336550
C	1.8196648	0.5676697	-3.5019456

C	1.3958884	0.5993080	-4.8242821
H	1.8581782	1.3080946	-5.5267078
C	0.3442771	-0.2421528	-5.2968945
C	-0.1391994	-0.1295904	-6.6345295
C	-0.2642665	-1.2098360	-4.4131663
C	-1.3616291	-1.9797821	-4.8987771
C	0.2429738	-1.3338617	-3.0693522
C	1.2053157	-0.4111248	-2.6619553
O	-0.7242957	-0.7797577	-0.4013964
O	1.6238036	-0.4477104	-1.3370207
P	0.5727052	0.2130397	-0.2638816
O	1.3054437	0.0127695	1.0868689
O	0.1511406	1.6173393	-0.6556184
C	0.1369334	-6.5729535	-3.1252213
C	0.6271021	-5.5850348	-4.0195334
H	-0.7623234	-6.9440136	-1.1909908
H	0.2052742	-7.6387771	-3.3910788
H	0.9336575	-3.4889701	-4.4035318
H	1.0887819	-5.8897068	-4.9711541
C	-1.8175234	-1.8317799	-6.2014016
C	-1.1950001	-0.9090527	-7.0826186
H	-1.8542196	-2.6907295	-4.2203806
H	-2.6727947	-2.4299916	-6.5509392
H	-1.5616116	-0.8029372	-8.1149120
H	0.3350782	0.6061165	-7.3029651
C	-0.5254780	-2.6309990	2.5772819
C	-1.4599603	-2.7039092	1.5080191
C	-1.0087117	-2.3577730	3.8711565
C	-2.8404841	-2.4579730	1.7409563
C	-3.2683709	-2.1772369	3.0536311
C	-2.3722121	-2.1479089	4.1381328
H	-0.2995026	-2.3318271	4.7133337
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H	-4.3417998	-2.0048437	3.2345622
C	-4.3031299	-1.0882760	0.1786630
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H	-3.4454764	-0.4679268	-0.1446873
C	-5.0652565	-3.3967846	0.9284128
H	-3.3478355	-2.9533842	-0.2737715
H	-5.6819925	-2.9790350	1.7516603
H	-4.7455126	-4.4146223	1.2309706
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C	-2.8531441	-1.9635391	5.5739277
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H	-3.8469975	-0.4900890	6.8639031
H	-4.4759824	-0.5336448	5.1903690
H	-2.8885979	0.2339753	5.5330144
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C	0.9641968	-2.8985452	2.3630984
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H	1.8617351	-2.4909605	4.3391255
H	1.5625251	-1.0255863	3.3459068
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H	1.2058957	-2.5842673	1.3268450
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H	4.9263856	-2.3731776	-1.4576661
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H	-0.3090978	4.8541963	-2.6139921
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H	4.6875497	3.4526735	1.4579073	C	-0.5038858	-3.0933996	-1.2367291
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C	1.5619815	4.1510722	-4.6470302	C	-0.8070632	-3.2906240	1.2374521
H	7.4242844	3.1786417	-1.1723727	C	-0.4781006	-4.6387003	1.1570659
C	3.4703030	3.6413452	-1.9675867	C	-0.0624922	-5.2408730	-0.0661685
C	6.9008166	3.4477936	-0.2326975	C	-0.0420899	-4.4598479	-1.2806048
H	7.5207227	4.1961448	0.3011230	C	0.3617277	-6.6032547	-0.1077589
H	3.2641893	4.7148706	-1.8361491	C	0.8238919	-7.1713647	-1.2855368
C	4.7225110	-1.3047998	-1.2391699	C	0.8884818	-6.3898447	-2.4701195
H	5.8747086	-1.6582860	-3.7442607	C	0.4641329	-5.0680038	-2.4683344
H	5.3633630	-0.0992506	-4.4764008	O	-1.1878883	-1.2151703	0.0910817
C	4.0118661	0.9138958	-2.3039453	P	0.0017989	-0.1021579	-0.0742572
C	0.7233487	4.5901538	-2.3120298	O	-0.7377411	1.2352957	-0.1360295
C	2.5600804	2.8634904	-2.7039474	Zn	-0.9793448	2.7805385	1.0571326
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C	4.4174521	-0.5414478	-2.5386232	C	-0.1840881	-2.3655052	3.5188731
C	2.8336864	1.4744801	-2.8751572	C	-0.5806688	-1.7767361	4.7320878
C	1.3030072	3.5287184	-3.2611406	C	-1.9154245	-1.4228439	5.0057746
H	3.8665286	-1.2580271	-0.5383126	C	-2.8657252	-1.6489598	3.9983805
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H	3.7770796	4.7694737	0.6574502	C	1.2938296	-2.6876481	3.2934434
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H	6.8555547	2.5433737	0.4089769	C	-3.6234879	-2.4039883	1.7140210
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H	5.7629933	1.2821428	-1.0922105	C	-2.1908567	-1.9051025	7.4630772
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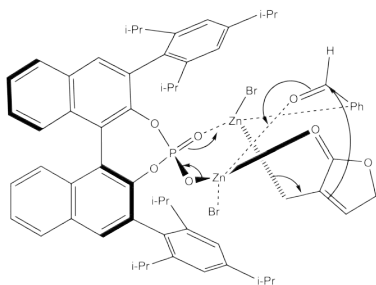


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C	2.6539726	2.4677813	-3.7384494	H	4.6055111	3.9004915	2.3649645
C	1.9212274	3.6668252	-3.6891457	H	0.2460026	3.8765670	-0.7117008
C	0.5191593	3.5779128	-3.6530432	H	-0.0425591	5.1264666	0.6620855
C	-0.1588445	2.3422583	-3.6667377	H	2.1726694	5.3187687	2.4853154
C	2.6209094	5.0220867	-3.6864241	H	-0.5183243	-5.2593992	2.0645864
C	3.5536362	5.1907829	-4.8986428	H	-0.7813736	-0.0802155	-5.7569741
C	2.8892591	-0.0467913	-3.8798449	H	0.3306940	-7.1913636	0.8229662
C	3.8840787	-0.1924860	-2.7179959	H	1.1559685	-8.2206062	-1.3013079
C	-1.6873672	2.3285521	-3.6737796	H	0.5274171	-4.4721997	-3.3895672
C	-2.3033441	3.2011094	-2.5708198	H	1.2836171	-6.8334727	-3.3967353
C	-0.0782284	-0.1839129	-3.7245483	H	-2.3147541	-4.4621954	-2.6104006
C	-0.7659785	-0.6718995	-4.8288655				
C	-1.4877180	-1.8989702	-4.7833783				
C	-1.4669955	-2.6957164	-3.5794110				
C	-0.6596144	-2.2596446	-2.4638291				
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H	-3.6590178	-5.1651708	-4.5669652	C	-0.1595034	2.3471317	-3.6482308
H	-3.6117617	-3.8263672	-6.6977826	C	2.6154554	5.0312703	-3.6792723
H	-2.2560160	-1.7274745	-6.8152185	C	3.5473406	5.2011423	-4.8916595
H	0.1840726	-1.5674323	5.4967461	C	2.8913808	-0.0363404	-3.8821398
H	-3.9138504	-1.3610295	4.1672075	C	3.9035520	-0.1763457	-2.7349526
H	-4.7644286	-0.5693759	2.1581410	C	-1.6881252	2.3285087	-3.6508008
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H	-5.2269750	-3.0215805	3.0945153	C	-1.4723439	-1.8973265	-4.7829844
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H	-5.4657577	-3.5513146	1.4009700	C	-0.6539372	-2.2575227	-2.4601593
H	-3.7636524	0.3941687	7.3855896	C	-0.0444008	-1.0003575	-2.5471291
H	-4.4656691	-0.8198382	6.2810724	C	-2.2642142	-3.8702031	-3.5399031
H	-3.7111571	0.6610936	5.6144387	C	-3.0116691	-4.2639212	-4.6410339
H	-1.4800367	-0.0684809	6.5858173	C	-2.9883984	-3.5039446	-5.8401947
H	-2.3738548	-1.4664688	8.4659025	C	-2.2373484	-2.3405626	-5.9031322
H	-1.1989558	-2.3993778	7.4805378	C	-0.5013510	-3.0918044	-1.2332085
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H	3.2629242	-1.7531607	3.4644417	C	-0.8102274	-3.2903263	1.2397600
H	2.2916905	-1.6303547	4.9589924	C	-0.4815274	-4.6381500	1.1589553
H	1.9068743	-0.5840975	3.5694918	C	-0.0627417	-5.2399390	-0.0629426
H	1.4574606	-2.7292934	2.1965595	C	-0.0383713	-4.4578195	-1.2762873
H	2.7474248	-4.2774154	3.7022652	C	0.3614050	-6.6017897	-0.1049969
H	1.0794342	-4.8826268	3.4576850	C	0.8269421	-7.1688461	-1.2812751
H	1.5128202	-4.0633620	4.9877824	C	0.8955092	-6.3863534	-2.4642613
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H	4.4679517	-1.1304496	-2.8178288	O	-0.7518416	1.2356610	-0.1352568
H	3.8853383	6.2557018	-2.3794167	Zn	-1.0061030	2.7868028	1.0379391
H	-3.4097411	3.1269800	-2.5856274	Br	-3.0875950	3.8279227	1.1734877
H	4.1432381	4.4913271	-2.1862828	C	-1.1821521	-2.6222776	2.5294098
H	3.0100125	5.0248714	-5.8504944	C	-0.1881297	-2.3615331	3.5193324
H	3.9885824	6.2114286	-4.9225490	C	-0.5857231	-1.7689509	4.7301490
H	-0.0674665	4.5110087	-3.6246794	C	-1.9206107	-1.4160655	5.0027907
H	4.1747777	-1.0320553	-5.3595271	C	-2.8709784	-1.6475803	3.9971293
H	2.8687255	-0.0320333	-6.0818688	C	-2.5282360	-2.2310401	2.7604165
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H	-1.9369292	3.7706164	-5.3129566	C	1.2900176	-2.6831879	3.2946643
H	3.3641083	-0.2196628	-1.7436265	C	1.6721823	-4.0535201	3.8873593
H	-1.9708399	2.8712961	-1.5701224	C	-3.6282645	-2.4152374	1.7166507
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H	2.6758701	5.2652020	-1.5048716	C	-2.2738263	-0.8152529	6.3604553
H	-2.0473603	4.2749687	-2.6858194	C	-2.2052904	-1.8950632	7.4594567
H	4.3979279	4.4711259	-4.8636703	C	-0.0261179	1.8172218	3.1058144
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H	-2.0121634	1.2866007	-3.4763904	C	-1.8950953	2.8192877	4.3109921
H	3.7545327	2.5094297	-3.7669315	C	-1.0673608	3.8892470	4.6887829
H	2.8639097	3.4449235	3.9491737	C	0.2771742	3.9223481	4.2916768
				C	0.8209887	2.8828604	3.5092728
				C	2.2787460	2.8539961	3.1871998
				C	2.5090058	4.4244690	1.8819729
				C	1.7684370	3.9704678	0.7569117
				C	2.6765384	2.9532069	0.1394231
				O	3.9516600	3.2197140	0.4927717
				C	3.9685629	4.2344479	1.5206460
				C	0.4652941	4.2081648	0.3152899
				O	2.3791577	1.9317810	-0.4702512
				O	2.8499097	1.8019373	2.7012232
				Zn	2.8832850	0.4038519	1.2843136
				O	1.0623329	-0.2957813	1.0204459
				Br	4.7947308	-0.8306679	0.9783368
				C	-4.2471474	-1.0654794	1.3055865
				C	-3.6253913	-0.0921871	6.3989334
				C	2.2316154	-1.6030408	3.8551720
				C	3.3677364	5.2829907	-2.3591365
				C	3.5779703	-0.0833929	-5.2605587
				C	-2.2301971	2.7037265	-5.0438780
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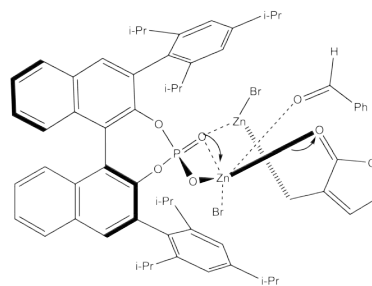
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H	0.9234004	4.7545545	4.6157557
H	-1.4757770	4.7068040	5.3016537
H	-2.9506629	2.8012551	4.6166115
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H	4.6086617	3.8445204	2.3381197
H	0.2369878	3.8777611	-0.7164609
H	-0.0402220	5.1241203	0.6628577
H	2.1958373	5.3026564	2.4669106
H	-0.5241035	-5.2578991	2.0670098
H	-0.7656174	-0.0753900	-5.7506255
H	0.3282201	-7.1904067	0.8253201
H	1.1592425	-8.2179595	-1.2967023
H	0.5381128	-4.4670992	-3.3822037
H	1.2938808	-6.8288191	-3.3899706
H	-2.3007125	-4.4640159	-2.6163456
H	-3.6322526	-5.1709872	-4.5804195
H	-3.5788272	-3.8305291	-6.7097180
H	-2.2306929	-1.7268897	-6.8176988
H	0.1791625	-1.5558581	5.4936452
H	-3.9198305	-1.3621880	4.1655920
H	-4.7783383	-0.5837930	2.1531245
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H	-3.4736198	-0.3612719	0.9409112
H	-3.1679440	-2.8553287	0.8093788
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H	-4.2518626	-4.3920005	2.4522028
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H	-2.3885610	-1.4564764	8.4622646
H	-1.2165615	-2.3951827	7.4787141
H	-2.9718335	-2.6780918	7.2818637
H	3.2584423	-1.7463500	3.4628298
H	2.2946686	-1.6361705	4.9630318
H	1.9011468	-0.5805216	3.5837969
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H	2.7439046	-4.2720203	3.7019931
H	1.0781962	-4.8790402	3.4511613
H	1.5052726	-4.0647889	4.9851159
H	1.8182989	5.8032205	-3.7596280
H	4.2837856	0.7639001	-5.3893644
H	-3.3378663	2.6401008	-5.0668622
H	4.4860789	-1.1144341	-2.8380438
H	3.8784368	6.2685615	-2.3732406
H	-3.4134988	3.1334118	-2.5710277
H	4.1377653	4.5043156	-2.1781283
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H	3.9792462	6.2229838	-4.9187559
H	-0.0718519	4.5154862	-3.6037963
H	4.1572425	-1.0225567	-5.3781569
H	2.8367787	-0.0294796	-6.0839629
H	-1.8318494	2.0360804	-5.8340003
H	-1.9439401	3.7420906	-5.3130588
H	3.4003035	-0.2003925	-1.7519033
H	-1.9708787	2.9132071	-1.5571714
H	4.6287345	0.6633739	-2.7144366
H	2.6697235	5.2762621	-1.4979725
H	-2.0643831	4.2919376	-2.7014899
H	4.3940275	4.4845779	-4.8560126
H	2.2163583	-0.9152457	-3.8319117
H	-2.0083834	1.2886362	-3.4351967
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C	-0.404777	-5.336804	-1.772946
C	0.311750	-4.113773	-1.754515
C	-1.795191	-5.331428	-1.621954
C	-0.385299	-2.884965	-1.672133
O	2.535709	-3.229219	-1.463307
H	-3.568926	-4.091163	-1.360936
H	0.143896	-6.286942	-1.872871
H	-2.319918	-1.935219	-1.486562
H	-2.352903	-6.279531	-1.607903
H	0.171120	-1.941103	-1.743973
Br	-3.537793	-1.123362	1.059177
Zn	-1.528993	-2.285765	1.451371
H	2.738962	-6.446169	2.363525
H	-1.262209	-3.831010	3.326602
C	0.881332	-5.629740	1.544515
C	2.366458	-5.586683	1.758224
H	0.363076	-6.465492	1.054131
C	0.308067	-4.531317	2.108175
C	-1.078274	-4.068878	2.255287
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O	2.615666	-4.374671	2.470223
O	1.364361	-2.644454	3.247688
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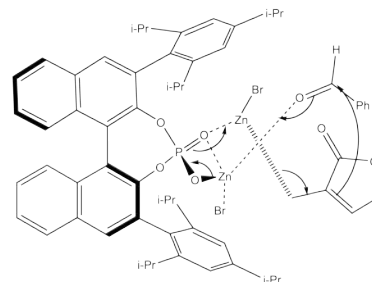
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C	-1.988646	-0.058196	-3.902110
C	-2.076377	-1.266557	-4.618773
C	-0.938005	-1.919404	-5.124162
H	1.211218	-1.825066	-5.298713
C	-3.267047	0.653940	-3.456945
H	-3.071844	-1.704386	-4.794950
C	-4.202911	-0.224532	-2.613608
H	-4.508234	-1.149010	-3.147438
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H	-3.738989	-0.510662	-1.649153
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H	-1.449693	-4.525976	-4.241826
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H	-1.531244	-1.787499	5.181062
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Zn	2.825956	-1.583030	-0.262507
Br	4.684515	-1.861638	0.997497
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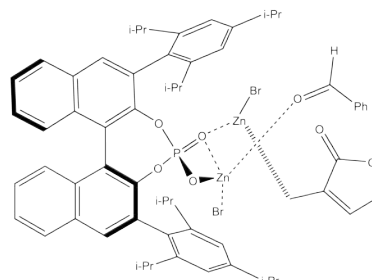


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C	-3.163825	6.376322	0.082216	C	3.950287	2.101450	1.097037
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H	-2.925808	2.936320	3.072799	H	2.747484	2.075666	-1.422990
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C	-6.541245	0.227921	-0.169942				
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H	-6.959166	0.498322	0.821181				
C	-5.054413	-2.427678	-4.563854				
C	-5.019476	-3.876140	-4.049147				
H	-5.462174	-4.571391	-4.792121				
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C	-1.478430	1.052844	-3.632017				
C	-0.482508	0.238516	-4.473706				
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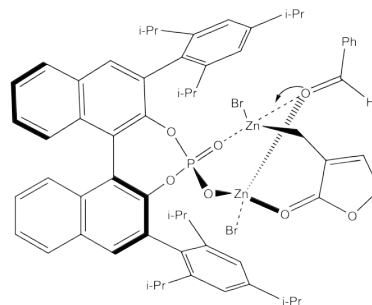
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C	-0.8661048	-2.9683460	-1.1258666
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H	-2.5651904	-1.9797481	-0.2369001
H	-2.4542843	-6.3087331	0.1703987
H	-0.4488753	-2.0454716	-1.5476267
Br	-1.9585101	-0.7139669	2.4891113
Zn	-0.0780186	-2.0252785	1.9818506
H	4.5343040	-5.7958523	1.0699207
H	0.5715137	-3.9462340	3.4235873
C	2.5436308	-4.9024712	0.8895418
C	4.0385575	-4.8103058	0.9147614
H	1.9933579	-5.5573290	0.2007404
C	2.0144155	-4.1319410	1.8801211
C	0.6337378	-3.8711164	2.3167813
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O	4.3444614	-3.9600307	2.0216584	H	0.9072872	-1.6520108	-3.8226062
O	3.1758217	-2.8003961	3.5809639	C	-0.7592578	0.7556852	-5.7440983
H	4.4656533	-4.3481957	-0.0054326	H	-0.0643377	0.6881569	-3.7018017
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C	-1.2741971	2.8332637	-0.6337597	H	-1.1595927	0.0808160	-6.5295629
C	-1.6348836	3.9968627	-1.4110215	H	5.7039253	-1.0380191	4.5661428
C	-1.3248629	5.3259463	-0.9925990	H	5.5417603	4.0729794	1.6677722
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P	0.6389349	0.2500923	-0.4132525	C	4.1970833	2.6514780	-0.3851381
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H	-3.2013788	4.8137514	-4.3942090	C	2.3460280	0.9335163	3.8261283
H	-2.6705946	7.1217075	-3.5889945	H	1.2135223	2.4249203	5.9210802
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H	-1.0830836	4.8968127	4.9824091	H	5.8477097	-1.8334548	2.2193492
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C	-2.5025098	0.0008222	-2.9324383	H	7.3737226	1.4069772	3.6572708
C	-2.1357927	-1.9268344	-4.3655874	H	2.6379770	3.5903970	0.7550727
C	-3.7083749	-0.5857496	-2.4569742	H	0.2126154	0.9738028	4.0903346
C	-4.0957783	-1.8382804	-2.9676435	Zn	2.4432192	-1.5859540	-1.1241194
C	-3.3309255	-2.5222205	-3.9291632	Br	4.6892988	-1.6011988	-0.7131313
H	-1.5302118	-2.4556055	-5.1185474	H	5.6341623	1.5857167	1.8018973
C	-4.6323334	0.1569913	-1.4890714	H	1.4350414	-5.2281456	-2.3860867
H	-5.0370533	-2.2864813	-2.6111158				
C	-5.0700122	-0.6789409	-0.2749379				
H	-5.5832147	-1.6175056	-0.5718060				
H	-5.7819416	-0.1006035	0.3483820				
H	-4.2115504	-0.9357804	0.3782576				
C	-5.8477704	0.7143608	-2.2560294				
H	-4.0729918	1.0273993	-1.0896638				
H	-6.4606509	-0.1058569	-2.6853426				
H	-5.5295461	1.3668270	-3.0941163				
H	-6.4991429	1.3109222	-1.5844798				
C	-3.7842724	-3.8628482	-4.4948540				
C	-3.7629087	-4.9674834	-3.4247493				
H	-4.0585056	-5.9462277	-3.8564725				
H	-4.4666184	-4.7391117	-2.5968992				
H	-2.7547766	-5.0759088	-2.9786750				
C	-5.1630271	-3.7620415	-5.1707985				
H	-3.0474821	-4.1445063	-5.2794507				
H	-5.4442464	-4.7270106	-5.6408266				
H	-5.1707215	-2.9801488	-5.9563392				
H	-5.9556632	-3.5073149	-4.4367235				
C	-0.4365769	-0.0317192	-4.4587507				
C	0.6998165	-1.0325478	-4.7153877				
H	1.6334343	-0.4912557	-4.9682474				
H	0.4764920	-1.7132298	-5.5634956				

7.2.3 Pathways starting from 14j-ma

7.2.3.1 to 15r-ma and 15r-2-ma

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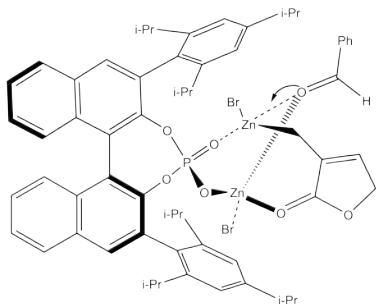


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C	0.7102933	-5.8017789	1.7921195	H	4.3350696	-0.0950798	4.7555582
C	-1.6801130	-5.4027837	1.3645949	H	6.1586260	-0.5942906	-2.9488767
C	-1.9723029	-6.6080742	2.0718069	C	4.9529672	3.7018566	1.7625071
C	-2.7278374	-4.5582229	0.8983586	H	1.2338517	-0.7381606	4.6502025
H	-3.7710021	-4.8598624	1.0777568	H	4.6434564	5.3697263	3.1383958
C	-2.4681804	-3.3347638	0.2935626	H	4.0472845	0.6155833	-3.7293292
C	3.2315350	-1.7440900	0.3848977	C	4.4552110	2.2972822	1.4346323
C	4.1382594	-2.6998981	-0.0615560	C	3.9745452	-1.0212209	4.2606873
H	5.2113542	-2.4574095	-0.0782441	C	4.3420776	4.3080081	3.0314748
C	3.7173923	-3.9685589	-0.5515958	H	4.6840558	3.7772081	3.9442643
C	4.6518983	-4.8882660	-1.1166759	C	3.8628995	1.4527433	2.3857034
C	2.3192222	-4.3220796	-0.5053388	C	5.9901527	-0.2097051	-1.9216309
C	1.9164243	-5.5606006	-1.0895064	H	6.9523714	3.3343088	0.9092194
C	1.3850717	-3.4057710	0.1051816	C	4.6284342	1.7892803	0.1348873
C	1.8548351	-2.1283962	0.4412759	C	6.4932830	3.7212187	1.8408908
O	-0.8566316	-1.8443472	-0.6852491	H	6.8710905	4.7513509	2.0085864
O	0.9794320	-1.1902637	0.9618258	H	5.0771621	2.4441902	-0.6299374
P	-0.2356647	-0.5306819	0.0805477	C	1.6449723	-0.0751746	3.8614119
O	-1.1956075	-0.0024626	1.1551202	H	3.5784671	-1.6919411	5.0512118
O	0.2570607	0.3870832	-1.0415228	H	4.8513107	-1.5168949	3.7962439
C	-0.9580731	-7.3786013	2.6198391	C	3.4570161	0.1385106	2.0792277
C	0.3921774	-6.9569405	2.4938046	C	3.9174188	1.0153973	-2.7036952
H	-3.0268133	-6.9028504	2.1911261	C	4.2439214	0.4876435	-0.2296273
H	-1.1973776	-8.3019651	3.1690573	H	6.4173184	-0.9420181	-1.2069800
H	1.7597208	-5.4872835	1.7156472	H	6.5691058	0.7317796	-1.8131658
H	1.1953963	-7.5468430	2.9612750	C	2.8866054	-0.7144411	3.2128189
C	2.8470223	-6.4234399	-1.6523370	C	3.6518377	-0.3566394	0.7591069
C	4.2294061	-6.0953155	-1.6531278	C	4.4897655	0.0352087	-1.6698140
H	0.8494277	-5.8236111	-1.1026395	H	0.8450385	0.0944731	3.1164796
H	2.5089563	-7.3671501	-2.1070493	H	2.8307856	1.1589713	-2.5532466
H	4.9589208	-6.7913778	-2.0944746	H	1.8786543	0.8990110	4.3388944
H	5.7173008	-4.6093558	-1.1349356	H	3.2340794	4.2683222	3.0211289
C	-4.1680257	-1.6594474	1.0967629	H	4.4202412	2.0039546	-2.6627867
C	-3.5347126	-2.3246541	0.0076679	H	6.8476125	3.0848835	2.6787884
C	-5.1081900	-0.6515987	0.8117773	H	2.5722861	-1.6882276	2.7883940
C	-3.8688940	-1.9770187	-1.3300387	H	3.9593193	-0.9256633	-1.8207956
C	-4.8096181	-0.9558607	-1.5568730	H	3.7148606	1.8158548	3.4134555
C	-5.4409539	-0.2752869	-0.4995036	Zn	-1.3970968	1.7964286	1.8734372
H	-5.6034578	-0.1314798	1.6478438	Br	-1.8257889	2.6331528	3.9828409
C	-3.2850332	-2.7324903	-2.5230320	C	2.9517124	5.9937727	-1.8950128
H	-5.0661970	-0.6934690	-2.5959245	C	0.8948940	3.6837761	1.3032390
C	-2.5530709	-1.8107470	-3.5093728	C	2.4852459	4.2727218	-2.0517713
H	-3.2249713	-1.0459669	-3.9507538	C	2.1326861	5.6414877	0.3907497
H	-2.1025938	-2.3856449	-4.3433821	C	1.6610624	4.3176979	0.2346763
H	-1.7204405	-1.2893446	-2.9959073	C	2.7827598	6.2762889	-0.6754778
C	-4.3763482	-3.5590545	-3.2300384	C	1.8496686	3.6278579	-0.9879084
H	-2.5372548	-3.4527366	-2.1323883	O	0.4105029	2.5487261	1.1781195
H	-5.1622505	-2.9044162	-3.6614819	H	3.4536044	6.0972968	-2.7357206
H	-4.8708707	-4.2561549	-2.5234153	H	1.9798371	6.1657938	1.3472380
H	-3.9425516	-4.1568312	-4.0582383	H	2.6199318	3.7475047	-3.0087355
C	-6.4439304	0.8452269	-0.7480670	H	3.1546606	7.3054867	-0.5626123
C	-5.7400739	2.1250011	-1.2364645	H	1.4801529	2.5931643	-1.0678455
H	-6.4602863	2.9651211	-1.3231865	Br	0.8112741	0.1545415	-4.5790577
H	-5.2807415	1.9695797	-2.2350077	Zn	-0.5635543	0.8575300	-2.8261134
H	-4.9307947	2.4248793	-0.5413450	H	-0.2572683	5.7423823	-1.2965216
C	-7.5726914	0.4271928	-1.7051327	C	-1.5560852	4.4893150	-2.5402111
H	-6.9075544	1.0776860	0.2359744	C	-1.3100714	5.3896605	-1.3770573
H	-8.3256982	1.2365526	-1.8010380	C	-1.9549494	3.2551670	-2.0996804
H	-8.0910583	-0.4850904	-1.3466360	C	-2.2341159	1.9808952	-2.7689988
H	-7.1849394	0.2165161	-2.7238481	C	-1.9834373	3.3597907	-0.6263402
C	-3.8982196	-2.0249574	2.5572869	O	-1.5966233	4.5837091	-0.2129825
C	-3.6049851	-0.8096438	3.4493278	O	-2.3152313	2.4785029	0.1799905
H	-3.3839686	-1.1355276	4.4863533	H	-1.9709029	6.2836986	-1.3392709
H	-4.4582827	-0.1030085	3.5037148	H	-1.4065586	4.8017408	-3.5825163
H	-2.7239916	-0.2511993	3.0846949	H	0.7107330	4.2732241	2.2383104
C	-5.0681754	-2.8525057	3.1260940	H	-2.5672964	2.1129531	-3.8160847
H	-2.9930894	-2.6638631	2.5833170	H	-2.9745280	1.3836925	-2.2003299
H	-4.8543131	-3.1741546	4.1665526				
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TS1-8-r



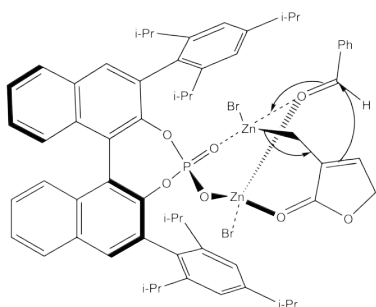
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C	0.7109644	-5.8003244	1.7806507
C	-1.6803455	-5.3964878	1.3658078
C	-1.9704624	-6.6018154	2.0727762
C	-2.7282281	-4.5497832	0.9048403
H	-3.7714614	-4.8485853	1.0883800
C	-2.4698914	-3.3270084	0.2987106
C	3.2264557	-1.7362435	0.3759026
C	4.1326880	-2.6898840	-0.0754470
H	5.2049778	-2.4444696	-0.0951776
C	3.7129251	-3.9583413	-0.5659393
C	4.6464224	-4.8760731	-1.1346123
C	2.3156516	-4.3138708	-0.5161795
C	1.9131643	-5.5521323	-1.1003203
C	1.3821597	-3.4002188	0.0986286
C	1.8507866	-2.1231706	0.4370942
O	-0.8606897	-1.8370769	-0.6845073
O	0.9757065	-1.1891841	0.9647628
P	-0.2403485	-0.5259224	0.0865742
O	-1.2020781	-0.0070471	1.1644390
O	0.2505507	0.4002640	-1.0285979
C	-0.9554165	-7.3750270	2.6140432
C	0.3943442	-6.9558927	2.4814227
H	-3.0249487	-6.8944552	2.1973501
H	-1.1937936	-8.2987002	3.1630334
H	1.7602156	-5.4871074	1.6983763
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H	0.8463862	-5.8156392	-1.1098551
H	2.5051737	-7.3567395	-2.1202315
H	4.9538890	-6.7772161	-2.1147882
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C	-4.1646317	-1.6443707	1.0999689
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H	-5.0701759	-0.6971544	-2.5954480
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H	-1.7310741	-1.3162293	-3.0178712
C	-4.3994732	-3.5770190	-3.2036996
H	-2.5519772	-3.4647791	-2.1211034
H	-5.1869212	-2.9250362	-3.6361716
H	-4.8915171	-4.2634677	-2.4852984
H	-3.9752176	-4.1860125	-4.0286191
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C	-5.7274020	2.1336872	-1.2490282
H	-6.4442536	2.9762582	-1.3397788
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H	-4.9169378	2.4340427	-0.5556338
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C	-3.8958836	-2.0069657	2.5614814
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H	-3.3881905	-1.1175810	4.4928031
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H	4.0397832	0.6387490	-3.7354135
C	4.4519647	2.3015538	1.4350491
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C	3.8617193	1.4542896	2.3843845
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H	6.9510061	3.3339529	0.9147931
C	4.6219605	1.7979797	0.1334399
C	6.4922562	3.7207715	1.8464301
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H	5.0699102	2.4549296	-0.6301436
C	1.6501058	-0.0812968	3.8631120
H	3.5918712	-1.6981878	5.0400618
H	4.8590271	-1.5167418	3.7803002
C	3.4556879	0.1409792	2.0748596
C	3.9160119	1.0379429	-2.7091462
C	4.2356785	0.4981614	-0.2350713
H	6.4003870	-0.9408916	-1.2172536
H	6.5627452	0.7326629	-1.8171469
C	2.8903688	-0.7160358	3.2078423
C	3.6465356	-0.3493980	0.7525574
C	4.4783752	0.0500371	-1.6772237
H	0.8466541	0.0894196	3.1224531
H	2.8303390	1.1907062	-2.5608251
H	1.8817596	0.8914732	4.3443103
H	3.2338982	4.2686961	3.0274997
H	4.4303633	2.0207764	-2.6666360
H	6.8445249	3.0807665	2.6820965
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H	3.9399221	-0.9055491	-1.8333036
H	3.7161738	1.8130967	3.4139749
Zn	-1.4118825	1.7858574	1.8903641
Br	-1.7935650	2.6764373	3.9760404
C	2.9610676	5.6195596	-1.8386903
C	0.8781035	3.6725380	1.3236559
C	2.5154166	4.2930598	-2.0043040
C	2.1056181	5.6514388	0.4335199
C	1.6546934	4.3224977	0.2685283
C	2.7635480	6.2974504	-0.6210508
C	1.8718832	3.6374544	-0.9511461
O	0.4142642	2.5334541	1.1847899
H	3.4700718	6.1313510	-2.6702074
H	1.9319370	6.1707724	1.3893153
H	2.6722990	3.7682540	-2.9580891
H	3.1203984	7.3311787	-0.5003539

H	1.5165372	2.5982537	-1.0392225
Br	0.8407392	0.1090578	-4.5684844
Zn	-0.5443020	0.8131388	-2.8446116
H	-0.2293809	5.6896151	-1.3557213
C	-1.5425584	4.4310986	-2.5816416
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C	-1.9443798	3.2026291	-2.1265323
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C	-1.9665023	3.3237436	-0.6521302
O	-1.5703583	4.5527165	-0.2550882
O	-2.2996747	2.4562024	0.1644684
H	-1.9407793	6.2413662	-1.3955070
H	-1.3976045	4.7294921	-3.6285727
H	0.6644076	4.2545079	2.2584692
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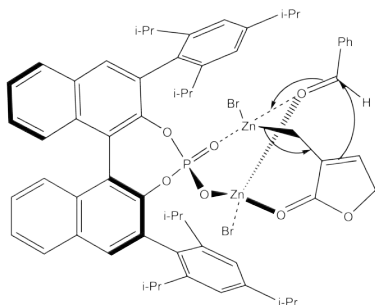
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C	4.8075284	3.7731654	1.2735929
C	2.6090009	4.8120203	1.6632405
C	3.2578927	6.0827747	1.7161613
C	1.1899438	4.7123740	1.7306541
H	0.5982017	5.6332313	1.8466500
C	0.5330267	3.4960752	1.5850422
C	3.8185735	-1.1738989	0.2895209
C	4.9439999	-1.3978177	1.0722243
H	5.5160408	-2.3298949	0.9480753
C	5.3348357	-0.4865936	2.0976510
C	6.4278363	-0.7883312	2.9652022
C	4.5741614	0.7222029	2.3184632
C	4.8963875	1.5234780	3.4543981
C	3.5072465	1.0520442	1.4007335
C	3.1687064	0.0931136	0.4431392
O	0.6598355	1.1082341	1.4470233
O	2.1401022	0.3769428	-0.4538702
P	0.5934145	0.2671605	0.0468375
O	-0.2294100	0.9780472	-1.0427280
O	0.1553326	-1.1480663	0.4250635
C	4.6303337	6.1909275	1.5508791
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C	5.9505853	1.1880950	4.2939232
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H	-3.7275605	2.1471116	3.0336117
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H	-7.0217079	4.4190395	0.9772175
H	-5.4764406	5.2477433	0.5889603
H	-5.8034318	4.7095659	2.2650911
C	-0.8039513	4.6116633	-0.8446330
C	-1.0818459	4.0237963	-2.2393165
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Zn	-1.3955816	0.1454532	-2.3366328
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C	-3.3499707	-6.0374511	-2.0312843
C	-4.1704360	-3.9733681	-3.7449214
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Br	-1.7973971	-3.9510097	1.6482099
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C	5.4051612	5.0343986	1.3071082
H	2.6384346	6.9871979	1.8676311
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C	5.9605581	1.1990047	4.2859833
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H	6.1857735	1.8330132	5.1570331
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H	7.0122244	-1.6969875	2.7729383
C	-1.5796042	3.9121465	0.2706118
C	-0.9521993	3.3961024	1.4435718
C	-2.9716169	3.7777087	0.1401004
C	-1.7338447	2.7471126	2.4375577
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C	-3.7687782	3.1480588	1.1110094
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H	-0.9107522	0.3041690	4.8178419
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C	-5.9330740	4.4291982	1.2167056
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C	-1.0801024	4.0248500	-2.2408761
H	-0.4886231	4.5653356	-3.0079190
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H	-0.7917987	2.9588092	-2.2818519
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H	2.7412513	-5.2937283	2.9652405
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C	4.8403984	-1.4937040	-3.5128044
C	-0.2010331	-4.0982451	-4.0691708
H	0.5752547	-4.0486384	-4.8613879
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C	2.4060146	-5.0820408	1.9296203
H	1.2939525	-6.5878849	-2.1028408
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TS2-8-r

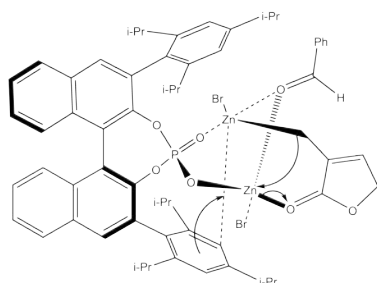


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C	2.6092916	4.8187900	1.6606754
C	3.2574547	6.0893993	1.7132008
C	1.1906744	4.7172678	1.7279338
H	0.5966610	5.6368164	1.8427075
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H	2.1624925	-1.6142820	2.3498033	O	2.3218468	0.5101908	-0.5007945
H	2.3456012	-0.5807826	-4.4287075	P	0.7540852	0.3744944	-0.0672452
H	-0.5821757	-3.0698598	-3.9109098	O	-0.0512959	1.1604133	-1.1072664
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H	1.8031987	-6.0485624	-3.7321647	C	4.5901605	6.2803338	1.8138154
H	4.1556347	-0.2010178	-1.9449448	C	5.4074622	5.1472870	1.5561350
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Zn	-1.3847103	0.1617427	-2.3482870	H	5.4919552	3.0155942	1.2450950
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C	-3.0480372	-4.7203344	-1.7611905	C	-1.4943331	3.8311722	0.1991730
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Br	-1.7825450	-4.0045609	1.5942391	C	-1.1427328	2.0734369	3.6452961
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C	-5.7231865	-1.0632292	-2.0424353	H	-0.9273097	0.1416438	4.6592250
C	-4.0539207	-0.6975735	-0.4386703	H	-0.9764739	0.0211196	2.8757974
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H	-5.0477500	-2.6851443	-0.5856123	C	-5.2051193	2.9411104	0.6860648
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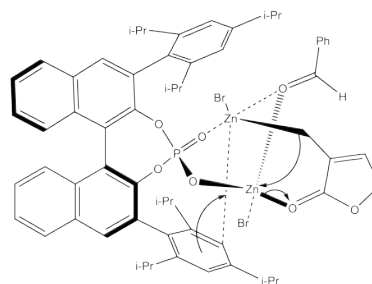
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C	1.5233590	-3.7370356	-2.1335570
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C	0.1561539	-4.0334534	-4.2865335
H	1.0025839	-4.0835423	-5.0030789
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H	5.7146140	-0.6234407	-3.9462195
H	5.7696544	-1.9783187	-2.7672368
C	3.1278714	-1.8836161	-1.9754318
C	1.8983627	-2.5816442	2.4400554
C	2.5748002	-3.2018726	0.0379400
H	2.9425324	-5.6957593	1.2242374
H	1.3117061	-5.1978558	1.7900748
C	3.9159174	-0.7921389	-2.6960957
C	3.2624351	-2.1085678	-0.5807315
C	2.7185866	-3.5209896	1.5328779
H	2.1548450	0.4661967	-3.1026912
H	2.1423308	-1.5153487	2.2760694
H	2.6804251	-0.5143405	-4.5042525
H	-0.1582831	-2.9729175	-4.2188338
H	0.8135824	-2.7062746	2.2530782
H	2.0080196	-6.0588709	-3.6679504
H	4.3404217	-0.1174850	-1.9246661
H	3.7863473	-3.3644459	1.7893436
H	2.1682524	-2.5159791	-3.8037926
Zn	-1.7114447	0.3262701	-1.8720223
Br	-1.5399561	0.4682948	-4.1975184
C	-5.2135463	-5.9945904	-2.7197598
C	-2.6396596	-2.6118899	-2.9173240
C	-4.1956577	-5.8529973	-1.7545815
C	-4.5101259	-3.9376222	-3.7976073
C	-3.4882059	-3.7877698	-2.8260053
C	-5.3731884	-5.0381180	-3.7392924
C	-3.3330923	-4.7558085	-1.8022625
O	-1.7574294	-2.2702966	-2.0985244
H	-5.8897167	-6.8623994	-2.6757882
H	-4.6230853	-3.1777000	-4.5870029
H	-4.0804257	-6.6046267	-0.9593937
H	-6.1702125	-5.1554813	-4.4883946
H	-2.5516800	-4.6234779	-1.0388497
Br	-1.9668894	-3.6440404	1.4043942
Zn	-1.3904867	-1.9316782	-0.0835763
H	-6.2104281	-2.7473136	-1.7380809
C	-4.9626788	-1.7885277	-0.2200028
C	-6.1437247	-1.8105257	-1.1384346
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C	-4.7933857	-0.0733386	-1.7258769
O	-5.9568488	-0.7074225	-2.0445850
O	-4.3543510	0.8900059	-2.3390106
H	-7.1148318	-1.6788843	-0.6114975
H	-4.7952479	-2.5225327	0.5807750
H	-2.7857840	-1.9436168	-3.8031613
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H	-2.8749954	0.8797551	-0.0714053



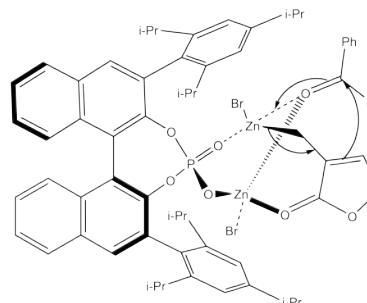
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C	4.8481975	3.8853578	1.4614587
C	2.6072683	4.8457927	1.8122894
C	3.2162471	6.1312594	1.9303596
C	1.1901115	4.7031965	1.8230879
H	0.5687646	5.6031080	1.9443820
C	0.5738386	3.4746638	1.6167290
C	3.9283980	-1.0867910	0.2935741
C	5.0265383	-1.3397802	1.1058630
H	5.5826676	-2.2820780	0.9850875
C	5.4058577	-0.4504667	2.1537418
C	6.4740685	-0.7786364	3.0415082
C	4.6497644	0.7600633	2.3796271
C	4.9480204	1.5326280	3.5417210
C	3.6111205	1.1182355	1.4415283
C	3.2988590	0.1923465	0.4411618
O	0.7917850	1.0918361	1.4341127
O	2.3135630	0.5185233	-0.4885030
P	0.7491416	0.3765248	-0.0454625
O	-0.0693486	1.1662453	-1.0714189
O	0.3425030	-1.0797120	0.2162323
C	4.5890879	6.2847164	1.8155227
C	5.4066191	5.1519868	1.5604176
H	2.5668903	7.0056531	2.0943701
H	5.0443033	7.2831467	1.9008088
H	5.4917137	3.0195610	1.2539761
H	6.4925796	5.2788487	1.4334052
C	5.9789081	1.1720720	4.3988233
C	6.7640221	0.0182853	4.1384899
H	4.3441260	2.4237651	3.7603111
H	6.1843905	1.7842791	5.2901465
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C	-1.4833754	3.8272329	0.1936484
C	-0.9039463	3.3338610	1.4030921
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C	-1.7203581	2.6682570	2.3559653
C	-3.1034842	2.5478972	2.1119658
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C	-1.1548125	2.0883682	3.6511624
H	-3.7263109	2.0416650	2.8644926
C	-1.4111784	0.5736970	3.7628203
H	-2.4958981	0.3429769	3.8164181
H	-0.9424016	0.1642546	4.6810353
H	-0.9804808	0.0303151	2.8993093
C	-1.6919256	2.8459566	4.8795542
H	-0.0559487	2.2353523	3.6366053
H	-2.7926411	2.7375954	4.9745920
H	-1.4669833	3.9295868	4.8126527
H	-1.2353480	2.4561791	5.8127791
C	-5.1967089	2.9401866	0.6582818
C	-5.9154229	1.8244576	1.4280001

TS2-8-r-transmetall

H	-6.9659112	1.7350567	1.0839253	Br	-1.9337382	-3.7156904	1.3643573
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H	-5.4257778	0.8401580	1.2856677	H	-6.1970570	-2.7520215	-1.7446604
C	-5.8704315	4.3028850	0.9169175	C	-4.9425475	-1.8374091	-0.2043429
H	-5.2942371	2.7181370	-0.4278374	C	-6.1301559	-1.8331762	-1.1170534
H	-6.9472965	4.2716429	0.6505534	C	-4.1465182	-0.7822189	-0.5213023
H	-5.3936042	5.1094760	0.3251367	C	-2.8420498	-0.2818465	-0.0699368
H	-5.7891798	4.5809930	1.9886904	C	-4.7891214	-0.0757634	-1.6606281
C	-0.6666698	4.5530137	-0.8770798	O	-5.9551520	-0.7038423	-1.9887611
C	-0.9800649	4.0937060	-2.3106559	O	-4.3544422	0.9048497	-2.2454626
H	-0.3091380	4.6083775	-3.0282193	H	-7.0987712	-1.7212576	-0.5795402
H	-2.0200855	4.3318720	-2.6146977	H	-4.7607840	-2.5962033	0.5699794
H	-0.8247006	3.0064386	-2.4358486	H	-2.7553975	-1.9503082	-3.8043651
C	-0.8583673	6.0783410	-0.7523934	H	-2.6187005	-0.5466579	0.9880447
H	0.4029547	4.3275183	-0.6918604	H	-2.8603688	0.8337033	-0.0063512
H	-0.2235142	6.6159240	-1.4866798				
H	-0.6014411	6.4510827	0.2589605				
H	-1.9150456	6.3573965	-0.9481794				
H	-0.3804327	-4.6627449	-2.2914814				
H	4.7347011	-2.0950993	-4.2445751				
H	2.7022269	-5.1964444	2.9245224				
C	0.5445623	-4.6094873	-2.9107428				
H	3.5988405	0.9357558	-4.0206485				
H	-0.6750593	-4.6304029	-4.7232047				
H	2.1141898	-2.8220762	3.5120181				
C	1.5187288	-3.7329011	-2.1279105				
C	5.0865340	-1.3942500	-3.4586089				
C	0.1558974	-4.0423840	-4.2820352				
H	1.0039887	-4.0939503	-4.9964328				
C	2.2564592	-2.7002300	-2.7221717				
C	2.4112967	-4.9838368	1.8758289				
H	1.3169143	-6.4924823	-2.0606864				
C	1.7116172	-3.9706676	-0.7523707				
C	1.0806136	-6.0480416	-3.0479318				
H	0.3385693	-6.7031521	-3.5502753				
H	1.1386052	-4.7810024	-0.2772573				
C	3.0178739	0.0788637	-3.6223602				
H	5.6901716	-0.6053530	-3.9539073				
H	5.7522053	-1.9621341	-2.7773988				
C	3.1154247	-1.8732849	-1.9732998				
C	1.9077114	-2.5847161	2.4479446				
C	2.5756434	-3.1968891	0.0402077				
H	2.9554313	-5.6919111	1.2182860				
H	1.3257501	-5.1996530	1.7942372				
C	3.8972626	-0.7784770	-2.6956102				
C	3.2569372	-2.1006939	-0.5799275				
C	2.7264237	-3.5186383	1.5339056				
H	2.1336186	0.4807997	-3.0910327				
H	2.1476473	-1.5171654	2.2869656				
H	2.6503880	-0.4978668	-4.4964258				
H	-0.1604958	-2.9820454	-4.2215204				
H	0.8223249	-2.7135037	2.2679610				
H	2.0121879	-6.0591429	-3.6514562				
H	4.3241511	-0.1046982	-1.9247039				
H	3.7948360	-3.3591071	1.7861087				
H	2.1508205	-2.5052763	-3.7983918				
Zn	-1.7312176	0.3456736	-1.8415900				
Br	-1.5749307	0.4505856	-4.1628005				
C	-5.2610138	-5.9738326	-2.7628004				
C	-2.6295494	-2.6279624	-2.9211770				
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C	-5.3951303	-5.0113233	-3.7798658				
C	-3.3718481	-4.7654390	-1.8212462				
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H	-4.6079396	-3.1573766	-4.6102016				
H	-4.1561829	-6.6038990	-0.9914426				
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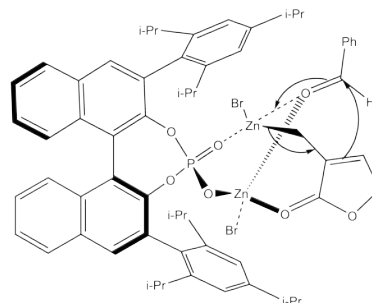


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C	2.5444718	4.7920951	1.4272309
C	3.2302661	6.0435448	1.4030910
C	1.1265070	4.7353282	1.5259933
H	0.5606628	5.6763014	1.5998557
C	0.4299990	3.5356366	1.4468447
C	3.7165777	-1.1635694	0.1390593
C	4.9041992	-1.3142768	0.8461677
H	5.5477549	-2.1819827	0.6357574
C	5.2843267	-0.4146538	1.8820877
C	6.4399788	-0.6555047	2.6844632
C	4.4632766	0.7387057	2.1587758
C	4.7999088	1.5548149	3.2797220
C	3.3322435	1.0130329	1.3035237
C	2.9633898	0.0306967	0.3776664
O	0.4934869	1.1274001	1.5244989
O	1.8472288	0.2406494	-0.4316716
P	0.3433300	0.1688078	0.2032184
O	-0.5531111	0.7930761	-0.8851659
O	-0.0398709	-1.2147662	0.7283301
C	4.5971253	6.1033444	1.1822511
C	5.3258409	4.9058332	0.9567427
H	2.6431473	6.9652399	1.5402099
H	5.1135350	7.0749605	1.1575825
H	5.2709554	2.7588409	0.8103045
H	6.4038152	4.9542176	0.7397057
C	5.9160330	1.2782966	4.0571945
C	6.7558240	0.1753699	3.7485071
H	4.1556345	2.4089359	3.5305518
H	6.1486415	1.9174908	4.9224778
H	7.6444096	-0.0279946	4.3652861
H	7.0657105	-1.5317908	2.4530581
C	-1.5982027	3.8284432	-0.0079656
C	-1.0570121	3.5129463	1.2754776

C	-2.9942392	3.8034835	-0.1674566	H	3.8224493	0.0402463	-1.9974156
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C	-3.3119153	3.2267714	2.1465130	H	2.1559497	-2.6392414	-4.0244025
C	-3.8747962	3.5191512	0.8961953	Zn	-2.4592982	0.5698968	-1.0600453
H	-3.4188587	4.0162362	-1.1604029	Br	-4.0707273	1.2098492	-2.5954359
C	-1.3735687	2.7933543	3.7203918	C	-4.1149496	-5.8807056	-3.5205901
H	-3.9700950	2.9808938	2.9923738	C	-3.7036579	-2.1350079	-1.4617579
C	-1.7240511	1.3314502	4.0577665	C	-5.2554523	-5.1272620	-3.1820203
H	-2.8219551	1.1869589	4.1365800	C	-2.6927742	-4.1972618	-2.4905166
H	-1.2742375	1.0340085	5.0276365	C	-3.8305393	-3.4436083	-2.1276366
H	-1.3429399	0.6489199	3.2737464	C	-2.8384366	-5.4081093	-3.1809329
C	-1.8370902	3.7592462	4.8248518	C	-5.1135028	-3.9174347	-2.4978260
H	-0.2667367	2.8623570	3.6711103	O	-2.5317452	-1.6529854	-1.1144077
H	-2.9403930	3.7418214	4.9460126	H	-4.2253336	-6.8339611	-4.0596932
H	-1.5425250	4.8032537	4.5952419	H	-1.6909039	-3.8204677	-2.2454397
H	-1.3910608	3.4825286	5.8025412	H	-6.2575820	-5.4862361	-3.4614249
C	-5.3773655	3.5226503	0.6317439	H	-1.9425199	-5.9843732	-3.4547230
C	-6.2209058	2.9398789	1.7706784	H	-6.0065596	-3.3238399	-2.2456845
H	-7.2887465	2.8988768	1.4746887	Br	-1.0353030	-4.9001937	0.4162849
H	-6.1591337	3.5634522	2.6875657	Zn	-1.4050800	-2.5858877	0.3606612
H	-5.9060979	1.9106025	2.0313643	H	-6.4242971	-1.3356856	-0.8161898
C	-5.8679302	4.9384214	0.2686167	C	-4.9429798	-2.4409399	0.4308082
H	-5.5234710	2.8726725	-0.2615335	C	-6.0083251	-1.3967236	0.2109400
H	-6.9438398	4.9275447	-0.0028796	C	-3.9696477	-1.8486657	1.2675907
H	-5.3074168	5.3624947	-0.5878799	C	-2.8799164	-2.3350736	1.9902811
H	-5.7385948	5.6291937	1.1282916	C	-4.1001712	-0.4023004	0.9427985
C	-0.7117066	4.2651492	-1.1777283	O	-5.3225522	-0.1329598	0.4493974
C	-1.0868888	3.6395751	-2.5296406	O	-3.2035430	0.4491595	0.9528425
H	-0.3709961	3.9708009	-3.3094814	H	-6.8586269	-1.4739066	0.9249359
H	-2.1008254	3.9336586	-2.8686994	H	-5.1703203	-3.5161705	0.4116075
H	-1.0502237	2.5353137	-2.4911930	H	-4.4491215	-1.3721470	-1.7703728
C	-0.7123849	5.8036395	-1.2901244	H	-2.8843865	-3.3819042	2.3291812
H	0.3250707	3.9430828	-0.9507220	H	-2.3036548	-1.6083164	2.5880147
H	-0.0258571	6.1405953	-2.0942487				
H	-0.3968251	6.2898384	-0.3463685				
H	-1.7300691	6.1762594	-1.5309894				
H	0.3719936	-5.5758370	-2.6663349				
H	4.4501933	-1.6280424	-4.5135402				
H	3.3246276	-5.5761097	2.5289949				
C	1.1883773	-5.1649612	-3.3047440				
H	2.7952924	1.0727656	-3.9818064				
H	-0.0227841	-5.4080614	-5.1086417				
H	2.3257852	-3.3851203	3.2455345				
C	1.8872392	-4.1091588	-2.4540266				
C	4.7117553	-0.9471831	-3.6765447				
C	0.5548293	-4.6165462	-4.5891097				
H	1.3248804	-4.2589720	-5.3041001				
C	2.3188958	-2.8769275	-2.9631352				
C	2.9990993	-5.3687590	1.4894288				
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C	2.1506469	-4.3899094	-1.0995193				
C	2.1494328	-6.3278069	-3.6231597				
H	1.6280275	-7.1382465	-4.1740805				
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H	5.1282410	-0.0164807	-4.1150814				
H	5.5111073	-1.4376314	-3.0847744				
C	2.9629351	-1.9217060	-2.1525781				
C	2.0629126	-3.1401799	2.1957321				
C	2.7864534	-3.4793606	-0.2414964				
H	3.6729065	-5.9221829	0.8041559				
H	1.9758918	-5.7834306	1.3802734				
C	3.4792577	-0.6390197	-2.8036261				
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C	3.0260746	-3.8550950	1.2283351				
H	1.5141866	0.3290196	-2.9719422				
H	2.0908205	-2.0402783	2.0852267				
H	2.0582470	-0.4735220	-4.4835058				
H	-0.1338672	-3.7719023	-4.3848824				
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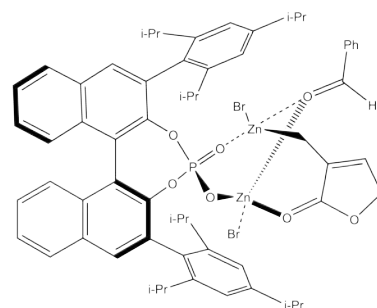


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C	2.5444718	4.7920951	1.4272309
C	3.2302661	6.0435448	1.4030910
C	1.1265070	4.7353282	1.5259933
H	0.5606628	5.6763014	1.5998557
C	0.4299990	3.5356366	1.4468447
C	3.7165777	-1.1635694	0.1390593
C	4.9041992	-1.3142768	0.8461677
H	5.5477549	-2.1819827	0.6357574
C	5.2843267	-0.4146538	1.8820877
C	6.4399788	-0.6555047	2.6844632
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C	3.3322435	1.0130329	1.3035237
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C	-5.3773655	3.5226503	0.6317439	H	-1.9425199	-5.9843732	-3.4547230
C	-6.2209058	2.9398789	1.7706784	H	-6.0065596	-3.3238399	-2.2456845
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C	0.5548293	-4.6165462	-4.5891097				
H	1.3248804	-4.2589720	-5.3041001				
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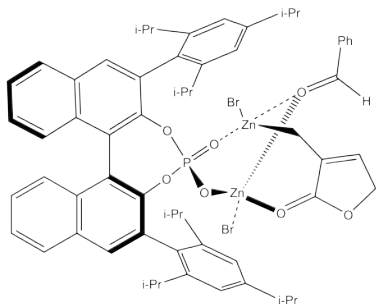


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C	3.9448372	6.4967187	1.6908442	C	3.3482857	-1.6451433	-2.0762658
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H	1.8733091	7.0592967	1.9783689	C	2.9099186	-3.1069310	-0.1358167
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C	6.5952882	0.5272667	4.1543923	C	3.0652889	-3.4744490	1.3462723
H	3.9368717	2.6578421	3.7260484	H	2.1857674	0.6826008	-3.0959480
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H	7.4278148	0.3461889	4.8513262	H	2.7835435	-0.2009055	-4.5296843
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C	-1.2642968	1.9835389	3.7960629	C	-4.4420141	-6.1330638	-2.9949949
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C	-5.6084711	2.3959050	1.1501119	H	-3.8553770	-6.3951669	-5.0778171
C	-6.1947936	1.3964784	2.1538732	H	-3.5022427	-3.5379176	-0.9601192
H	-7.2619195	1.1993043	1.9247587	Br	-1.2206763	-4.4676457	0.6346955
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H	-2.8165151	3.8895422	-2.4416616	H	-5.6169605	-1.9899100	0.8958030
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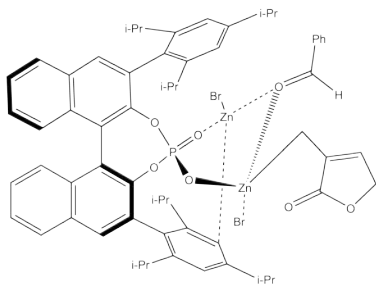
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O	0.5591598	1.0178131	1.3570710
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H	5.9248453	5.6326281	1.3249066
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C	6.6010821	0.5189147	4.1452807
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H	7.4360227	0.3353954	4.8385849
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H	4.9984652	-1.5854894	-4.3248036
H	3.2362747	-5.2153969	2.6426301
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H	3.6026566	1.2990380	-3.9929000
H	0.0346755	-4.6882210	-5.1173908
H	2.2961802	-2.9776637	3.3253333
C	1.9391285	-3.6404586	-2.3517813
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C	0.7760009	-4.0425569	-4.6033467
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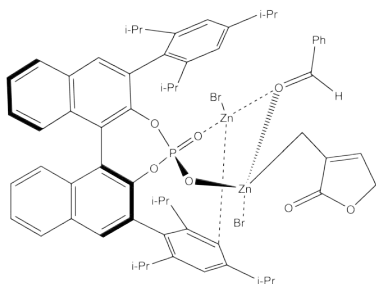
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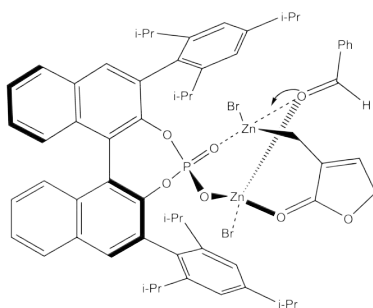
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H	-5.2634219	-5.4871079	-4.8841462	C	1.3018291	-5.1077456	-0.0688232
H	-2.2660835	-4.9224289	-0.8970128	H	1.5419077	-5.9039829	0.6523878
Br	-1.6532016	-4.0225766	1.4584402	C	0.7499213	-3.9188313	0.3909101
Zn	-0.4774509	-2.7777990	-0.1543867	C	0.1499863	0.2682843	-3.7431658
H	-5.8801628	-3.0663368	-2.1181578	C	-0.6114468	-0.0916849	-4.8489578
C	-4.5909714	-2.0669644	-0.6412582	H	-0.8366143	0.6616404	-5.6187161
C	-5.9103282	-2.2990387	-1.3099374	C	-1.1456641	-1.4048967	-4.9985063
C	-4.2859619	-0.7243307	-0.7100630	C	-2.0024767	-1.7292822	-6.0932690
C	-3.1639355	0.0404526	-0.2333095	C	-0.8414269	-2.4219077	-4.0190685
C	-5.3683408	-0.0766152	-1.5333288	C	-1.4589098	-3.7010003	-4.1556940
O	-6.2843474	-1.0404061	-1.8855165	C	0.0453560	-2.0942905	-2.9291019
O	-5.4838908	1.0859263	-1.8561088	C	0.4461573	-0.7629092	-2.8015571
H	-6.7015090	-2.6149298	-0.5911483	O	-0.2074587	-1.7770543	-0.0987669
H	-4.0755633	-2.8163617	-0.0231421	O	1.2381850	-0.4070200	-1.7157250
H	-3.0925155	-1.8102136	-3.0914227	P	0.5219259	-0.3020246	-0.2507730
H	-2.5969038	-0.4260465	0.5928923	O	1.7003137	-0.1256861	0.7147208
H	-3.4122915	1.0979878	-0.0189228	O	-0.6437477	0.6906650	-0.1993005
				C	2.5470258	-6.6957706	-3.2310229
				C	2.2426692	-5.6781845	-4.1743120
				H	2.4781499	-7.2835675	-1.1477287
				H	3.0509217	-7.6173645	-3.5600394
				H	1.3786713	-3.7339809	-4.5172255
				H	2.5255003	-5.8090135	-5.2300305
				C	-2.3028416	-3.9778640	-5.2226989
				C	-2.5676609	-2.9905748	-6.2091435
				H	-1.2692706	-4.4703391	-3.3940440
				H	-2.7752282	-4.9690187	-5.3005893
				H	-3.2330100	-3.2236501	-7.0544100
				H	-2.2196264	-0.9482947	-6.8389219
				C	1.4651571	-3.1389835	2.6981900
				C	0.4623258	-3.6768076	1.8421790
				C	1.1470071	-2.9311350	4.0507446
				C	-0.8284200	-3.9737276	2.3502664
				C	-1.0955120	-3.7404946	3.7147379
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				H	1.9138630	-2.5167741	4.7236401
				C	-1.9400239	-4.5175549	1.4539231
				H	-2.1013327	-3.9667676	4.0989479
				C	-3.0610606	-3.4819137	1.2557207
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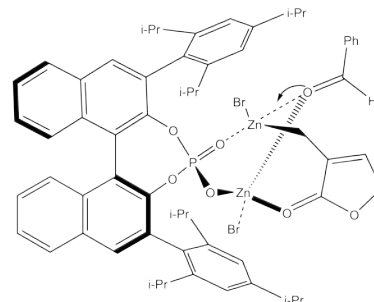
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Br	-4.1881771	0.1520553	-0.4103958
H	-1.0635748	-0.9627590	2.8723483

H	-2.6695503	-2.5424997	0.8181671
C	-2.4937937	-5.8568487	1.9711663
H	-1.4981478	-4.7143681	0.4557461
H	-2.9918127	-5.7425164	2.9566845
H	-1.6861560	-6.6079941	2.0876677
H	-3.2460488	-6.2663931	1.2658109
C	-0.4035569	-2.9088432	6.0513674
C	-0.6300466	-1.3949999	6.2428210
H	-0.7407443	-1.1412803	7.3176828
H	-1.5501043	-1.0700885	5.7143121
H	0.2149822	-0.8062549	5.8324649
C	-1.5602972	-3.7140230	6.6563256
H	0.5216896	-3.1758603	6.6104271
H	-1.6338416	-3.5270681	7.7468341
H	-1.4275209	-4.8041097	6.5027150
H	-2.5355566	-3.4253606	6.2109811
C	2.8630227	-2.8082422	2.1756738
C	3.5210111	-1.6240260	2.9025408
H	4.3855458	-1.2428680	2.3233924
H	3.8962295	-1.9091663	3.9076783
H	2.8054756	-0.7920488	3.0418940
C	3.7880291	-4.0401203	2.2288266
H	2.7468772	-2.5132005	1.1118625
H	4.7961328	-3.7890599	1.8384554
H	3.3924363	-4.8817729	1.6283531
H	3.9047336	-4.3949377	3.2744374
H	1.2606158	6.2939418	-2.3561994
H	4.3530888	2.0637888	-5.1256013
H	-3.5532035	2.8097341	-4.4156037
C	2.1192219	5.7077807	-2.7541574
H	4.7963633	-0.1456995	-2.8277485
H	3.5236620	6.8365212	-1.5041510
H	-3.4875062	2.8168288	-1.8451151
C	1.6129353	4.2883329	-2.9806398
C	3.7927039	1.1053619	-5.1374537
C	3.2616520	5.7818508	-1.7268076
H	4.1808750	5.2881365	-2.1039515
C	2.4993242	3.2298582	-3.2420409
C	-2.4630460	3.0154367	-4.4416181
H	1.6964430	6.3520966	-4.8154155
C	0.2377907	4.0015290	-2.9730455
C	2.5334073	6.3578854	-4.0884823
H	2.8552992	7.4094289	-3.9375693
H	-0.4698374	4.8186472	-2.7585378
C	4.1146073	0.7095896	-2.6406641
H	4.5163045	0.2959184	-5.3675197
H	3.0577635	1.1558131	-5.9665752
C	2.0515274	1.9222408	-3.4970258
C	-2.4192070	3.1024933	-1.9118761
C	-0.2683595	2.7089891	-3.2177618
H	-2.0487673	2.5499043	-5.3584619
H	-2.3262934	4.1134859	-4.5377215
C	3.0963314	0.8460346	-3.7880189
C	0.6509549	1.6580711	-3.4979778
C	-1.7799478	2.4877566	-3.1656851
H	3.6067739	0.5415553	-1.6711609
H	-1.9213208	2.7205922	-1.0019892
H	4.7438751	1.6185030	-2.5410371
H	2.9989174	5.2823485	-0.7714808
H	-2.3604178	4.2110812	-1.9066738
H	3.3805162	5.8056959	-4.5467683
H	2.5726988	-0.1260750	-3.8824131
H	-1.9596214	1.3951676	-3.1053826
H	3.5828858	3.4254844	-3.2508227
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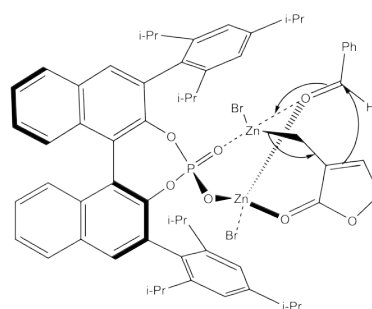
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Br	3.9906173	2.6368095	1.8021129
H	-1.6483034	3.9504692	4.4141898
Br	-4.2082393	0.1340261	-0.4089735
H	-1.0880561	-0.9939754	2.8757108
Zn	-2.2952551	0.1175755	0.9036393
C	-2.3590967	1.8792721	4.2605336
C	-1.4785403	2.9352188	4.8411108
C	-1.5963285	0.9358292	3.6233217
C	-1.9228604	-0.2652940	2.8532923
C	-0.1944181	1.3851424	3.8043960
O	-0.1386207	2.5361338	4.5013477
O	0.8408482	0.8282647	3.4103133
H	-1.5379328	3.0244714	5.9492024
H	-2.8485665	-0.7524329	3.2165716
H	-3.4544711	1.8919575	4.3430756
C	-2.9247226	5.2534630	1.1345685
C	-1.8360422	4.3904007	1.2734097
C	-0.5616290	4.7835032	0.7975777
C	-0.3906098	6.0471283	0.1906344
C	-1.4855244	6.9097152	0.0545968
C	-2.7496150	6.5112337	0.5236654
H	-3.9208654	4.9441042	1.4846417
H	-1.9502934	3.3927236	1.7244962
H	0.5765608	3.8744286	0.9093511
H	0.6049364	6.3406939	-0.1764851
H	-1.3579373	7.8929583	-0.4222005
H	-3.6119412	7.1858046	0.4079200
O	0.4829474	2.7649031	1.4539516
C	0.3961338	-2.9458054	-0.5739050
C	0.5546694	-3.1187308	-1.9544340
C	1.2475873	-4.3024485	-2.4073467
C	1.6265727	-4.5019726	-3.7693758
C	1.6055756	-5.3181958	-1.4461802
C	2.2618448	-6.5034553	-1.8941027
C	1.3182294	-5.1126907	-0.0665753
H	1.5598098	-5.9095988	0.6534191
C	0.7555838	-3.9302523	0.3963310
C	0.1369384	0.2707196	-3.7185673
C	-0.6202292	-0.0904653	-4.8266537
H	-0.8503161	0.6662097	-5.5916087
C	-1.1421774	-1.4069919	-4.9850197
C	-1.9934718	-1.7338099	-6.0826492
C	-0.8294257	-2.4262547	-4.0110422
C	-1.4333039	-3.7105913	-4.1566966
C	0.0519256	-2.0962076	-2.9175303
C	0.4409411	-0.7618940	-2.7813813
O	-0.2154671	-1.7936789	-0.0903320
O	1.2287139	-0.4043960	-1.6933232
P	0.5123567	-0.3162964	-0.2264627
O	1.6905484	-0.1548900	0.7414369
O	-0.6531763	0.6750886	-0.1648220
C	2.5900985	-6.6768613	-3.2296569
C	2.2817644	-5.6580679	-4.1694552

TS1-8-d

H	2.5172617	-7.2740539	-1.1497980
H	3.1026389	-7.5930509	-3.5602251
H	1.4034919	-3.7188871	-4.5068776
H	2.5694730	-5.7822551	-5.2245984
C	-2.2714261	-3.9896391	-5.2270457
C	-2.5448332	-2.9996636	-6.2075517
H	-1.2367407	-4.4817709	-3.3988706
H	-2.7331832	-4.9851671	-5.3117172
H	-3.2064952	-3.2342200	-7.0552186
H	-2.2180721	-0.9501169	-6.8231884
C	1.4557214	-3.1586911	2.7108077
C	0.4594092	-3.6960152	1.8470426
C	1.1279507	-2.9553444	4.0613788
C	-0.8333792	-3.9985366	2.3461229
C	-1.1097666	-3.7690803	3.7091596
C	-0.1451964	-3.2492792	4.5854119
H	1.8898127	-2.5413044	4.7400217
C	-1.9374016	-4.5450781	1.4419531
H	-2.1171392	-4.0000925	4.0862602
C	-3.0613077	-3.5141526	1.2363453
H	-3.5629212	-3.2601566	2.1936389
H	-3.8363333	-3.8980197	0.5420039
H	-2.6723953	-2.5727376	0.8012234
C	-2.4889048	-5.8869650	1.9546412
H	-1.4877613	-4.7397537	0.4467908
H	-2.9950453	-5.7757666	2.9362841
H	-1.6790912	-6.6343926	2.0781606
H	-3.2341414	-6.3002009	1.2441027
C	-0.4348315	-2.9388851	6.0514917
C	-0.6514860	-1.4240850	6.2467860
H	-0.7677724	-1.1725986	7.3216403
H	-1.5655675	-1.0907495	5.7131866
H	0.2002678	-0.8399628	5.8438581
C	-1.6017552	-3.7374486	6.6450011
H	0.4838629	-3.2152892	6.6170046
H	-1.6835290	-3.5539908	7.7354734
H	-1.4759383	-4.8277628	6.4886070
H	-2.5713486	-3.4402456	6.1930658
C	2.8560376	-2.8217250	2.1988033
C	3.5067399	-1.6399448	2.9361892
H	4.3715211	-1.2497028	2.3637888
H	3.8802377	-1.9299567	3.9405882
H	2.7872365	-0.8122102	3.0810727
C	3.7845075	-4.0508326	2.2512370
H	2.7460543	-2.5210836	1.1360234
H	4.7945288	-3.7942649	1.8698611
H	3.3967399	-4.8896143	1.6420698
H	3.8945456	-4.4124899	3.2951019
H	1.2022026	6.3243044	-2.4234529
H	4.3234638	2.0800476	-5.1253961
H	-3.6074426	2.7610442	-4.3310922
C	2.0625498	5.7398899	-2.8210195
H	4.7880685	-0.0997669	-2.8024859
H	3.4734778	6.9168804	-1.6215778
H	-3.4883905	2.7936842	-1.7620122
C	1.5700847	4.3096106	-3.0064456
C	3.7692946	1.1180356	-5.1241411
C	3.2202969	5.8541688	-1.8149124
H	4.1401479	5.3639351	-2.1945335
C	2.4642472	3.2551406	-3.2556287
C	-2.5208534	2.9791844	-4.3825051
H	1.5977201	6.3274156	-4.8895352
C	0.1983349	4.0095865	-2.9779853
C	2.4460854	6.3629177	-4.1771884
H	2.7571357	7.4219184	-4.0587987
H	-0.5151048	4.8229908	-2.7682599
C	4.0993524	0.7513842	-2.6231310
H	4.4979310	0.3114127	-5.3477534
H	3.0319471	1.1550109	-5.9516023
C	2.0265491	1.9399556	-3.4878597
C	-2.4258867	3.0926192	-1.8559669

C	-0.2977802	2.7089658	-3.1975364
H	-2.1210150	2.5090840	-5.3032396
H	-2.3985580	4.0774735	-4.4935800
C	3.0785399	0.8686129	-3.7701490
C	0.6285996	1.6641516	-3.4756283
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H	3.5956964	0.5870839	-1.6509536
H	-1.9029047	2.7253988	-0.9538546
H	4.7215734	1.6658475	-2.5311498
H	2.9821837	5.3728263	-0.8439633
H	-2.3796787	4.2019932	-1.8639602
H	3.2916922	5.8098357	-4.6366683
H	2.5615521	-0.1079746	-3.8530891
H	-1.9738290	1.3782531	-3.0412097
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TS2-8-d; COSMO

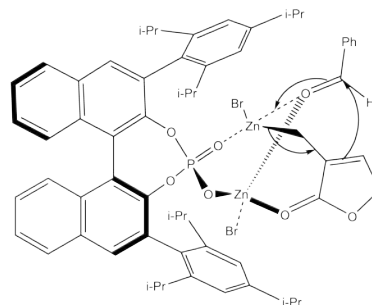


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Br	-2.6830964	3.9525632	-1.0696850
H	-0.7547197	2.0791123	2.4657710
Zn	-1.0185776	2.5137049	-0.2710666
C	0.4351301	5.1393496	1.2217297
C	1.6100891	5.7697932	1.9222883
C	0.1843808	3.9177510	1.8917983
C	-0.8794305	3.0112920	1.8880097
C	1.5276278	3.5533511	2.4318215
O	2.2914348	4.6512691	2.5554701
O	1.9746923	2.4200907	2.6421756
H	1.3047939	6.4912124	2.7111356
H	-1.9029672	3.4123694	1.8008032
H	-0.3414139	5.7443183	0.7307648
C	0.0682140	5.2199062	-3.8463623
C	0.3277562	4.4334176	-2.7172832
C	1.0913801	4.9504286	-1.6462933
C	1.6041108	6.2660760	-1.7420380
C	1.3371860	7.0520228	-2.8682727
C	0.5629353	6.5322295	-3.9227482
H	-0.5242662	4.8012927	-4.6741665
H	-0.0257587	3.3935150	-2.6855067
C	1.4254630	4.1072106	-0.4815874
H	2.2287250	6.6715474	-0.9310359
H	1.7418824	8.0734241	-2.9318010
H	0.3555357	7.1497324	-4.8099623
O	1.0271867	2.8482511	-0.4599742
C	-1.1455859	-2.4942202	1.4299996
C	-1.0744798	-3.5961857	0.5694995
C	-0.7834695	-4.8837249	1.1579911
C	-0.5134128	-6.0509230	0.3811627
C	-0.7228769	-4.9964841	2.5969042
C	-0.4797350	-6.2730774	3.1884920
C	-0.8411730	-3.8290082	3.4039065

H	-0.7566220	-3.9291674	4.4967781	H	4.0788714	3.8420213	-3.9167319
C	-0.9898733	-2.5636243	2.8472352	H	-3.5229926	1.2867948	-3.9976819
C	-0.4252145	-2.2640909	-2.9839254	C	1.9047995	1.1342982	-4.3460236
C	-1.2168082	-3.1157261	-3.7455711	C	3.3511972	-3.0253766	-3.9401187
H	-1.2021691	-3.0308868	-4.8427423	C	3.6104019	2.8768368	-3.6340609
C	-2.0937980	-4.0649637	-3.1431547	H	4.4269919	2.1639450	-3.3986655
C	-2.9696374	-4.8624487	-3.9401870	C	2.5273956	0.0113033	-3.7731328
C	-2.1340002	-4.1991659	-1.7051331	C	-2.0988690	-0.2187367	-5.8616911
C	-3.1012470	-5.0798099	-1.1347385	H	2.8558795	1.7533639	-6.8768367
C	-1.2223302	-3.4156456	-0.9051269	C	0.5147145	1.0831844	-4.5355942
C	-0.4526985	-2.4543963	-1.5678236	C	3.5148120	2.0800479	-6.0469868
O	-1.4198238	-1.2343862	0.9002988	H	4.0621497	2.9877696	-6.3765054
O	0.3933360	-1.6362113	-0.8211801	H	0.0160548	1.9500370	-4.9986321
P	-0.2647559	-0.4393688	0.0673376	C	3.4888581	-1.9472990	-1.6393167
O	0.8687033	0.0580102	0.9789808	H	3.8700528	-3.9278240	-3.5549511
O	-1.0186729	0.6090582	-0.7641521	H	2.6772773	-3.3398300	-4.7629418
C	-0.2603414	-7.3941792	2.4027104	C	1.8023613	-1.1231022	-3.3716446
C	-0.2590043	-7.2737498	0.9873813	C	-2.4209353	1.3301267	-3.8790566
H	-0.4502479	-6.3445123	4.2871609	C	-0.2658390	-0.0207789	-4.1392558
H	-0.0671205	-8.3710096	2.8716131	H	-1.6775775	-1.1792449	-6.2221094
H	-0.4970061	-5.9749865	-0.7144141	H	-1.6737354	0.5867484	-6.4969242
H	-0.0482100	-8.1558859	0.3636880	C	2.5687962	-2.3218551	-2.8137987
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C	-3.8777480	-5.7313385	-3.3536308	C	-1.7754108	0.0271040	-4.3750065
H	-3.1755050	-5.1563971	-0.0409823	H	2.9266203	-1.4366680	-0.8342988
H	-4.6954855	-6.4922836	-1.4734207	H	-2.2060318	1.5038649	-2.8086806
H	-4.5517290	-6.3344247	-3.9809074	H	4.3090345	-1.2693553	-1.9523536
H	-2.9210449	-4.7599205	-5.0357381	H	3.0371296	3.0304387	-2.6996911
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C	-0.8994998	-1.3141511	3.6692065	H	4.2633512	1.2778832	-5.8757631
C	0.4128202	0.1797094	5.0773057	H	1.8289160	-3.0554840	-2.4344060
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C	-1.9045941	0.6692131	4.6739026	H	3.6184602	0.0194674	-3.6264514
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C	-3.3914017	-0.7837371	3.2400466				
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H	-5.3963662	-1.4106685	3.8735004				
C	-0.5570939	2.2126637	6.2421076				
C	0.3010531	3.3205245	5.5997373				
H	0.4830449	4.1461035	6.3183402				
H	-0.2191020	3.7469751	4.7167521				
H	1.2830397	2.9338592	5.2636451				
C	-1.8911032	2.7826825	6.7388868				
H	0.0023057	1.8455891	7.1326985				
H	-1.7148610	3.5771106	7.4919319				
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H	-2.4717554	3.2410153	5.9107536				
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C	1.9832474	-2.5506839	5.3722818				
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H	2.8711904	-3.1976479	5.2160515				
H	1.1493482	-3.1922251	5.7224910				
H	2.2226819	-1.8407583	6.1916674				
H	1.9712381	3.1594423	-4.9989065				
H	4.1201899	-2.3521711	-4.3738479				
H	-3.1958131	-0.2393340	-6.0290374				
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TS2-8-d

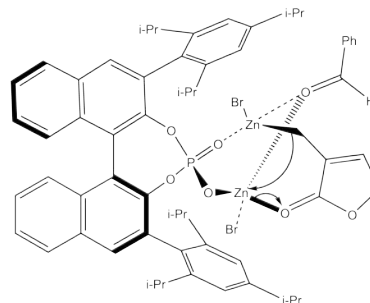


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H	-0.7726124	2.0781956	2.4575380
Zn	-1.0310865	2.5129171	-0.2888388
C	0.4203294	5.1351302	1.2079336
C	1.5943977	5.7648476	1.9109388
C	0.1666862	3.9163225	1.8817408
C	-0.8967222	3.0105593	1.8801374
C	1.5078740	3.5512494	2.4279042
O	2.2730537	4.6523903	2.5500003
O	1.9512984	2.4206868	2.6461610
H	1.2899412	6.4920887	2.6962797
H	-1.9204665	3.4068093	1.7788097
H	-0.3530085	5.7336939	0.7041240
C	0.0855826	5.2403850	-3.8521444
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C	1.6620866	6.2397723	-1.7581596	H	-2.5262468	1.9922042	7.2152056
C	1.4108803	7.0346074	-2.8811877	H	-2.4818455	3.2307835	5.9198782
C	0.6156166	6.5381278	-3.9305803	C	1.6201855	-1.7987736	4.0788872
H	-0.5252808	4.8388249	-4.6748487	C	2.8101707	-0.9645072	3.5733293
H	-0.0527946	3.4159203	-2.6935133	H	3.7010756	-1.6099362	3.4324477
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H	2.3065283	6.6239686	-0.9520296	H	2.5767341	-0.4958068	2.6004783
H	1.8450298	8.0436663	-2.9471240	C	1.9850624	-2.5480464	5.3748632
H	0.4197751	7.1623817	-4.8156537	H	1.4125201	-2.5608270	3.3012203
O	1.0184709	2.8387889	-0.4674186	H	2.8739389	-3.1938558	5.2198216
C	-1.1461998	-2.4964225	1.4337050	H	1.1524490	-3.1901539	5.7268261
C	-1.0742284	-3.5981760	0.5727101	H	2.2233029	-1.8374727	6.1938773
C	-0.7825075	-4.8858003	1.1605297	H	1.9627006	3.1657510	-5.0030111
C	-0.5128583	-6.0523675	0.3830017	H	4.1195643	-2.3361925	-4.3685720
C	-0.7211953	-4.9998081	2.5991182	H	-3.2029420	-0.2357866	-6.0163786
C	-0.4776826	-6.2766578	3.1888141	C	2.6993163	2.3644625	-4.7730861
C	-0.8395890	-3.8328684	3.4063103	H	3.9597085	-2.8404631	-1.2021011
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C	-0.9895150	-2.5673851	2.8508968	H	-3.5305152	1.2890595	-3.9828244
C	-0.4245856	-2.2591958	-2.9776097	C	1.8980792	1.1425551	-4.3434331
C	-1.2147389	-3.1105737	-3.7407133	C	3.3527773	-3.0109163	-3.9336796
H	-1.1999008	-3.0216421	-4.8375434	C	3.6139886	2.8855938	-3.6529653
C	-2.0901122	-4.0627796	-3.1413355	H	4.4327339	2.1739210	-3.4220424
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C	-2.1306809	-4.2000915	-1.7038292	C	-2.1060082	-0.2136223	-5.8494467
C	-3.0959916	-5.0841747	-1.1361049	H	2.8269199	1.7492216	-6.8832808
C	-1.2209760	-3.4166474	-0.9018576	C	0.5077735	1.0896217	-4.5289752
C	-0.4518512	-2.4532436	-1.5620169	C	3.4938573	2.0787786	-6.0612137
O	-1.4217443	-1.2368231	0.9065121	H	4.0406490	2.9833873	-6.3999280
O	0.3924941	-1.6363878	-0.8134476	H	0.0070291	1.9550180	-4.9925525
P	-0.2680695	-0.4391823	0.0736001	C	3.4892136	-1.9326477	-1.6324803
O	0.8637641	0.0586873	0.9870357	H	3.8746355	-3.9120442	-3.5496219
O	-1.0208477	0.6059072	-0.7615400	H	2.6792388	-3.3263415	-4.7562114
C	-0.2591360	-7.3969535	2.4026068	C	1.8001080	-1.1127700	-3.3646213
C	-0.2587761	-7.2753636	0.9879746	C	-2.4285002	1.3330789	-3.8657555
H	-0.4470275	-6.3486642	4.2874097	C	-0.2708019	-0.0144038	-4.1301055
H	-0.0656560	-8.3739984	2.8708322	H	-1.6829453	-1.1724697	-6.2119745
H	-0.4975171	-5.9745000	-0.7123465	H	-1.6826475	0.5922433	-6.4851718
H	-0.0486684	-8.1569059	0.3633043	C	2.5698008	-2.3093702	-2.8066752
C	-3.9447252	-5.8309509	-1.9414051	C	0.3847456	-1.1292095	-3.5328096
C	-3.8696033	-5.7328863	-3.3558813	C	-1.7809775	0.0317203	-4.3631214
H	-3.1693515	-5.1628022	-0.0425366	H	2.9263231	-1.4242627	-0.8264558
H	-4.6856784	-6.5001471	-1.4780939	H	-2.2151659	1.5065495	-2.7952394
H	-4.5417298	-6.3361064	-3.9849268	H	4.3077052	-1.2518825	-1.9433040
H	-2.9152030	-4.7549423	-5.0348585	H	3.0518165	3.0427839	-2.7127274
C	0.3488995	-0.9678292	4.2686324	H	-2.0807116	2.2234699	-4.4301967
C	-0.9003384	-1.3184564	3.6734929	H	4.2417071	1.2753578	-5.8940652
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C	-2.0305464	-0.4789341	3.8605577	H	-2.2371598	-0.7925895	-3.7789971
C	-1.9086287	0.6622537	4.6787065	H	3.6135597	0.0325058	-3.6221135
C	-0.7043816	1.0031971	5.3158739	H	2.4215415	4.2754393	-0.0269524
H	1.3704378	0.4401399	5.5520223				
C	-3.3941116	-0.7956024	3.2484027				
H	-2.7990847	1.2888573	4.8340371				
C	-3.8972466	0.3403129	2.3388676				
H	-4.0580446	1.2807669	2.9062807				
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H	-3.1789055	0.5476185	1.5216591				
C	-4.4234842	-1.1435279	4.3401141				
H	-3.2811293	-1.6981138	2.6147131				
H	-4.6087170	-0.2811728	5.0142002				
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H	-5.3955139	-1.4295688	3.8876506				
C	-0.5622435	2.2095797	6.2435811				
C	0.2890836	3.3206769	5.5979809				
H	0.4709822	4.1475887	6.3152280				
H	-0.2364232	3.7440299	4.7166235				
H	1.2708375	2.9381660	5.2568338				
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TS2-8-d-transmetall; COSMO

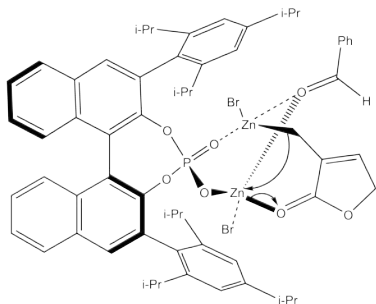


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Br	-1.1413463	4.3981640	-1.8130992

H	0.2077797	2.2804055	2.2695340	H	-4.6686435	1.2409119	1.0483384
Zn	0.0064449	2.6919235	-0.7176502	H	-2.8962212	1.4165128	0.8835366
C	0.0943863	5.6155887	1.7416606	C	-4.7674140	0.6788750	3.7644254
C	0.8900575	6.5352592	2.6173549	H	-3.4658041	-0.4190705	2.4670317
C	0.5223810	4.3443084	1.9455573	H	-4.9387424	1.7040335	4.1542999
C	0.1582521	3.0139313	1.4285677	H	-4.6336005	0.0061697	4.6358067
C	1.6338391	4.4061478	2.9252810	H	-5.6868518	0.3674647	3.2267517
O	1.8132480	5.6934971	3.3336245	C	-0.8651272	4.0247301	5.5103946
O	2.3114316	3.4674142	3.3203790	C	-1.7904108	5.0995646	4.9264757
H	0.2620133	7.0811548	3.3562925	H	-1.5593491	6.0893531	5.3701602
H	-0.9304428	2.9671139	1.1922527	H	-2.8572093	4.8865317	5.1476867
H	-0.7009010	5.9515378	1.0619918	H	-1.6819990	5.1796110	3.8261680
C	1.6500597	3.7874939	-5.3286290	C	-1.0798088	3.8896595	7.0321947
C	1.6685862	3.2800809	-4.0278710	H	0.1847088	4.3612066	5.3567557
C	2.9097572	3.0499630	-3.3829535	H	-0.9261191	4.8628898	7.5428994
C	4.1241678	3.3321623	-4.0575168	H	-0.3801416	3.1539699	7.4768329
C	4.0969749	3.8458095	-5.3582436	H	-2.1129557	3.5460842	7.2497508
C	2.8608111	4.0708662	-5.9920996	C	1.1548228	-0.5294717	4.6837873
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H	0.7295874	3.0635511	-3.5000850	H	3.3199248	-0.6579889	4.4118293
C	2.9833169	2.5337062	-2.0278419	H	2.7477217	1.0119236	4.7132217
H	5.0830136	3.1465010	-3.5488016	H	2.4870632	0.2433030	3.1213265
H	5.0368478	4.0676925	-5.8847692	C	1.2324213	-0.9539926	6.1635292
H	2.8393566	4.4698008	-7.0180020	H	0.9726420	-1.4423429	4.0817174
O	2.0035281	2.3269274	-1.2803871	H	2.0457901	-1.6927796	6.3182911
C	-1.3648292	-1.6454604	1.8562999	H	0.2835588	-1.4103547	6.5117240
C	-1.4844186	-2.9257651	1.3038604	H	1.4400830	-0.0806645	6.8168357
C	-1.4645682	-4.0516296	2.2067631	H	3.0167898	1.1797171	-5.7521034
C	-1.3997757	-5.4049055	1.7567109	H	3.5782509	-4.3919700	-3.7676614
C	-1.4754637	-3.8049960	3.6296265	H	-3.1858174	-0.5938517	-5.6102808
C	-1.4844916	-4.9133643	4.5295725	C	3.3175692	0.1093572	-5.7325193
C	-1.4450844	-2.4662074	4.1149599	H	3.5283121	-3.8573606	-0.6114407
H	-1.4659692	-2.2962329	5.2022205	H	5.4166221	0.7016893	-5.8350669
C	-1.3448474	-1.3752574	3.2584149	H	-2.7079637	1.4028589	-4.0880417
C	-0.6757218	-2.6647068	-2.4506603	C	2.3102169	-0.6024940	-4.8366135
C	-1.6602260	-3.4783865	-2.9982663	C	2.6943998	-4.6738047	-3.1576798
H	-1.6662188	-3.6618883	-4.0834249	C	4.7638821	0.0434571	-5.2264366
C	-2.6918316	-4.0507208	-2.1993768	H	5.1784374	-0.9838804	-5.2970495
C	-3.7452299	-4.8095577	-2.7933151	C	2.6673078	-1.6575718	-3.9824794
C	-2.6970436	-3.8334085	-0.7715461	C	-2.1192032	-0.8945077	-5.5495631
C	-3.8003367	-4.3354581	-0.0173450	H	2.1852143	-0.3236241	-7.5723040
C	-1.6118575	-3.0915980	-0.1728907	C	0.9546081	-0.2279853	-4.8812242
C	-0.6818831	-2.4979082	-1.0322886	C	3.2172167	-0.4170357	-7.1783638
O	-1.3207482	-0.5467443	1.0072292	H	3.8962443	0.1436708	-7.8543050
O	0.3549350	-1.7400460	-0.4953562	H	0.6628360	0.6114700	-5.5329855
P	0.0374047	-0.2629014	0.1251360	C	3.2601451	-3.0271422	-1.2969953
O	1.2604763	0.0686377	0.9904040	H	2.9917570	-5.5233392	-2.5084163
O	-0.4181559	0.7614329	-0.9281534	H	1.9068007	-5.0307834	-3.8522393
C	-1.4485323	-6.2167313	4.0573196	C	1.7184392	-2.3412329	-3.1983711
C	-1.3904027	-6.4601173	2.6588134	C	-1.6359771	1.1182346	-4.0889238
H	-1.5039997	-4.7102057	5.6118952	C	-0.0349866	-0.8755829	-4.1209765
H	-1.4485821	-7.0618998	4.7623974	H	-2.0684737	-1.9975489	-5.6468079
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H	-1.3312898	-7.4941288	2.2859956	C	2.1959842	-3.4883009	-2.3097916
C	-4.8194538	-5.0533037	-0.6286302	C	0.3522922	-1.9586829	-3.2788868
C	-4.7870420	-5.3082079	-2.0257093	C	-1.4853943	-0.4047684	-4.2329961
H	-3.8451312	-4.1383868	1.0625994	H	2.8889603	-2.1819053	-0.6849943
H	-5.6624434	-5.4226924	-0.0248363	H	-1.1976002	1.4738570	-3.1385221
H	-5.5962563	-5.8859525	-2.4977803	H	4.1929836	-2.7027998	-1.8038388
H	-3.7214448	-4.9774112	-3.8816096	H	4.8443302	0.3667891	-4.1688621
C	-0.0233128	0.4197281	4.4587127	H	-1.1551816	1.6688772	-4.9244789
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C	-3.7423970	1.5220767	1.5905468				
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TS2-8-d-transmetall



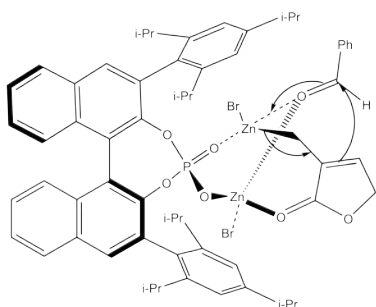
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Br	4.3452755	2.1075919	1.1173511
H	1.4480036	7.3005597	2.0203624
Br	-1.1330569	4.4003184	-1.8553674
H	0.1725835	2.2928815	2.2490407
Zn	-0.0201046	2.6937103	-0.7347935
C	0.0633622	5.6265319	1.7029565
C	0.8539742	6.5468852	2.5851063
C	0.4848372	4.3554146	1.9190127
C	0.1203925	3.0245974	1.4070105
C	1.5870331	4.4176234	2.9128553
O	1.7640489	5.7090098	3.3161084
O	2.2520262	3.4787346	3.3217685
H	0.2179665	7.0988914	3.3136430
H	-0.9674639	2.9773089	1.1674764
H	-0.7203060	5.9578890	1.0075256
C	1.6741420	3.8129969	-5.3354432
C	1.6776205	3.2955639	-4.0380336
C	2.9112775	3.0453365	-3.3878764
C	4.1322781	3.3185835	-4.0524056
C	4.1202683	3.8411837	-5.3496559
C	2.8912726	4.0855958	-5.9897586
H	0.7164299	4.0086994	-5.8404322
H	0.7322662	3.0918278	-3.5159587
C	2.9675736	2.5165227	-2.0338248
H	5.0852978	3.1175057	-3.5383534
H	5.0662962	4.0553336	-5.8684684
H	2.8815824	4.4922752	-7.0129052
O	1.9788348	2.3143757	-1.3011084
C	-1.3756980	-1.6452841	1.8561353
C	-1.4953556	-2.9255071	1.3033224
C	-1.4752984	-4.0520061	2.2052981
C	-1.4127584	-5.4049074	1.7544821
C	-1.4839864	-3.8067572	3.6282017
C	-1.4946879	-4.9158815	4.5264219
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H	-1.4643668	-2.2980104	5.2011873
C	-1.3489891	-1.3770024	3.2586007
C	-0.6763702	-2.6601985	-2.4478285
C	-1.6571695	-3.4758167	-2.9986508
H	-1.6582121	-3.6576637	-4.0840958
C	-2.6902524	-4.0508431	-2.2041620
C	-3.7396532	-4.8121162	-2.8008487
C	-2.7007311	-3.8336856	-0.7765642
C	-3.8053066	-4.3381948	-0.0263821
C	-1.6190780	-3.0905435	-0.1737536
C	-0.6869720	-2.4941721	-1.0292448
O	-1.3372170	-0.5461681	1.0082672
O	0.3454599	-1.7347532	-0.4891592
P	0.0211237	-0.2565918	0.1273280
O	1.2384957	0.0839446	0.9952448
O	-0.4362064	0.7593583	-0.9333313
C	-1.4626946	-6.2185495	4.0535551
C	-1.4057250	-6.4605813	2.6553835

H	-1.5119837	-4.7133305	5.6088933
H	-1.4642011	-7.0641218	4.7580688
H	-1.3587319	-5.6069875	0.6758712
H	-1.3492011	-7.4942672	2.2814018
C	-4.8200250	-5.0586751	-0.6408402
C	-4.7823293	-5.3135577	-2.0372026
H	-3.8525974	-4.1411575	1.0533786
H	-5.6638451	-5.4303443	-0.0396999
H	-5.5883692	-5.8932757	-2.5121591
H	-3.7119982	-4.9793349	-3.8891517
C	-0.0137874	0.4127175	4.4508836
C	-1.2059279	0.0235046	3.7698625
C	0.0709438	1.7169005	4.9700515
C	-2.2560603	0.9657203	3.5917055
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C	-0.9738736	2.6510585	4.8497854
H	0.9962819	2.0262420	5.4808678
C	-3.5506693	0.6255785	2.8539974
H	-2.9473144	2.9686105	4.0125253
C	-3.7584872	1.5220316	1.6188951
H	-3.8469278	2.5925059	1.8994103
H	-4.6899091	1.2425227	1.0848917
H	-2.9198428	1.4155218	0.9033831
C	-4.7632310	0.6775098	3.8021122
H	-3.4739888	-0.4190677	2.4913666
H	-4.9308925	1.7018424	4.1955360
H	-4.6209417	0.0044623	4.6716494
H	-5.6884659	0.3672238	3.2738393
C	-0.8400970	4.0146479	5.5209156
C	-1.7676568	5.0938057	4.9488479
H	-1.5306597	6.0818118	5.3936150
H	-2.8331362	4.8838688	5.1791938
H	-1.6691220	5.1765495	3.8477196
C	-1.0406041	3.8753358	7.0440896
H	0.2088474	4.3491209	5.3580563
H	-0.8793927	4.8458219	7.5577328
H	-0.3392429	3.1358367	7.4791302
H	-2.0719632	3.5328197	7.2709071
C	1.1656280	-0.5378352	4.6634574
C	2.5040961	0.0488991	4.1848077
H	3.3288728	-0.6672579	4.3770834
H	2.7625142	1.0020201	4.6875979
H	2.4906026	0.2380242	3.0957247
C	1.2521814	-0.9672010	6.1412992
H	0.9785365	-1.4483527	4.0592688
H	2.0662529	-1.7065166	6.2892217
H	0.3056164	-1.4240427	6.4950256
H	1.4640854	-0.0964542	6.7964974
H	3.0257394	1.1745394	-5.7538396
H	3.5818738	-4.3861216	-3.7444707
H	-3.1760261	-0.5973739	-5.6220085
C	3.3248314	0.1036119	-5.7275989
H	3.5217121	-3.8424254	-0.5878718
H	5.4260596	0.6917462	-5.8314978
H	-2.7043502	1.4050297	-4.1028507
C	2.3159904	-0.6024653	-4.8286465
C	2.6965537	-4.6660348	-3.1358803
C	4.7706522	0.0387401	-5.2200052
H	5.1839090	-0.9893871	-5.2845614
C	2.6708648	-1.6534352	-3.9690620
C	-2.1095874	-0.8971888	-5.5559083
H	2.1944089	-0.3411376	-7.5651867
C	0.9607869	-0.2284424	-4.8784010
C	3.2260202	-0.4316574	-7.1701186
H	3.9059959	0.1232194	-7.8499621
H	0.6705200	0.6086910	-5.5339574
C	3.2555668	-3.0144012	-1.2766470
H	2.9927864	-5.5140747	-2.4842704
H	1.9114970	-5.0247143	-3.8321587
C	1.7200345	-2.3347856	-3.1856998
C	-1.6329122	1.1191981	-4.0988587

C	-0.0309947	-0.8738499	-4.1195449
H	-2.0578591	-2.0002548	-5.6510037
H	-1.5808685	-0.4654871	-6.4318247
C	2.1956352	-3.4787532	-2.2921618
C	0.3539913	-1.9539359	-3.2728718
C	-1.4810959	-0.4038885	-4.2382638
H	2.8826285	-2.1686958	-0.6667265
H	-1.1995675	1.4787115	-3.1478871
H	4.1907782	-2.6912678	-1.7798417
H	4.8510101	0.3662068	-4.1637653
H	-1.1491940	1.6683831	-4.9338035
H	3.5046597	-1.5055260	-7.2078105
H	1.3237947	-3.8442025	-1.7131481
H	-2.0483968	-0.8593215	-3.4012780
H	3.7237958	-1.9642774	-3.8996987
H	3.9708269	2.2852185	-1.5956963

TS2-8d-2; COSMO



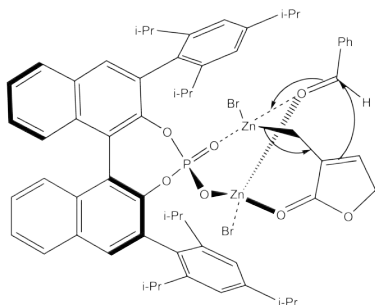
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Br	-1.4459977	3.8142339	-2.6936374
H	-0.4951734	2.8812343	1.5435340
Zn	-0.3026339	2.4273825	-1.1949713
C	1.5703505	5.0543348	-0.2838796
C	2.7702154	5.6342386	0.4184899
C	0.9395163	4.1997338	0.6522469
C	-0.3090651	3.5741682	0.7047476
C	2.0711151	3.7745453	1.5282241
O	3.0651218	4.6760561	1.4725613
O	2.1896954	2.7093046	2.1444365
H	2.5607932	6.6213054	0.8852144
H	-1.1800736	4.1193103	0.3044189
H	1.0369585	5.6054079	-1.0724546
C	3.3899476	5.2887030	-4.5014094
C	3.3161875	4.8880741	-3.1629760
C	2.4961192	3.7990370	-2.7835074
C	1.7725907	3.1062422	-3.7805070
C	1.8543308	3.5047665	-5.1203824
C	2.6544036	4.6002146	-5.4845109
H	4.0314300	6.1368204	-4.7847382
H	3.9109789	5.4178600	-2.4028221
C	2.4683006	3.3432405	-1.3794163
H	1.1790601	2.2216529	-3.5106484
H	1.2886775	2.9521478	-5.8859870
H	2.7150584	4.9137219	-6.5378480
O	1.7691884	2.2677958	-1.0652196
C	-1.9090724	-1.5831592	1.8410593
C	-2.0204798	-2.8995505	1.3775832
C	-2.1481083	-3.9457912	2.3664655
C	-2.0954709	-5.3349553	2.0404209
C	-2.2979792	-3.5794531	3.7558155
C	-2.4697761	-4.6047477	4.7345980
C	-2.2083205	-2.2111432	4.1404819

H	-2.2890535	-1.9541280	5.2076398
C	-1.9528182	-1.2039968	3.2166382
C	-0.6159133	-3.0006006	-2.2057286
C	-1.5004756	-3.8771937	-2.8229741
H	-1.3291191	-4.1701160	-3.8698663
C	-2.6604271	-4.3680346	-2.1546143
C	-3.6073724	-5.1893491	-2.8379603
C	-2.9112249	-3.9999806	-0.7801507
C	-4.1363613	-4.4194170	-0.1804369
C	-1.9336482	-3.1981739	-0.0826708
C	-0.8656902	-2.6951039	-0.8321900
O	-1.7803236	-0.5458133	0.9188504
O	0.0646998	-1.8662816	-0.2075873
P	-0.3654066	-0.3325347	0.1353519
O	0.7375483	0.1986194	1.0650151
O	-0.7133076	0.5048879	-1.1045374
C	-2.4526157	-5.9440943	4.3763301
C	-2.2441080	-6.3082538	3.0192650
H	-2.5964122	-4.3080350	5.7876267
H	-2.5789873	-6.7247110	5.1418891
H	-1.9236437	-5.6358767	0.9981829
H	-2.1932180	-7.3717567	2.7401006
C	-5.0460602	-5.2006573	-0.8803062
C	-4.7747874	-5.6045957	-2.2147873
H	-4.3625312	-4.1070667	0.8486319
H	-5.9875446	-5.5043304	-0.3976261
H	-5.4991040	-6.2315149	-2.7567926
H	-3.3987443	-5.4732168	-3.8814728
C	-0.4283022	0.4639620	4.3361196
C	-1.6434256	0.2014471	3.6340806
C	-0.1718641	1.7751676	4.7716583
C	-2.5312761	1.2699285	3.3380713
C	-2.2194397	2.5667930	3.7947470
C	-1.0560902	2.8429910	4.5321338
H	0.7571971	1.9750018	5.3299861
C	-3.8431144	1.0575029	2.5841117
H	-2.9282864	3.3796046	3.5785969
C	-3.9139072	1.9034509	1.2993939
H	-3.8898801	2.9908744	1.5215573
H	-4.8550561	1.6991409	0.7488605
H	-3.0706422	1.6709818	0.6195802
C	-5.0559414	1.3165585	3.4977671
H	-3.8921368	-0.0073225	2.2797873
H	-5.0917999	2.3736226	3.8348615
H	-5.0201122	0.6764489	4.4027034
H	-6.0039067	1.1027116	2.9619825
C	-0.7221215	4.2316340	5.0764904
C	0.4552450	4.8686988	4.3120829
H	0.7511846	5.8329777	4.7743536
H	0.1668058	5.0708157	3.2594053
H	1.3421389	4.2052922	4.3019108
C	-1.9182130	5.1901987	5.1232351
H	-0.3795482	4.0730995	6.1244286
H	-1.6370443	6.1336905	5.6331656
H	-2.7789401	4.7512235	5.6670082
H	-2.2636598	5.4611680	4.1032491
C	0.5980862	-0.6266026	4.6514867
C	2.0181013	-0.2636512	4.1824988
H	2.7179771	-1.0971450	4.3966328
H	2.4122068	0.6411204	4.6887285
H	2.0369984	-0.0781723	3.0933947
C	0.5883234	-0.9746458	6.1525034
H	0.3024451	-1.5387003	4.0952553
H	1.2975719	-1.7999248	6.3700208
H	-0.4183072	-1.2891133	6.4947128
H	0.8894363	-0.0997986	6.7662589
H	3.3213817	0.8204019	-5.2264387
H	3.8883482	-4.4742854	-2.5778106
H	-2.3787038	-1.5910454	-6.1998922
C	3.7924245	0.0225014	-4.6110075
H	3.2151313	-3.8478319	0.4971789

H	5.3685868	1.4077361	-3.9790836
H	-2.5498463	0.5588892	-4.8165017
C	2.6573638	-0.8029604	-4.0194909
C	2.9251548	-4.7917849	-2.1261107
C	4.6336414	0.7120094	-3.5243275
H	5.1989056	-0.0209557	-2.9129433
C	2.8959996	-1.7726898	-3.0296568
C	-1.3424666	-1.7402171	-5.8313059
H	4.0709368	-1.2890620	-6.3572533
C	1.3348337	-0.6298590	-4.4572117
C	4.6709126	-0.8301686	-5.5454468
H	5.4691757	-0.2148711	-6.0105983
H	1.1362390	0.1154679	-5.2444357
C	3.0539897	-3.0593386	-0.2666857
H	3.1434940	-5.5993114	-1.3967197
H	2.2987789	-5.2183303	-2.9359229
C	1.8605738	-2.5349374	-2.4633795
C	-1.4960442	0.4141159	-4.5018905
C	0.2546081	-1.3549282	-3.9163198
H	-1.1419121	-2.8304644	-5.7999910
H	-0.6499191	-1.2988133	-6.5787321
C	2.2189488	-3.6081924	-1.4360743
C	0.5207239	-2.3154142	-2.8982404
C	-1.1512172	-1.0822104	-4.4507777
H	2.5481745	-2.2052144	0.2226584
H	-1.3746460	0.8894716	-3.5112137
H	4.0533204	-2.7087474	-0.5965044
H	3.9957809	1.2888274	-2.8274875
H	-0.8639438	0.9702636	-5.2254810
H	5.1626668	-1.6523869	-4.9841337
H	1.2746505	-4.0052128	-1.0113332
H	-1.8736799	-1.5507419	-3.7527221
H	3.9263810	-1.9381777	-2.6787270
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TS2-8d-2



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number of imaginary frequencies: 1

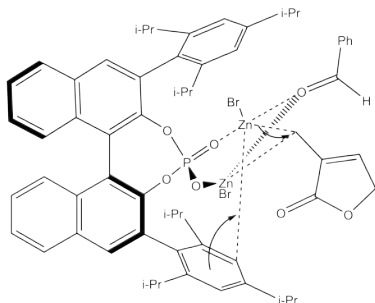
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Br	-1.4241847	3.8218039	-2.7164567
H	-0.5107137	2.8715913	1.5229166
Zn	-0.3152360	2.4129424	-1.2243975
C	1.5342972	5.0547180	-0.3144710
C	2.7300111	5.6444938	0.3863849
C	0.9101005	4.1999089	0.6247299
C	-0.3328880	3.5644798	0.6827476
C	2.0434852	3.7868512	1.5047669
O	3.0326001	4.6983495	1.4445381
O	2.1673476	2.7292816	2.1284795
H	2.5171810	6.6348312	0.8471461
H	-1.2095565	4.0924667	0.2733794
H	0.9994451	5.5879590	-1.1144189
C	3.4656061	5.2461191	-4.5083541
C	3.3718672	4.8401390	-3.1733324

C	2.5136491	3.7781472	-2.8024468
C	1.7730647	3.1149161	-3.8066990
C	1.8739328	3.5189666	-5.1432033
C	2.7111759	4.5889137	-5.4977854
H	4.1381923	6.0726136	-4.7845681
H	3.9840295	5.3409759	-2.4072750
C	2.4654450	3.3215811	-1.4006193
H	1.1486620	2.2499105	-3.5450803
H	1.2909863	2.9904948	-5.9128578
H	2.7865697	4.9064848	-6.5488921
O	1.7581056	2.2576588	-1.0839857
C	-1.9075356	-1.5819084	1.8479624
C	-2.0237159	-2.8981106	1.3842241
C	-2.1625793	-3.9430365	2.3730514
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C	-2.3205886	-3.5760490	3.7610794
C	-2.5053622	-4.6003469	4.7377960
C	-2.2261307	-2.2082933	4.1454797
H	-2.3138587	-1.9487737	5.2113956
C	-1.9573298	-1.2034335	3.2235842
C	-0.6058355	-2.9995989	-2.1936535
C	-1.4899816	-3.8743090	-2.8140422
H	-1.3159642	-4.1636063	-3.8615239
C	-2.6524503	-4.3649606	-2.1506010
C	-3.5982728	-5.1838669	-2.8374664
C	-2.9079811	-3.9973714	-0.7770887
C	-4.1363862	-4.4145205	-0.1831094
C	-1.9312372	-3.1985785	-0.0752686
C	-0.8585692	-2.6980934	-0.8197262
O	-1.7702974	-0.5436491	0.9295764
O	0.0709337	-1.8739824	-0.1895091
P	-0.3548923	-0.3367665	0.1444128
O	0.7498406	0.1944119	1.0722883
O	-0.6991158	0.4902813	-1.1021626
C	-2.4931978	-5.9393469	4.3801182
C	-2.2766163	-6.3044140	3.0251964
H	-2.6375719	-4.3026974	5.7898712
H	-2.6295803	-6.7189988	5.1448623
H	-1.9372357	-5.6331079	1.0066397
H	-2.2295359	-7.3680744	2.7461901
C	-5.0442096	-5.1938739	-0.8866791
C	-4.7684662	-5.5975693	-2.2196919
H	-4.3650605	-4.1019218	0.8452119
H	-5.9880705	-5.4959657	-0.4077829
H	-5.4915683	-6.2228011	-2.7651657
H	-3.3860839	-5.4667752	-3.8805158
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C	-2.5322598	1.2700603	3.3565468
C	-2.2169266	2.5643096	3.8172160
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C	-3.8460249	1.0602667	2.6053866
H	-2.9268563	3.3786678	3.6102174
C	-3.9143019	1.9016331	1.3176193
H	-3.8822068	2.9897559	1.5354954
H	-4.8580416	1.7028029	0.7697031
H	-3.0752199	1.6600459	0.6362200
C	-5.0570252	1.3260090	3.5190888
H	-3.8979909	-0.0054655	2.3042948
H	-5.0905572	2.3842279	3.8524905
H	-5.0217133	0.6902403	4.4268611
H	-6.0065167	1.1127949	2.9858666
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C	0.4251461	4.8817646	4.2875835
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H	0.0965736	5.0698952	3.2441492
H	1.3251227	4.2374416	4.2502536
C	-1.9161193	5.1628327	5.2041194
H	-0.3217900	4.0569744	6.1256000

H	-1.6308133	6.0998165	5.7236583
H	-2.7509027	4.6996715	5.7674937
H	-2.3013840	5.4508572	4.2033827
C	0.6062444	-0.6347741	4.6313460
C	2.0305392	-0.2524466	4.1926028
H	2.7213587	-1.1067540	4.3430956
H	2.4352370	0.6055716	4.7670415
H	2.0554727	0.0161038	3.1217187
C	0.5813801	-1.0247549	6.1215182
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H	-0.4226803	-1.3683057	6.4413847
H	0.8553117	-0.1606637	6.7622680
H	3.3120188	0.8300455	-5.2295094
H	3.9067889	-4.4448066	-2.5622429
H	-2.3664123	-1.5982202	-6.2045207
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H	3.2387481	-3.8165240	0.5120277
H	5.3774113	1.4098624	-4.0114870
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C	2.6561655	-0.7914011	-4.0155510
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C	4.6469017	0.7166127	-3.5460976
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C	2.8993948	-1.7518788	-3.0183254
C	-1.3307367	-1.7413596	-5.8320891
H	4.0356113	-1.2848534	-6.3683293
C	1.3327877	-0.6284673	-4.4536032
C	4.6486870	-0.8273288	-5.5657946
H	5.4440513	-0.2170500	-6.0423098
H	1.1299448	0.1104518	-5.2458850
C	3.0686221	-3.0297916	-0.2515375
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H	3.9302748	-1.9083561	-2.6651290
H	3.4044338	3.4605015	-0.8220264

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Zn	0.3290391	2.3689322	-0.6764462
C	1.1903774	4.7754976	2.0562927
C	1.9671070	5.5921626	3.0395590
C	0.9260443	3.5499011	2.5999458
C	0.2686451	2.3552993	2.0806140
C	1.5596149	3.5313102	3.9612247
O	2.1695038	4.7422055	4.1762057
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H	1.4248425	6.5080903	3.3667295
H	-0.5368418	2.5871189	1.3493381
H	0.8299309	5.1616511	1.0924303
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C	4.3346418	5.5431041	0.1003115
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C	3.8237057	7.2489654	-1.5482833
H	2.1919525	6.8051275	-2.9246885
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C	3.0972950	3.4331903	0.1954083
H	4.9368135	5.1731085	0.9451923
H	5.4038290	7.4244988	-0.0587066
H	4.0289353	8.2355132	-1.9915371
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C	-1.5872545	-2.7344445	2.3001067
C	-0.1913714	-2.1716216	-3.3426466
C	-0.9769340	-2.8811375	-4.2419544
H	-0.9203707	-2.6410958	-5.3150141
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C	-1.1889299	-3.4735364	-1.4542714
C	-0.2708687	-2.5537414	-1.9678752
O	-1.2865708	-1.3223386	0.3861609
O	0.6501824	-1.9623328	-1.1049927
P	0.1697616	-0.7647274	-0.1095879
O	1.2432877	-0.6922042	0.9794209
O	-0.1750068	0.5350659	-0.8638175
C	-1.2984319	-7.6080998	1.8071188
C	-0.9872042	-7.4613504	0.4286754
H	-1.7718101	-6.5837176	3.6552936
H	-1.3161961	-8.6099929	2.2624192
H	-0.7200648	-6.1052099	-1.2270523
H	-0.7499593	-8.3500481	-0.1758901
C	-4.0171958	-5.5341545	-2.9160965
C	-3.8069423	-5.3378115	-4.3066725
H	-3.3721041	-5.0842673	-0.9114411
H	-4.8498158	-6.1668421	-2.5725676
H	-4.4652391	-5.8313116	-5.0377794
H	-2.6378340	-4.3079902	-5.8105538
C	-0.6071211	-1.2898903	4.1294419
C	-1.6302135	-1.5096868	3.1604729
C	-0.6533137	-0.1169871	4.9075231
C	-2.6700920	-0.5490396	3.0012401
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C	-1.6790223	0.8352641	4.7817484
H	0.1479724	0.0730935	5.6387165
C	-3.8081431	-0.7270102	1.9969240
H	-3.4960314	1.3203967	3.7045240
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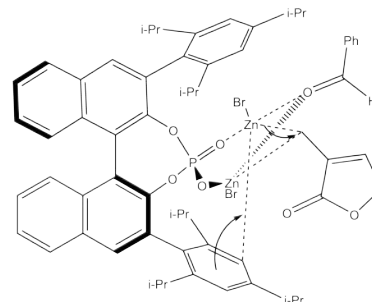


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Br	-0.9298717	4.2152133	-1.2722303

H	-4.6689870	0.2610526	0.2396405
H	-2.9362594	0.6329337	0.5082468
C	-5.1464350	-0.9742963	2.7185911
H	-3.5983065	-1.6343056	1.3959852
H	-5.4372387	-0.1023001	3.3409733
H	-5.0851079	-1.8576852	3.3862334
H	-5.9610529	-1.1519399	1.9860236
C	-1.7107398	2.0512166	5.7001519
C	-2.1083248	3.3523382	4.9861684
H	-2.0402893	4.2116706	5.6842165
H	-3.1531427	3.3183164	4.6122049
H	-1.4482396	3.5622232	4.1214533
C	-2.6302031	1.7811553	6.9074326
H	-0.6747007	2.1850466	6.0779688
H	-2.6102252	2.6318688	7.6200742
H	-2.3204058	0.8669971	7.4530055
H	-3.6809953	1.6362288	6.5780891
C	0.5311339	-2.2798091	4.3813844
C	1.9190991	-1.6346871	4.2416135
H	2.7158841	-2.3627307	4.4984402
H	2.0494115	-0.7521715	4.9004575
H	2.0983205	-1.3072394	3.2005041
C	0.3634417	-2.9560841	5.7562908
H	0.4706750	-3.0749295	3.6120833
H	1.1456279	-3.7277538	5.9117216
H	-0.6272892	-3.4457163	5.8542709
H	0.4503984	-2.2164895	6.5795614
H	1.9837173	3.6566461	-3.9324670
H	4.2838916	-1.8091885	-4.8808345
H	-3.1641901	0.3776148	-5.7994914
C	2.6393040	2.8589787	-4.3494430
H	4.2996340	-2.8678804	-1.8496337
H	4.4082015	4.0173210	-3.7968042
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C	1.9359183	1.5350316	-4.0699227
C	3.5618628	-2.5798111	-4.5378480
C	4.0181680	2.9851992	-3.6900551
H	4.7578913	2.3038769	-4.1592387
C	2.6376873	0.3562419	-3.7665350
C	-2.0642493	0.4313975	-5.6622512
H	1.7320610	3.0715534	-6.3464907
C	0.5345914	1.4547468	-4.1818303
C	2.7317191	3.1053192	-5.8690219
H	3.1841909	4.0958151	-6.0838780
H	-0.0301407	2.3733079	-4.4125310
C	3.7813550	-1.9170096	-2.0897726
H	4.1302003	-3.5125821	-4.3417803
H	2.8568275	-2.7745715	-5.3714673
C	1.9828393	-0.8736037	-3.5692790
C	-2.3944621	1.2995866	-3.2960583
C	-0.1691799	0.2481175	-4.0111754
H	-1.5997989	-0.3524765	-6.2950192
H	-1.7229297	1.4153002	-6.0473214
C	2.8160130	-2.1175133	-3.2709952
C	0.5693716	-0.9317647	-3.6947993
C	-1.6898657	0.2560555	-4.1778693
H	3.2442820	-1.5824849	-1.1804245
H	-2.1598761	1.1366938	-2.2266197
H	4.5660920	-1.1666850	-2.3208057
H	3.9785021	2.7451151	-2.6091742
H	-2.1002809	2.3383799	-3.5501147
H	3.3616539	2.3283341	-6.3506352
H	2.1162478	-2.9318656	-2.9929963
H	-2.0706862	-0.7335527	-3.8591698
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TS3-8-d-transmetall



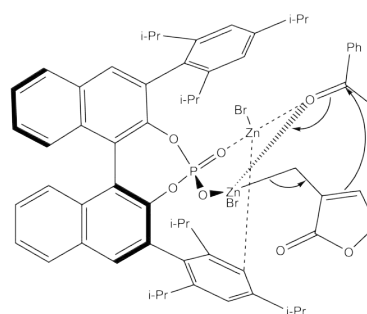
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Br	-0.8787167	4.2142280	-1.3408936
H	-0.2130601	1.7413488	2.8527807
Zn	0.3424213	2.3600284	-0.7006467
C	1.2059019	4.7587961	2.0257487
C	1.9755560	5.5741859	3.0173708
C	0.9245804	3.5388571	2.5751210
C	0.2648918	2.3497859	2.0551281
C	1.5397415	3.5240851	3.9482211
O	2.1565125	4.7340699	4.1604403
O	1.5066333	2.6441579	4.7809960
H	1.4356820	6.4976618	3.3297724
H	-0.5327399	2.5805667	1.3149120
H	0.8542902	5.1411361	1.0571113
C	2.8537708	6.4658691	-2.0214510
C	2.5716606	5.2080513	-1.4848777
C	3.3247521	4.7214276	-0.3890755
C	4.3714887	5.5157482	0.1480516
C	4.6517398	6.7728929	-0.3973095
C	3.8917635	7.2492766	-1.4808672
H	2.2602786	6.8414608	-2.8683500
H	1.7535347	4.6011114	-1.8946022
C	3.1102814	3.4168677	0.2128978
H	4.9642811	5.1264315	0.9910603
H	5.4657094	7.3851875	0.0183659
H	4.1117137	8.2388052	-1.9103507
O	2.2978283	2.5208576	-0.1634810
C	-1.3607643	-2.6194504	0.8874381
C	-1.2641294	-3.7136315	0.0162074
C	-1.2604370	-5.0328496	0.6015828
C	-0.9687983	-6.2100490	-0.1507842
C	-1.5259460	-5.1728970	2.0136227
C	-1.5559575	-6.4783038	2.5901309
C	-1.7138113	-4.0111119	2.8153619
H	-1.9206285	-4.1347587	3.8894389
C	-1.5854599	-2.7281516	2.2942299
C	-0.1892155	-2.1835444	-3.3452517
C	-0.9729730	-2.8961799	-4.2432553
H	-0.9181464	-2.6543552	-5.3160465
C	-1.9231380	-3.8632469	-3.8033738
C	-2.7792199	-4.5223350	-4.7357177
C	-2.0916944	-4.1129074	-2.3898746
C	-3.1771304	-4.9453170	-1.9821450
C	-1.1837024	-3.4844729	-1.4555945
C	-0.2656622	-2.5648172	-1.9698173
O	-1.2852700	-1.3248308	0.3731139
O	0.6548091	-1.9726275	-1.1088094
P	0.1757237	-0.7707241	-0.1169503
O	1.2397162	-0.6968620	0.9792562
O	-0.1593143	0.5252833	-0.8826331
C	-1.2976141	-7.6038881	1.8233862
C	-0.9854331	-7.4632924	0.4451013

H	-1.7708631	-6.5710394	3.6663229
H	-1.3157838	-8.6035814	2.2833671
H	-0.7166885	-6.1137487	-1.2159792
H	-0.7479703	-8.3545502	-0.1555122
C	-4.0052333	-5.5552087	-2.9145536
C	-3.7949806	-5.3615473	-4.3049003
H	-3.3618861	-5.0985442	-0.9106507
H	-4.8359182	-6.1897181	-2.5698658
H	-4.4512610	-5.8584876	-5.0354123
H	-2.6284748	-4.3315048	-5.8098882
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H	-4.1952045	1.3948708	1.5158315
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H	-2.9378085	0.6282244	0.4901358
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H	-3.5970266	-1.6351407	1.3883580
H	-5.4371066	-0.0979161	3.3282083
H	-5.0822106	-1.8513690	3.3805659
H	-5.9606815	-1.1531950	1.9781719
C	-1.7112327	2.0672422	5.6783537
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H	-2.0495855	4.2263236	5.6582392
H	-3.1639373	3.3269196	4.5940644
H	-1.4625073	3.5751200	4.0946507
C	-2.6241095	1.7954125	6.8899478
H	-0.6740923	2.2074138	6.0502464
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H	-2.3079033	0.8836225	7.4354517
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C	1.9227981	-1.6265292	4.2363399
H	2.7167165	-2.3561471	4.4970016
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H	2.1073583	-1.3059497	3.1942022
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H	4.2801965	-1.7819309	-4.8939495
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C	2.5982157	2.8720516	-4.3381938
H	4.3080034	-2.8544562	-1.8661204
H	4.3639211	4.0387804	-3.7887569
H	-3.5173907	1.1854753	-3.3962047
C	1.9070868	1.5404829	-4.0637956
C	3.5644843	-2.5591151	-4.5527975
C	3.9808955	3.0034590	-3.6880730
H	4.7219440	2.3314271	-4.1683588
C	2.6190592	0.3661842	-3.7680775
C	-2.0905634	0.4166946	-5.6471789
H	1.6758425	3.0921552	-6.3272474
C	0.5063975	1.4499551	-4.1718650
C	2.6781454	3.1309229	-5.8561815
H	3.1218733	4.1260258	-6.0682145
H	-0.0666826	2.3655828	-4.3930615
C	3.7823158	-1.9065518	-2.1013525
H	4.1404433	-3.4883957	-4.3627950
H	2.8599871	-2.7545184	-5.3864963
C	1.9745973	-0.8694888	-3.5746731
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C	-0.1871538	0.2371916	-4.0060859
H	-1.6224279	-0.3587676	-6.2874490
H	-1.7584590	1.4052436	-6.0281048
C	2.8175499	-2.1082125	-3.2826530
C	0.5617653	-0.9379961	-3.6974785
C	-1.7086289	0.2347494	-4.1656690
H	3.2450019	-1.5817119	-1.1889164
H	-2.1775028	1.0980974	-2.2064480
H	4.5621918	-1.1501144	-2.3289712
H	3.9510130	2.7537381	-2.6092116
H	-2.1343005	2.3099727	-3.5201981
H	3.3094569	2.3618820	-6.3482016
H	2.1234511	-2.9283451	-3.0073193
H	-2.0802923	-0.7599937	-3.8522609
H	3.7145839	0.4049933	-3.6813310
H	3.7920602	3.1251481	1.0483238

TS4-8-d-transmetall; COSMO

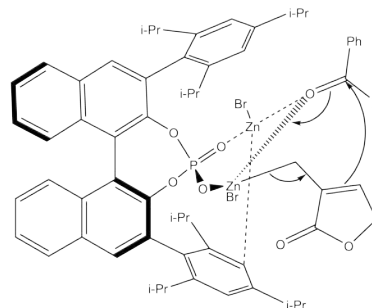


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Zn	2.2542831	1.4304243	0.5611252
Br	4.4828284	1.3745081	-0.1539507
H	2.6860445	6.4438318	-0.1108417
Br	-2.1023263	3.7283985	-1.2833056
H	1.2260620	2.1955083	2.6938765
Zn	-0.5718742	2.0071562	-1.7654407
C	1.2368876	4.9371861	0.5906048
C	2.1668997	6.0916223	0.8090643
C	1.5715215	3.9250729	1.4739364
C	1.0253761	2.6181494	1.6902569
C	2.8323339	4.3619086	2.1721408
O	3.1586385	5.6198946	1.7378631
O	3.4899674	3.7622272	2.9982846
H	1.6515377	6.9723902	1.2546931
H	-0.0168174	2.4652237	1.3579490
H	0.2864743	5.0157210	0.0440498
C	0.7683258	6.4171949	-3.7014985
C	0.7551629	5.3041971	-2.8552637
C	1.9595077	4.8371820	-2.2774191
C	3.1683984	5.5280913	-2.5506597
C	3.1773919	6.6321999	-3.4133736
C	1.9775427	7.0780882	-3.9926337
H	-0.1761487	6.7785795	-4.1360024
H	-0.1984293	4.8183071	-2.6004083
C	2.0825596	3.6647960	-1.4076912
H	4.1076408	5.1716761	-2.0986488
H	4.1241570	7.1490369	-3.6306795
H	1.9807436	7.9500962	-4.6643982
O	1.3585258	2.6080446	-1.3865669
C	-0.5961678	-2.6105945	1.6456256
C	-0.6819772	-3.7877844	0.8865297
C	-0.2349490	-5.0145595	1.5017197
C	-0.0924726	-6.2369912	0.7780847
C	0.1266911	-5.0032629	2.8994921
C	0.5396735	-6.2195232	3.5230970

C	0.1074130	-3.7779923	3.6248215	H	3.6260556	-2.5483920	-2.9104185
H	0.3822935	-3.7898589	4.6903063	H	2.0535690	3.9320837	-5.4585794
C	-0.1970751	-2.5645675	3.0167221	H	-4.8099408	0.2604207	-1.8323740
C	-1.1604778	-2.5634686	-2.7223711	C	0.0305856	1.3082559	-4.3023428
C	-2.0991704	-3.4585311	-3.2171668	C	1.9594918	-2.5848589	-5.1632044
H	-2.4734091	-3.3458818	-4.2465713	C	1.8775014	2.8951165	-5.1106680
C	-2.6664325	-4.4699199	-2.3856448	H	2.3419708	2.2114062	-5.8510004
C	-3.6900018	-5.3314498	-2.8833180	C	0.9526313	0.2509724	-4.2092559
C	-2.2750230	-4.5666482	-0.9963652	C	-4.0360017	-0.4060265	-4.4161813
C	-2.9974506	-5.4666280	-0.1567297	H	-1.4217032	2.6024106	-6.2616757
C	-1.1993486	-3.7314238	-0.5121566	C	-1.3032653	1.0595984	-3.8695365
C	-0.6779841	-2.7837413	-1.3955932	C	-0.3233428	2.7196798	-6.3474361
O	-0.9503715	-1.3935086	1.0628892	H	-0.1202787	3.7019191	-6.8206572
O	0.3854578	-1.9930569	-0.9912056	H	-2.0625704	1.8476325	-4.0117218
P	0.1148081	-0.7239695	0.0144805	C	2.9207554	-1.6954816	-2.9770105
O	1.4896272	-0.4202445	0.6038456	H	2.6916306	-3.4179538	-5.1502227
O	-0.6713305	0.4133929	-0.6478453	H	1.0459911	-2.9368918	-5.6841464
C	0.6352593	-7.3972653	2.7973543	C	0.5861590	-1.0274322	-3.7516952
C	0.3323990	-7.3982113	1.4093258	C	-3.7575002	0.5223437	-2.0635598
H	0.8000783	-6.1981711	4.5929724	C	-1.7277409	-0.2286522	-3.4450959
H	0.9628455	-8.3260428	3.2887407	H	-3.6700609	-1.1428342	-5.1602271
H	-0.3110645	-6.2511731	-0.2986885	H	-3.9986280	0.5972035	-4.8902346
H	0.4417374	-8.3255913	0.8265568	C	1.6461057	-2.1229024	-3.7257864
C	-4.0027836	-6.2762101	-0.6684758	C	-0.7654769	-1.2762372	-3.3779215
C	-4.3410034	-6.2257161	-2.0467352	C	-3.2032188	-0.4453831	-3.1193234
H	-2.7543710	-5.5123030	0.9134514	H	2.6979829	-1.3568287	-1.9468500
H	-4.5452925	-6.9590992	0.0029865	H	-3.1743574	0.4646344	-1.1235450
H	-5.1325723	-6.8797526	-2.4429382	H	3.4530933	-0.8718066	-3.4960633
H	-3.9682922	-5.2561035	-3.9463110	H	2.4114802	2.7687731	-4.1492783
C	1.1791434	-0.7984565	4.2023252	H	-3.7466266	1.5773381	-2.4038645
C	-0.0923883	-1.2599039	3.7465583	H	0.0525722	1.9266324	-7.0269282
C	1.2372788	0.3930938	4.9482739	H	1.2169110	-2.9935680	-3.1907030
C	-1.2570114	-0.4861657	4.0104081	H	-3.3024340	-1.4632373	-2.6979192
C	-1.1370564	0.7005703	4.7591970	H	1.9923569	0.4187394	-4.5205785
C	0.0949817	1.1533810	5.2584826	H	3.0837854	3.5543450	-0.9332954
H	2.2160907	0.7423070	5.3160344				
C	-2.6527756	-0.9193492	3.5630187				
H	-2.0495522	1.2759670	4.9747561				
C	-3.3186723	0.1355644	2.6603187				
H	-3.5190747	1.0773941	3.2125869				
H	-4.2914768	-0.2373833	2.2778161				
H	-2.6781030	0.3777975	1.7897907				
C	-3.5391792	-1.2711658	4.7727420				
H	-2.5504353	-1.8464448	2.9648405				
H	-3.7075173	-0.3875063	5.4230771				
H	-3.0735874	-2.0623490	5.3951473				
H	-4.5326283	-1.6362137	4.4385302				
C	0.2326687	2.4204859	6.0994240				
C	0.7524965	3.5994369	5.2536284				
H	0.8953916	4.5013492	5.8846142				
H	0.0280246	3.8547470	4.4518706				
H	1.7214625	3.3673141	4.7692608				
C	-1.0495327	2.8089080	6.8478462				
H	1.0119399	2.1987895	6.8632700				
H	-0.8501440	3.6503479	7.5419384				
H	-1.4548443	1.9633717	7.4400897				
H	-1.8443340	3.1462187	6.1498243				
C	2.4828657	-1.5554250	3.9395910				
C	3.5665718	-0.6682101	3.3034833				
H	4.4944877	-1.2513123	3.1324682				
H	3.8325628	0.2026906	3.9366721				
H	3.2403085	-0.2857913	2.3190777				
C	3.0057266	-2.2137404	5.2315481				
H	2.2645396	-2.3640030	3.2131653				
H	3.9171845	-2.8125482	5.0265593				
H	2.2502570	-2.8847124	5.6885082				
H	3.2690394	-1.4470687	5.9900640				
H	-0.0604453	3.4393087	-4.3434829				
H	2.3965405	-1.7603408	-5.7645624				
H	-5.0990582	-0.6355801	-4.1983133				
C	0.3744362	2.6334544	-4.9737189				

TS4-8-d-transmetall

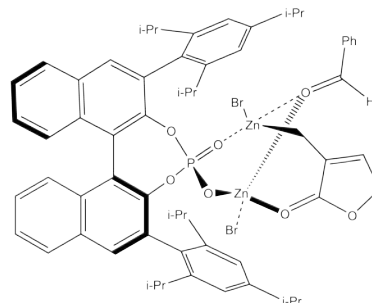


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number of imaginary frequencies: 1

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Br	4.5069793	1.3436308	-0.1671447
H	2.7097926	6.4133498	-0.1018647
Br	-2.0915624	3.7568035	-1.4113888
H	1.2253889	2.1687502	2.6943594
Zn	-0.5499262	2.0226038	-1.7559441
C	1.2581691	4.8973566	0.5751072
C	2.1807071	6.0567060	0.8110613
C	1.5819977	3.8901892	1.4696855
C	1.0391722	2.5840183	1.6847536
C	2.8323195	4.3331408	2.1882131
O	3.1592244	5.5931022	1.7529434
O	3.4734700	3.7369660	3.0260270
H	1.6513213	6.9347420	1.2477031
H	0.0046724	2.4200146	1.3346454
H	0.3127265	4.9734061	0.0192348
C	0.8851384	6.4400037	-3.6745401

C	0.8424692	5.3172809	-2.8422386	H	0.9812487	2.2165387	6.8540315
C	2.0311217	4.8221655	-2.2568360	H	-0.8840607	3.6721952	7.5151435
C	3.2558387	5.4891381	-2.5160016	H	-1.4895714	1.9857716	7.4126817
C	3.2948757	6.5999564	-3.3694603	H	-1.8676153	3.1665706	6.1172940
C	2.1091639	7.0790862	-3.9501868	C	2.4712221	-1.5441755	3.9498530
H	-0.0491347	6.8256761	-4.1105220	C	3.5623355	-0.6608551	3.3216498
H	-0.1224873	4.8464432	-2.6009635	H	4.4900818	-1.2455883	3.1570670
C	2.1211164	3.6414458	-1.3900387	H	3.8262784	0.2128066	3.9515096
H	4.1824941	5.1082607	-2.0576476	H	3.2474149	-0.2827575	2.3319807
H	4.2540061	7.0987299	-3.5748162	C	2.9817845	-2.1986135	5.2487126
H	2.1356163	7.9587193	-4.6114630	H	2.2589616	-2.3542773	3.2234518
O	1.3813784	2.5964360	-1.3919618	H	3.8948096	-2.7985025	5.0545892
C	-0.5963494	-2.6048349	1.6358825	H	2.2222222	-2.8672048	5.7022764
C	-0.6703752	-3.7849622	0.8801674	H	3.2384791	-1.4300538	6.0073515
C	-0.2178244	-5.0070299	1.5002332	H	-0.1357516	3.4422438	-4.3287239
C	-0.0638479	-6.2301930	0.7807359	H	2.3835484	-1.7203176	-5.7879872
C	0.1354940	-4.9901777	2.8997107	H	-5.1462778	-0.6726093	-4.1133675
C	0.5520412	-6.2022832	3.5279415	C	0.2959032	2.6479901	-4.9766335
C	0.1034584	-3.7632648	3.6210144	H	3.6256397	-2.5018369	-2.9380877
H	0.3726518	-3.7689601	4.6879459	H	1.9601630	3.9625969	-5.4764930
C	-0.2039832	-2.5527929	3.0087937	H	-4.7997068	0.2210962	-1.7513561
C	-1.1593464	-2.5742686	-2.7314258	C	-0.0265853	1.3117976	-4.3135814
C	-2.0894330	-3.4790457	-3.2239442	C	1.9573706	-2.5520764	-5.1887960
H	-2.4675605	-3.3683773	-4.2522486	C	1.7946898	2.9221035	-5.1341762
C	-2.6456130	-4.4950770	-2.3911802	H	2.2524257	2.2465560	-5.8862458
C	-3.6601266	-5.3684084	-2.8855384	C	0.9102556	0.2661396	-4.2283122
C	-2.2537370	-4.5829587	-1.0016317	C	-4.0901827	-0.4366227	-4.3567600
C	-2.9688034	-5.4861532	-0.1593857	H	-1.5192611	2.6189408	-6.2379053
C	-1.1857266	-3.7367616	-0.5192389	C	-1.3530422	1.0433801	-3.8752790
C	-0.6715018	-2.7870572	-1.4052389	C	-0.4232224	2.7455106	-6.3381744
O	-0.9525222	-1.3923975	1.0454222	H	-0.2349700	3.7338833	-6.8047721
O	0.3858207	-1.9872654	-1.0091821	H	-2.1185739	1.8293443	-3.9879286
P	0.1259723	-0.7240686	0.0080054	C	2.9079753	-1.6589640	-2.9994591
O	1.4978759	-0.4401134	0.6084192	H	2.7005298	-3.3754074	-5.1806282
O	-0.6472251	0.4249902	-0.6511162	H	1.0486848	-2.9136185	-5.7115573
C	0.6587369	-7.3809342	2.8062354	C	0.5637863	-1.0176042	-3.7708343
C	0.3639428	-7.3870271	1.4170736	C	-3.7544810	0.4873770	-2.0088878
H	0.8066506	-6.1764211	4.5990984	C	-1.7569060	-0.3464043	-3.4433639
H	0.9892460	-8.3063216	3.3019167	H	-3.7395959	-1.1688385	-5.1126750
H	-0.2769538	-6.2470579	-0.2970154	H	-4.0716863	0.5675820	-4.8299049
H	0.4820780	-8.3150305	0.8371174	C	1.6386769	-2.0990840	-3.7499625
C	-3.9653369	-6.3073472	-0.6686197	C	-0.7818052	-1.2830026	-3.3884249
C	-4.3027745	-6.2658462	-2.0467771	C	-3.2233535	-0.4741089	-3.0828097
H	-2.7252474	-5.5246674	0.9108370	H	2.6845568	-1.3310020	-1.9662944
H	-4.5015912	-6.9926141	0.0053634	H	-3.1477813	0.4260328	-1.0843047
H	-5.0874566	-6.9290336	-2.4413233	H	3.4300148	-0.8250388	-3.5125516
H	-3.9385890	-5.2992842	-3.9489465	H	2.3430878	2.7935497	-4.1813715
C	1.1655236	-0.7858987	4.2001165	H	-3.7551175	1.5446897	-2.3420292
C	-0.1034847	-1.2468519	3.7363875	H	-0.0532949	1.9625483	-7.0324526
C	1.2188925	0.4069345	4.9438646	H	1.2200661	-2.9766144	-3.2174237
C	-1.2694707	-0.4732322	3.9931213	H	-3.3057183	-1.4940623	-2.6625677
C	-1.1535543	0.7146625	4.7400443	H	1.9468143	0.4486843	-4.5417432
C	0.0753284	1.1683407	5.2452746	H	3.1130034	3.5121764	-0.9005210
H	2.1958514	0.7581652	5.3143663				
C	-2.6626569	-0.9073839	3.5387156				
H	-2.0670667	1.2908127	4.9487878				
C	-3.3223181	0.1440699	2.6276554				
H	-3.5256611	1.0885656	3.1740526				
H	-4.2929065	-0.2288794	2.2397561				
H	-2.6760552	0.3829397	1.7606643				
C	-3.5564758	-1.2545013	4.7441356				
H	-2.5568001	-1.8368613	2.9447390				
H	-3.7284867	-0.3689630	5.3907507				
H	-3.0947824	-2.0428591	5.3726554				
H	-4.5482736	-1.6203708	4.4060581				
C	0.2084518	2.4376926	6.0833470				
C	0.7369947	3.6132812	5.2385202				
H	0.8766736	4.5168672	5.8677212				
H	0.0188430	3.8673745	4.4307276				
H	1.7097515	3.3788913	4.7631882				
C	-1.0784893	2.8291980	6.8216397				

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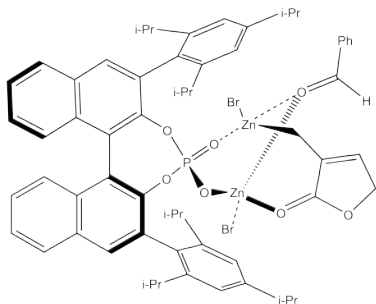


Energy(Hartree) = -11970.0475287

Zn	2.6758207	1.2869402	-0.0642540
Br	4.0899358	0.9325406	-1.8777066
H	2.8040227	6.1867290	2.6616956

Br	-2.3413749	4.1795770	1.3013699	H	-2.2027519	0.9068217	4.8926580
H	1.1494278	1.2259971	2.6748415	H	-3.5374180	0.0479913	4.0622508
Zn	-0.6577629	2.5381502	1.3099173	H	-2.0547380	0.4862342	3.1546679
C	1.6126569	4.5260347	3.4691951	C	-2.3693354	-1.7692057	5.8300833
C	2.9005812	5.2324309	3.2260996	H	-2.0921506	-1.9484954	3.7129304
C	1.6349209	3.2979000	2.8640502	H	-2.1495103	-1.0876615	6.6782939
C	0.6571525	2.2093337	2.8014365	H	-1.9367064	-2.7606628	6.0745482
C	2.9493039	3.2209047	2.1915819	H	-3.4717480	-1.8799834	5.7700924
O	3.6785028	4.3255992	2.4185450	C	2.4420545	0.6901408	6.5825544
O	3.4350597	2.3040388	1.5006168	C	2.7401683	2.0834369	5.9948626
H	3.4766136	5.4484751	4.1533508	H	3.3199874	2.7031303	6.7105177
H	0.0297972	2.1777392	3.7133127	H	1.7973417	2.6183897	5.7584848
H	0.7933456	4.9466606	4.0674487	H	3.3199949	2.0089618	5.0527403
C	-0.6890699	6.5195476	-1.6184523	C	1.6865507	0.8077852	7.9131225
C	-0.0060926	5.3872327	-1.1704532	H	3.4218828	0.2058946	6.7938495
C	0.7813372	4.6374325	-2.0772718	H	2.2997000	1.3511067	8.6605807
C	0.8975697	5.0527813	-3.4268516	H	1.4357323	-0.1879076	8.3315205
C	0.2167346	6.1913820	-3.8683401	H	0.7391449	1.3748652	7.7973854
C	-0.5804111	6.9196414	-2.9648327	C	2.8244687	-2.3109693	2.5192006
H	-1.3215046	7.0859306	-0.9188760	C	3.9566628	-1.3811301	2.0458833
H	-0.1079493	5.0565104	-0.1269963	H	4.3937288	-1.7512207	1.0967171
C	1.4657785	3.4253289	-1.6684928	H	4.7809553	-1.3182767	2.7866515
H	1.5213565	4.4692399	-4.1202122	H	3.5890394	-0.3512505	1.8763637
H	0.3001633	6.5134122	-4.9169523	C	3.4109357	-3.6517294	3.0011556
H	-1.1243087	7.8108747	-3.3144484	H	2.1800584	-2.5143693	1.6388861
O	1.4221767	2.9452560	-0.5124156	H	4.0535339	-4.1021670	2.2163707
C	-0.7883504	-2.3380205	1.4522879	H	2.6202930	-4.3845897	3.2530177
C	-1.3704712	-3.1802134	0.4982091	H	4.0344835	-3.5020941	3.9076598
C	-1.2054539	-4.6048721	0.6674971	H	0.9211203	3.3572375	-5.9971256
C	-1.6035282	-5.5559217	-0.3205476	H	1.2171331	-2.5384177	-6.0804680
C	-0.5798097	-5.0968409	1.8722377	H	-4.7912573	2.1939422	-3.7178072
C	-0.4470511	-6.5049590	2.0661377	C	1.3275556	2.3270912	-6.1107638
C	-0.0674343	-4.1736539	2.8283262	H	2.2716507	-3.3398817	-3.1595490
H	0.3992914	-4.5632799	3.7457631	H	3.3651630	3.1013113	-6.3534218
C	-0.1112841	-2.8000018	2.6204491	H	-3.3826025	3.3259383	-1.8886037
C	-1.9283352	-1.2076551	-2.7489960	C	0.5070576	1.4269509	-5.1948243
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H	-3.5937860	-1.3508198	-4.1090944	C	2.8192994	2.3586964	-5.7359072
C	-3.9623692	-2.5183010	-2.3042779	H	3.3002419	1.3729130	-5.9018649
C	-5.2835213	-2.9073138	-2.6797966	C	0.8842401	0.0937907	-4.9591977
C	-3.4202892	-2.9895532	-1.0510611	C	-3.8646803	1.8077169	-4.1909991
C	-4.2521975	-3.7875239	-0.2097176	H	0.0652826	1.9478377	-7.8729994
C	-2.0776334	-2.6093184	-0.6846478	C	-0.6734163	1.8900444	-4.5898920
C	-1.4238101	-1.6815972	-1.5006618	C	1.1359008	1.9257154	-7.5860423
O	-0.9152978	-0.9606272	1.3064280	H	1.6903793	2.6108713	-8.2607382
O	-0.1639489	-1.2228217	-1.1249937	H	-0.9750031	2.9374720	-4.7534967
P	-0.0752442	-0.1806414	0.1320985	C	1.9892517	-2.2852210	-3.3581723
O	1.4195872	-0.1070186	0.4797817	H	0.8278254	-4.0414726	-5.1869595
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C	-0.8745809	-7.4021203	1.0990314	C	0.1131721	-0.7743345	-4.1681615
C	-1.4415887	-6.9186484	-0.1104047	C	-2.4758884	2.9856815	-2.4280881
H	0.0205975	-6.8644178	2.9962923	C	-1.4810795	1.0662954	-3.7797884
H	-0.7595328	-8.4851888	1.2577158	H	-4.1071972	0.8444000	-4.6833307
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C	-5.5398556	-4.1331673	-0.5971372	C	-1.0921608	-0.2880135	-3.5842561
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H	-3.8652695	-4.1200580	0.7638421	H	2.0230802	-1.7283415	-2.4021892
H	-6.1656476	-4.7417028	0.0734627	H	-1.6742204	2.8753879	-1.6756817
H	-7.0778043	-3.9883051	-2.1473067	H	2.7642315	-1.8515392	-4.0236270
H	-5.6820983	-2.5499344	-3.6423236	H	2.9773645	2.6107350	-4.6671696
C	1.9338446	-1.6612819	3.5790468	H	-2.1859420	3.7942860	-3.1313763
C	0.5205677	-1.8418955	3.5856484	H	1.5109792	0.8963197	-7.7654447
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C	-0.2806972	-1.1403714	4.5232279	H	-3.0899649	0.9373937	-2.3755607
C	0.3485157	-0.3307576	5.4899273	H	1.8114110	-0.2904477	-5.4122022
C	1.7439571	-0.1888939	5.5490415	H	2.0736205	2.8947530	-2.4433477
H	3.6043541	-0.7158148	4.5836661				
C	-1.8054189	-1.2266551	4.5049925				
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C	-2.4332501	0.1303515	4.1333129				

int1-8-d



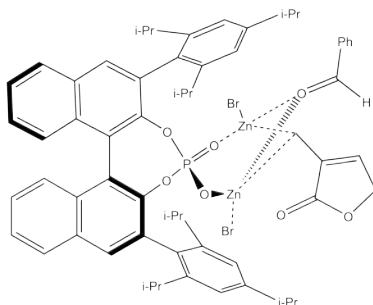
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Zn	-0.6753587	2.5427149	1.3216229
C	1.5543767	4.5208291	3.4608336
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C	1.5953369	3.2848394	2.8723061
C	0.6338639	2.1849596	2.8172102
C	2.9075921	3.2224253	2.1890049
O	3.6182278	4.3451737	2.3989598
O	3.4012531	2.3090053	1.5046510
H	3.4087420	5.4874432	4.1176259
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H	0.7256783	4.9357620	4.0497542
C	-0.6382093	6.5222057	-1.6716412
C	0.0304620	5.3843428	-1.2153785
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C	0.9628807	5.0464072	-3.4584505
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H	-1.2810870	7.0858206	-0.9793239
H	-0.0958813	5.0493868	-0.1755865
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C	-0.7839186	-2.3357816	1.4577801
C	-1.3665888	-3.1760809	0.5020785
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C	-1.5983015	-5.5489899	-0.3241468
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C	-1.9284052	-1.1967199	-2.7392423
C	-3.1806660	-1.6558310	-3.1292594
H	-3.5925539	-1.3376902	-4.0990460
C	-3.9608228	-2.5105632	-2.2971036
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C	-4.2472324	-3.7871051	-0.2071467
C	-2.0755643	-2.6029366	-0.6784456
C	-1.4230347	-1.6724149	-1.4920830
O	-0.9113430	-0.9584109	1.3172128
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P	-0.0746326	-0.1736923	0.1430055
O	1.4200719	-0.1012428	0.4900879
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C	-1.4354954	-6.9118823	-0.1188286
H	0.0303787	-6.8675500	2.9849365
H	-0.7505620	-8.4826276	1.2423991

H	-2.0307275	-5.1884011	-1.2672897
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H	-7.0719856	-3.9886618	-2.1445021
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C	0.5217910	-1.8475727	3.5949078
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C	-0.2824503	-1.1652664	4.5434018
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C	1.7352199	-0.1931352	5.5617909
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H	-0.2897937	0.1622150	6.2500722
C	-2.4561893	0.0726150	4.1643783
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H	-3.5597773	-0.0244383	4.1048092
H	-2.0930908	0.4299719	3.1806708
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H	-1.9031871	-2.8077066	6.1066135
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H	1.7917804	2.6159444	5.7608304
H	3.3150048	2.0008868	5.0628750
C	1.6690893	0.8142851	7.9217082
H	3.4074228	0.2044480	6.8131047
H	2.2796596	1.3585544	8.6704909
H	1.4130957	-0.1788797	8.3424103
H	0.7239452	1.3838348	7.8001043
C	2.8249706	-2.2850763	2.5142113
C	3.9563381	-1.3483253	2.0528613
H	4.3870620	-1.6986709	1.0934654
H	4.7861891	-1.3029516	2.7887845
H	3.5917258	-0.3135940	1.9083260
C	3.4127946	-3.6312664	2.9786808
H	2.1811714	-2.4778173	1.6311571
H	4.0597483	-4.0683015	2.1900901
H	2.6233114	-4.3701934	3.2152287
H	4.0317984	-3.4941543	3.8901433
H	0.9251624	3.3601919	-5.9925544
H	1.2010014	-2.5362214	-6.0798058
H	-4.7822114	2.2175024	-3.6779914
C	1.3187446	2.3261995	-6.1186907
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H	3.3598594	3.0835700	-6.3919555
H	-3.3539391	3.3410853	-1.8539815
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H	0.0187649	1.9702761	-7.8577600
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C	1.0942449	1.9348420	-7.5919617
H	1.6441418	2.6152074	-8.2752323
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H	-3.5685524	2.5392267	-4.9584263
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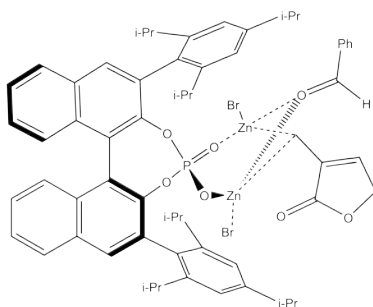
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O	0.1395288	1.1213074	1.3909263
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C	3.8253523	6.3881738	1.7139598
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H	4.2601887	7.3981819	1.7612646
H	4.8029030	3.1171149	1.3376166
H	5.7570814	5.4022424	1.4325512
C	5.0534877	1.4894257	4.7182068
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H	3.4357343	2.6403662	3.8800471
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H	-1.4566547	-0.0541638	2.9611945
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H	3.2130176	-4.8888373	2.7870382
C	2.2099965	-4.8771621	-3.6779055
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H	0.7329738	-4.3384314	2.5041183
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C	5.5205674	-0.5779482	-2.9465688
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H	3.0551191	-6.7460747	-4.4730974
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C	3.2236418	0.4468788	-3.3531935
H	6.0060656	0.3845495	-3.2102078
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C	3.4680730	-1.6553503	-1.9407476
C	0.9186176	-4.1399433	1.4287254
C	2.6349693	-3.2210350	-0.2293368
H	4.4235182	-4.2523140	1.6245811
H	3.3301261	-5.5799032	1.1355379
C	4.1117380	-0.3386830	-2.3713052
C	3.2305187	-1.9735739	-0.5760695
C	2.3485516	-3.6163877	1.2194374
H	2.2172563	0.6235927	-2.9256786
H	0.1705720	-3.3988930	1.0916874
H	3.1011411	-0.0923305	-4.3157632
H	1.1600773	-3.4826841	-5.0176886
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C	-1.4042552	-6.2115920	-4.2742771	H	3.4551820	2.6420725	3.8825150
C	-1.2503224	-4.8009331	-1.8290838	H	5.1808973	2.1477860	5.5888383
O	-1.6123589	-1.9282805	-2.0674556	H	6.6922679	0.1516497	5.3355464
H	-1.1028103	-7.9914100	-3.0629147	H	6.3973129	-1.3887339	3.3883051
H	-1.6818450	-4.2683665	-5.2131696	C	-2.3488873	3.8248819	0.4467444
H	-0.9674254	-6.7344396	-0.8977536	C	-1.6136477	3.3103370	1.5544164
H	-1.4592665	-6.7699977	-5.2202523	C	-3.7461104	3.6566900	0.4258053
H	-1.1912541	-4.2428159	-0.8847410	C	-2.2963649	2.6117114	2.5911687
Br	-3.0082173	-3.4585915	1.1844854	C	-3.6953371	2.4752855	2.5178532
Zn	-2.1401962	-1.6282053	0.0359107	C	-4.4446347	2.9949037	1.4494046
H	-7.0149615	-1.8677222	-2.3785242	H	-4.3179249	4.0314265	-0.4368048
C	-5.5826001	-1.4272012	-0.7880772	C	-1.5767307	2.0333817	3.8095185
C	-6.8680310	-1.1830172	-1.5128293	H	-4.2147510	1.9457013	3.3313946
C	-4.8251773	-0.3034813	-0.8393088	C	-1.7976936	0.5150769	3.9421353
C	-3.4843476	0.0376418	-0.2991398	H	-2.8661359	0.2680744	4.1139784
C	-5.5999950	0.7196594	-1.6084471	H	-1.2239964	0.1101956	4.8011035
O	-6.7941267	0.1644540	-1.9933388	H	-1.4598912	-0.0196288	3.0326807
O	-5.2976316	1.8695391	-1.8632255	C	-1.9811227	2.7786236	5.0954621
H	-7.7619212	-1.2820404	-0.8559294	H	-0.4884649	2.1961541	3.6767212
H	-5.3265086	-2.3772463	-0.2962751	H	-3.0617275	2.6526634	5.3155310
H	-1.6936785	-2.1639833	-4.0761785	H	-1.7824059	3.8659426	5.0079183
H	-3.4651666	-0.0582193	0.8141560	H	-1.4140594	2.3936104	5.9682397
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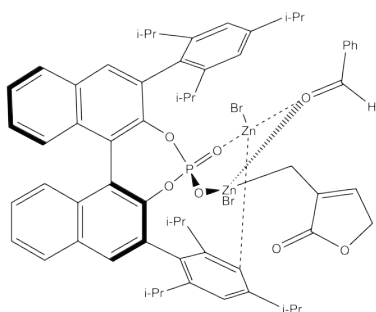


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C	4.1441360	3.9723850	1.4818529	C	5.4974377	-0.5594902	-2.9390470
C	1.8799510	4.9143472	1.7264268	C	1.9363294	-4.2840244	-5.0706456
C	2.4668455	6.2141397	1.7816474	H	2.8535805	-3.8610616	-5.5306247
C	0.4657421	4.7457890	1.7603340	C	3.1132267	-2.5855207	-2.9261037
H	-0.1730865	5.6358380	1.8675189	C	3.3750930	-4.6401507	1.7216289
C	-0.1293885	3.4972033	1.6196689	H	3.5001409	-6.4033735	-2.7583943
C	3.5373935	-0.9811740	0.5053678	C	2.3019565	-4.1203132	-1.2620683
C	4.5584421	-1.1604351	1.4298548	C	3.3283086	-5.9357055	-3.7484939
H	5.2032273	-2.0493027	1.3547856	H	3.0714070	-6.7392053	-4.4701951
C	4.7682907	-0.2461202	2.5021428	H	1.8398152	-5.0875054	-1.0055698
C	5.7648991	-0.4931075	3.4932418	C	3.1946904	0.4604863	-3.3293109
C	3.9393626	0.9313954	2.6136940				
C	4.1097073	1.7687065	3.7570642				
C	2.9536552	1.1947236	1.5907914				
C	2.7577644	0.2103727	0.6168261				
O	0.1388683	1.1246876	1.4289017				
O	1.7906409	0.4011637	-0.3651706				
P	0.2069609	0.3017030	0.0137499				

H	5.9792886	0.4058174	-3.1987440
H	6.1509829	-1.0867191	-2.2147588
C	3.4526484	-1.6493552	-1.9312647
C	0.9042526	-4.1543991	1.4232635
C	2.6209793	-3.2232495	-0.2273044
H	4.4086939	-4.2499676	1.6306202
H	3.3249290	-5.5811199	1.1340217
C	4.0902897	-0.3281891	-2.3568727
C	3.2152120	-1.9739220	-0.5682820
C	2.3319154	-3.6232215	1.2195821
H	2.1909496	0.6351447	-2.8952762
H	0.1526412	-3.4184044	1.0836914
H	3.0668242	-0.0736684	-4.2940003
H	1.1784127	-3.4757665	-5.0307181
H	0.7305172	-5.1089550	0.8832281
H	4.2864671	-5.4778513	-4.0719082
H	4.2186039	0.2956560	-1.4493907
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H	3.3081560	-2.3253377	-3.9771415
Zn	-2.1503303	0.2397785	-1.9642325
Br	-2.7576870	0.5039563	-4.1791248
C	-1.2233697	-6.8947631	-3.1221771
C	-1.5570122	-2.6553589	-3.0714485
C	-1.1499268	-6.2128530	-1.8919783
C	-1.5099384	-4.7939464	-4.2999881
C	-1.4389653	-4.1024662	-3.0649041
C	-1.4032027	-6.1878389	-4.3260175
C	-1.2545427	-4.8206161	-1.8566736
O	-1.5667491	-1.9425985	-2.0447401
H	-1.1364513	-7.9921454	-3.1435196
H	-1.6479532	-4.2251572	-5.2329660
H	-1.0098174	-6.7714832	-0.9545608
H	-1.4563236	-6.7289677	-5.2821866
H	-1.2025182	-4.2796292	-0.9017813
Br	-3.0134351	-3.5188684	1.1330450
Zn	-2.1450517	-1.6516085	0.0535862
H	-6.9924184	-1.8808758	-2.4311244
C	-5.5811583	-1.4647778	-0.8134528
C	-6.8599247	-1.2111125	-1.5505309
C	-4.8306348	-0.3363374	-0.8372929
C	-3.4983750	0.0045455	-0.2786533
C	-5.6041122	0.6995799	-1.5956498
O	-6.7914280	0.1425158	-2.0032211
O	-5.3049884	1.8546636	-1.8185064
H	-7.7617303	-1.3305684	-0.9067529
H	-5.3213906	-2.4205441	-0.3341767
H	-1.6562940	-2.1326630	-4.0556973
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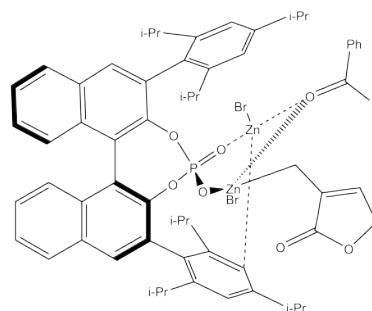


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Br	-1.1932240	3.8908882	-2.0029915
H	0.5899536	2.2893702	2.8694783
Zn	0.0850389	1.9172146	-1.9820602

C	1.3830264	4.9302211	0.9092743
C	2.3354963	6.0147501	1.2994365
C	1.5116562	3.8797896	1.7728405
C	0.8761818	2.5653356	1.8334576
C	2.5934450	4.2498475	2.7411330
O	3.0572059	5.5074671	2.4312959
O	3.0431794	3.6036315	3.6685586
H	1.8231316	6.9591668	1.5932992
H	-0.0051104	2.4758003	1.1696717
H	0.6670911	5.0113624	0.0784529
C	2.5473244	6.2591341	-3.2168403
C	2.2216152	5.0406724	-2.6176340
C	3.1536535	4.4054050	-1.7613793
C	4.4076774	5.0185354	-1.5097900
C	4.7336502	6.2330324	-2.1258464
C	3.8045375	6.8519842	-2.9803853
H	1.8166742	6.7590925	-3.8702978
H	1.2282360	4.5928942	-2.7673501
C	2.9118131	3.1290046	-1.1011421
H	5.1224471	4.5271388	-0.8304757
H	5.7101844	6.7025134	-1.9356949
H	4.0562136	7.8103723	-3.4601749
O	1.9804211	2.3128628	-1.2926306
C	-1.2171989	-2.4750470	1.4724795
C	-1.2240667	-3.6729036	0.7407489
C	-1.0855498	-4.9084973	1.4735700
C	-0.8813667	-6.1692787	0.8357051
C	-1.1141406	-4.8707292	2.9162736
C	-1.0136183	-6.0923862	3.6485607
C	-1.1969119	-3.6179289	3.5876012
H	-1.2187521	-3.6086553	4.6879014
C	-1.1926011	-2.4082693	2.9000861
C	-0.6840983	-2.5661932	-2.8964769
C	-1.5521030	-3.3983182	-3.5899537
H	-1.6572282	-3.2906823	-4.6806283
C	-2.3965137	-4.3212322	-2.9048709
C	-3.3462333	-5.1097411	-3.6218667
C	-2.3676856	-4.3866845	-1.4605496
C	-3.3616149	-5.1755134	-0.8065985
C	-1.3644533	-3.6310421	-0.7436226
C	-0.5523986	-2.7713890	-1.4887458
O	-1.2762472	-1.2603423	0.7923868
O	0.4594757	-2.0677088	-0.8568783
P	0.0971553	-0.7458421	0.0541293
O	1.2905141	-0.5983488	0.9886479
O	-0.3654065	0.4446713	-0.7956590
C	-0.8492920	-7.3044930	2.9953056
C	-0.7651887	-7.3371134	1.5773871
H	-1.0497351	-6.0490604	4.7484452
H	-0.7646299	-8.2380172	3.5721694
H	-0.8029415	-6.2091345	-0.2596338
H	-0.5997935	-8.2952980	1.0614743
C	-4.2862716	-5.9139390	-1.5331122
C	-4.2684905	-5.9005002	-2.9530306
H	-3.3967368	-5.1909876	0.2909448
H	-5.0432917	-6.5103273	-1.0013647
H	-4.9996566	-6.4982971	-3.5181268
H	-3.3461172	-5.0592250	-4.7221309
C	0.0227988	-0.7739731	4.4018988
C	-1.1249335	-1.0933916	3.6150095
C	0.0341731	0.4355446	5.1206351
C	-2.2039507	-0.1686284	3.5395747
C	-2.1356819	1.0272545	4.2801385
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H	0.9125738	0.6763390	5.7419852
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H	-2.9882386	1.7208461	4.2309324
C	-3.7286495	0.6394183	1.6735068
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H	-4.6020385	0.3711111	1.0434121
H	-2.8512054	0.7617596	1.0090422

C	-4.6892259	-0.6303709	3.6620627
H	-3.3367640	-1.4060325	2.1971975
H	-4.9087352	0.2964182	4.2322012
H	-4.5150977	-1.4430131	4.3965440
H	-5.5956984	-0.8857475	3.0746612
C	-0.9710501	2.6207588	5.9335368
C	-0.1414107	3.7137385	5.2317532
H	-0.0513079	4.6117319	5.8779352
H	-0.6256092	4.0249814	4.2822497
H	0.8821819	3.3668376	4.9884256
C	-2.3479638	3.1599067	6.3456749
H	-0.4265882	2.3468617	6.8652069
H	-2.2343332	3.9996860	7.0608401
H	-2.9700295	2.3785788	6.8279167
H	-2.9117125	3.5523017	5.4733443
C	1.2330106	-1.7020716	4.5295467
C	2.5548465	-1.0059587	4.1650932
H	3.4111637	-1.6982721	4.2987799
H	2.7520065	-0.1083293	4.7859277
H	2.5593586	-0.6998419	3.1021672
C	1.3079585	-2.3165943	5.9410212
H	1.1026447	-2.5331037	3.8082118
H	2.1458830	-3.0407929	6.0101299
H	0.3720965	-2.8480414	6.2088178
H	1.4748833	-1.5334454	6.7099337
H	1.1401795	3.2542468	-4.5156798
H	3.5046800	-2.1677027	-5.1096537
H	-4.1129168	-0.4686073	-5.0757362
C	1.6454347	-2.3903910	-5.0024265
H	4.0105628	-2.8376210	-2.0018211
H	3.4657050	3.5679507	-5.2207130
H	-4.1706633	0.6090749	-2.7684705
C	1.0958028	1.1302524	-4.3427304
C	2.8890990	-2.9237118	-4.5784430
C	3.1603672	2.5672000	-4.8569979
H	3.7143536	1.8136459	-5.4540675
C	1.9003923	0.0224445	-4.0252512
C	-3.0131197	-0.3303024	-5.1126026
H	0.1370786	2.3528160	-6.6181000
C	-0.3094595	1.0019573	-4.1468585
C	1.2361238	2.4123081	-6.4908035
H	1.5861480	3.3473745	-6.9734493
H	-0.9645471	1.8324179	-4.4591269
C	3.4076377	-1.9495344	-2.2795935
H	3.5396719	-3.7950786	-4.3602487
H	2.0889053	-3.2560138	-5.2705403
C	1.3557739	-1.1982135	-3.5816442
C	-3.0762671	0.7785495	-2.8239499
C	-0.9044448	-0.2268363	-3.7548907
H	-2.5835707	-1.1501433	-5.7235021
H	-2.8104247	0.6247352	-5.6413334
C	2.3024298	-2.3515988	-3.2727931
C	-0.0558857	-1.3353643	-3.4721693
C	-2.4273345	-0.3146128	-3.6862972
H	2.9900199	-1.5194686	-1.3485910
H	-2.6767635	0.7610837	-1.7907037
H	4.1054234	-1.2038753	-2.7140012
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H	1.6891707	1.5557453	-7.0319154
H	1.7044856	-3.1575254	-2.8022710
H	-2.6822461	-1.2827150	-3.2154240
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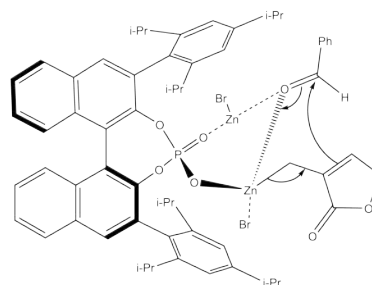
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H	0.6791470	2.2057821	2.8830542
Zn	0.0946705	1.9404842	-1.9416958
C	1.4349344	4.8726715	0.9133850
C	2.3745784	5.9597333	1.3318987
C	1.5454056	3.8224161	1.7852595
C	0.9072636	2.5179314	1.8432874
C	2.6211820	4.1881573	2.7690524
O	3.0902750	5.4456965	2.4611099
O	3.0505134	3.5393757	3.7001316
H	1.8452719	6.8929150	1.6348079
H	0.0040728	2.4307723	1.2104507
H	0.7108610	4.9657826	0.0908851
C	2.5367770	6.2731087	-3.2672380
C	2.1960033	5.0837527	-2.6189649
C	3.1153874	4.4767159	-1.7300616
C	4.3718471	5.0917320	-1.4966868
C	4.7135319	6.2748063	-2.1637694
C	3.7971251	6.8652737	-3.0506366
H	1.8124763	6.7502524	-3.9447643
H	1.1982902	4.6400924	-2.7540324
C	2.8669096	3.2230561	-1.0240336
H	5.0777716	4.6224128	-0.7927512
H	5.6938627	6.7421680	-1.9876108
H	4.0608780	7.7995120	-3.5699603
O	1.9700757	2.3691125	-1.2359383
C	-1.2230509	-2.4779589	1.4641394
C	-1.2354627	-3.6778688	0.7359688
C	-1.0878796	-4.9111151	1.4706415
C	-0.8921357	-6.1738305	0.8345060
C	-1.0962513	-4.8687596	2.9133719
C	-0.9845377	-6.0879704	3.6471571
C	-1.1722227	-3.6141283	3.5815554
H	-1.1790473	-3.6000190	4.6820088
C	-1.1816939	-2.4064747	2.8911325
C	-0.7080403	-2.5767243	-2.9043709
C	-1.5815987	-3.4066574	-3.5933134
H	-1.6902599	-3.2988428	-4.6838550
C	-2.4247952	-4.3280837	-2.9049327
C	-3.3778666	-5.1165860	-3.6165756
C	-2.3893396	-4.3939871	-1.4607952
C	-3.3791932	-5.1839764	-0.8025699
C	-1.3836301	-3.6386732	-0.7478333
C	-0.5726998	-2.7808150	-1.4963784
O	-1.2886140	-1.2653407	0.7805185
O	0.4405061	-2.0785565	-0.8693156
P	0.0859825	-0.7543620	0.0413084
O	1.2789089	-0.6057330	0.9726931
O	-0.3747667	0.4343054	-0.8142250
C	-0.8294922	-7.3019089	2.9961661
C	-0.7657989	-7.3390080	1.5779288
H	-1.0045482	-6.0408006	4.7472772

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H	-0.8290257	-6.2163492	-0.2616147	H	-2.8026961	0.7203567	-5.6358330
H	-0.6076161	-8.2986730	1.0626143	C	2.2816367	-2.3761378	-3.2579009
C	-4.3064015	-5.9227218	-1.5246228	C	-0.0723367	-1.3493275	-3.4787347
C	-4.2960687	-5.9080758	-2.9440589	C	-2.4378988	-0.3169852	-3.7252186
H	-3.4066625	-5.1999375	0.2951368	H	2.9699709	-1.5746049	-1.3201876
H	-5.0597411	-6.5205147	-0.9893444	H	-2.6917773	0.6584373	-1.7772308
H	-5.0294343	-6.5060001	-3.5060648	H	4.0898518	-1.2445463	-2.6768904
H	-3.3830896	-5.0658977	-4.7168472	H	3.4823128	2.4529188	-3.6935750
C	0.0320906	-0.7527079	4.3757206	H	-2.9074556	1.7742093	-3.1610504
C	-1.1189795	-1.0888385	3.6009333	H	1.7597302	1.5791576	-6.9762908
C	0.0348156	0.4597853	5.0888028	H	1.6765849	-3.1826947	-2.7975956
C	-2.2097890	-0.1779133	3.5322166	H	-2.7051418	-1.3053834	-3.3064929
C	-2.1494051	1.0213957	4.2672924	H	2.9881176	0.0873492	-4.0698230
C	-1.0480851	1.3568424	5.0708517	H	3.6430462	2.9403879	-0.2703759
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H	-4.6362328	0.3234793	1.0550701				
H	-2.8916074	0.7383719	1.0065928				
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H	-3.3399828	-1.4333953	2.2042508				
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H	0.4186903	-2.8001519	6.1985054				
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H	1.1520828	3.2469136	-4.4527192				
H	3.4900730	-2.1832140	-5.0898732				
H	-4.1148721	-0.3886898	-5.1321921				
C	1.6667362	2.3878353	-4.9380179				
H	3.9845986	-2.8866518	-1.9894954				
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C	2.8684150	-2.9401670	-4.5671398				
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C	1.8959760	0.0087704	-3.9821263				
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C	3.3859545	-1.9926472	-2.2569586				
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C	1.3419736	-1.2152842	-3.5631944				
C	-3.0820656	0.7367966	-2.8108184				
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7.2.3.3 to 15n-ma

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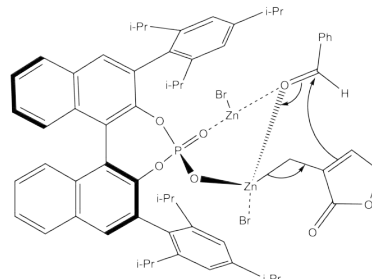


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C	2.2475402	6.3637770	1.9095933
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C	-0.0791481	3.4361776	1.5706411
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H	5.6382298	-1.6837160	1.5339945
C	5.1041730	0.1134088	2.6468314
C	6.1336593	-0.0424226	3.6236686
C	4.1825908	1.2187714	2.7613744
C	4.2932031	2.0705301	3.9019591
C	3.1683318	1.3936644	1.7472280
C	3.0313767	0.3856533	0.7823843
O	0.3850610	1.0806271	1.6045930
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P	0.4751948	0.2485025	0.1875828
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O	0.1309438	-1.1949484	0.5484614
C	3.6036276	6.6523518	1.8755629
C	4.5460606	5.5985683	1.7401436
H	1.5045554	7.1738148	1.9787627
H	3.9498091	7.6955699	1.9319490
H	4.8664734	3.4738641	1.5684639
H	5.6200700	5.8304777	1.6756334
C	5.2926932	1.8794595	4.8464680
C	6.2345622	0.8264409	4.6996185
H	3.5660978	2.8828676	4.0382246
H	5.3502716	2.5469148	5.7198782
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H	6.8370238	-0.8829242	3.5145337	H	0.3675350	-4.0871051	-3.4113808
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C	-3.1736708	2.8468360	-0.5746281	H	4.3798974	0.4094589	-1.3936097
C	-2.2549693	2.2185317	2.0170261	H	3.1630970	-2.4960240	2.2479066
C	-3.4706516	1.7055886	1.5400655	H	3.3930141	-2.4243295	-3.6623972
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C	-1.8450612	1.9214003	3.4552874	C	-3.7508862	-3.6004569	-5.1483061
H	-4.0670230	1.0508575	2.1916100	C	-3.8097431	-1.4957609	-1.4297003
C	-1.8881619	0.4231814	3.7969805	C	-2.5409222	-3.2964918	-4.5004466
H	-2.9208304	0.0204101	3.7633438	C	-4.9908912	-2.5436632	-3.3483831
H	-1.4950025	0.2559390	4.8202747	C	-3.7773465	-2.2570444	-2.6716534
H	-1.2648480	-0.1594650	3.0912880	C	-4.9775243	-3.2157823	-4.5731287
C	-2.7227922	2.7464664	4.4186095	C	-2.5491686	-2.6288164	-3.2721944
H	-0.8010588	2.2695830	3.5887537	O	-2.7296374	-1.0212887	-0.8676906
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H	-2.6556438	3.8315531	4.1998572	H	-5.9483066	-2.2074735	-2.9209786
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C	-5.3795851	1.5601001	-0.1148735	H	-5.9232589	-3.4294283	-5.0934604
C	-6.4091053	2.1879453	0.8487168	H	-1.6059350	-2.3700851	-2.7750932
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H	-6.3969063	3.2950079	0.7708444	Zn	-1.4635947	-2.3243409	0.2363121
H	-6.2102156	1.9088356	1.9014436	H	-6.5235501	-2.5392129	-0.9361209
C	-5.7740779	1.8143130	-1.5728713	H	-2.4078730	-3.7911037	1.8407816
H	-5.4188169	0.4643692	0.0693121	C	-4.6661102	-3.2205953	0.0635365
H	-6.7699126	1.3729769	-1.7768565	C	-6.1273850	-2.8858633	0.0405546
H	-5.0539616	1.3775970	-2.2943673	H	-4.2272759	-4.0536912	-0.5036182
H	-5.8465350	2.9003124	-1.7908128	C	-4.1074150	-2.6443142	1.2033864
C	-1.2125626	4.4028213	-1.0180166	C	-2.8198450	-2.7663373	1.7944345
C	-0.9989730	3.9250498	-2.4606041	O	-5.1329212	-1.6793122	1.7262602
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C	-1.9507792	5.7568671	-0.9801337	H	-2.6619899	-2.1622807	2.7027276
H	-0.2066104	4.5614376	-0.5845827	H	-4.7656356	-0.9888248	-1.1855621
H	-1.3895365	6.5190476	-1.5583864				
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C	2.8081263	-3.8530300	-2.1397510				
C	5.6310284	-0.5145973	-2.8670783				
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H	1.5491464	-3.5710220	-4.6655267				
C	3.3040373	-2.6130550	-2.5803911				
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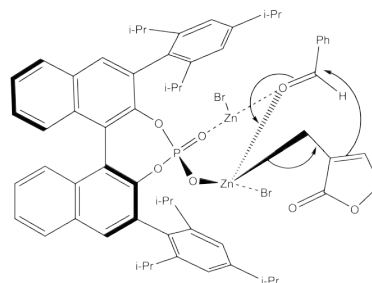
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P	0.4747302	0.2566253	0.1854922	C	3.2805455	0.3816324	-3.2398462
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C	3.6097416	6.6563881	1.8749173	C	3.6729407	-1.5995423	-1.6838463
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H	-1.2601420	-0.1531254	3.0902611	C	-4.9647173	-3.2086191	-4.5875016
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H	-6.2018376	1.8104700	1.9218926	H	-6.4912783	-2.5931797	-0.9574841
C	-5.7887473	1.8582857	-1.5557722	H	-2.3846783	-3.7860325	1.8549543
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C	3.2918435	-2.6141301	-2.5767575				
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H	4.3474045	-5.8397634	-3.2957413				
C	2.7029750	-4.0658234	-0.7510777				

7.2.3.4 to 15q-ma

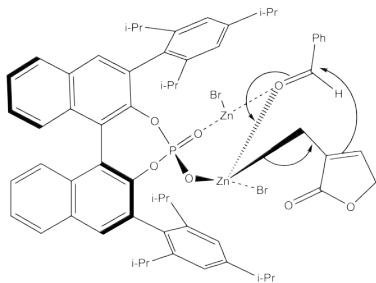
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C	3.0285735	3.7566450	1.8102164	H	0.5002867	-4.8668025	-3.4077607
C	4.4280065	3.9031003	1.5713129	H	5.0586947	-1.0581745	-3.9665782
C	2.2311692	4.9538963	1.9563533	H	2.7052577	-4.7419350	2.7491283
C	2.8775807	6.2265335	1.9319533	C	1.3647220	-4.3070369	-3.8292623
C	0.8115817	4.8587170	2.0594295	H	3.6499711	1.7251531	-3.2176536
H	0.2218508	5.7857101	2.1277108	H	0.3182251	-4.1549279	-5.7445194
C	0.1559463	3.6345411	2.0105778	H	0.1175758	-4.0938114	2.3372442
C	3.4178880	-0.9883431	0.5516463	C	1.9080409	-3.4392161	-2.7007661
C	4.5360895	-1.2574005	1.3303276	C	5.2593346	-0.5634769	-2.9931564
H	5.1293833	-2.1626499	1.1309735	C	0.8534393	-3.4963205	-5.0299001
C	4.9318544	-0.3967570	2.3963438	H	1.6870937	-3.0237632	-5.5900574
C	6.0318919	-0.7326564	3.2417670	C	2.6510353	-2.2741279	-2.9465257
C	4.1987809	0.8229046	2.6460375	C	2.9454420	-4.4395226	1.7086614
C	4.5671475	1.6138258	3.7758370	H	2.7434889	-5.9725790	-3.4106829
C	3.1055408	1.1754628	1.7718888	C	1.6942764	-3.8095966	-1.3607791
C	2.7249437	0.2353950	0.8063863	C	2.4142791	-5.3479290	-4.2655787
O	0.3221848	1.2399217	2.0263140	H	2.0069546	-6.0208130	-5.0489927
O	1.6291240	0.5022724	-0.0151388	H	1.1033912	-4.7184194	-1.1622155
P	0.1426528	0.3760412	0.6557986	C	3.0930052	0.7790787	-3.0552492
O	-0.8570131	0.9723951	-0.3242317	H	5.8453988	0.3558583	-3.2001134
O	-0.1392581	-1.0539404	1.1803083	H	5.8929434	-1.2477399	-2.3925024
C	4.2464711	6.3304232	1.7346112	C	3.1685300	-1.4828252	-1.9046388
C	5.0222414	5.1575554	1.5358784	C	0.4849323	-4.1344373	1.2930987
H	2.2602854	7.1302376	2.0558780	C	2.1820267	-3.0504542	-0.2807987
H	4.7294653	7.3191579	1.7124661	H	3.9460085	-3.9669786	1.7164681
H	5.0398189	3.0059437	1.4049409	H	3.0112560	-5.3583664	1.0892526
H	6.1030801	5.2422335	1.3455580	C	3.9508443	-0.2195892	-2.2578414
C	5.6304046	1.2482038	4.5902665	C	2.9367645	-1.8754478	-0.5585143
C	6.3808617	0.0739047	4.3148730	C	1.8719940	-3.4843187	1.1517740
C	3.9890409	2.5199450	4.0045810	H	2.1503063	1.0121607	-2.5235795
H	5.8898524	1.8716871	5.4594555	H	-0.2532619	-3.6249040	0.6316261
H	7.2273119	-0.2013521	4.9622798	H	2.8159730	0.3775882	-4.0519024
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C	-1.9756057	3.8236911	0.6710367	H	0.4708624	-5.1955918	0.9696702
C	-1.3264479	3.4607499	1.8880970	H	3.3133415	-4.8457429	-4.6805353
C	-3.3332333	3.4913234	0.5092872	H	4.2385298	0.2768151	-1.3085768
C	-2.0587852	2.7959501	2.9105109	H	1.8682225	-2.5667497	1.7742611
C	-3.4138508	2.4893844	2.6939142	H	2.8217390	-1.9520536	-3.9847145
C	-4.0696062	2.0099892	1.4934908	Zn	-1.8888181	0.3258043	-1.9137889
H	-3.8376668	3.7544255	-0.4349486	Br	-0.7658420	0.3126453	-3.9603406
C	-1.4268264	2.4297830	4.2521196	C	-2.4759161	-6.8897386	-2.5041573
H	-3.9698847	1.9704542	3.4891418	C	-2.0284579	-2.6447716	-2.3073726
C	-1.6298538	0.9491451	4.6191791	C	-2.4121143	-6.2719420	-1.2393829
H	-2.6988948	0.7104134	4.7978134	C	-2.3018517	-4.7190725	-3.5779950
H	-1.0787138	0.7014626	5.5497455	C	-2.2232711	-4.0874519	-2.3090225
H	-1.2609487	0.2838922	3.8140057	C	-2.4234425	-6.1106809	-3.6724211
C	-1.9458994	3.3628225	5.3631962	C	-2.2866112	-4.8842953	-1.1393398
H	-0.3342266	2.6032295	4.1713950	O	-1.6547208	-1.9222854	-1.3190126
H	-3.0415253	3.2482973	5.5020546	H	-2.5692956	-7.9839961	-2.5759112
H	-1.7485159	4.4265186	5.1193830	H	-2.2317103	-4.1056433	-4.4895868
H	-1.4560486	3.1343655	6.3326285	H	-2.4658697	-6.8803559	-0.3242213
C	-5.5389598	2.4785473	1.2597241	H	-2.4701966	-6.5905430	-4.6612394
C	-5.9728440	1.1392440	1.8746127	H	-2.2737500	-4.4174887	-0.1441227
H	-7.0056449	0.8854714	1.5603397	Br	-3.5919676	-2.6809514	1.8114411
H	-5.9713175	1.1763006	2.9840242	Zn	-1.7119856	-2.0168993	0.6881911
H	-5.3069780	0.3068321	1.5685101	H	-4.6149858	-3.5620223	-3.8740055
C	-6.4349062	3.6313862	1.7544385	C	-4.5667166	-2.1727091	-2.1657302
H	-5.6736664	2.4005983	0.1577735	C	-5.1769188	-2.7127897	-3.4223610
H	-7.5041315	3.4276545	1.5371204	C	-4.3958870	-0.8078867	-2.3037935
H	-6.1610240	4.5911002	1.2716546	C	-3.8834669	0.2011973	-1.4199012
H	-6.3279987	3.7651591	2.8516327	C	-4.7687923	-0.4692770	-3.7238815
C	-1.2579136	4.5613786	-0.4604800	O	-5.1865289	-1.6187131	-4.3501098
C	-1.4718465	3.9294145	-1.8459702	O	-4.7462307	0.6085530	-4.2768980
H	-0.9130623	4.4954736	-2.6189362	H	-6.2228217	-3.0631916	-3.2664746
H	-2.5377939	3.9257028	-2.1544629	H	-4.5250123	-2.7331940	-1.2213320
H	-1.0982201	2.8880074	-1.8706998	H	-1.9779364	-2.1512675	-3.3030975
C	-1.6647912	6.0484362	-0.4656222	H	-3.9475859	-0.0150982	-0.3386981
H	-0.1692041	4.5159517	-0.2567934	H	-4.2200786	1.2242081	-1.6788901
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TS3-8-q



Energy(Hartree)= -11970.00679487
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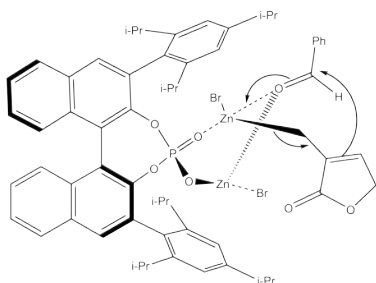
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C	2.2315535	4.9525945	1.9566487
C	2.8787654	6.2242670	1.9318228
C	0.8121691	4.8574809	2.0587713
H	0.2220532	5.7843275	2.1255990
C	0.1558869	3.6339508	2.0105688
C	3.4180148	-0.9892789	0.5539705
C	4.5374257	-1.2567679	1.3310596
H	5.1311967	-2.1613409	1.1298142
C	4.9342042	-0.3961465	2.3964628
C	6.0355946	-0.7298272	3.2402415
C	4.2003690	0.8226925	2.6469384
C	4.5700831	1.6142609	3.7754914
C	3.1055274	1.1743176	1.7745878
C	2.7242246	0.2337765	0.8098458
O	0.3206943	1.2401605	2.0284880
O	1.6284233	0.4991364	-0.0102937
P	0.1409547	0.3739372	0.6596490
O	-0.8541693	0.9714750	-0.3239716
O	-0.1432695	-1.0546917	1.1857212
C	4.2473258	6.3278659	1.7356881
C	5.0224121	5.1550361	1.5384519
H	2.2615740	7.1282125	2.0543667
H	4.7304731	7.3164552	1.7132431
H	5.0390044	3.0034578	1.4088485
H	6.1034093	5.2390761	1.3489659
C	5.6348827	1.2502898	4.5879494
C	6.3857857	0.0771132	4.3120024
H	3.9911995	2.5198396	4.0039260
H	5.8952229	1.8745926	5.4562241
H	7.2336762	-0.1971121	4.9578948
H	6.5951741	-1.6549771	3.0304640
C	-1.9741151	3.8207404	0.6686988
C	-1.3263026	3.4601913	1.8869323
C	-3.3308322	3.4861848	0.5061617
C	-2.0588536	2.7960795	2.9093167
C	-3.4128446	2.4872951	2.6913455
C	-4.0675655	2.8053636	1.4900366
H	-3.8343477	3.7475846	-0.4390520
C	-1.4282209	2.4337767	4.2524955
H	-3.9688538	1.9679996	3.4862659
C	-1.6279232	0.9535375	4.6224720
H	-2.6963502	0.7119503	4.8004956
H	-1.0775163	0.7091445	5.5541933
H	-1.2559743	0.2873369	3.8198030
C	-1.9508610	3.3685746	5.3602456
H	-0.3358914	2.6095455	4.1727201
H	-3.0463621	3.2526132	5.4977614
H	-1.7558144	4.4318669	5.1139140
H	-1.4624293	3.1439358	6.3311938
C	-5.5364140	2.4722432	1.2552181
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H	-7.0026375	0.8786468	1.5565801
H	-5.9709866	1.1725575	2.9807604
H	-5.3041233	0.3005807	1.5685893
C	-6.4336020	3.6256405	1.7462625
H	-5.6696302	2.3916526	0.1531602
H	-7.5026206	3.4214843	1.5282791
H	-6.1592638	4.5845506	1.2626098
H	-6.3279173	3.7619908	2.8430668
C	-1.2563509	4.5585594	-0.4626882
C	-1.4665550	3.9259356	-1.8485187
H	-0.9073584	4.4920865	-2.6207934
H	-2.5314791	3.9205891	-2.1601880
H	-1.0911383	2.8853692	-1.8734375
C	-1.6662081	6.0447506	-0.4686059
H	-0.1678479	4.5154139	-0.2573119
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H	0.5011797	-4.8655596	-3.4075175
H	5.0523423	-1.0510663	-3.9663465
H	2.7127436	-4.7461957	-2.7476933
C	1.3632813	-4.3024026	-3.8296594
H	3.6430902	1.7310699	-3.2107264
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H	0.1219262	-4.0998917	-2.3375729
C	1.9070811	-3.4360797	-2.7002361
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H	2.7482315	-5.9644714	-3.4187624
C	1.6959379	-3.8093001	-1.3609382
C	2.4146503	-5.3390896	-4.2710158
H	2.0082945	-6.0113206	-5.0555082
H	1.1063316	-4.7193010	-1.1636342
C	3.0869435	0.7845696	-3.0490859
H	5.8392941	0.3619236	-3.1995773
H	5.8888583	-1.2428302	-2.3944590
C	3.1660210	-1.4797736	-1.9024146
C	0.4895521	-4.1398105	1.2934492
C	2.1840253	-3.0516136	-0.2804066
H	3.9503576	-3.9680827	1.7146058
H	3.0180559	-5.3600074	1.0865645
C	3.9464888	-0.2152639	-2.2548531
C	2.9365697	-1.8752607	-0.5568485
C	1.8757936	-3.4877525	1.1519513
H	2.1449915	1.0172210	-2.5163871
H	-0.2494990	-3.6318459	0.6325912
H	2.8079040	0.3858609	-4.0461110
H	0.1620164	-2.6756771	-4.7130258
H	0.4775450	-5.2012317	0.9701723
H	3.3112014	-4.8333328	-4.6860964
H	4.2357733	0.2793126	-1.3050665
H	1.8703597	-2.5708055	1.7754595
H	2.8156377	-1.9446208	-3.9821553
Zn	-1.8822465	0.3231005	-1.9146045
Br	-0.7610508	0.2906924	-3.9585894
C	-2.5031554	-6.8856123	-2.5052415
C	-2.0325941	-2.6392663	-2.3045194
C	-2.4427006	-6.2674212	-1.2411764
C	-2.3086433	-4.7150482	-3.5763837
C	-2.2337053	-4.0831297	-2.3076827
C	-2.4387880	-6.1060245	-3.6719743
C	-2.3088886	-4.8803652	-1.1394373
O	-1.6561901	-1.9202342	-1.3140615
H	-2.6032803	-7.9792952	-2.5778746
H	-2.2265365	-4.1018011	-4.4872627
H	-2.5062263	-6.8748852	-0.3259052
H	-2.4826518	-6.5850088	-4.6614260
H	-2.2997729	-4.4139920	-0.1438488

Br	-3.5936443	-2.6900287	1.8106237
Zn	-1.7151310	-2.0182281	0.6924931
H	-4.5929894	-3.5686796	-3.8674458
C	-4.5453921	-2.1776352	-2.1603860
C	-5.1560109	-2.7183419	-3.4180412
C	-4.3819270	-0.8107563	-2.3007409
C	-3.8778771	0.2000551	-1.4190051
C	-4.7574296	-0.4723760	-3.7232842
O	-5.1711363	-1.6289752	-4.3467140
O	-4.7404851	0.6042459	-4.2715872
H	-6.2009777	-3.0729697	-3.2593128
H	-4.5029697	-2.7353421	-1.2142139
H	-1.9721756	-2.1448927	-3.2993595
H	-3.9403804	-0.0122598	-0.3369248
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7.2.3.5 to 15j-ma

TS1-8-j; COSMO



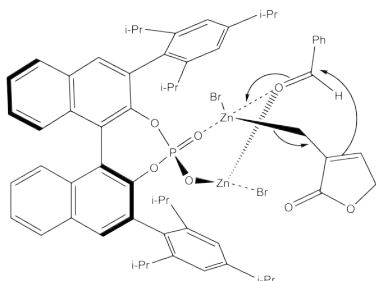
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Br	-2.3877684	2.8011915	-3.5691163
H	-1.4425717	4.3015233	-0.2867467
Zn	-0.7850400	2.5193828	-1.8393188
C	1.9798376	4.7339096	-0.3457694
C	2.8273445	4.2577946	0.8044175
C	0.6801043	4.3064198	-0.1413141
C	-0.5246095	4.3694357	-0.9040992
C	0.6848447	3.4526639	1.0918639
O	1.9793185	3.3749448	1.5655919
O	-0.2489508	2.8924682	1.6184479
H	3.1537886	5.0917359	1.4665431
H	-0.5848325	5.1199683	-1.7102116
H	2.3053925	5.5166661	-1.0417333
C	0.9891655	4.6801470	-5.3360585
C	1.0990714	3.8153425	-4.2418480
C	2.2071279	3.9139630	-3.3667772
C	3.2223159	4.8699715	-3.6334421
C	3.1141046	5.7214995	-4.7348004
C	1.9916565	5.6339889	-5.5832335
H	0.1148261	4.6016517	-5.9992727
H	0.3211163	3.0541947	-4.0836628
C	2.3561612	3.0437191	-2.2148347
H	4.0947416	4.9361664	-2.9638018
H	3.9035985	6.4600537	-4.9391453
H	1.9048718	6.3106204	-6.4472058
O	1.5260241	2.0961634	-1.9350196
C	-1.7692712	-1.3244969	1.9854223
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C	-2.0637460	-3.6836069	2.5170845
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C	-1.8298263	-1.9782771	4.2983557
H	-1.7864127	-1.7263814	5.3688722
C	-1.6348296	-0.9708306	3.3614329
C	-0.8162152	-3.0663513	-2.0920965
C	-1.7568735	-3.9694122	-2.5767773
H	-1.6139010	-4.4265213	-3.5667826
C	-2.9314793	-4.3007934	-1.8376953
C	-3.9409514	-5.1396797	-2.3992331
C	-3.1178173	-3.7783695	-0.5039195
C	-4.3301810	-4.0809993	0.1834413
C	-2.0799610	-2.9588001	0.0725103
C	-1.0436531	-2.5587551	-0.7743128
O	-1.7067078	-0.2645591	1.0732493
O	-0.0900693	-1.6791296	-0.2885463
P	-0.4646382	-0.1244545	0.0391756
O	0.8512564	0.3648706	0.6982245
O	-0.9677608	0.6587094	-1.1718015
C	-2.2149696	-5.6967062	4.5360327
C	-2.1797055	-6.0501230	3.1610855
H	-2.1194065	-4.0719127	5.9648996
H	-2.2854287	-6.4811133	5.3049182
H	-2.0658301	-5.3718008	1.1242427
H	-2.2040969	-7.1108513	2.8680120
C	-5.3014049	-4.8829294	-0.4008677
C	-5.1019146	-5.4290188	-1.6971011
H	-4.4935529	-3.6596092	1.1857747
H	-6.2348920	-5.0930220	0.1431625
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H	-3.7859050	-5.5415913	-3.4129036
C	0.0768511	0.6678840	4.2147788
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H	2.8841374	-3.5429037	0.9344089
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C	2.7836912	-2.0939830	-2.8947342
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TS1-8-j



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Zn	-0.7968387	2.5109321	-1.8539201
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C	2.8180445	4.2418804	0.8086997
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H	3.1442376	5.0735570	1.4749377
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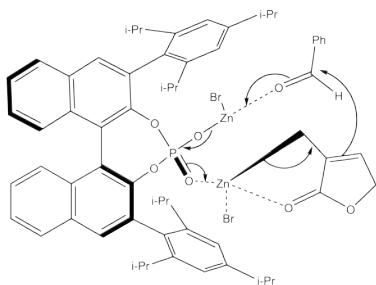
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C	-2.0105590	-2.6301946	1.5283890
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C	-2.1077347	-5.0717647	2.1899924
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H	-1.6052532	-4.4468863	-3.5580598
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C	-1.2638231	0.4162406	3.7951458
C	0.3801782	1.9289233	4.7492201
C	-2.2355495	1.4456820	3.8535242
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H	-2.6329487	3.4881040	4.4368148
C	-3.8838556	2.1529819	2.0799481
H	-3.8552759	3.2265502	2.3608984
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H	1.2335716	-0.7662554	-5.6270679
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C	1.6853804	-2.7149350	-2.2731780
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H	-0.8403241	1.9966729	3.5025315
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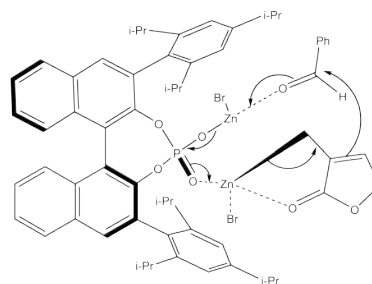
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TS1-8-o; COSMO



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H	0.2219631	-4.9213524	-5.6035419
H	1.0971801	-4.5773775	2.1474032
C	2.3111735	-3.7349711	-3.0644157
C	5.0005021	-0.2804190	-3.5675743
C	0.5914587	-4.1802607	-4.8645169
H	0.8051067	-3.2383856	-5.4117470
C	2.7374735	-2.4338328	-3.3813374
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H	3.8671879	-5.4354349	-4.6288733
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C	2.9736289	-5.0296588	-5.1450285
H	2.6351086	-5.7786318	-5.8908142
H	1.9837869	-5.1268601	-1.4506361
C	2.6211743	0.6196465	-3.6855473
H	5.4007938	0.7176739	-3.8418716
H	5.7530107	-0.7900597	-2.9319213
C	3.1381189	-1.5154236	-2.3952400
C	1.2415247	-4.4538595	1.0559215
C	2.6606482	-3.2192103	-0.6775081
H	4.7142442	-4.0471619	1.0484726
H	3.7854253	-5.4943777	0.5646173
C	3.6512897	-0.1455662	-2.8360050
C	3.0950883	-1.9073748	-1.0272369
C	2.5483325	-3.6945105	0.7727275
H	1.6597950	0.7228252	-3.1456621
H	0.3611552	-3.9121787	0.6535461
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H	1.2354602	-5.4651595	0.5996233
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H	3.8402305	0.4579593	-1.9257837
H	2.5406883	-2.7955798	1.4226444
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C	-1.0849492	-5.6337945	-1.6505449
C	-3.6246199	-4.8822506	-2.5763015
C	-2.7542788	-3.9078753	-2.0380199
C	-3.2260348	-6.2199948	-2.6501509
C	-1.4723468	-4.2877099	-1.5850601
O	-2.3034754	-1.5842297	-1.7294196
H	-1.6405532	-7.6520099	-2.2307538
H	-4.6190521	-4.5791860	-2.9419434
H	-0.0896263	-5.9313467	-1.2937679
H	-3.9030841	-6.9727972	-3.0789598
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Br	0.2142460	-2.1981997	3.9207510
Zn	-0.8957961	-2.0276269	1.8864246
H	-5.2657372	-0.8410769	-1.2903560
H	-2.6432156	-4.5057824	1.2476462
C	-4.4409610	-2.6345517	-0.2316071
C	-5.1591242	-1.3010218	-0.2850249
H	-4.9762318	-3.5587616	-0.4892118
C	-3.5432277	-2.5612462	0.8611896
C	-2.6862782	-3.4448573	1.5314913
C	-3.4157332	-1.1102618	1.1665097
O	-4.3146607	-0.3947093	0.4824596
O	-2.5439431	-0.5831399	1.8652326
H	-6.1625194	-1.3252468	0.1938698
H	-2.5336450	-3.2557483	2.6153024
H	-4.0881850	-2.2386318	-2.5603700



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C	2.1441385	2.3704190	1.4574722
C	2.7875224	3.6610593	1.5314971
C	4.1971318	3.8385404	1.3877160
C	1.9726675	4.8352582	1.7262755
C	2.5997594	6.1119981	1.8440929
C	0.5562781	4.7080815	1.7394188
H	-0.0558055	5.6148984	1.8591571
C	-0.0811798	3.4888052	1.5367057
C	3.4703239	-0.9483805	0.0520012
C	4.5565277	-1.1710605	0.8917373
H	5.2126678	-2.0319876	0.6977074
C	4.8146876	-0.3586061	2.0309437
C	5.8686670	-0.6730045	2.9403781
C	3.9682429	0.7775581	2.2989251
C	4.1755659	1.5060723	3.5081833
C	2.9352341	1.1143898	1.3500803
C	2.6907785	0.2229351	0.3004366
O	0.1044216	1.0923474	1.3513142
O	1.6530931	0.5046339	-0.5948120
P	0.1310303	0.2504510	-0.0559037
O	-0.7761130	0.9080967	-1.1143130
O	-0.0992045	-1.2214300	0.2991123
C	3.9750814	6.2433127	1.7356145
C	4.7749314	5.0962727	1.4874966
H	1.9626989	6.9959353	2.0049690
H	4.4463983	7.2341611	1.8219011
H	4.8302873	2.9640827	1.1860147
H	5.8636403	5.2048055	1.3670848
C	5.1954757	1.1609948	4.3835657
C	6.0617211	0.0736950	4.0921630
H	3.5061716	2.3433056	3.7492279
H	5.3286667	1.7312040	5.3154712
H	6.8716617	-0.1852683	4.7909212
H	6.5136401	-1.5374905	2.7177604
C	-2.1175168	3.8773749	0.1197414
C	-1.5637832	3.4107843	1.3446427
C	-3.5169808	3.8474897	-0.0371620
C	-2.4078174	2.9062093	2.3737389
C	-3.7971537	2.9001789	2.1611937
C	-4.3755567	3.3830495	0.9715669
H	-3.9594799	4.2145232	-0.9768506
C	-1.8163029	2.4812194	3.7187500
H	-4.4523039	2.5212739	2.9592292
C	-2.6600892	1.4598137	4.4934257
H	-3.6095749	1.9008947	4.8637864
H	-2.0992199	1.1032946	5.3807797
H	-2.8991182	0.5795576	3.8684981
C	-1.5431405	3.7214500	4.5949989
H	-0.8416038	1.9932304	3.5076696
H	-2.4923711	4.2483176	4.8269646
H	-0.8698630	4.4431840	4.0921804
H	-1.0706331	3.4276096	5.5551681
C	-5.8873985	3.4257350	0.7726082
C	-6.4669198	2.0322985	0.4720439

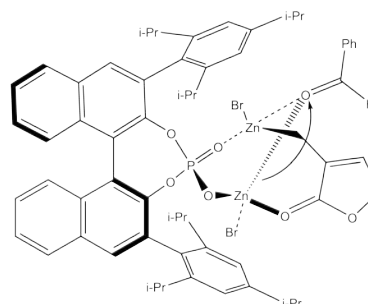
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H	-6.2858118	1.3381670	1.3189329
H	-5.9946655	1.6005188	-0.4321186
C	-6.6139091	4.0911147	1.9535983
H	-6.0676195	4.0546839	-0.1269895
H	-7.6964704	4.2014431	1.7365965
H	-6.2007051	5.0970190	2.1690646
H	-6.5251342	3.4866771	2.8803363
C	-1.2538667	4.4836474	-0.9897708
C	-1.5692343	3.9418167	-2.3923761
H	-0.8847563	4.3943091	-3.1390277
H	-2.6062844	4.1668416	-2.7135656
H	-1.4336851	2.8455126	-2.4369948
C	-1.3663079	6.0214160	-0.9750213
H	-0.1982108	4.2214774	-0.7748315
H	-0.6987370	6.4737502	-1.7374867
H	-1.0950274	6.4463022	0.0116494
H	-2.4052128	6.3422278	-1.1988854
H	1.5855688	-5.6615609	-3.6311843
H	4.8956504	-0.8734654	-4.4999977
H	3.6687605	-4.8696850	2.2496695
C	1.8626497	-4.7146257	-4.1458387
H	2.9851726	1.6325973	-3.9261007
H	0.2412647	-4.9433005	-5.6087864
H	1.0986642	-4.5822812	2.1477093
C	2.3166806	-3.7424512	-3.0644483
C	4.9963361	-0.2818139	-3.5660780
C	0.6049593	-4.1994255	-4.8698986
H	0.8156051	-3.2574411	-5.4180555
C	2.7384445	-2.4402448	-3.3818981
C	3.7504851	-4.5689482	1.1848997
H	3.8858730	-5.4375269	-4.6191207
C	2.3059718	-4.1106951	-1.7103406
C	2.9923203	-5.0378484	-5.1394678
H	2.6610638	-5.7896226	-5.8854850
H	1.9934042	-5.1338812	-1.4497227
C	2.6150811	0.6136093	-3.6901162
H	5.3956596	0.7164774	-3.8410479
H	5.7480522	-0.7894961	-2.9282875
C	3.1347083	-1.5194719	-2.3967147
C	1.2445603	-4.4622331	1.0561708
C	2.6607340	-3.2229412	-0.6776266
H	4.7151431	-4.0418600	1.0536248
H	3.7937129	-5.4929391	0.5704257
C	3.6451276	-0.1487710	-2.8381917
C	3.0913758	-1.9102154	-1.0286044
C	2.5482777	-3.6972963	0.7730026
H	1.6522676	0.7155817	-3.1529025
H	0.3623110	-3.9249854	0.6517612
H	2.4216187	0.1019505	-4.6560967
H	-0.2158141	-3.9961460	-4.1534571
H	1.2439525	-5.4752771	0.6025769
H	3.3077842	-4.1318905	-5.6981723
H	3.8308373	0.4561287	-1.9282818
H	2.5351615	-2.7984026	1.4229643
H	2.7656828	-2.1276523	-4.4381102
Zn	-2.4838198	0.3739953	-1.8136659
Br	-4.2541288	1.2479495	-2.9903655
C	-1.9558047	-6.5826263	-2.1743578
C	-3.1837258	-2.4769174	-1.9597523
C	-1.0855693	-5.6151288	-1.6479290
C	-3.6221910	-4.8652596	-2.5833710
C	-2.7524418	-3.8886856	-2.0453559
C	-3.2253779	-6.2042833	-2.6514849
C	-1.4715129	-4.2677631	-1.5874007
O	-2.3031814	-1.5666782	-1.7296065
H	-1.6421193	-7.6366496	-2.2229013
H	-4.6151282	-4.5619743	-2.9547934
H	-0.0904154	-5.9100912	-1.2874647
H	-3.9022754	-6.9591439	-3.0796937
H	-0.7903265	-3.4867701	-1.2173446

Br	0.2094298	-2.2299777	3.9166604
Zn	-0.8937900	-2.0308161	1.8918373
H	-5.2641835	-0.8243958	-1.2870101
H	-2.6526970	-4.4992601	1.2431810
C	-4.4493449	-2.6228743	-0.2271817
C	-5.1617347	-1.2870277	-0.2821873
H	-4.9805389	-3.5465417	-0.4929994
C	-3.5499826	-2.5536977	0.8633262
C	-2.6932755	-3.4394086	1.5310249
C	-3.4179930	-1.1036819	1.1708524
O	-4.3176613	-0.3853477	0.4871690
O	-2.5461220	-0.5791355	1.8685403
H	-6.1670344	-1.3055190	0.1931290
H	-2.5347357	-3.2539938	2.6142312
H	-4.0850265	-2.2155556	-2.5667140

7.2.3.7 to 15c-ma

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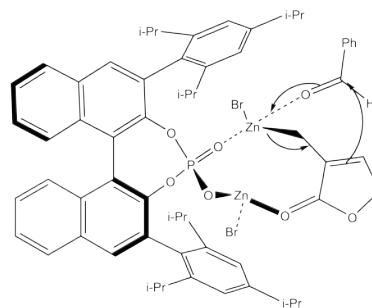


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C	4.423740	3.948213	0.648880
C	2.252876	5.025705	1.095463
C	2.912095	6.290169	1.045995
C	0.842683	4.937430	1.282633
H	0.268688	5.862582	1.444240
C	0.179150	3.718530	1.244503
C	3.482745	-0.916820	-0.272496
C	4.584198	-1.157207	0.541117
H	5.174379	-2.072790	0.389267
C	4.947159	-0.282394	1.604783
C	6.025382	-0.602363	2.482527
C	4.194868	0.928611	1.828986
C	4.518707	1.727581	2.964859
C	3.125677	1.255917	0.919469
C	2.787891	0.312943	-0.053444
O	0.282651	1.336237	1.130190
O	1.696701	0.590004	-0.881427
P	0.243684	0.334069	-0.181845
O	-0.747489	0.838138	-1.254711
O	0.108961	-1.058254	0.412104
C	4.273920	6.377336	0.801023
C	5.030239	5.194594	0.587889
H	2.309986	7.201257	1.189589
H	4.766958	7.360223	0.755933
H	5.017756	3.040655	0.474537
H	6.106114	5.265038	0.366571
C	5.561749	1.377145	3.810815
C	6.333864	0.211834	3.561297
H	3.919437	2.624274	3.175324
H	5.786251	2.003716	4.687451

H	7.163159	-0.052362	4.235023	H	2.228681	0.121774	-4.940935
H	6.597421	-1.524671	2.295362	H	-0.739712	-4.180099	-3.677717
C	-2.156857	3.731104	0.251198	H	1.048323	-5.300710	0.477873
C	-1.306241	3.564088	1.381792	H	2.200113	-3.825356	-6.125458
C	-3.538599	3.506462	0.409424	H	3.799421	0.422879	-2.296851
C	-1.851149	3.183685	2.636145	H	2.674815	-2.783137	1.197396
C	-3.239747	2.966723	2.737815	H	2.388224	-2.106495	-4.676652
C	-4.104490	3.126455	1.642739	Zn	-2.647761	0.621325	-1.392339
H	-4.212652	3.655727	-0.449817	Br	-4.029043	0.267803	-3.197352
C	-0.973237	3.056530	3.882354	H	-4.830553	-3.560169	-0.135059
H	-3.655212	2.676944	3.715712	Br	1.478545	-1.548024	3.589286
C	-0.943116	1.630773	4.453911	Zn	-0.474823	-1.452804	2.297662
H	-1.951662	1.290630	4.769936	C	-4.254023	-2.852347	1.859158
H	-0.280239	1.576352	5.341089	C	-5.050759	-2.753810	0.601121
H	-0.546040	0.907999	3.716777	C	-3.426720	-1.766500	1.972382
C	-1.385057	4.079588	4.957149	C	-2.401711	-1.342783	2.920605
H	0.065044	3.304282	3.581578	C	-3.691803	-0.962092	0.771136
H	-2.410308	3.884166	5.335663	O	-4.645685	-1.503082	0.001185
H	-1.364553	5.114989	4.561160	O	-3.124757	0.104214	0.458760
H	-0.695711	4.028021	5.825064	H	-6.152754	-2.718629	0.747822
C	-5.610829	2.904847	1.757741	C	-3.086683	-6.501859	-1.427368
C	-5.981315	1.422951	1.554059	C	-2.564841	-5.248469	-1.097750
H	-7.079344	1.278050	1.627485	C	-2.821331	-4.145973	-1.941296
H	-5.502298	0.787388	2.329014	C	-3.603225	-4.293580	-3.103666
H	-5.654160	1.055954	0.562193	C	-4.137738	-5.548829	-3.420860
C	-6.205981	3.446702	3.067171	C	-3.875346	-6.649273	-2.585947
H	-6.075780	3.474153	0.922264	H	-2.884807	-7.370414	-0.782363
H	-7.312709	3.374059	3.049657	H	-1.952967	-5.084207	-0.196727
H	-5.933363	4.508573	3.231300	C	-2.338745	-2.807790	-1.557521
H	-5.858241	2.868798	3.948686	H	-3.799143	-3.409974	-3.733170
C	-1.602033	4.232398	-1.083468	H	-4.761087	-5.671361	-4.318908
C	-2.325298	3.683315	-2.316871	H	-4.290630	-7.636318	-2.839184
H	-1.779883	3.945340	-3.244701	O	-1.895207	-2.546903	-0.447165
H	-3.361205	4.065976	-2.417948	H	-2.482979	-0.247957	3.083429
H	-2.393286	2.576012	-2.319189	H	-2.469773	-1.866772	3.891966
C	-1.624647	5.773575	-1.141264	H	-4.326904	-3.700109	2.552937
H	-0.544295	3.899741	-1.142657	H	-2.458444	-2.009236	-2.344220
H	-1.196225	6.134514	-2.099019				
H	-1.046959	6.229340	-0.315633				
H	-2.667646	6.146877	-1.070551				
H	1.279312	-5.633283	-3.788113				
H	4.622732	-1.033223	-4.886366				
H	3.774391	-4.932099	1.832619				
C	1.324247	-4.632956	-4.273840				
H	2.920429	1.620623	-4.257504				
H	-0.602361	-4.930704	-5.297621				
H	1.224317	-4.493021	2.066506				
C	1.941311	-3.681337	-3.255575				
C	4.816752	-0.430547	-3.974461				
C	-0.122945	-4.215939	-4.596126				
H	-0.151922	-3.208062	-5.060953				
C	2.419418	-2.411205	-3.618814				
C	3.714418	-4.628295	0.767085				
H	3.205499	-5.072153	-5.324157				
C	2.008115	-4.036300	-1.899739				
C	2.162314	-4.775898	-5.553701				
H	1.724242	-5.542693	-6.225308				
H	1.639889	-5.030947	-1.600217				
C	2.499425	0.629058	-3.991292				
H	5.270703	0.530498	-4.294147				
H	5.563296	-0.978642	-3.364616				
C	2.947787	-1.511444	-2.676182				
C	1.212841	-4.318914	0.971517				
C	2.512158	-3.172145	-0.909650				
H	4.685594	-4.171677	0.488712				
H	3.601546	-5.547537	0.153653				
C	3.520050	-0.186771	-3.179107				
C	2.989980	-1.886743	-1.302343				
C	2.535195	-3.661968	0.536504				
H	1.571654	0.794048	-3.409981				
H	0.347182	-3.669825	0.726582				

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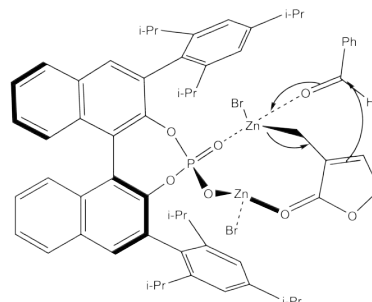


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C	3.1243800	3.7996450	0.8776269
C	4.5358210	3.9048172	0.6896466
C	2.3752840	5.0133734	1.0998821
C	3.0688704	6.2579805	1.1827325
C	0.9570467	4.9514106	1.2241613
H	0.4012804	5.8744730	1.4500306
C	0.2634108	3.7610440	1.0524384
C	3.5188654	-0.9804102	-0.3325836
C	4.5695577	-1.2245765	0.5451779
H	5.1486166	-2.1539119	0.4568826
C	4.8917705	-0.3332953	1.6100384
C	5.9057013	-0.6662707	2.5578533
C	4.1462302	0.8900889	1.7784445
C	4.3985467	1.6815051	2.9376827
C	3.1583114	1.2371152	0.7850002

C	2.8673480	0.2914241	-0.1974405	C	0.5111855	-4.7473009	-5.0013659
O	0.2860737	1.4085586	0.6490288	H	-0.3037889	-5.2750936	-5.5389422
O	1.9093182	0.6206363	-1.1519730	H	0.9060426	-4.7544825	-1.1991343
P	0.3246155	0.5984381	-0.7814564	C	2.7024956	0.4129695	-4.2363146
O	-0.2816117	1.4076977	-1.9505614	H	5.3640218	-0.3219988	-4.4986783
O	-0.2765611	-0.7759909	-0.4815410	H	5.3554799	-1.7164090	-3.3648720
C	4.4446944	6.3205623	1.0191889	C	2.7138479	-1.6089305	-2.6482168
C	5.1787902	5.1334090	0.7554981	C	1.6312960	-4.5986456	1.2656369
H	2.4844178	7.1733544	1.3664338	C	2.3279544	-3.1729675	-0.7790986
H	4.9666442	7.2877758	1.0786490	H	4.8085271	-4.0737550	-0.1058348
H	5.1153564	2.9959289	0.4767376	H	3.7702518	-5.5174585	-0.2090907
H	6.2667204	5.1871356	0.5969287	C	3.5250031	-0.4935982	-3.3068062
C	5.3755892	1.3174685	3.8548700	C	2.9138075	-1.9680089	-1.2821424
C	6.1509959	0.1443420	3.6564418	C	2.7173765	-3.7626807	0.5756469
H	3.7984333	2.5851582	3.1112592	H	1.8129861	0.8207223	-3.7178515
H	5.5442972	1.9403807	4.7466058	H	0.6802925	-4.0452972	1.3647931
H	6.9290989	-0.1300597	4.3850264	H	2.3562111	-0.1270541	-5.1421854
H	6.4757642	-1.5972029	2.4109390	H	-1.5347659	-2.6580663	-3.0481741
C	-2.0792832	3.9527878	0.0936106	H	1.4217347	-5.5443216	0.7221607
C	-1.2256448	3.6577633	1.1900062	H	0.9184031	-3.9769400	-5.6889447
C	-3.4688952	3.8277468	0.2676093	H	3.9427144	0.1449409	-2.5022004
C	-1.7735771	3.2122988	2.4241221	H	2.9485575	-2.9161080	1.2557325
C	-3.1712820	3.0811728	2.5374669	H	1.6315405	-2.0424328	-4.4686595
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C	-0.6793913	4.2080627	4.4584797	C	-2.7581739	-0.6408223	1.6615208
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TS2-8-c

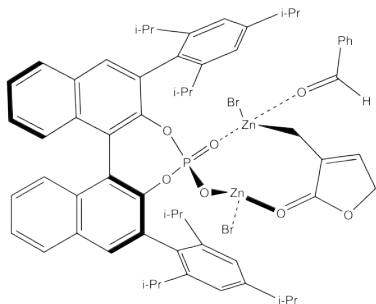


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H	-0.3404381	5.0792705	3.8740122	O	-2.9203490	0.6030260	-1.0387568
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C	-5.5412192	3.1402552	1.5421938	C	-3.2301918	-7.0394890	1.0047833
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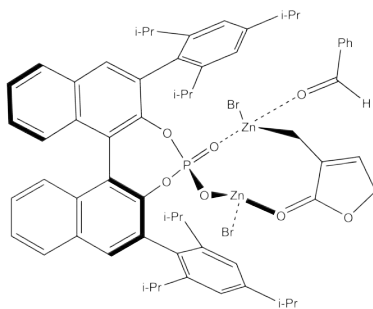
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H	3.3170945	1.3603677	-4.3391160
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H	1.6158121	-5.4799250	0.7420499
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H	-4.6663475	-5.1961932	-3.3242602
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O	-1.4572392	-3.4002321	1.1299254
H	-2.4552031	0.4078571	2.1987812
H	-2.8356118	-0.8881557	3.4157876
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int1-8-c



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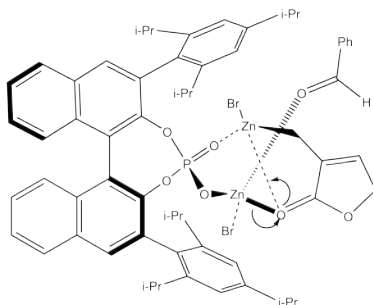
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C	2.1431791	5.0384302	0.6376065
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C	4.9612311	-0.0767607	1.7430123
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P	0.3188461	0.3057157	-0.5664778
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H	4.6178093	7.4140965	0.2950917
H	4.9873234	3.0941396	0.3291414
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C	5.3223401	1.7784098	3.8476660
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H	3.6720130	2.8786497	2.9988951
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C	-1.7929651	3.7484724	-1.5275299
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H	-2.6537208	5.7438746	-1.8382224
H	1.5996224	-5.7853581	-3.6307021
H	5.0216420	-1.3964893	-4.6827499
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C	1.3434464	-4.7463270	-3.9391151
H	3.3531665	1.3478722	-4.3580403
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C	3.8440341	-0.3879821	-3.1218609
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H	1.9313121	0.5962131	-3.5614528
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C	-5.3991102	-2.2038336	0.2742298	H	4.329234	7.149519	1.299064
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H	-4.3983360	-7.3531267	0.4660909	C	-3.752404	2.854921	2.882276
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H	-4.7085456	-5.2053822	-3.3018242	H	-4.181186	2.477352	3.823555
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				C	-6.127016	3.080596	1.961610
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				C	2.631551	-4.334016	-1.759699
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7.2.3.8 to 15p-ma

TS1-8-p; woelfling data



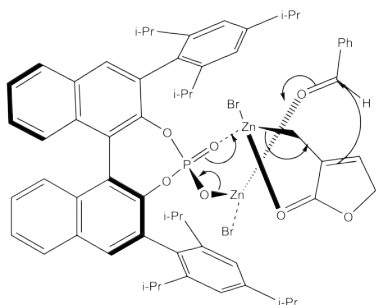
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C	0.363975	4.741910	1.522361
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H	4.761025	-2.245979	1.030990
C	4.341747	-0.469652	2.220062
C	5.280332	-0.788383	3.245501
C	3.569372	0.744242	2.317887
C	3.739157	1.557883	3.477361
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C	2.421731	0.109338	0.265072

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H	1.970872	0.463296	-3.200884
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H	2.939653	-0.138833	-4.591554
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H	0.394126	-5.215405	-0.132157
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H	1.821267	-2.823234	1.203353
H	3.823736	-2.411179	-4.308005
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O	-2.895269	-0.995957	-2.205234
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H	-4.092146	-4.291655	-3.994382
H	0.856496	-3.951600	-3.295979
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H	-0.631342	-2.108944	-2.521278
Br	0.709378	-1.445949	3.363155
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O	-5.018569	-0.624850	-0.198910
O	-3.228491	0.191533	0.937561
H	-6.714127	-1.826575	-0.091276
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H	4.538722	-2.434985	1.647862
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C	4.900659	-0.964119	3.894214
C	3.298837	0.583230	2.814152
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O	-0.305533	0.958777	1.367762
O	1.461999	0.243926	-0.395146
P	-0.165449	0.317404	-0.126701
O	-0.663159	1.333800	-1.172974
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C	3.598071	6.041642	1.892768
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H	1.591939	6.841821	2.037735
H	4.082543	7.027145	1.966160
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H	2.766321	2.315437	4.036263
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H	5.622785	-0.393818	5.849656
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C	-2.789836	3.485924	0.581272
C	-1.987367	3.167026	1.709532
C	-4.169712	3.224030	0.638642
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C	-3.967075	2.348206	2.868862
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H	-4.801395	3.443991	-0.236570
C	-1.759738	2.268843	4.112770
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C	-6.275544	2.354068	1.750255
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H	-1.817656	6.038395	-1.621448
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H	-3.332296	5.951193	-0.656779
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H	6.131743	-1.403306	-3.253672

TS2-8-p; woelfling data

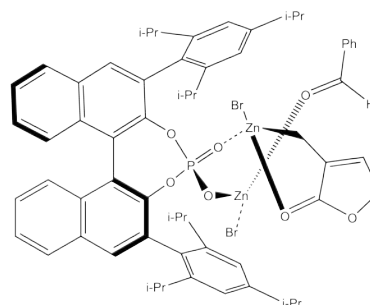


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C	3.794567	3.623245	1.658274

H	1.250467	-4.670770	2.756832
C	3.543287	-5.536368	-3.347748
H	4.247706	1.080121	-3.168262
H	3.776703	-6.156181	-5.431739
H	-0.737874	-4.291318	1.199776
C	3.274797	-4.332834	-2.443507
C	5.989590	-0.887315	-2.281264
C	3.539369	-5.239706	-4.854793
H	4.290476	-4.472024	-5.132960
C	3.919437	-3.093348	-2.616061
C	1.947283	-4.569275	1.899945
H	4.881409	-6.491523	-1.879160
C	2.427318	-4.470458	-1.330355
C	4.872495	-6.209449	-2.950363
H	5.044019	-7.125673	-3.553262
H	1.882514	-5.418974	-1.197938
C	3.754084	0.100307	-3.002795
H	6.484872	0.101809	-2.362358
H	6.521416	-1.475865	-1.506484
C	3.796728	-2.047381	-1.676859
C	-0.027422	-4.274734	0.348807
C	2.262994	-3.455979	-0.366579
H	2.895491	-4.140615	2.280552
H	2.167491	-5.585823	1.510080
C	4.502518	-0.716704	-1.930673
C	2.997760	-2.248110	-0.516447
C	1.315658	-3.685870	0.808311
H	2.706848	0.299837	-2.701236
H	-0.467184	-3.668356	-0.468355
H	3.736082	-0.436086	-3.975122
H	2.549555	-4.891710	-5.204544
H	0.071466	-5.317194	-0.018034
H	5.726281	-5.522145	-3.126097
H	4.458585	-0.135572	-0.986374
H	1.096451	-2.698122	1.265418
H	4.564004	-2.937291	-3.495255
Zn	-1.266973	1.557085	-2.963743
Br	-0.219612	2.274216	-4.866752
C	0.578860	-2.984342	-4.727075
C	-2.900305	-0.715285	-3.983577
C	0.571204	-2.098065	-3.635932
C	-1.778250	-2.588366	-5.131269
C	-1.766346	-1.609611	-4.109309
C	-0.596468	-3.264984	-5.446624
C	-0.602208	-1.414829	-3.329851
O	-2.890508	0.394922	-3.403052
H	1.521479	-3.471952	-5.004932
H	-2.705205	-2.776428	-5.696111
H	1.480182	-1.943819	-3.036658
H	-0.580106	-3.999250	-6.265551
H	-0.647280	-0.764910	-2.448855
Br	-1.933315	-2.555139	3.073166
Zn	-2.293180	-2.063820	0.807256
H	-5.370929	0.170174	-3.271589
H	-3.230931	-3.818869	-1.135508
C	-5.006324	-1.822169	-2.351318
C	-5.656286	-0.468813	-2.407122
H	-5.167094	-2.607075	-3.103767
C	-4.326775	-1.949902	-1.172858
C	-3.571391	-2.995027	-0.481618
C	-4.410831	-0.612914	-0.512240
O	-5.215804	0.219101	-1.220497
O	-3.811933	-0.259502	0.498754
H	-6.767122	-0.541650	-2.392486
H	-4.200901	-3.429080	0.329052
H	-3.823056	-0.999456	-4.541698

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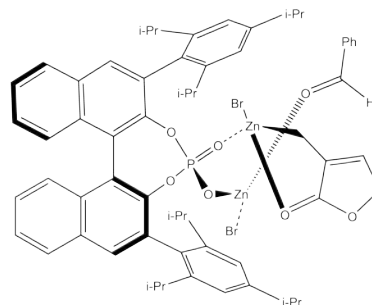


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C	3.8234979	3.3168406	1.6532400
C	1.6697316	4.5176244	1.7036838
C	2.3925015	5.7331182	1.8948367
C	0.2452121	4.5003497	1.6486750
H	-0.3078635	5.4352240	1.8302359
C	-0.4661449	3.3333865	1.3934390
C	2.9781092	-1.4091401	0.3679172
C	3.7306706	-1.7464888	1.4879614
H	4.3240951	-2.6736589	1.4718192
C	3.7455663	-0.9407535	2.6603108
C	4.4505527	-1.3499382	3.8316163
C	3.0310760	0.3117080	2.6676376
C	3.0166557	1.0751404	3.8734553
C	2.3254996	0.7171843	1.4777157
C	2.2444706	-0.1876081	0.4165342
O	-0.4213799	0.9880369	0.8691170
O	1.4739233	0.1428790	-0.6956288
P	-0.1622382	0.2447947	-0.5675550
O	-0.5023643	1.1772811	-1.7557881
O	-0.8752714	-1.1005144	-0.4947366
C	3.7784761	5.7370871	1.9576059
C	4.4971898	4.5184364	1.8263723
H	1.8253809	6.6729327	1.9860509
H	4.3234078	6.6826557	2.1009900
H	4.3887639	2.3799839	1.5461827
H	5.5974730	4.5268351	1.8582054
C	3.6975923	0.6410352	5.0023946
C	4.4324143	-0.5747804	4.9813248
H	2.4399826	2.0098544	3.9103387
H	3.6600519	1.2408545	5.9246541
H	4.9723488	-0.9056804	5.8816450
H	4.9983762	-2.3051864	3.8080958
C	-2.7940589	3.6280011	0.4018565
C	-1.9617882	3.3002007	1.4991952
C	-4.1860539	3.6921138	0.5956353
C	-2.5390259	2.9668962	2.7545702
C	-3.9354224	3.0397257	2.8968311
C	-4.7789061	3.4141767	1.8370378
H	-4.8417734	3.9516771	-0.2510403
C	-1.6874164	2.5339656	3.9460366
H	-4.3794675	2.7849124	3.8724404
C	-2.1649234	1.1971912	4.5373071
H	-3.1703929	1.2848340	5.0003953
H	-1.4640611	0.8511623	5.3243608
H	-2.2036663	0.4127087	3.7566234
C	-1.6165087	3.6445864	5.0096882
H	-0.6540543	2.3663839	3.5808547
H	-2.6238041	3.8732075	5.4177717
H	-1.2049863	4.5833094	4.5849998
H	-0.9690989	3.3383595	5.8577237
C	-6.2914024	3.4716030	2.0125431
C	-6.8782751	2.0675751	2.2491723
H	-7.9851767	2.1058356	2.3234702

H	-6.4920993	1.6277874	3.1926017	Zn	-1.8629276	-1.8682459	1.1540117
H	-6.6019686	1.3831156	1.4232391	H	-5.7050484	-0.1025576	-2.2114611
C	-6.7087369	4.4497580	3.1245293	H	-3.7061238	-3.7223604	0.3275378
H	-6.7118024	3.8519358	1.0551802	C	-5.5295596	-1.7330834	-0.7545396
H	-7.8140728	4.5226978	3.1927920	C	-5.8802043	-0.3264362	-1.1352465
H	-6.3066713	5.4665274	2.9398567	H	-6.0526726	-2.6110956	-1.1597927
H	-6.3364567	4.1162645	4.1157891	C	-4.5015468	-1.7205164	0.1389548
C	-2.2040586	3.8915698	-0.9786414	C	-3.6690266	-2.7315546	0.8204885
C	-2.9821921	3.1499632	-2.0789828	C	-4.1588184	-0.2863683	0.3500445
H	-2.4507237	3.2344565	-3.0565207	O	-4.9943970	0.5124666	-0.3693246
H	-3.9887494	3.5730957	-2.2732804	O	-3.2319573	0.1544635	1.0202038
H	-3.1843789	2.0944918	-1.7684933	H	-6.9313184	-0.0506676	-0.8954582
C	-2.1099000	5.3942441	-1.2939142	H	-4.0178570	-2.8658033	1.8701269
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H	-1.6590486	5.5665355	-2.2935399				
H	-1.4829476	5.9137302	-0.5422560				
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H	3.0504875	-5.9273902	-4.0046537				
H	6.2471896	-1.0186691	-3.2403260				
H	1.2805380	-5.2440509	2.0241742				
C	3.8877742	-5.1929370	-3.9874843				
H	4.1527055	1.3277753	-3.2457862				
H	4.2080041	-5.4659264	-6.1341815				
H	-0.6713334	-4.4852630	0.5410930				
C	3.5258308	-4.1369639	-2.9482055				
C	5.9677978	-0.5459726	-2.2755405				
C	4.0583900	-4.6393819	-5.4102557				
H	4.9450018	-3.9765643	-5.4874374				
C	4.0618672	-2.8378425	-2.9860540				
C	1.9861672	-5.0444754	1.1917024				
H	5.0152461	-6.4064032	-2.5372853				
C	2.6736208	-4.4614641	-1.8770773				
C	5.1503003	-5.9588279	-3.5422948				
H	5.3962285	-6.7732959	-4.2551819				
H	2.2050382	-5.4597109	-1.8557659				
C	3.7423059	0.2982500	-3.1877482				
H	6.3852791	0.4819563	-2.2793923				
H	6.4649054	-1.1156505	-1.4642888				
C	3.8319107	-1.9019011	-1.9586490				
C	0.0495633	-4.3343960	-0.2906423				
C	2.4006481	-3.5584672	-0.8328505				
H	2.9564028	-4.7451333	1.6371960				
H	2.1468897	-5.9950154	0.6395094				
C	4.4428164	-0.5071713	-2.0758959				
C	3.0327237	-2.2854993	-0.8471109				
C	1.4262401	-3.9449811	0.2744603				
H	2.6542760	0.3758942	-2.9931284				
H	-0.3477314	-3.5360542	-0.9473411				
H	3.8869097	-0.1784415	-4.1804655				
H	3.1758470	-4.0527375	-5.7389583				
H	0.0845665	-5.2773089	-0.8764245				
H	6.0221573	-5.2733632	-3.4902276				
H	4.2578587	0.0236921	-1.1200907				
H	1.2618110	-3.0478100	0.9048318				
H	4.7019672	-2.5425922	-3.8315513				
Zn	-1.8063132	1.1031917	-3.1556732				
Br	-1.6094311	1.5242431	-5.4110407				
C	0.3124958	-4.1057429	-4.3053897				
C	-2.9082391	-1.7146904	-2.8944204				
C	0.5313974	-2.7261980	-4.1185128				
C	-1.9737805	-3.8731669	-3.5459521				
C	-1.7737979	-2.4797835	-3.3760612				
C	-0.9365804	-4.6815520	-4.0192529				
C	-0.5052363	-1.9142072	-3.6633624				
O	-3.0023884	-0.4786375	-2.7421471				
H	1.1334918	-4.7398397	-4.6691456				
H	-2.9555533	-4.3105077	-3.3046084				
H	1.5257837	-2.2958824	-4.3070723				
H	-1.0936602	-5.7613702	-4.1565230				
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int1-8-p



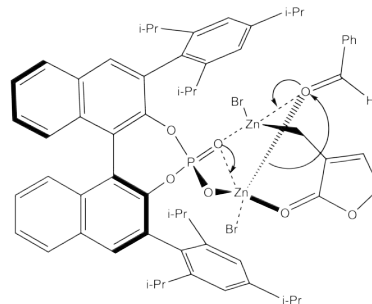
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C	3.8035007	3.3528279	1.6021347
C	1.6372817	4.5287000	1.6815192
C	2.3491043	5.7522563	1.8578713
C	0.2125252	4.4949705	1.6482259
H	-0.3490725	5.4243964	1.8318841
C	-0.4902375	3.3197588	1.4072801
C	2.9728704	-1.3968945	0.3512387
C	3.7451577	-1.7216121	1.4614260
H	4.3407964	-2.6472672	1.4415415
C	3.7762244	-0.9074811	2.6268689
C	4.5018936	-1.3037104	3.7893342
C	3.0544937	0.3404048	2.6360136
C	3.0540101	1.1119569	3.8366917
C	2.3286211	0.7341045	1.4541392
C	2.2347342	-0.1781483	0.3996618
O	-0.4245141	0.9752257	0.8887406
O	1.4485691	0.1386203	-0.7054027
P	-0.1858931	0.2596538	-0.5633292
O	-0.5261646	1.2263870	-1.7233410
O	-0.9134827	-1.0797193	-0.5139030
C	3.7351568	5.7724857	1.8999912
C	4.4654400	4.5621974	1.7621628
H	1.7726465	6.6858015	1.9546183
H	4.2709714	6.7247559	2.0324684
H	4.3764753	2.4213034	1.4905895
H	5.5658414	4.5831473	1.7785688
C	3.7557352	0.6900106	4.9569051
C	4.4976571	-0.5206692	4.9329696
H	2.4711419	2.0425611	3.8764412
H	3.7282390	1.2958944	5.8754370
H	5.0532208	-0.8421851	5.8270411
H	5.0535623	-2.2566108	3.7640871
C	-2.8161529	3.6681652	0.4416001
C	-1.9845906	3.2720912	1.5158571

C	-4.2071433	3.7347459	0.6437169	H	4.2432660	0.0068172	-1.1706008
C	-2.5614553	2.8550184	2.7473840	H	1.2469731	-3.0126650	0.9214783
C	-3.9555172	2.9346487	2.8976701	H	4.6857840	-2.6159850	-3.8271277
C	-4.7976712	3.3895958	1.8680231	Zn	-1.7747722	1.1951946	-3.1659168
H	-4.8627491	4.0491741	-0.1846042	Br	-1.5761950	1.7109868	-5.3897354
C	-1.7005107	2.3361476	3.8977305	C	0.4086654	-3.9967652	-4.3086176
H	-4.4010291	2.6162242	3.8525959	C	-2.8523866	-1.6431228	-2.9253541
C	-2.3167216	1.1167158	4.6005714	C	0.5968093	-2.6083180	-4.1620789
H	-3.2280368	1.3806377	5.1774566	C	-1.8722107	-3.7959249	-3.5268956
H	-1.5892438	0.6784537	5.3128544	C	-1.7041226	-2.3944636	-3.3982267
H	-2.5765627	0.3290752	3.8669951	C	-0.8228965	-4.5928837	-3.9909902
C	-1.3744932	3.4649190	4.8935199	C	-0.4532005	-1.8079233	-3.7170610
H	-0.7393445	1.9896707	3.4661811	O	-2.9756706	-0.4081267	-2.8000268
H	-2.3019581	3.8633953	5.3564888	H	1.2401554	-4.6196576	-4.6663803
H	-0.8582465	4.3097467	4.3938354	H	-2.8396692	-4.2486522	-3.2573037
H	-0.7174586	3.0952067	5.7081498	H	1.5787227	-2.1611586	-4.3740204
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C	-6.9104981	2.0382616	2.1793465	H	-0.2887572	-0.7275870	-3.6023981
H	-8.0165574	2.0809870	2.2631074	Br	-0.3532115	-1.8837421	2.9417484
H	-6.5238054	1.5195562	3.0814499	Zn	-1.8830085	-1.8433383	1.1600445
H	-6.6449728	1.4190094	1.3001107	H	-5.6596000	-0.0937281	-2.3045143
C	-6.7135866	4.3421328	3.2393377	H	-3.7512400	-3.6931686	0.3627549
H	-6.7275043	3.9098163	1.1298647	C	-5.5162856	-1.7114922	-0.8245830
H	-7.8177633	4.4233269	3.3157136	C	-5.8596219	-0.3084944	-1.2303479
H	-6.2983258	5.3647803	3.1356471	H	-6.0313171	-2.5961503	-1.2257076
H	-6.3448379	3.9272576	4.2005143	C	-4.5131228	-1.6871820	0.0970031
C	-2.2324853	3.9790502	-0.9324392	C	-3.7012638	-2.6844121	0.8159320
C	-2.9994982	3.2442685	-2.0463934	C	-4.1742842	-0.2490766	0.2964145
H	-2.4752787	3.3556177	-3.0242070	O	-4.9951987	0.5400068	-0.4546802
H	-4.0176386	3.6483970	-2.2210319	O	-3.2632773	0.2006830	0.9779287
H	-3.1725745	2.1777727	-1.7582517	H	-6.9169871	-0.0324889	-1.0170555
C	-2.1697678	5.4891580	-1.2163129	H	-4.0545704	-2.7713873	1.8689254
H	-1.1952197	3.5864553	-0.9459118	H	-3.7408552	-2.2594013	-2.6432732
H	-1.7290893	5.6928921	-2.2145787				
H	-1.5485823	6.0052073	-0.4578373				
H	-3.1821796	5.9434916	-1.1873900				
H	3.0182252	-5.9806415	-3.9579700				
H	6.2049056	-1.0542894	-3.3081360				
H	1.2614693	-5.1770463	2.0881458				
C	3.8820480	-5.2779664	-3.9105828				
H	4.0986910	1.2767341	-3.3170487				
H	4.2956093	-5.6064241	-6.0338918				
H	-0.6890475	-4.4532457	0.5920646				
C	3.5108909	-4.1904363	-2.9071136				
C	5.9373601	-0.5723285	-2.3445830				
C	4.1468358	-4.7609430	-5.3321992				
H	5.0651690	-4.1397331	-5.3760519				
C	4.0438512	-2.8919269	-2.9767423				
C	1.9641302	-5.0042710	1.2476697				
H	4.8867362	-6.5050448	-2.3838104				
C	2.6537568	-4.4884048	-1.8319353				
C	5.0889758	-6.0841167	-3.3887778				
H	5.3385892	-6.9216647	-4.0730351				
H	2.1857892	-5.4863199	-1.7863237				
C	3.6933189	0.2471899	-3.2332681				
H	6.3503825	0.4570320	-2.3673921				
H	6.4501172	-1.1303204	-1.5352488				
C	3.8115526	-1.9321426	-1.9717957				
C	0.0277507	-4.3169772	-0.2454871				
C	2.3800317	-3.5622742	-0.8090931				
H	2.9379483	-4.7006719	1.6817301				
H	2.1165617	-5.9688758	0.7179415				
C	4.4159524	-0.5377976	-2.1209553				
C	3.0144961	-2.2911369	-0.8513179				
C	1.4073390	-3.9224602	0.3082008				
H	2.6090820	0.3274932	-3.0200515				
H	-0.3697523	-3.5275533	-0.9130215				
H	3.8223278	-0.2450974	-4.2207562				
H	3.3101731	-4.1413972	-5.7160998				
H	0.0574908	-5.2694233	-0.8164252				
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7.2.3.9 to 15b-ma

TS1-8-b; woelfling data

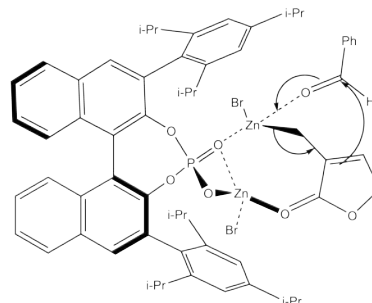


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C	2.924444	3.814030	0.785816
C	4.322078	3.944950	0.527455
C	2.138128	5.016508	0.929855
C	2.790243	6.284072	0.864333
C	0.727554	4.919117	1.111451
H	0.146015	5.840967	1.266084
C	0.071708	3.694542	1.091774
C	3.488491	-0.887266	-0.387113
C	4.557821	-1.122480	0.468287
H	5.177960	-2.018118	0.314863
C	4.860538	-0.257219	1.557586
C	5.913977	-0.563517	2.469137
C	4.083016	0.941813	1.758438
C	4.363487	1.748447	2.900564
C	3.036839	1.254214	0.817614

C	2.744375	0.311308	-0.169130	C	3.210032	-4.815199	-5.697716
O	0.199097	1.306917	0.952025	H	2.910030	-5.526485	-6.495122
O	1.671800	0.569266	-1.031201	H	1.811923	-4.926495	-2.110715
P	0.191947	0.336616	-0.383037	C	2.958617	0.830909	-4.026740
O	-0.772508	0.861889	-1.471876	H	5.750768	0.780491	-4.109606
O	-0.038864	-1.064658	0.162499	H	5.986748	-0.805587	-3.300258
C	4.154069	6.375082	0.631399	C	3.318628	-1.395402	-2.852369
C	4.920959	5.193899	0.448781	C	0.949786	-4.241423	0.364315
H	2.182045	7.194147	0.986701	C	2.578206	-3.099229	-1.230009
H	4.641566	7.360075	0.573418	H	4.439798	-4.077942	0.627092
H	4.923103	3.037611	0.376617	H	3.457048	-5.469575	0.080889
H	5.998398	5.267737	0.236204	C	3.927076	-0.038922	-3.205232
C	5.384928	1.412497	3.778184	C	3.126030	-1.814433	-1.505705
C	6.177955	0.255641	3.555751	C	2.329043	-3.586099	0.195343
H	3.748249	2.639298	3.089348	H	1.994594	0.955974	-3.496956
H	5.576474	2.044291	4.658829	H	0.162056	-3.595003	-0.059646
H	6.989606	0.003067	4.254919	H	2.751148	0.382155	-5.020703
H	6.504845	-1.477150	2.298850	H	-0.012771	-3.611214	-4.980020
C	-2.298387	3.633512	0.172145	H	0.886623	-5.238011	-0.122347
C	-1.408577	3.539470	1.279164	H	3.624960	-3.913913	-6.195720
C	-3.672331	3.436626	0.395516	H	4.128605	0.499910	-2.257289
C	-1.909661	3.247852	2.576362	H	2.332333	-2.698254	0.859390
C	-3.294693	3.041289	2.739860	H	3.110899	-1.936321	-4.934867
C	-4.196038	3.137723	1.666377	C	-3.555381	-6.774239	0.070702
H	-4.374369	3.526991	-0.448836	C	-2.921627	-5.530821	0.094036
C	-0.986372	3.191919	3.796178	C	-3.124683	-4.623492	-0.969218
H	-3.677134	2.816384	3.747497	C	-3.960312	-4.958084	-2.053473
C	-0.818811	1.768897	4.355910	C	-4.608161	-6.201112	-2.062875
H	-1.786906	1.352960	4.704758	C	-4.403386	-7.104935	-1.005026
H	-0.124211	1.767978	5.220449	H	-3.396813	-7.488529	0.892656
H	-0.398984	1.074723	3.602788	H	-2.266745	-5.218250	0.922217
C	-1.441343	4.169696	4.894876	C	-2.537406	-3.278346	-0.867885
H	0.016927	3.526651	3.462657	H	-4.116924	-4.224001	-2.861124
H	-2.424502	3.881193	5.322230	H	-5.278960	-6.467398	-2.893140
H	-1.534604	5.203953	4.506188	H	-4.911309	-8.081046	-1.015409
H	-0.711145	4.179175	5.730116	O	-2.024385	-2.863897	0.165947
C	-5.698756	2.928336	1.832964	Zn	-2.564702	0.202950	-1.696909
C	-6.075910	1.442261	1.677457	Br	-3.662925	-0.567143	-3.553260
H	-7.172618	1.299495	1.774425	H	-5.192308	-3.605982	0.510765
H	-5.581089	0.825121	2.457060	Br	1.328335	-1.733626	3.334853
H	-5.768002	1.052345	0.687867	Zn	-0.626289	-1.391907	2.078941
C	-6.257314	3.510367	3.139890	C	-4.450764	-2.490350	2.248143
H	-6.183680	3.475542	0.993810	C	-5.312980	-2.633660	1.039478
H	-7.364670	3.447075	3.151455	C	-3.568607	-1.456624	2.069082
H	-5.972402	4.574367	3.264961	C	-2.451889	-0.912820	2.826430
H	-5.891239	2.955717	4.028768	C	-3.854995	-0.938884	0.721946
C	-1.797243	4.031103	-1.216086	O	-4.866109	-1.594999	0.134688
C	-2.587710	3.411514	-2.375624	O	-3.252722	-0.010143	0.146659
H	-2.073098	3.584520	-3.341040	H	-6.399154	-2.479102	1.224291
H	-3.614768	3.819539	-2.463528	H	-4.514821	-3.158375	3.117361
H	-2.692257	2.309508	-2.279941	H	-2.636073	-2.623500	-1.780920
C	-1.803431	5.565893	-1.372110	H	-2.439032	0.192495	2.737581
H	-0.748330	3.677764	-1.302543	H	-2.456342	-1.210057	3.891463
H	-1.405171	5.865389	-2.363448				
H	-1.191004	6.059788	-0.594298				
H	-2.838517	5.957601	-1.284833				
H	1.638918	-5.399329	-4.344843				
H	5.170348	-0.722607	-4.890977				
H	3.251754	-4.818508	1.744230				
C	2.012528	-4.455419	-4.800233				
H	3.391436	1.838081	-4.200010				
H	0.527278	-4.544788	-6.418205				
H	0.732190	-4.381653	1.443520				
C	2.417802	-3.540599	-3.651171				
C	5.283583	-0.207127	-3.914281				
C	0.860302	-3.847415	-5.621405				
H	1.174542	-2.903240	-6.113592				
C	2.960701	-2.267143	-3.894487				
C	3.433949	-4.538364	0.686082				
H	4.028500	-5.278607	-5.111025				
C	2.242851	-3.933016	-2.314804				

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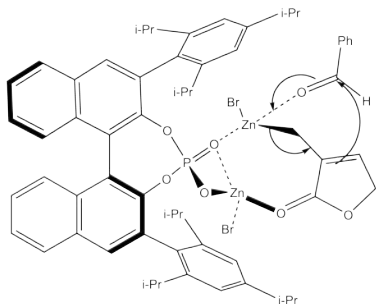


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C	4.2429815	3.8789219	0.5679862	H	5.8687311	-0.5671108	-4.7564203
C	2.0491743	4.9554629	0.8867862	H	2.7134946	-4.7629149	1.3380217
C	2.7134280	6.2181560	0.9251979	C	2.3041919	-3.9224076	-5.3697719
C	0.6319632	4.8647758	1.0033721	H	4.2839740	2.0696862	-3.9203514
H	0.0522219	5.7805009	1.1966171	H	0.7382552	-3.7624275	-6.9075270
C	-0.0340647	3.6511916	0.8883501	H	0.2825912	-4.4186053	0.5723284
C	3.5272311	-0.9096537	-0.5010687	C	2.7215293	-3.1907764	-4.1002612
C	4.5342276	-1.1406769	0.4264094	C	5.9332864	-0.1818152	-3.7173009
H	5.2074476	-2.0002527	0.2896105	C	1.1025836	-3.2060057	-6.0186441
C	4.7150261	-0.2977160	1.5618233	H	1.3879418	-2.1849574	-6.3495378
C	5.6875717	-0.6061100	2.5591294	C	3.4618620	-1.9973472	-4.1429413
C	3.8996504	0.8830460	1.7173102	C	3.0794774	-4.4278811	0.3455003
C	4.0619407	1.6701885	2.8952630	H	4.3211766	-4.6192274	-5.9042113
C	2.9237056	1.1947668	0.7014267	C	2.2946865	-3.6543280	-2.8442982
C	2.7193257	0.2478496	-0.2994936	C	3.4542264	-4.1096872	-6.3715277
O	0.0598100	1.2781641	0.5604756	H	3.1226555	-4.7182796	-7.2378984
O	1.7073747	0.4664879	-1.2441753	H	1.7089669	-4.5855596	-2.8030406
P	0.1511631	0.3830850	-0.8002824	C	3.7404871	1.1021368	-3.9004622
O	-0.6446687	0.8776175	-2.0291609	H	6.5066696	0.7678551	-3.7493965
O	-0.4104972	-1.0108584	-0.3819681	H	6.5150969	-0.9152981	-3.1228430
C	4.0904222	6.3043185	0.7848187	C	3.7574824	-1.2613808	-2.9808278
C	4.8565786	5.1239266	0.5913508	C	0.6907552	-4.2069757	-0.4351846
H	2.1058076	7.1272074	1.0570747	C	2.5586478	-2.9563503	-1.6515149
H	4.5895176	7.2849648	0.8097051	H	4.0540907	-3.9247493	0.4973833
H	4.8475715	2.9753593	0.4087510	H	3.2582114	-5.3274927	-0.2806458
H	5.9462167	5.1958657	0.4534542	C	4.5373479	0.0465266	-3.1105069
C	5.0036331	1.3308573	3.8569448	C	3.2978356	-1.7442006	-1.7250227
C	5.8341081	0.1917129	3.6841045	C	2.0476871	-3.4970180	-0.3195191
H	3.4151186	2.5453608	3.0481287	H	2.7451408	1.2721011	-3.4447187
H	5.1010169	1.9456212	4.7647801	H	-0.0459524	-3.5853998	-0.9824896
H	6.5811626	-0.0642102	4.4508615	H	3.5833982	0.7840524	-4.9525052
H	6.3098406	-1.5048194	2.4252302	H	0.2610952	-3.1023046	-5.3034659
C	-2.4184386	3.5551589	0.0019169	H	0.7736809	-5.1791009	-0.9645477
C	-1.5113981	3.5070237	1.0974013	H	3.8098171	-3.1377391	-6.7729755
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C	-1.9880415	3.2757247	2.4142143	H	1.9099096	-2.6269574	0.3578192
C	-3.3703817	3.0747093	2.6110185	C	3.8053854	-1.6102166	-5.1153300
C	-4.2865138	3.1073506	1.5485239	H	-3.9354448	-6.8326662	2.6307248
H	-4.4961287	3.3952962	-0.5839325	C	-3.2987763	-5.6048556	2.4126824
C	-1.0513381	3.2393862	3.6224111	C	-3.3601349	-4.9911506	1.1425359
H	-3.7305140	2.8853985	3.6329824	C	-4.0454136	-5.6372508	0.0906905
C	-0.9577126	1.8342527	4.2426487	C	-4.6806998	-6.8695880	0.3127937
H	-1.9504179	1.4754774	4.5877574	H	-4.6327481	-7.4656646	1.5836847
H	-0.2800417	1.8412019	5.1212645	C	-3.8850072	-7.3071875	3.6229293
H	-0.5518891	1.0948114	3.5243946	H	-2.7361111	-5.1047222	3.2156696
C	-1.4445221	4.2971531	4.6697110	C	-2.6829737	-3.6878079	0.8936284
H	-0.0344265	3.5018033	3.2668340	H	-4.0506681	-5.1847150	-0.9147453
H	-2.4395356	4.0858019	5.1143623	H	-5.2060321	-7.3715007	-0.5141456
H	-1.4849808	5.3115937	4.2229707	H	-5.1298736	-8.4322774	1.7580560
H	-0.7080288	4.3154360	5.4993971	O	-1.6723034	-3.3624175	1.6297240
C	-5.7807092	2.8493555	1.7311760	Zn	-1.9127493	-0.6603556	-2.1135747
C	-6.1559254	1.4478800	1.2071843	Br	-2.4356878	-2.5559289	-3.2858848
H	-7.2501857	1.2762575	1.2759038	H	-5.4298048	-3.4541955	-0.0576134
H	-5.6478018	0.6639667	1.8078359	Br	1.1450809	-1.3234858	2.8931817
H	-5.8557658	1.3159555	0.1486222	Zn	-0.7514735	-1.6356684	1.5651209
C	-6.2820533	3.0441748	3.1670598	C	-4.2318645	-2.4030500	1.4874513
H	-6.3072013	3.5898203	1.0872486	C	-5.3192944	-2.4751643	0.4513651
H	-7.3864818	2.9547456	3.2068096	C	-3.5574095	-1.1690076	1.2840618
H	-6.0045478	4.0396153	3.5687736	C	-2.5808145	-0.5063724	2.0357567
H	-5.8679348	2.2746714	3.8520415	C	-3.8997776	-0.7866664	-0.1061498
C	-1.9263724	3.8633002	-1.4107107	O	-4.9249020	-1.5075737	-0.5611540
C	-2.7790194	3.2242137	-2.5169529	O	-3.3265007	0.0472400	-0.8328269
H	-2.2624759	3.3117723	-3.4936810	H	-6.3149550	-2.1708079	0.8403866
H	-3.7644229	3.7247583	-2.6211385	H	-4.3883579	-2.8365644	2.4852824
H	-2.9589983	2.1511277	-2.3174330	H	-2.6825693	-3.3824740	-0.1834282
C	-1.8164171	5.3856318	-1.6290125	H	-2.2634195	0.4931609	1.6915369
H	-0.9053816	3.4357971	-1.5000151	H	-2.5602508	-0.6760111	3.1242972
H	-1.4342829	5.6097969	-2.6465649				
H	-1.1321226	5.8584333	-0.8977474				
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TS2-8-b



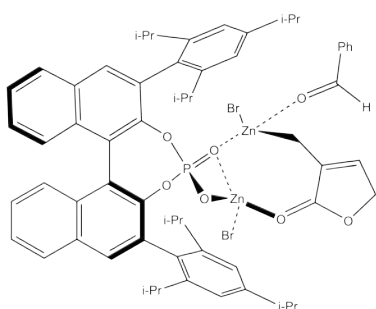
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C	2.8279106	3.7540270	0.7297972
C	4.2399915	3.8832375	0.5669367
C	2.0453896	4.9571931	0.8842727
C	2.7083365	6.2201004	0.9203104
C	0.6287319	4.8640582	1.0013358
H	0.0463099	5.7784879	1.1929157
C	-0.0357995	3.6496066	0.8891593
C	3.5295928	-0.9076421	-0.4971248
C	4.5395217	-1.1338710	0.4280822
H	5.2126443	-1.9932686	0.2901172
C	4.7222989	-0.2892639	1.5614979
C	5.6973806	-0.5937096	2.5568520
C	3.9048629	0.8897749	1.7173553
C	4.0686071	1.6787908	2.8935832
C	2.9257180	1.1977503	0.7034808
C	2.7204351	0.2489697	-0.2955886
O	0.0606715	1.2766645	0.5669093
O	1.7064813	0.4647449	-1.2384472
P	0.1514862	0.3784892	-0.7928228
O	-0.6503237	0.8717096	-2.0182275
O	-0.4064497	-1.0165064	-0.3704255
C	4.0846549	6.3080107	0.7798707
C	4.8518126	5.1286303	0.5885172
H	2.0994395	7.1285780	1.0502553
H	4.5822806	7.2893933	0.8029914
H	4.8446249	2.9794478	0.4100501
H	5.9413736	5.2014288	0.4508846
C	5.0134083	1.3429752	3.8527838
C	5.8453693	0.2057346	3.6797528
H	3.4195400	2.5521765	3.0463352
H	5.1112405	1.9589594	4.7596410
H	6.5941747	-0.0482519	4.4453262
H	6.3198341	-1.4922817	2.4233963
C	-2.4199840	3.5516997	0.0033311
C	-1.5129911	3.5059319	1.0987745
C	-3.7868801	3.3591522	0.2589672
C	-1.9895066	3.2806215	2.4164936
C	-3.3718583	3.0823929	2.6141320
C	-4.2878233	3.1125714	1.5519405
H	-4.4973182	3.3932576	-0.5813402
C	-1.0532069	3.2497964	3.6252146
H	-3.7318979	2.8985527	3.6370988
C	-0.9589423	1.8482275	4.2530363
H	-1.9514435	1.4912770	4.6008602
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H	-0.5519072	1.1040080	3.5405134
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H	-0.0363109	3.5104759	3.2682643
H	-2.4417542	4.1047827	5.1124774
H	-1.4884887	5.3251339	4.2144729
H	-0.7110954	4.3367195	5.4966004
C	-5.7824271	2.8577244	1.7356636

C	-6.1600906	1.4547265	1.2177441
H	-7.2547045	1.2845165	1.2865455
H	-5.6526036	0.6731300	1.8220939
H	-5.8590260	1.3166586	0.1603465
C	-6.2838376	3.0599122	3.1703661
H	-6.3077201	3.5967542	1.0889540
H	-7.3883788	2.9728718	3.2117871
H	-6.0040949	4.0562937	3.5676299
H	-5.8713250	2.2928218	3.8589388
C	-1.9282009	3.8527094	-1.4109217
C	-2.7843658	3.2128722	-2.5138850
H	-2.2676990	3.2928647	-3.4909763
H	-3.7673048	3.7177394	-2.6209041
H	-2.9701601	2.1418453	-2.3093881
C	-1.8124523	5.3735111	-1.6356344
H	-0.9094592	3.4203023	-1.5005687
H	-1.4305382	5.5920775	-2.6543716
H	-1.1249198	5.8464209	-0.9077680
H	-2.8045013	5.8602173	-1.5292978
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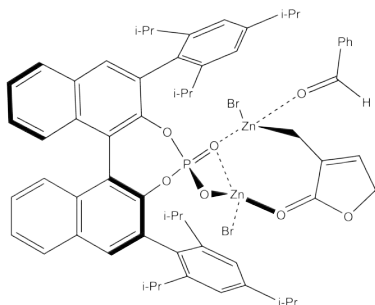
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C	-0.1430487	3.5550298	0.9257374
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C	4.6304983	-1.0388639	0.5541580
H	5.3489920	-1.8627128	0.4285061
C	4.7476354	-0.1911263	1.6939443
C	5.7162550	-0.4496753	2.7090578
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int1-8-b



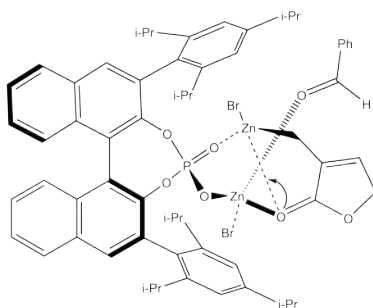
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C	4.6391710	-1.0357609	0.5565575
H	5.3538371	-1.8622077	0.4266826
C	4.7635814	-0.1893485	1.6961321
C	5.7363178	-0.4494778	2.7061977
C	3.8901007	0.9498403	1.8407727
C	4.0013552	1.7471770	3.0174515
C	2.9144254	1.2134955	0.8122497
C	2.7631152	0.2572878	-0.1896507
O	0.0569871	1.1866850	0.6467778
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C	1.0621917	-4.3090181	-0.2387519	C	0.290640	4.819916	2.462857
C	2.8472322	-2.9923751	-1.4971560	H	-0.294318	5.745286	2.580115
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H	-4.6706354	-7.3425225	2.2460905	H	5.627071	5.147504	2.336370
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C	-2.2557781	-3.7642242	0.4591010	C	5.451990	0.056741	5.230458
H	-3.7023103	-4.3917783	-1.7027181	H	3.074367	2.455575	4.604943
H	-5.4337095	-6.2143995	-1.8818724	H	4.747560	1.818858	6.314114
H	-5.9084218	-7.6781989	0.0952139	H	6.194844	-0.215358	5.995629
O	-1.6048437	-3.4840721	1.4758203	H	5.883711	-1.650069	3.967586
Zn	-1.7665934	-0.9053237	-2.0151474	C	-2.329804	4.007747	0.667211
Br	-2.0373830	-2.6732872	-3.4553160	C	-1.827015	3.502014	1.902139
H	-5.7449603	-3.4191498	0.4888254	C	-3.628710	3.628642	0.274856
Br	1.1870281	-1.5823737	2.9727389	C	-2.669256	2.746042	2.760721
Zn	-0.8234616	-1.5063221	1.7810044	C	-3.959585	2.400933	2.322199
C	-4.7559462	-2.0064169	1.8536295	C	-4.450611	2.804618	1.068294
C	-5.6791221	-2.3340820	0.7326389	H	-4.022590	3.987324	-0.687759
C	-3.7575558	-1.1690879	1.4148794	C	-2.230607	2.387104	4.178255
C	-2.6157815	-0.5516134	2.0681111	H	-4.597493	1.800318	2.988033
C	-4.0085857	-1.0167541	-0.0357853	C	-2.413560	0.904273	4.514450
O	-5.1196288	-1.6700352	-0.4183371	H	-3.478861	0.595651	4.502264
O	-3.3294594	-0.3925125	-0.8699173	H	-2.023509	0.677502	5.527722
H	-6.7151368	-1.9519349	0.8763215	H	-1.879526	0.255240	3.797811
H	-4.8997737	-2.3704605	2.8795823	C	-2.959293	3.291420	5.192122
H	-2.1150633	-3.1761150	-0.4852345	H	-1.147990	2.617273	4.261882
H	-2.4200763	0.4609079	1.6611564	H	-4.055631	3.118978	5.160741
H	-2.7478294	-0.4937208	3.1645741	H	-2.782331	4.366000	4.982259
				H	-2.614195	3.077257	6.225011
				C	-5.830381	2.382020	0.571100
				C	-5.777062	0.996463	-0.101805
				H	-6.783676	0.691336	-0.457929
				H	-5.411967	0.223061	0.606243
				H	-5.103478	1.004943	-0.980516
				C	-6.905937	2.410852	1.668465
				H	-6.123726	3.115684	-0.212032
				H	-7.910184	2.233426	1.232012
				H	-6.925673	3.384370	2.198271
				H	-6.737879	1.616703	2.425515
				C	-1.509298	4.947866	-0.223378
				C	-0.724778	4.216867	-1.328074
				H	-0.098509	4.937680	-1.894225
				H	-1.415677	3.732879	-2.049418
				H	-0.065704	3.432242	-0.910685
				C	-2.361427	6.085210	-0.811486
				H	-0.751739	5.426674	0.426602
				H	-1.709875	6.832439	-1.309525
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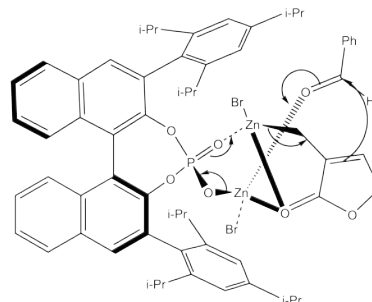
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H	5.088904	-1.204228	-3.278842
H	2.551105	-4.834708	3.593075
C	2.498268	-5.310504	-2.853014
H	3.070684	1.215708	-3.092010
H	1.042276	-6.080141	-4.316765
H	0.061157	-4.231802	2.964509
C	2.593321	-4.154594	-1.865505
C	5.063507	-0.585738	-2.357117
C	1.182238	-5.212611	-3.637159
H	1.197838	-4.292248	-4.252877
C	2.995428	-2.863430	-2.249992
C	2.852979	-4.638324	2.544146
H	4.652957	-5.476591	-3.267114
C	2.226374	-4.354865	-0.526331
C	3.692356	-5.404787	-3.814295
H	3.598168	-6.296731	-4.467533
H	1.878015	-5.355190	-0.220230
C	2.683345	0.216388	-2.803096
H	5.478332	0.411001	-2.613246
H	5.741083	-1.060141	-1.618485
C	3.104236	-1.808866	-1.323370
C	0.441818	-4.188813	1.924564
C	2.304897	-3.335091	0.437631
H	3.892005	-4.253065	2.551391
H	2.863641	-5.611376	2.009189
C	3.634567	-0.457078	-1.797094
C	2.783038	-2.054587	0.039508
C	1.880618	-3.653781	1.870783
H	1.675290	0.353576	-2.365029
H	-0.223871	-3.521235	1.346585
H	2.582013	-0.383615	-3.732575
H	0.305952	-5.151117	-2.958827
H	0.350737	-5.203432	1.483592
H	3.748899	-4.518859	-4.480758
H	3.695731	0.208207	-0.912691
H	1.892223	-2.706633	2.446011
H	3.270178	-2.671906	-3.299630
C	-0.834658	-3.588498	-5.750865
C	-0.918051	-2.527928	-4.844276
C	-1.192658	-1.223624	-5.318346
C	-1.345745	-0.991864	-6.704337
C	-1.216186	-2.052562	-7.610496
C	-0.969781	-3.350369	-7.131428
H	-0.651800	-4.608891	-5.388472
H	-0.787146	-2.680369	-3.761267
C	-1.397242	-0.125333	-4.370511
H	-1.571312	0.024795	-7.062852
H	-1.316773	-1.875143	-8.691309
H	-0.877803	-4.190322	-7.837053
O	-1.257487	-0.259468	-3.146484
Zn	-2.344379	0.947436	-1.727598
Br	-3.627766	2.256481	-3.173505
H	-3.451679	-3.187069	-4.376221
Br	-2.835250	-2.485939	3.666995
Zn	-2.222963	-2.303469	1.418220
C	-3.678949	-3.980476	-2.349753
C	-4.067512	-3.062858	-3.458023
C	-3.278656	-3.263727	-1.262267
C	-2.792683	-3.683146	0.075062
C	-3.384066	-1.845135	-1.676512
O	-3.837062	-1.737798	-2.941930
O	-3.095798	-0.843917	-1.003154
H	-5.137802	-3.140870	-3.750295
H	-3.594709	-4.251587	0.595523
H	-1.957784	-4.406408	-0.050016
H	-3.719906	-5.076367	-2.423624
H	-1.749888	0.854015	-4.786917



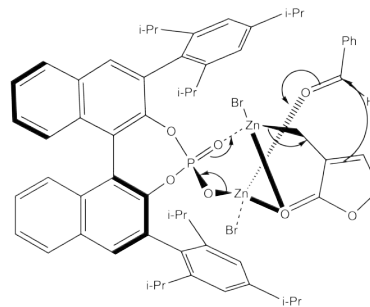
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C	3.6499618	3.8662529	2.2148186
C	1.3781499	4.7802522	2.4819219
C	1.9513289	6.0845269	2.5764993
C	-0.0341488	4.5973538	2.4701096
H	-0.6826637	5.4803050	2.5780191
C	-0.6127881	3.3492404	2.2661245
C	3.0766945	-1.1320023	1.3609629
C	4.1219144	-1.2515178	2.2695618
H	4.7615521	-2.1465979	2.2357316
C	4.3419822	-0.2898105	3.2952357
C	5.3561404	-0.4855669	4.2808484
C	3.4850273	0.8680859	3.3804795
C	3.6368170	1.7343763	4.5053227
C	2.4942354	1.0818645	2.3501431
C	2.3049026	0.0687555	1.4028034
O	-0.3247237	0.9563773	2.1826444
O	1.3404028	0.2392803	0.4048164
P	-0.2461839	0.0901308	0.8055804
O	-1.0164422	0.7371134	-0.3454238
O	-0.6186996	-1.3512102	1.1902081
C	3.3228671	6.2687568	2.4861759
C	4.1745114	5.1498792	2.2840746
H	1.2771833	6.9464624	2.7014206
H	3.7515499	7.2804070	2.5514187
H	4.3208994	3.0112557	2.0531548
H	5.2595521	5.3008858	2.1772859
C	4.6181465	1.5045069	5.4599651
C	5.5001556	0.3974986	5.3399101
H	2.9571941	2.5894859	4.6212839
H	4.7080866	2.1841073	6.3211362
H	6.2806764	0.2318910	6.0980437
H	6.0099355	-1.3675262	4.1931673
C	-2.6340706	3.6707065	0.7907934
C	-2.0666781	3.1448915	1.9919758
C	-3.9509282	3.3016265	0.4620975
C	-2.8538344	2.3367611	2.8588259
C	-4.1619678	1.9980218	2.4734269
C	-4.7190010	2.4390944	1.2624782
H	-4.3945270	3.6685948	-0.4733941
C	-2.3436088	1.8807992	4.2249524
H	-4.7607532	1.3557708	3.1382101
C	-2.5343016	0.3742239	4.4689713
H	-3.6078512	0.0994060	4.5302652
H	-2.0660191	0.0766926	5.4297500
H	-2.0711736	-0.2243871	3.6606000
C	-3.0013402	2.7186679	5.3393527
H	-1.2550506	2.0877808	4.2702429
H	-4.1010888	2.5670634	5.3554534
H	-2.8143903	3.8019171	5.1921033
H	-2.6043998	2.4320389	6.3355015
C	-6.0956984	1.9734839	0.8092476
C	-6.0939948	0.4565412	0.5397423
H	-7.0810931	0.1241084	0.1560228

TS2-8-I; COSMO

H	-5.8843127	-0.1146490	1.4684692	Br	-2.0345310	-4.9772489	0.3387756
H	-5.3213559	0.1806193	-0.2046695	Zn	-1.4434122	-2.7598931	0.0796078
C	-7.2021935	2.3701551	1.8019732	C	-2.3905807	-2.0824139	-4.0669697
H	-6.3052229	2.4833108	-0.1564420	C	-3.9015762	-2.0522194	-4.0260924
H	-8.1999028	2.0714212	1.4188141	C	-1.9529230	-2.0795981	-2.7153814
H	-7.2147739	3.4648824	1.9791341	C	-0.6911239	-2.0692951	-2.1450210
H	-7.0622437	1.8715012	2.7841771	C	-3.1567036	-1.8446488	-1.8877764
C	-1.8477494	4.5841190	-0.1611402	O	-4.2579821	-1.8214590	-2.6310713
C	-0.9151653	3.8060141	-1.1093702	O	-3.1798562	-1.7621794	-0.6451852
H	-0.2904884	4.4976400	-1.7104110	H	-4.3778798	-3.0111221	-4.3214721
H	-1.5330928	3.2341165	-1.8455791	H	-0.4976818	-1.4269345	-1.2711305
H	-0.2463874	3.1085435	-0.5720441	H	0.2077328	-2.3608435	-2.6980777
C	-2.7364747	5.5424686	-0.9691525	H	-1.8817715	-2.6365824	-4.8664392
H	-1.1831679	5.2139608	0.4622862	H	-2.5973057	0.2510320	-4.7227016
H	-2.1072568	6.2782371	-1.5099158				
H	-3.4360102	6.1015411	-0.3159798				
H	-3.3364457	5.0037883	-1.7313025				
H	1.4455633	-6.4229161	-1.5405809				
H	5.1130173	-2.0105833	-2.7304686				
H	2.9191938	-4.7454083	4.0948780				
C	1.6430655	-5.5577567	-2.2106313				
H	3.2986690	0.6552297	-3.0590219				
H	0.0509621	-6.2022377	-3.5716845				
H	0.4693072	-4.1932816	3.9917927				
C	2.0027547	-4.3869420	-1.3006625				
C	5.0745504	-1.2284513	-1.9433265				
C	0.3468658	-5.2971051	-3.0017577				
H	0.4856397	-4.4740391	-3.7353367				
C	2.5970552	-3.2127166	-1.7991471				
C	2.9847016	-4.6408509	2.9920669				
H	3.7353830	-6.1294045	-2.5916122				
C	1.7529759	-4.4583513	0.0822312				
C	2.7955208	-5.9474292	-3.1511428				
H	2.5440117	-6.8703899	-3.7127873				
H	1.2841002	-5.3702187	0.4842562				
C	2.8403916	-0.3018641	-2.7358814				
H	5.5908120	-0.3272785	-2.3346318				
H	5.6475407	-1.6020416	-1.0703981				
C	2.9360099	-2.1326872	-0.9627671				
C	0.5205366	-4.0737071	2.8899760				
C	2.1101836	-3.4244830	0.9708143				
H	4.0167874	-4.3251972	2.7376641				
H	2.8255173	-5.6447821	2.5457634				
C	3.6197600	-0.9030110	-1.5558537				
C	2.7038055	-2.2452222	0.4339861				
C	1.9335697	-3.6371352	2.4762443				
H	1.7830275	-0.1016074	-2.4712961				
H	-0.2322719	-3.3165282	2.5994322				
H	2.8523882	-0.9796621	-3.6151851				
H	-0.4888207	-5.0233010	-2.3278753				
H	0.2214240	-5.0387296	2.4343953				
H	2.9969153	-5.1538981	-3.9011082				
H	3.6615262	-0.1281129	-0.7643465				
H	2.1255071	-2.6674752	2.9767773				
H	2.8134058	-3.1347109	-2.8767050				
C	1.1916597	-1.2187135	-6.9685340				
C	0.5262489	-0.8143792	-5.8029826				
C	-0.8614792	-0.5570706	-5.8279512				
C	-1.5686077	-0.7000589	-7.0427887				
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C	0.4814954	-1.3639027	-8.1735940				
H	2.2743896	-1.4176723	-6.9400144				
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C	-1.5725259	-0.1627059	-4.5879396				
H	-2.6508859	-0.4921314	-7.0696445				
H	-1.4573259	-1.2017195	-9.1519333				
H	1.0049948	-1.6790865	-9.0892983				
O	-0.8544838	0.2900273	-3.5957439				
Zn	-1.8300303	1.0286230	-2.0627652				
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TS2-8-1

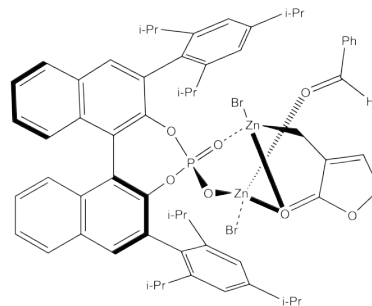


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C	3.6446682	3.8621776	2.3214614
C	1.3726190	4.7770851	2.5749564
C	1.9481710	6.0775410	2.6968862
C	-0.0395924	4.5987034	2.5381732
H	-0.6883678	5.4816082	2.6456508
C	-0.6192414	3.3560299	2.3077180
C	3.0915052	-1.1033851	1.3467133
C	4.1382580	-1.2335197	2.2517964
H	4.7903128	-2.1182885	2.1915406
C	4.3448841	-0.2984459	3.3044217
C	5.3595379	-0.5078033	4.2860525
C	3.4761947	0.8480442	3.4181603
C	3.6193448	1.6880734	4.5634444
C	2.4836486	1.0785716	2.3932757
C	2.3016909	0.0841450	1.4246518
O	-0.3381331	0.9653330	2.2107880
O	1.3325735	0.2625648	0.4347627
P	-0.2527996	0.1011963	0.8337958
O	-1.0176823	0.7478802	-0.3225938
O	-0.6212779	-1.3391414	1.2230800
C	3.3205573	6.2601691	2.6268072
C	4.1712814	5.1428405	2.4172716
H	1.2744106	6.9391483	2.8262792
H	3.7504252	7.2696544	2.7133017
H	4.3150804	3.0080617	2.1543223
H	5.2578592	5.2923149	2.3256131
C	4.6020941	1.4446811	5.5126303
C	5.4942600	0.3497672	5.3664456
H	2.9311191	2.5335413	4.6977021
H	4.6849820	2.1040535	6.3900002
H	6.2757865	0.1728102	6.1208967
H	6.0220089	-1.3808928	4.1773026
C	-2.6006429	3.7027443	0.7866675

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C	-3.9124969	3.3492149	0.4237953	H	3.6311683	-0.0015253	-0.7360962
C	-2.8803898	2.3499394	2.8349107	H	2.2413008	-2.7451076	2.9118862
C	-4.1818600	2.0274128	2.4154229	H	2.8009152	-2.9231852	-2.9693692
C	-4.7084785	2.4892111	1.1988510	C	1.1520734	-1.8496297	-6.7154532
H	-4.3310481	3.7292612	-0.5179592	C	0.5028873	-1.2565680	-5.6245539
C	-2.4061746	1.8760172	4.2078720	C	-0.8314558	-0.8100842	-5.7455814
H	-4.8016514	1.3839583	3.0593065	C	-1.4964436	-0.9539546	-6.9836978
C	-2.6132446	0.3686986	4.4321526	C	-0.8418526	-1.5388914	-8.0752868
H	-3.6896034	0.1002346	4.4638934	C	0.4828485	-1.9938616	-7.9432972
H	-2.1717717	0.0579970	5.4013057	H	2.1913891	-2.1983844	-6.6099218
H	-2.1339445	-0.2264862	3.6309662	H	1.0137333	-1.1210963	-4.6613658
C	-3.0835871	2.7081133	5.3146044	C	-1.5339716	-0.2380595	-4.5760049
H	-1.3173832	2.0740962	4.2805604	H	-2.5358837	-0.6009197	-7.0850431
H	-4.1845153	2.5661022	5.3029087	H	-1.3651716	-1.6404651	-9.0384569
H	-2.8854485	3.7911077	5.1822884	H	0.9941910	-2.4571209	-8.8009415
H	-2.7134615	2.4090413	6.3173687	O	-0.8152342	0.1914750	-3.5816707
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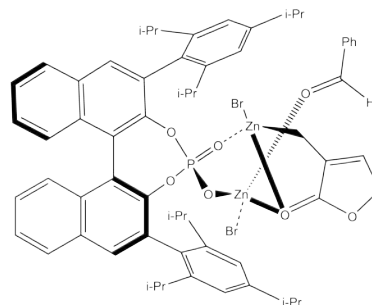


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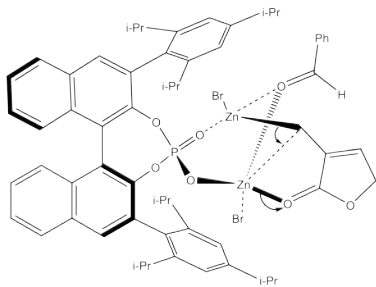
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C	1.9734321	-5.2917262	-2.6512818				

7.2.4 Pathways starting from 14d-ma

7.2.4.1 to 15r-ma and 15r-2-ma

TS1-8-r-transmetall; COSMO



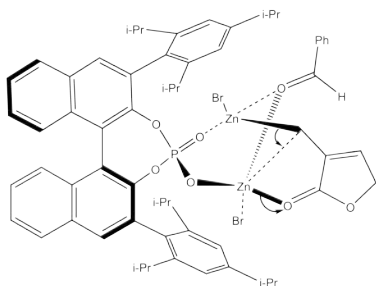
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C	4.9242007	3.7270574	1.5499223
C	2.7076629	4.7512981	1.8756963
C	3.3528706	6.0166683	2.0207143
C	1.2865530	4.6526872	1.8609238
H	0.6912785	5.5696512	1.9852780
C	0.6374593	3.4462303	1.6262804
C	3.9007737	-1.1963390	0.3088496
C	4.9785417	-1.4834042	1.1370272
H	5.5196109	-2.4339309	1.0131379
C	5.3542147	-0.6164806	2.2052604
C	6.3976641	-0.9804068	3.1091018
C	4.6199491	0.6072136	2.4332963
C	4.9118811	1.3579059	3.6114243
C	3.6070270	1.0002329	1.4805750
C	3.2923741	0.0919792	0.4654520
O	0.7824214	1.0612131	1.4173412
O	2.3266801	0.4478222	-0.4754266
P	0.7540529	0.3364596	-0.0567748
O	-0.0335929	1.1255369	-1.1090360
O	0.3050088	-1.1082425	0.2041172
C	4.7319693	6.1294567	1.9304504
C	5.5192158	4.9751284	1.6741205
H	2.7276128	6.9083140	2.1854779
H	5.2158954	7.1123442	2.0361574
H	5.5455048	2.8453428	1.3415656
H	6.6105280	5.0703953	1.5663960
C	5.9175447	0.9631440	4.4839525
C	6.6826900	-0.2044703	4.2229370
H	4.3235164	2.2592542	3.8309725
H	6.1184561	1.5585406	5.3876764
H	7.4846599	-0.5025257	4.9153885
H	6.9590468	-1.9078717	2.9149107
C	-1.3778172	3.8683966	0.1650869
C	-0.8400228	3.3543318	1.3847434
C	-2.7591821	3.7450129	-0.0651858
C	-1.6979171	2.7184582	2.3211018
C	-3.0795902	2.6457760	2.0495771
C	-3.6353962	3.1487312	0.8624738
H	-3.1756641	4.1203879	-1.0135598
C	-1.1767643	2.1147607	3.6241126
H	-3.7335429	2.1596227	2.7886178
C	-1.4745873	0.6061653	3.7175072
H	-2.5659700	0.4021859	3.7304067
H	-1.0496844	0.1805633	4.6497275
H	-1.0257633	0.0557883	2.8675429
C	-1.7221742	2.8752490	4.8470461
H	-0.0742304	2.2333226	3.6349548
H	-2.8269094	2.7915785	4.9180690
H	-1.4703235	3.9538549	4.7937378
H	-1.2943036	2.4674778	5.7861673
C	-5.1257948	3.0831343	0.5394129
C	-5.9078552	2.0559086	1.3674005
H	-6.9531051	1.9863572	1.0038624

H	-5.9537004	2.3421259	2.4391859
H	-5.4590451	1.0442182	1.3042772
C	-5.7634602	4.4817832	0.6628184
H	-5.1953718	2.7772681	-0.5294490
H	-6.8295580	4.4601008	0.3558600
H	-5.2400553	5.2258170	0.0297090
H	-5.7147667	4.8402560	1.7125919
C	-0.5121786	4.5599391	-0.8895581
C	-0.8222683	4.1141244	-2.3279264
H	-0.1081919	4.5867075	-3.0330010
H	-1.8404640	4.4128211	-2.6523749
H	-0.7305484	3.0186189	-2.4444982
C	-0.6365125	6.0922504	-0.7666689
H	0.5430462	4.2865832	-0.6862499
H	0.0322540	6.6000249	-1.4921327
H	-0.3761797	6.4528411	0.2481682
H	-1.6768814	6.4183226	-0.9773051
H	-0.4571266	-4.6185280	-2.3822958
H	4.7715843	-2.1409170	-4.2261123
H	2.5454295	-5.3377977	2.8291382
C	0.4580458	-4.5407694	-3.0128343
H	3.7017300	0.9167325	-3.9673093
H	-0.8042943	-4.4334168	-4.7927682
H	2.0356848	-2.9577411	3.4676920
C	1.4553689	-3.7209638	-2.1995544
C	5.1234279	-1.4615638	-3.4213247
C	0.0526539	-3.8914266	-4.3426432
H	0.8813118	-3.9260058	-5.0805660
C	2.2351900	-2.7018537	-2.7634842
C	2.2692403	-5.0921711	1.7836331
H	1.2188573	-6.4762474	-2.2805516
C	1.6286434	-3.9993843	-0.8292549
C	0.9754695	-5.9749590	-3.2387063
H	0.2193965	-6.5923094	-3.7672134
H	1.0257669	-4.8030311	-0.3799334
C	3.0942904	0.0631355	-3.6025016
H	5.7553115	-0.6787156	-3.8904281
H	5.7615075	-2.0555425	-2.7357718
C	3.1096942	-1.9185496	-1.9861709
C	1.8407895	-2.6917645	2.4080346
C	2.5061812	-3.2702355	-0.0093876
H	2.7946381	-5.8028292	1.1136795
H	1.1777841	-5.2705387	1.6892218
C	3.9328068	-0.8309099	-2.6725335
C	3.2245048	-2.1792232	-0.5957929
C	2.6347690	-3.6307090	1.4775506
H	2.2043801	0.4695595	-3.0834849
H	2.1132074	-1.6287155	2.2700246
H	2.7392241	-0.4883883	-4.4978442
H	-0.2345541	-2.8283628	-4.2173711
H	0.7530226	-2.7828394	2.2202780
H	1.8989816	-5.9615443	-3.8547609
H	4.3590314	-0.1808304	-1.8811647
H	3.7063826	-3.5132992	1.7396419
H	2.1477549	-2.4810399	-3.8365210
Zn	-1.6715422	0.2943732	-1.9151553
Br	-1.5836556	0.5656252	-4.2237490
C	-5.2470299	-5.9083898	-2.5990249
C	-2.7238872	-2.4960626	-2.8825860
C	-4.1875272	-5.7634931	-1.6805434
C	-4.6202721	-3.8321345	-3.6875826
C	-3.5539725	-3.6807062	-2.7649055
C	-5.4667084	-4.9430075	-3.5990367
C	-3.3408891	-4.6557363	-1.7581139
O	-1.8273577	-2.1429039	-2.0800527
H	-5.9102943	-6.7847018	-2.5326461
H	-4.7822310	-3.0633261	-4.4593386
H	-4.0264676	-6.5196788	-0.8978118
H	-6.2986368	-5.0611683	-4.3090001
H	-2.5273106	-4.5213020	-1.0301402
Br	-2.0768166	-3.5400744	1.4638469

Zn	-1.5001808	-1.8189080	-0.0070037
H	-6.2017958	-2.8986531	-1.3187488
H	-2.6742038	-0.1619893	0.9620474
C	-4.9725477	-1.6943794	0.0229728
C	-6.1639771	-1.8829165	-0.8615937
H	-4.7660746	-2.3100822	0.9092711
C	-4.2023295	-0.6940058	-0.4822681
C	-2.8935515	-0.1176293	-0.1280672
C	-4.8838365	-0.1952756	-1.7067265
O	-6.0283721	-0.9148794	-1.9140678
O	-4.5110954	0.7011613	-2.4461614
H	-7.1329051	-1.7128170	-0.3411530
H	-2.9166965	0.9904876	-0.2810169
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TS1-8-r-transmetall



Energy(Hartree)= -11970.00805767
number of imaginary frequencies: 1

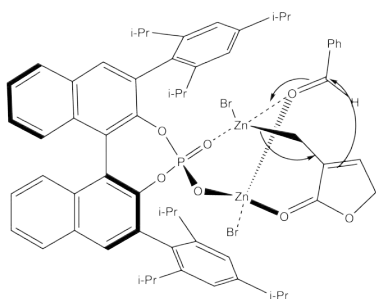
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C	2.7008647	4.7520744	1.8661803
C	3.3425016	6.0188349	2.0105742
C	1.2804087	4.6485028	1.8495975
H	0.6813259	5.5632261	1.9720542
C	0.6351371	3.4400193	1.6161302
C	3.9105958	-1.1959824	0.3130598
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C	5.3584801	-0.6104107	2.2122095
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C	4.6229965	0.6133631	2.4350466
C	4.9119385	1.3674945	3.6114097
C	3.6123434	1.0032411	1.4787923
C	3.3017830	0.0928348	0.4644122
O	0.7878608	1.0558623	1.4073682
O	2.3397864	0.4459046	-0.4801114
P	0.7659898	0.3324489	-0.0684561
O	-0.0189261	1.1232415	-1.1210126
O	0.3185048	-1.1133100	0.1896869
C	4.7209800	6.1354959	1.9235495
C	5.5117150	4.9833389	1.6711132
H	2.7143185	6.9089906	2.1722183
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H	5.5441978	2.8529730	1.3421852
H	6.6029855	5.0813487	1.5659903
C	5.9157071	0.9761498	4.4870139
C	6.6817996	-0.1913268	4.2314065
H	4.3224031	2.2691156	3.8262077
H	6.1142791	1.5745532	5.3892049
H	7.4824011	-0.4869850	4.9263870
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C	-1.3862560	3.8544985	0.1602643
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C	-1.1671262	2.1053208	3.6203286
H	-3.7269223	2.1424481	2.7946729
C	-1.4590431	0.5958847	3.7171086
H	-2.5495131	0.3874582	3.7347602
H	-1.0291098	0.1725656	4.6479437
H	-1.0116254	0.0454847	2.8666053
C	-1.7096035	2.8663390	4.8441234
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H	-2.8137411	2.7801022	4.9201100
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C	-5.1301561	3.0593646	0.5491796
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H	-6.9531475	1.9581829	1.0215244
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H	-1.8602039	4.3970901	-2.6574827
H	-0.7434100	3.0083766	-2.4548940
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H	-0.8008335	-4.4265536	-4.7832405
H	2.0327798	-2.9433784	3.4738564
C	1.4621025	-3.7190422	-2.1909070
C	5.1406502	-1.4799524	-3.4135646
C	0.0585648	-3.8875411	-4.3338361
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C	2.2464151	-2.7048995	-2.7568721
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H	1.2124866	-6.4729042	-2.2656656
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C	0.9707963	-5.9729905	-3.2248092
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H	1.0260620	-4.7946106	-0.3690935
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H	5.7772715	-0.7020151	-3.8843265
H	5.7744090	-2.0753580	-2.7254884
C	3.1231745	-1.9234149	-1.9808208
C	1.8417468	-2.6799091	2.4130414
C	2.5122615	-3.2675042	-0.0011604
H	2.7891236	-5.7974180	1.1301713
H	1.1724835	-5.2574801	1.7003435
C	3.9518449	-0.8411779	-2.6689438
C	3.2350434	-2.1808905	-0.5897635
C	2.6355449	-3.6237223	1.4872102
H	2.2308367	0.4678081	-3.0870768
H	2.1178685	-1.6180570	2.2739019
H	2.7628770	-0.4967508	-4.4974109
H	-0.2224368	-2.8224071	-4.2126870
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H	2.1603447	-2.4856134	-3.8302751
Zn	-1.6557044	0.2958687	-1.9324000
Br	-1.5705943	0.5497112	-4.2392285
C	-5.3003806	-5.8552422	-2.6160674
C	-2.7256868	-2.4777610	-2.8967224
C	-4.2374452	-5.7272145	-1.6999415
C	-4.6464034	-3.7845644	-3.6989165
C	-3.5757682	-3.6512745	-2.7796491
C	-5.5083920	-4.8837244	-3.6121865
C	-3.3747429	-4.6313912	-1.7762269
O	-1.8240562	-2.1429545	-2.0949746
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H	-4.8005067	-3.0089951	-4.4655221
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H	-6.3436708	-4.9876285	-4.3205741
H	-2.5590379	-4.5089987	-1.0479231
Br	-2.0646611	-3.5607686	1.4308103
Zn	-1.4857344	-1.8256102	-0.0198079
H	-6.1864723	-2.9023041	-1.3080308
H	-2.6494534	-0.1627003	0.9577354
C	-4.9508140	-1.6982697	0.0291127
C	-6.1464553	-1.8858620	-0.8517145
H	-4.7361449	-2.3156881	0.9124819
C	-4.1837871	-0.6972950	-0.4791914
C	-2.8744422	-0.1222949	-0.1312137
C	-4.8706049	-0.1974311	-1.7024305
O	-6.0173223	-0.9201009	-1.9040905
O	-4.5009813	0.6977867	-2.4411874
H	-7.1133315	-1.7152127	-0.3262340
H	-2.8941373	0.9843739	-0.2937222
H	-2.8931697	-1.8024801	-3.7735613

O	-0.4093700	0.6562435	-0.8964763
O	0.0597639	-1.3355684	0.7428329
C	4.5744569	6.0175100	1.7018275
C	5.3270335	4.8297821	1.5017264
H	2.5906973	6.8598720	1.9173393
H	5.0849527	6.9914564	1.7493287
H	5.3007762	2.6897357	1.2861158
H	6.4188793	4.8889085	1.3751890
C	5.7520597	1.0641992	4.4627125
C	6.6302769	-0.0052606	4.1416084
H	4.0053600	2.1973327	3.8938563
H	5.9194878	1.6538520	5.3769355
H	7.4833976	-0.2313693	4.7992993
H	7.0536516	-1.6255762	2.7682844
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C	-1.0463993	3.4120399	1.2091531
C	-2.8264931	3.6989028	-0.4239721
C	-2.0141514	3.1410465	2.2046777
C	-3.3808869	3.1951379	1.8634182
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H	-3.1475694	3.8896889	-1.4593697
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H	-4.1233529	2.9840134	2.6466577
C	-1.9735820	1.3011378	3.9393022
H	-3.0711111	1.1403911	3.8929719
H	-1.6322199	1.0193841	4.9570079
H	-1.4960743	0.6189363	3.2094253
C	-2.1951112	3.7321492	4.6707214
H	-0.5035705	2.8488735	3.6900734
H	-3.3044609	3.6930404	4.6871553
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H	-1.8390095	3.4729508	5.6892370
C	-5.2823038	3.4858807	0.1459096
C	-6.2469913	2.9710610	1.2197702
H	-7.2821631	2.9439761	0.8230303
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H	-6.7454706	4.8910276	-0.6990464
H	-5.0499482	5.2687973	-1.1380506
H	-5.6407389	5.6185617	0.5153697
C	-0.4413096	4.0732269	-1.2170148
C	-0.7356428	3.4655275	-2.5969830
H	0.0786860	3.7260479	-3.3037264
H	-1.6818898	3.8461271	-3.0329449
H	-0.8019187	2.3632480	-2.5522692
C	-0.3336211	5.6077958	-1.3341118
H	0.5490625	3.6872864	-0.8981795
H	0.4376923	5.8921575	-2.0796950
H	-0.0660601	6.0816562	-0.3698090
H	-1.3022799	6.0405536	-1.6616331
H	0.2897966	-5.2784546	-2.6747825
H	4.6920152	-1.4516170	-4.3544559
C	3.4073948	-5.7712917	2.2911866
H	0.8701685	-4.6132971	-3.3529095
H	3.2157076	1.3482204	-3.7077194
H	-0.8745572	-4.3955734	-4.6614861
H	2.5405446	-3.5990843	3.2432534
C	1.7752825	-3.7752323	-2.4585148
C	4.9752949	-0.8320177	-3.4775999
C	-0.1335425	-3.7551532	-4.1413683
H	0.3728946	-3.1408972	-4.9145358
C	2.3514336	-2.5775857	-2.9116470
C	3.0394012	-5.4598518	1.2923716
H	2.3812068	-6.1702302	-3.7190946
C	2.0709665	-4.1965702	-1.1493528
C	1.6934478	-5.5155172	-4.2914043
H	1.0322175	-6.1614264	-4.9062970
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C	2.7429037	0.3873512	-3.4173191

TS1-8r-2; COSMO



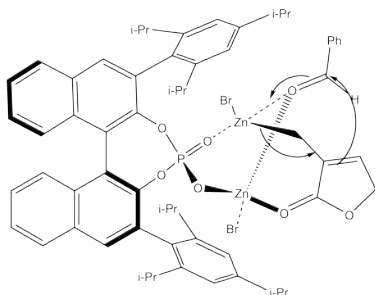
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C	4.6992033	3.5923410	1.4548939
C	2.5173792	4.6899733	1.7333964
C	3.1938225	5.9452409	1.8043833
C	1.0966066	4.6269502	1.6983489
H	0.5221968	5.5646433	1.7425408
C	0.4175531	3.4271419	1.5264412
C	3.8431021	-1.1776647	0.2829077
C	4.9923313	-1.3501543	1.0444196
H	5.6679156	-2.1907418	0.8254320
C	5.2873728	-0.5061206	2.1547235
C	6.3968779	-0.7756881	3.0118114
C	4.4275981	0.6151185	2.4499914
C	4.6800125	1.3692071	3.6345521
C	3.3416738	0.9213194	1.5476365
C	3.0479681	-0.0167553	0.5535306
O	0.4794432	1.0185653	1.5799871
O	1.9676733	0.2054369	-0.2976073
P	0.4354657	0.0620207	0.2479148

H	5.4693268	0.0870179	-3.8563739
H	5.7188258	-1.4058800	-2.8878762
C	3.1143376	-1.7563954	-2.0643750
C	2.2364844	-3.2592188	2.2314883
C	2.8400109	-3.4236712	-0.2598194
H	3.6538424	-5.9739333	0.5254291
H	1.9954710	-5.8234615	1.2012707
C	3.7379984	-0.4804253	-2.6278272
C	3.3158913	-2.1566723	-0.7147367
C	3.1204100	-3.9308725	1.1615682
H	1.8429829	0.6143741	-2.8132828
H	2.3096083	-2.1556652	2.2064793
H	2.4150348	-0.1095121	-4.3543098
H	-0.6890295	-3.0651241	-3.4741836
H	1.1730117	-3.5273255	2.0805213
H	2.3095804	-4.9029743	-4.9830246
H	4.0996509	0.1268084	-1.7725744
H	4.1690674	-3.6530516	-1.3925587
H	2.1809410	-2.2541095	-3.9496841
Zn	-2.2763275	0.3449280	-1.2213316
Br	-3.7198709	0.9698658	-2.9228196
C	-4.3323314	-6.1167232	-3.3730682
C	-3.6080427	-2.3100875	-1.5190538
C	-3.0846968	-5.8636377	-2.7796394
C	-5.0835075	-3.8947557	-2.7355603
C	-3.8320935	-3.6359589	-2.1210947
C	-5.3316842	-5.1246894	-3.3528072
C	-2.8341884	-4.6324121	-2.1600745
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H	-4.5268346	-7.0844100	-3.8603577
H	-5.8612622	-3.1144988	-2.7390249
H	-2.2943285	-6.6295263	-2.7990037
H	-6.3052292	-5.3115776	-3.8308464
H	-1.8547861	-4.4435612	-1.7043279
Br	-0.9269553	-4.9850740	0.7710399
Zn	-1.3466780	-2.6872244	0.4267569
H	-6.3340357	-1.4302878	-1.0633356
H	-2.9651393	-3.3389358	2.3374802
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C	-5.9535127	-1.4316358	-0.0217625
H	-5.1685747	-3.5447505	0.3386279
C	-3.9682524	-1.8507063	1.1437926
C	-2.9182987	-2.3152480	1.9360009
C	-4.0584788	-0.4256823	0.7272419
O	-5.2498153	-0.1717510	0.1645454
O	-3.1415935	0.4061646	0.7237816
H	-6.8265147	-1.4532593	0.6665390
H	-2.3596073	-1.5665649	2.5240602
H	-4.2784271	-1.5147555	-1.9069810

C	3.1886844	5.9586759	1.7839799
C	1.0962376	4.6318666	1.6923619
H	0.5169328	5.5665663	1.7358670
C	0.4207786	3.4292617	1.5272128
C	3.8507417	-1.1712670	0.2849230
C	5.0043996	-1.3367824	1.0410170
H	5.6780795	-2.1790846	0.8226412
C	5.3059919	-0.4855694	2.1435994
C	6.4210038	-0.7471471	2.9952362
C	4.4460079	0.6356017	2.4375726
C	4.7042341	1.3964405	3.6162216
C	3.3548205	0.9352828	1.5395920
C	3.0578596	-0.0078983	0.5513431
O	0.4924869	1.0216034	1.5840703
O	1.9755998	0.2104700	-0.2978669
P	0.4442695	0.0702161	0.2492776
O	-0.3988570	0.6742284	-0.8915912
O	0.0623368	-1.3278296	0.7374142
C	4.5679680	6.0362488	1.6749553
C	5.3238674	4.8513718	1.4746763
H	2.5823970	6.8712016	1.8969493
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H	5.3043086	2.7104759	1.2646393
H	6.4148589	4.9141754	1.3431753
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H	4.0291446	2.2245101	3.8739800
H	5.9540367	1.6945759	5.3481985
H	7.5182522	-0.1904655	4.7716531
H	7.0777017	-1.5973863	2.7527505
C	-1.4603995	3.7028550	-0.1165160
C	-1.0445888	3.4078939	1.2175613
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C	-2.0050593	3.1226532	2.2160607
C	-3.3737513	3.1724347	1.8833119
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H	-3.1640958	3.8915720	-1.4350703
C	-1.5899495	2.7397894	3.6338711
H	-4.1105772	2.9536787	2.6697885
C	-1.9534234	1.2748007	3.9430619
H	-3.0515724	1.1153062	3.9074034
H	-1.6028063	0.9877151	4.9560333
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C	-2.1667212	3.7038355	4.6848510
H	-0.4840240	2.8213500	3.6889149
H	-3.2760826	3.6706193	4.7059934
H	-1.8676967	4.7510209	4.4764504
H	-1.8077692	3.4387875	5.7008211
C	-5.2866633	3.4684019	0.1792833
C	-6.2428823	2.9380087	1.2530340
H	-7.2801287	2.9087114	0.8620465
H	-6.2504864	3.5889011	2.1528195
H	-5.9763160	1.9114244	1.5716641
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H	-5.3640589	2.7923060	-0.7032841
H	-6.7604398	4.8780743	-0.6403105
H	-5.0691881	5.2669494	-1.0844514
H	-5.6505979	5.5953838	0.5755883
C	-0.4595963	4.0962848	-1.2069779
C	-0.7464613	3.4846865	-2.5867840
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H	-0.7799879	2.3808098	-2.5463357
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H	0.5390745	3.7293492	-0.8920953
H	0.3826749	5.9340833	-2.0670937
H	-0.1234221	6.1101997	-0.3567488
H	-1.3592197	6.0477262	-1.6467932
H	0.2795337	-5.3045098	-2.5957853
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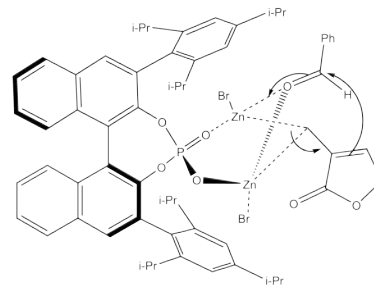
TS1-8r-2



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C	2.5165344	4.7012865	1.7197722

C	0.8571702	-4.6526299	-3.2890430
H	3.1946780	1.3109702	-3.7323823
H	-0.8935861	-4.4569411	-4.5936902
H	2.5418203	-3.5621690	3.2751953
C	1.7681275	-3.8009275	-2.4134867
C	4.9561161	-0.8659991	-3.4827216
C	-0.1511558	-3.8084274	-4.0858436
H	0.3495866	-3.2040690	-4.8704077
C	2.3331350	-2.6041892	-2.8820346
C	3.0576791	-5.4415579	1.3478760
H	2.3671009	-6.2148830	-3.6348323
C	2.0798203	-4.2100005	-1.1045824
C	1.6753884	-5.5718102	-4.2151598
H	1.0119534	-6.2293952	-4.8151531
H	1.6635993	-5.1608859	-0.7446811
C	2.7237599	0.3537383	-3.4276299
H	5.4488347	0.0478312	-3.8754352
H	5.7016972	-1.4330143	-2.8893486
C	3.1031135	-1.7740107	-2.0504241
C	2.2416146	-3.2340962	2.2585720
C	2.8499965	-3.4245910	-0.2277821
H	3.6740093	-5.9620730	0.5869502
H	2.0152835	-5.8104755	1.2623390
C	3.7223512	-0.5042329	-2.6322932
C	3.3176623	-2.1606588	-0.6989299
C	3.1321919	-3.9139546	1.1993745
H	1.8262024	0.5886994	-2.8233379
H	2.3113280	-2.1305896	2.2237500
H	2.3911682	-0.1535925	-4.3572411
H	-0.7053293	-3.1100912	-3.4264633
H	1.1798233	-3.5083187	2.1068788
H	2.2882465	-4.9723653	-4.9208119
H	4.0875610	0.1135650	-1.7861369
H	4.1787889	-3.6279972	1.4299154
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Br	-3.7290638	0.9958821	-2.9059975
C	-4.3803414	-6.0523984	-3.4755467
C	-3.5760131	-2.2905244	-1.5655078
C	-3.1702355	-5.8763166	-2.7846626
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O	-2.3843008	-1.8823934	-1.1835113
H	-4.5974175	-7.0080760	-3.9768289
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H	-1.9411563	-4.5382857	-1.6097130
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Zn	-1.3199610	-2.6940638	0.3978630
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H	-2.9580921	-3.3716437	2.2862618
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H	-5.1531025	-3.5537222	0.2670588
C	-3.9628849	-1.8694469	1.1088331
C	-2.9188560	-2.3410580	1.9029156
C	-4.0495867	-0.4393427	0.7096295
O	-5.2400837	-0.1783414	0.1421692
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H	-6.8221749	-1.4649393	0.6013987
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H	-4.2337825	-1.4810754	-1.9468938



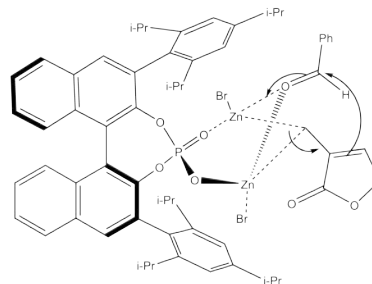
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C	4.8341036	3.8910194	1.1139729
C	2.6163654	4.8946209	1.5027781
C	3.2450944	6.1754249	1.5567564
C	1.2014387	4.7656949	1.6041420
H	0.5964409	5.6709264	1.7660190
C	0.5622661	3.5395384	1.4532692
C	3.8369820	-1.1639946	0.3605196
C	4.9002140	-1.3779118	1.2288299
H	5.4217387	-2.3473850	1.2174832
C	5.2855615	-0.4045184	2.1962386
C	6.3197105	-0.6833708	3.1400598
C	4.5643692	0.8444399	2.2862907
C	4.8559724	1.7095619	3.3835905
C	3.5640660	1.1451426	1.2863074
C	3.2548279	0.1441890	0.3622236
O	0.7359488	1.1652497	1.1819342
O	2.3224762	0.4228853	-0.6393853
P	0.7372229	0.3919387	-0.2634018
O	0.0115610	1.1364544	-1.3892717
O	0.2512222	-1.0275813	0.0704994
C	4.6157126	6.3051704	1.3903483
C	5.4117233	5.1527457	1.1514852
H	2.6138946	7.0637349	1.7165865
H	5.0862854	7.2995043	1.4261336
H	5.4593056	3.0082935	0.9196676
H	6.4949773	5.2608017	0.9887390
C	5.8518564	1.3975626	4.2997325
C	6.6071641	0.2023039	4.1678284
H	4.2766828	2.6342651	3.5075389
H	6.0524556	2.0819357	5.1381514
H	7.4019327	-0.0290269	4.8932887
H	6.8709793	-1.6324068	3.0481398
C	-1.6741196	3.9869971	0.3601103
C	-0.9285490	3.4036761	1.4270091
C	-3.0741748	3.8417061	0.3551786
C	-1.6062557	2.6783715	2.4484389
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C	-3.7676159	3.1522778	1.3650025
H	-3.6540331	4.2686128	-0.4782541
C	-0.8756079	2.0263004	3.6219781
H	-3.5245432	2.0273262	3.2010394
C	-1.1503283	0.5125771	3.6998444
H	-2.2155642	0.3004233	3.9287174
H	-0.5397490	0.0454246	4.4999741
H	-0.8953553	0.0109114	2.7462116
C	-1.2175064	2.7318036	4.9478675
H	0.2137960	2.1553829	3.4646879
H	-2.2969192	2.6385355	5.1898906
H	-0.9761878	3.8131881	4.9009057
H	-0.6449975	2.2870315	5.7881365
C	-5.2894060	3.0821908	1.3287593
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H	-6.9563717	1.7169206	1.6881737

TS2-8-r-transmetall; COSMO

H	-5.6952310	1.6398583	2.9484960	Zn	-1.3240719	-2.0425464	-0.2839336
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C	-5.8941892	4.2852641	2.0792506	H	-2.7481296	-0.6395358	0.5564248
H	-5.5779763	3.1645350	0.2591966	C	-4.8841541	-1.6353446	-1.0830992
H	-7.0019455	4.2817874	2.0086181	C	-6.1504925	-1.4652311	-1.8603730
H	-5.5259237	5.2451992	1.6643298	H	-4.5559469	-2.5932710	-0.6549467
H	-5.6196541	4.2564646	3.1550590	C	-4.2816854	-0.4195044	-0.9332861
C	-1.0226764	4.7749378	-0.7774853	C	-3.0199571	-0.0075694	-0.3197477
C	-1.3894056	4.2199220	-2.1633578	C	-5.1400036	0.5828982	-1.6480242
H	-0.9173304	4.8273973	-2.9627408	O	-6.2212921	-0.0711092	-2.1850304
H	-2.4831332	4.2190560	-2.3466842	O	-4.9781587	1.7818055	-1.7528961
H	-1.0278944	3.1815349	-2.2826205	H	-7.0573735	-1.7470318	-1.2790027
C	-1.3655308	6.2732559	-0.6671281	H	-3.0687346	1.0289826	0.0809810
H	0.0764410	4.6766253	-0.6751037	H	-3.0157377	-1.5154129	-3.7977864
H	-0.8423183	6.8546111	-1.4542844				
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H	-2.4556099	6.4440818	-0.7895527				
H	-0.1771681	-5.2952739	-2.0079653				
H	4.8401810	-2.6442389	-4.0140668				
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C	0.7058567	-5.0838515	-2.6514743				
H	3.7756663	0.3927791	-4.1562694				
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H	1.7243967	-2.5002482	3.6246662				
C	1.5481377	-4.0591150	-1.8999860				
C	5.1702679	-1.8801533	-3.2790733				
C	0.1911659	-4.5922866	-4.0105050				
H	1.0129524	-4.5058006	-4.7512793				
C	2.3146188	-3.0860795	-2.5577669				
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H	1.8049906	-6.8009449	-1.8167671				
C	1.6328117	-4.1269819	-0.4948530				
C	1.4791829	-6.4093888	-2.8012640				
H	0.8514581	-7.1829893	-3.2908743				
H	1.0405283	-4.8954610	0.0244993				
C	3.1475797	-0.3900787	-3.6838681				
H	5.8169251	-1.1533018	-3.8132132				
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C	3.1198634	-2.1720811	-1.8516579				
C	1.5993640	-2.3874148	2.5278719				
C	2.4396589	-3.2580494	0.2612265				
H	2.7618352	-5.5974304	1.7418466				
H	1.0899235	-5.0749004	2.1396077				
C	3.9621387	-1.1695680	-2.6374327				
C	3.1699197	-2.2424874	-0.4347514				
C	2.4885504	-3.4070986	1.7884574				
H	2.2702503	0.1066801	-3.2251918				
H	1.8451342	-1.3418997	2.2640052				
H	2.7823267	-1.0501744	-4.4980156				
H	-0.2905257	-3.5981941	-3.9283181				
H	0.5303977	-2.5496140	2.2842678				
H	2.3873474	-6.2608385	-3.4222776				
H	4.3687306	-0.4317484	-1.9162312				
H	3.5337800	-3.1999871	2.0952507				
H	2.2895740	-3.0272291	-3.6556836				
Zn	-1.8241107	0.5285796	-1.9297645				
Br	-2.3372425	1.0357265	-4.1521918				
C	-4.4958202	-6.1105451	-3.4824458				
C	-2.6913779	-2.2791048	-3.0505645				
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C	-4.2521087	-3.7967811	-4.1721937				
C	-3.2916947	-3.5954892	-3.1463872				
C	-4.8498076	-5.0506707	-4.3373973				
C	-2.9399046	-4.6710666	-2.2933188				
O	-1.7673557	-1.9197488	-2.2646868				
H	-4.9655474	-7.0976402	-3.6123464				
H	-4.5128360	-2.9604827	-4.8399576				
H	-3.2715457	-6.7509716	-1.7955740				
H	-5.5914801	-5.2073168	-5.1345221				
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TS2-8-r-transmetall

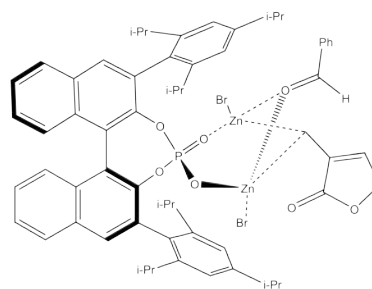


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C	2.6145077	4.8933763	1.5032738
C	3.2426325	6.1739975	1.5564099
C	1.1998256	4.7631327	1.6017805
H	0.5926501	5.6676707	1.7591573
C	0.5614321	3.5366024	1.4529084
C	3.8368393	-1.1630132	0.3600798
C	4.9029357	-1.3760705	1.2246883
H	5.4244058	-2.3455985	1.2096238
C	5.2907133	-0.4040031	2.1919706
C	6.3278027	-0.6814908	3.1322243
C	4.5683039	0.8437923	2.2850971
C	4.8626517	1.7084478	3.3817624
C	3.5649943	1.1446431	1.2883664
C	3.2533116	0.1448049	0.3636407
O	0.7377522	1.1612657	1.1913748
O	2.3193908	0.4236850	-0.6347285
P	0.7345753	0.3888899	-0.2553775
O	0.0013977	1.1321529	-1.3751138
O	0.2596301	-1.0348943	0.0788379
C	4.6128941	6.3047982	1.3923359
C	5.4095872	5.1530921	1.1557903
H	2.6102488	7.0619278	1.7135452
H	5.0824704	7.2995609	1.4277280
H	5.4581570	3.0084247	0.9257367
H	6.4929684	5.2614500	0.9944297
C	5.8617778	1.3973178	4.2939755
C	6.6177000	0.2034714	4.1591906
H	4.2824008	2.6323189	3.5066675
H	6.0644074	2.0817218	5.1318051
H	7.4151375	-0.0275122	4.8817400
H	6.8800002	-1.6297832	3.0380177
C	-1.6732360	3.9765033	0.3530624
C	-0.9291016	3.4002373	1.4247195

C	-3.0729438	3.8294909	0.3470403	H	4.3595336	-0.4309349	-1.9167718
C	-1.6071819	2.6812023	2.4498051	H	3.5392358	-3.2008551	2.0977830
C	-3.0099828	2.5828965	2.4015214	H	2.2773640	-3.0274749	-3.6491391
C	-3.7674142	3.1490968	1.3621902	Zn	-1.8339155	0.5395652	-1.9253374
H	-3.6522644	4.2480172	-0.4909575	Br	-2.3877183	1.0321960	-4.1332426
C	-0.8768758	2.0364147	3.6275752	C	-4.4975758	-6.0889154	-3.5340438
H	-3.5260227	2.0373014	3.2060471	C	-2.6981505	-2.2576534	-3.0365446
C	-1.1501486	0.5230728	3.7143318	C	-3.5492843	-5.9101163	-2.5077844
H	-2.2152041	0.3106204	3.9435983	C	-4.2545667	-3.7636402	-4.1845094
H	-0.5402662	0.0603008	4.5174249	C	-3.2987667	-3.5755828	-3.1525578
H	-0.8940051	0.0156463	2.7641524	C	-4.8492389	-5.0159291	-4.3727520
C	-1.2191348	2.7500271	4.9488333	C	-2.9485872	-4.6641930	-2.3168452
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H	-2.2984716	2.6588496	5.1915169	H	-4.9650824	-7.0746056	-3.6816665
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H	-0.6473089	2.3111617	5.7926193	H	-3.2787900	-6.7506623	-1.8513082
C	-5.2893014	3.0829573	1.3271408	H	-5.5868611	-5.1608185	-5.1760809
C	-5.8648416	1.7686294	1.8736528	H	-2.2221363	-4.5174463	-1.5057247
H	-6.9600705	1.7273978	1.7043366	Br	-2.1412074	-3.7153972	1.1028933
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H	-5.4100466	0.8864212	1.3797457	H	-6.1382317	-2.0841667	-2.8159801
C	-5.8894527	4.2982497	2.0611537	H	-2.7310019	-0.6519551	0.5608683
H	-5.5782001	3.1498604	0.2567827	C	-4.8508908	-1.6639780	-1.0948787
H	-6.9972072	4.2984838	1.9910999	C	-6.1234831	-1.5001965	-1.8656495
H	-5.5176709	5.2508702	1.6331991	H	-4.5095940	-2.6189424	-0.6703985
H	-5.6143588	4.2846190	3.1370251	C	-4.2711483	-0.4383774	-0.9249683
C	-1.0206828	4.7624116	-0.7854022	C	-3.0210648	-0.0153730	-0.3055451
C	-1.3860118	4.2092279	-2.1721880	C	-5.1504066	0.5623270	-1.6235902
H	-0.9114803	4.8163725	-2.9701665	O	-6.2190925	-0.1069557	-2.1720520
H	-2.4789074	4.2097589	-2.3597348	O	-5.0124955	1.7636124	-1.7015934
H	-1.0241333	3.1714672	-2.2940149	H	-7.0231842	-1.8052527	-1.2830865
C	-1.3637341	6.2606907	-0.6741955	H	-3.0750784	1.0215741	0.0928805
H	0.0783501	4.6637209	-0.6819148	H	-3.0249226	-1.4799875	-3.7692429
H	-0.8407495	6.8431549	-1.4606197				
H	-1.0739813	6.6772567	0.3123031				
H	-2.4536279	6.4315965	-0.7968714				
H	-0.1796377	-5.3005510	-1.9923116				
H	4.8298507	-2.6454142	-4.0128896				
H	2.3840875	-4.9129433	3.3638920				
C	0.7010606	-5.0875354	-2.6388872				
H	3.7619450	0.3922922	-4.1558591				
H	-0.5619662	-5.3104806	-4.4101432				
H	1.7374788	-2.4962150	3.6327161				
C	1.5430056	-4.0600224	-1.8907704				
C	5.1599665	-1.8800114	-3.2794226				
C	0.1801262	-4.5981572	-3.9962722				
H	0.9989136	-4.5100161	-4.7401476				
C	2.3062942	-3.0868161	-2.5513977				
C	2.1649385	-4.8263830	2.2804405				
H	1.8090795	-6.8000024	-1.8072234				
C	1.6314873	-4.1269744	-0.4861341				
C	1.4776625	-6.4107375	-2.7905597				
H	0.8519162	-7.1874274	-3.2778850				
H	1.0408308	-4.8948756	0.0357503				
C	3.1354266	-0.3906286	-3.6817464				
H	5.8057823	-1.1540712	-3.8157000				
H	5.7783980	-2.3935505	-2.5155862				
C	3.1130980	-2.1721737	-1.8484703				
C	1.6083155	-2.3836458	2.5365154				
C	2.4401705	-3.2575722	0.2669872				
H	2.7586369	-5.5970279	1.7480775				
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H	2.2592551	0.1071782	-3.2224865				
H	1.8555040	-1.3387599	2.2720859				
H	2.7690007	-1.0501484	-4.4958367				
H	-0.3032295	-3.6051280	-3.9126402				
H	0.5379895	-2.5444498	2.2985090				
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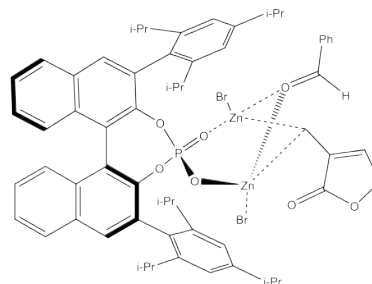


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C	4.8313442	3.6988090	1.1958439
C	2.6344094	4.7565724	1.5606770
C	3.2971234	6.0179390	1.6524882
C	1.2155475	4.6631227	1.6462090
H	0.6329208	5.5785300	1.8323955
C	0.5459314	3.4579684	1.4599996
C	3.7765042	-1.3073807	0.3493828
C	4.7988313	-1.5472014	1.2588245
H	5.3190953	-2.5172825	1.2442998
C	5.1479213	-0.5973798	2.2623908
C	6.1370612	-0.9040458	3.2450473
C	4.4411274	0.6604585	2.3390885
C	4.7010332	1.5082134	3.4578678
C	3.4846535	0.9880759	1.3044191
C	3.1937826	-0.0000750	0.3610218
O	0.6604804	1.0948091	1.0989511
O	2.2941059	0.2952929	-0.6667852
P	0.7002200	0.3197622	-0.3472322

O	0.0524142	1.1123667	-1.4982526	H	6.0506565	-1.1102215	-3.6671517
O	0.1083522	-1.0681046	-0.0567252	H	5.9393896	-2.4151002	-2.4374277
C	4.6738997	6.1124085	1.5154042	C	3.2316052	-2.2291747	-1.9439290
C	5.4426769	4.9428938	1.2703264	C	1.3970518	-2.6475266	2.3005185
H	2.6879056	6.9201782	1.8194483	C	2.4084911	-3.4077950	0.0660621
H	5.1709240	7.0922644	1.5805683	H	2.6703357	-5.8029953	1.4678835
H	5.4357009	2.8023931	0.9978765	H	0.9658138	-5.3249636	1.7683312
H	6.5317724	5.0236271	1.1326654	C	4.1207835	-1.1882730	-2.6210891
C	5.6524584	1.1693171	4.4109160	C	3.1709184	-2.3553912	-0.5304733
C	6.3940820	-0.0361384	4.2956901	C	2.3538839	-3.6211850	1.5853094
H	4.1314798	2.4404541	3.5698214	H	2.4719424	0.1201819	-3.2487546
H	5.8280468	1.8402750	5.2656390	H	1.6502461	-1.5886745	2.1047153
H	7.1539170	-0.2889050	5.0508317	H	3.0574848	-0.9783101	-4.5426238
H	6.6781948	-1.8597885	3.1630231	H	-0.3128829	-3.4925389	-3.9759818
C	-1.7030295	4.0238363	0.4469584	H	0.3519696	-2.8036860	1.9663973
C	-0.9483859	3.3625185	1.4598190	H	2.6019469	-5.9470975	-4.1090483
C	-3.1083995	3.9444688	0.4869760	H	4.4753161	-0.4861927	-1.8391138
C	-1.6257129	2.6172714	2.4692323	H	3.3719073	-3.4124389	1.9731084
C	-3.0329231	2.5793211	2.4629007	H	2.5481719	-3.0171570	-3.8382160
C	-3.7985154	3.2364796	1.4850344	Zn	-1.7486960	0.5471403	-2.1186370
H	-3.6948398	4.4319959	-0.3073030	Br	-2.5091828	1.1203867	-4.2393012
C	-0.8931054	1.8733209	3.5861771	C	-4.0774003	-6.2172498	-2.8182509
H	-3.5457316	2.0109837	3.2540827	C	-2.6925846	-2.2044530	-3.0297165
C	-1.2091920	0.3656934	3.5691888	C	-3.0783973	-5.7878485	-1.9227635
H	-2.2785108	0.1645209	3.7881306	C	-4.1533852	-4.0155059	-3.8344402
H	-0.6076487	-0.1707859	4.3315665	C	-3.1528913	-3.5742481	-2.9308008
H	-0.9690851	-0.0829815	2.5857481	C	-4.6154495	-5.3335388	-3.7734754
C	-1.1931412	2.4976939	4.9618763	C	-2.6133571	-4.4720628	-1.9743458
H	0.1966978	1.9830853	3.4188353	O	-1.8508932	-1.6796119	-2.2521541
H	-2.2689797	2.4122818	5.2215281	H	-4.4387822	-7.2562095	-2.7732499
H	-0.9272971	3.5741460	4.9803944	H	-4.5589792	-3.3123444	-4.5792200
H	-0.6142895	1.9860862	5.7585437	H	-2.6632361	-6.4869443	-1.1817659
C	-5.3218832	3.2232796	1.4925464	H	-5.3927210	-5.6800434	-4.4704806
C	-5.9249461	1.8774825	1.9221349	H	-1.8311711	-4.1254802	-1.2848532
H	-7.0270742	1.8912251	1.7991742	Br	-2.7160175	-3.0301931	1.2769110
H	-5.7190883	1.6510279	2.9891920	Zn	-1.8297774	-1.3622289	-0.0875059
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C	-5.8599553	4.3749390	2.3644971	H	-3.1088930	0.2273994	0.6911235
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H	-6.9686160	4.4155626	2.3296341	C	-6.3253360	-0.8927016	-1.9280432
H	-5.4683969	5.3544871	2.0234933	H	-4.7761145	-2.1046622	-0.7416464
H	-5.5556402	4.2414545	3.4242797	C	-4.3899287	0.0463228	-1.0391230
C	-1.0591298	4.8026000	-0.7009091	C	-3.0940837	0.3897165	-0.4137635
C	-1.4448708	4.2202425	-2.0719177	C	-5.2069177	1.0979660	-1.7288438
H	-1.0019675	4.8214557	-2.8923656	O	-6.3276179	0.5014878	-2.2525660
H	-2.5421934	4.1886898	-2.2288816	O	-4.9947604	2.2901524	-1.8161188
H	-1.0593098	3.1886433	-2.1799287	H	-7.2416461	-1.1295910	-1.3415930
C	-1.3943353	6.3030500	-0.6101845	H	-2.9426017	1.4958699	-0.4452644
H	0.0405776	4.7023809	-0.6089012	H	-3.0800348	-1.5737051	-3.8663053
H	-0.8739907	6.8691387	-1.4100844				
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H	0.0653790	-5.4834831	-2.4118552				
H	5.0961480	-2.5901136	-4.0079403				
H	2.1646712	-5.1960462	3.0794870				
C	0.8842153	-5.0857488	-3.0517403				
H	4.0308755	0.4435147	-4.0751498				
H	-0.4792305	-5.0975111	-4.7655433				
H	1.4393801	-2.8100538	3.3975798				
C	1.6845866	-4.1213118	-2.1848007				
C	5.3725266	-1.8636064	-3.2149855				
C	0.2352880	-4.4095373	-4.2690923				
H	0.9909750	-4.1171420	-5.0273204				
C	2.4932645	-3.1200842	-2.7438110				
C	2.0231358	-5.0672581	1.9872546				
H	2.1756603	-6.8095743	-2.5985240				
C	1.6727153	-4.2529311	-0.7841631				
C	1.7525830	-6.2851624	-3.4789048				
H	1.1609837	-7.0175584	-4.0671879				
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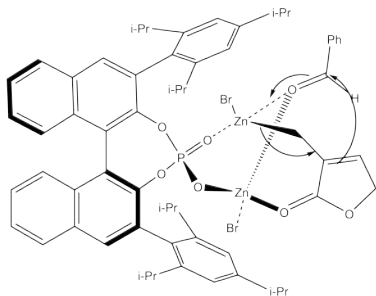
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C	2.6276307	4.7652490	1.5561153
C	3.2826837	6.0301985	1.6465750
C	1.2099370	4.6618314	1.6438447

H	0.6203414	5.5728137	1.8297502	H	-0.4934361	-5.1246363	-4.7070918
C	0.5474649	3.4527345	1.4586998	H	1.4558533	-2.7549476	3.4241606
C	3.7930035	-1.2964050	0.3534053	C	1.6814378	-4.1269766	-2.1428792
C	4.8181343	-1.5306119	1.2607396	C	5.3748106	-1.8957575	-3.2095783
H	5.3368063	-2.5016626	1.2489651	C	0.2261026	-4.4347908	-4.2204968
C	5.1705811	-0.5761207	2.2582075	H	0.9811999	-4.1565978	-4.9845412
C	6.1634695	-0.8759534	3.2384356	C	2.4923168	-3.1357403	-2.7156009
C	4.4612548	0.6802609	2.3321828	C	2.0282454	-5.0294021	2.0367641
C	4.7228779	1.5323013	3.4470334	H	2.1592495	-6.8215967	-2.5230679
C	3.5013015	1.0023364	1.2990152	C	1.6731087	-4.2431200	-0.7412966
C	3.2108964	0.0113818	0.3581805	C	1.7361391	-6.3074923	-3.4092428
O	0.6775881	1.0903806	1.0976083	H	1.1413692	-7.0452766	-3.9875901
O	2.3122979	0.3023044	-0.6704526	H	1.0490172	-5.0289259	-0.2889242
P	0.7175609	0.3216898	-0.3530864	C	3.3812026	-0.3847576	-3.6806412
O	0.0649068	1.1183989	-1.4967449	H	6.0552563	-1.1505947	-3.6716699
O	0.1339883	-1.0711071	-0.0690360	H	5.9412672	-2.4427259	-2.4287981
C	4.6580879	6.1338037	1.5076972	C	3.2372144	-2.2396764	-1.9281577
C	5.4336999	4.9696762	1.2617696	C	1.4107040	-2.6049914	2.3255507
H	2.6676324	6.9284237	1.8137059	C	2.4158404	-3.3929256	0.0971042
H	5.1486086	7.1169378	1.5719200	H	2.6693106	-5.7735465	1.5219069
H	5.4391238	2.8288911	0.9894294	H	0.9683431	-5.2832746	1.8266179
H	6.5220300	5.0572146	1.1226401	C	4.1280276	-1.2090855	-2.6186276
C	5.6786146	1.1997101	4.3973471	C	3.1812099	-2.3511730	-0.5136591
C	6.4225649	-0.0037710	4.2842904	C	2.3632893	-3.5889132	1.6187177
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H	-3.5344837	1.9826617	3.2537220	C	-2.7082244	-2.1651300	-3.0558615
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TS1-8d-2; COSMO



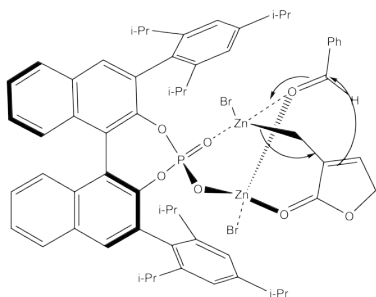
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H	0.8251662	-5.2614264	1.0272640
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TS1-8d-2



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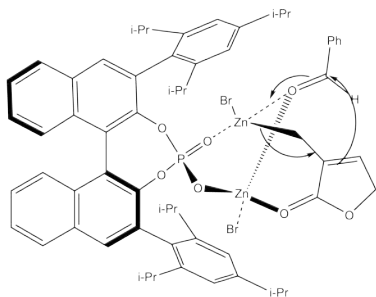
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H	-4.7234226	-4.1653141	-3.2665034
H	-1.0884517	-6.6313259	-0.8644813
H	-4.6647781	-6.6555674	-3.3308367
H	-1.1365185	-4.1473549	-0.8125642
Br	-2.6104340	-3.7684823	1.9116074
Zn	-1.8749910	-1.9402927	0.6599851
H	-5.7534892	-2.2168605	-2.9029774
H	-3.8424306	-1.0274556	1.7338041
C	-4.8506906	-1.9962524	-0.8801266
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H	-5.0357466	-2.9030460	-0.2855472
C	-4.2848146	-0.8081340	-0.3587522
C	-3.5697987	-0.5042653	0.8023963
C	-4.3068643	0.1166391	-1.5320181
O	-5.2486200	-0.2753567	-2.4120955
O	-3.5319730	1.0454511	-1.7749827
H	-6.8185264	-1.4461698	-1.6787781
H	-3.1701601	0.5200224	0.8995007
H	-3.3957438	-2.0426081	-2.9150893

C	3.0460956	1.1194985	1.8495851
C	2.7912553	0.1911100	0.8344009
O	0.2101384	1.1366263	1.8197469
O	1.7496793	0.4328518	-0.0600630
P	0.2139347	0.2431474	0.4553635
O	-0.6628404	0.8616425	-0.6451221
O	-0.1210947	-1.1877268	0.9028065
C	4.0974011	6.2745327	2.0431832
C	4.9020131	5.1153007	1.8825519
H	2.0788562	7.0435999	2.1943534
H	4.5683101	7.2679531	2.0957952
H	4.9616591	2.9713445	1.6906171
H	5.9946078	5.2157428	1.7944239
C	5.3297775	1.2189463	4.8667421
C	6.1677245	0.1007729	4.6106074
H	3.6681731	2.4202041	4.1956876
H	5.4820729	1.8195130	5.7765002
H	6.9751234	-0.1592929	5.3142943
H	6.5781319	-1.5651174	3.2894572
C	-1.8862591	3.8133497	0.2180225
C	-1.4184130	3.3977149	1.5012438
C	-3.2447201	3.6347779	-0.0905120
C	-2.3180059	2.8018077	2.4241828
C	-3.6729975	2.6578138	2.0650447
C	-4.1601692	3.0645790	0.8119613
H	-3.6076688	3.9346020	-1.0866456
C	-1.8704415	2.3350749	3.8078354
H	-4.3627468	2.2039030	2.7921005
C	-2.1843446	0.8469780	4.0484053
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H	-1.7188656	0.2092000	3.2710849
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H	-3.5820327	3.1562888	4.9235013
H	-2.2054634	4.2901149	4.7585094
H	-2.1060960	2.9164603	5.9113914
C	-5.6266204	2.9434984	0.4090441
C	-6.4088666	1.8729793	1.1807909
H	-7.4286700	1.7617005	0.7598332
H	-6.5278081	2.1442266	2.2507267
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H	-5.6287936	2.6550749	-0.6668242
H	-7.3727156	4.2585672	0.1587060
H	-5.7969093	5.0865218	-0.0786529
H	-6.3402948	4.6592584	1.5731079
C	-0.9733003	4.4560438	-0.8287192
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H	-0.3843848	4.2995003	-2.9276443
H	-2.0989496	3.8807079	-2.6477945
H	-0.8063368	2.7343823	-2.1765800
C	-1.2403217	5.9719042	-0.9142221
H	0.0745003	4.3209685	-0.4932404
H	-0.5420118	6.4563871	-1.6278036
H	-1.1210324	6.4653938	0.0715117
H	-2.2753431	6.1726619	-1.2625300
H	0.9872900	-5.3155440	-3.1297702
H	4.9157257	-0.9283392	-3.9558872
H	3.7472502	-5.1631201	2.4975848
C	1.5082668	-4.4773370	-3.6424729
H	3.2187530	1.7189226	-3.3004135
H	-0.0306031	-4.4488795	-5.2016841
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H	0.9286721	-2.9398909	-5.1135019
C	2.6111593	-2.3155755	-2.8439930
C	3.7229739	-4.8014915	1.4485881
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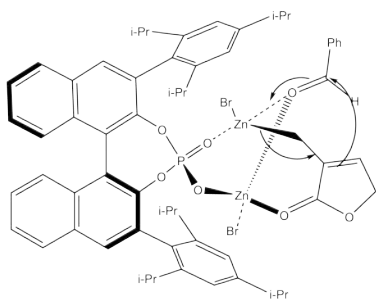


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C	4.3232865	3.8544654	1.8270652
C	2.0896415	4.8709477	2.0300626
C	2.7177727	6.1508628	2.1057531
C	0.6705407	4.7575786	1.9758061
H	0.0638900	5.6756980	1.9999114
C	0.0400277	3.5296842	1.8153210
C	3.5604558	-0.9901354	0.5992073
C	4.6361049	-1.2185567	1.4494888
H	5.2777004	-2.0975073	1.2852031
C	4.9037387	-0.3728916	2.5658243
C	5.9520876	-0.6803582	3.4849078
C	4.0836514	0.7933416	2.7991091
C	4.3145530	1.5574439	3.9821443

C	2.1200450	-4.0133756	-1.2137257
C	2.6284391	-5.0841031	-4.5080776
H	2.2107324	-5.7707476	-5.2736781
H	1.7235966	-5.0128053	-0.9719323
C	2.7757991	0.7223045	-3.0964455
H	5.5493156	0.6058710	-3.2774318
H	5.7928353	-0.9394135	-2.3940544
C	3.1399392	-1.4761167	-1.8493548
C	1.2387986	-4.3338992	1.6567323
C	2.6239134	-3.2091756	-0.1723875
H	4.7218926	-4.3858215	1.2048822
H	3.5622524	-5.6810767	0.7901718
C	3.7462995	-0.1372640	-2.2685834
C	3.1348793	-1.9192359	-0.4943287
C	2.6050643	-3.7587506	1.2537759
H	1.8186118	0.8748690	-2.5623446
H	0.4349860	-3.5847291	1.5349600
H	2.5387372	0.2580426	-4.0755384
H	-0.3110179	-3.2685280	-3.8777099
H	0.9627161	-5.2283710	1.0599715
H	3.1919849	-4.2882848	-5.0392065
H	3.9902894	0.4320090	-1.3488442
H	2.8095349	-2.9145451	1.9424291
H	2.6063458	-1.9607793	-3.8862467
Zn	-1.4399815	0.0736164	-2.2309179
Br	-0.9585752	0.0613053	-4.4825232
C	-2.3145099	-6.8982491	-2.3690787
C	-2.6765976	-2.6192335	-2.2461427
C	-1.4434938	-6.1432193	-1.5664850
C	-3.4319050	-4.8579630	-3.0746903
C	-2.5739228	-4.0907285	-2.2508445
C	-3.3068538	-6.2502584	-3.1286311
C	-1.5707767	-4.7501760	-1.5051574
O	-1.7960349	-1.9061536	-1.5704244
H	-2.2142130	-7.9934298	-2.4138586
H	-4.1946891	-4.3556860	-3.6896774
H	-0.6544120	-6.6416650	-0.9830896
H	-3.9789329	-6.8361037	-3.7737357
H	-0.8570319	-4.1644010	-0.9099341
Br	-2.5786681	-3.9115881	1.6937123
Zn	-1.8566672	-2.0266687	0.5063963
H	-5.3640591	-2.4736428	-3.4285359
H	-3.9771634	-1.2514793	1.3846230
C	-4.6772175	-2.2329448	-1.3235892
C	-5.4957345	-1.8438157	-2.5258509
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C	-4.2313842	-1.0244987	-0.7381782
C	-3.6427116	-0.7022512	0.4886591
C	-4.1924542	-0.0867262	-1.8984352
O	-5.0158995	-0.5144868	-2.8705005
O	-3.4478176	0.8880592	-2.0557566
H	-6.5838939	-1.7821282	-2.3057687
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TS1-8-n

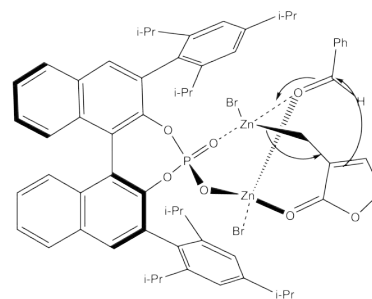


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C	2.0918663	4.8711899	2.0373474
C	2.7222205	6.1493800	2.1144472
C	0.6730680	4.7593787	1.9806125
H	0.0665055	5.6776175	2.0021202
C	0.0408746	3.5327680	1.8193942
C	3.5530310	-0.9886020	0.5976363
C	4.6305408	-1.2187685	1.4448290
H	5.2703655	-2.0982096	1.2763417
C	4.9016994	-0.3761427	2.5622668
C	5.9517617	-0.6852462	3.4781292
C	4.0831346	0.7900537	2.7997894
C	4.3181874	1.5519547	3.9831144
C	3.0433457	1.1186667	1.8538549
C	2.7848800	0.1923313	0.8376599
O	0.2062496	1.1402007	1.8294424
O	1.7412208	0.4355969	-0.0526201
P	0.2067036	0.2433497	0.4669293
O	-0.6726612	0.8609901	-0.6319789
O	-0.1225051	-1.1875223	0.9162625
C	4.1015534	6.2712167	2.0538075
C	4.9040424	5.1112501	1.8932043
H	2.0844632	7.0430126	2.2023743
H	4.5737016	7.2639267	2.1075861
H	4.9599122	2.9672333	1.6996489
H	5.9968601	5.2097889	1.8063634
C	5.3355051	1.2116603	4.8639291
C	6.1714213	0.0935736	4.6040127
H	3.6727665	2.4148695	4.1984364
H	5.4908426	1.8109842	5.7739303
H	6.9805213	-0.1621009	5.3049409
H	6.5761310	-1.5704985	3.2796427
C	-1.8772054	3.8143658	0.2129641
C	-1.4164406	3.4031069	1.4998967
C	-3.2341620	3.6364825	-0.1009851
C	-2.3208012	2.8120712	2.4207633
C	-3.6739967	2.6683278	2.0557345
C	-4.1544204	3.0713392	0.7991707
H	-3.5915573	3.9312647	-1.1005704
C	-1.8795994	2.3512328	3.8083999
H	-4.3679135	2.2189649	2.7816982
C	-2.1938317	0.8643183	4.0545736
H	-3.2864248	0.6680134	4.0491343
H	-1.8071676	0.5419025	5.0429767
H	-1.7228114	0.2227649	3.2840202
C	-2.4873059	3.2470031	4.9041225
H	-0.7784712	2.4691653	3.8687834
H	-3.5953959	3.1798590	4.9124326
H	-2.2181725	4.3111404	4.7472385
H	-2.1246844	2.9439960	5.9082069
C	-5.6193872	2.9536486	0.3900881
C	-6.4064841	1.8824055	1.1558692
H	-7.4254671	1.7738223	0.7320859
H	-6.5295716	2.1509811	2.2259513
H	-5.9080736	0.8932472	1.1108397
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H	-5.6173972	2.6674024	-0.6863582
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H	-6.3336197	4.6679193	1.5555894
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H	0.0879586	4.3131902	-0.4921807
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H	0.9911887	-5.3184725	-3.1361708
H	4.8896531	-0.9123030	-3.9631374
H	3.7480426	-5.1686431	2.4868577
C	1.5079445	-4.4763741	-3.6470963
H	3.1849063	1.7285767	-3.2955903
H	-0.0277117	-4.4566849	-5.2098184
H	1.2471901	-4.6486832	2.7195552
C	2.0763586	-3.5821269	-2.5532012
C	5.0516937	-0.3479889	-3.0211201
C	0.4640933	-3.7497264	-4.5104475
H	0.9193157	-2.9410439	-5.1179298
C	2.5971732	-2.3095794	-2.8450783
C	3.7201987	-4.8043240	1.4389259
H	3.3608060	-5.6400770	-3.8931609
C	2.1165302	-4.0116629	-1.2174883
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H	2.2224991	-5.7638307	-5.2783003
H	1.7251532	-5.0133175	-0.9765408
C	2.7470232	0.7298542	-3.0914961
H	5.5207977	0.6225645	-3.2852658
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C	3.1246861	-1.4698424	-1.8504391
C	1.2374353	-4.3338803	1.6561904
C	2.6186699	-3.2076162	-0.1755686
H	4.7188752	-4.3902361	1.1918184
H	3.5572549	-5.6824103	0.7792580
C	3.7242813	-0.1279619	-2.2697418
C	3.1248471	-1.9156732	-0.4964004
C	2.6030626	-3.7599290	1.2497037
H	1.7918449	0.8786744	-2.5530522
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H	-0.3193901	-3.2793315	-3.8862015
H	0.9569489	-5.2267201	1.0590426
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Zn	-1.4460529	0.0764877	-2.2212091
Br	-0.9973835	0.0345823	-4.4720341
C	-2.3005324	-6.9006690	-2.3932882
C	-2.6665066	-2.6225493	-2.2328544
C	-1.4365691	-6.1528224	-1.5775822
C	-3.4104984	-4.8545980	-3.0893543
C	-2.5603527	-4.0941153	-2.2517608
C	-3.2858517	-6.2459977	-3.1553300
C	-1.5632754	-4.7604280	-1.5048298
O	-1.7917786	-1.9105452	-1.5522206
H	-2.2005401	-7.9954642	-2.4465449
H	-4.1658659	-4.3456805	-3.7083928
H	-0.6535102	-6.6552988	-0.9897894
H	-3.9519070	-6.8258388	-3.8119772
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Br	-2.5888216	-3.9389490	1.6711711
Zn	-1.8469896	-2.0456328	0.5245910
H	-5.3550426	-2.4901357	-3.3972304
H	-3.9602291	-1.2829985	1.4169628
C	-4.6637333	-2.2558942	-1.2945092
C	-5.4902611	-1.8645144	-2.4913090
H	-4.8428733	-3.1856948	-0.7346836
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O	-5.0278859	-0.5311880	-2.8307181
O	-3.4693440	0.8823401	-2.0116172
H	-6.5796623	-1.8160856	2.2691376
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H	-3.0210567	-2.1604674	-3.1797437



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H	3.4574700	5.8710136	0.3243148
Br	-1.4005204	3.9613485	-2.6711273
H	-1.4032384	4.1502583	0.3341888
Zn	-0.3698286	2.5264176	-1.1343054
C	1.3662906	5.1635867	0.0273989
C	2.4887277	5.7429889	0.8476303
C	0.6729842	4.2703387	0.8796919
C	-0.5584238	3.6146098	0.7984526
C	1.7277902	3.844231	1.8453732
O	2.7079165	4.7613968	1.8985984
O	1.8077375	2.7662547	2.4470528
H	2.2219995	6.7137667	1.3194589
H	-0.7991536	2.8863417	1.5920181
H	0.8944723	5.7261934	-0.7916765
C	2.1256605	3.8303862	-4.8037835
C	1.9177026	3.3754150	-3.4958792
C	2.5521360	4.0149056	-2.4072350
C	3.4162849	5.1063609	-2.6624320
C	3.6175004	5.5626805	-3.9695731
C	2.9670883	4.9288319	-5.0449756
H	1.6268672	3.1926250	-5.6413344
H	1.2938210	2.4880771	-3.3215448
C	2.3914158	3.5052689	-1.0310030
H	3.9468813	5.5920714	-1.8288707
H	4.2929336	6.4113895	-4.1555737
H	3.1275153	5.2862805	-6.0735570
O	1.6834532	2.4098373	-0.8226279
C	-2.0428865	-1.7503016	1.5844118
C	-2.0613277	-3.0321795	1.0240025
C	-2.2074279	-4.1518140	1.9272486
C	-2.0743214	-5.5110039	1.5106177
C	-2.4610291	-3.8929069	3.3259345
C	-2.6540744	-4.9918744	4.2166813
C	-2.4415298	-2.5544050	3.8135709
H	-2.5841373	-2.3802623	4.8910340
C	-2.1706301	-1.4760211	2.9801347
C	-0.3578028	-2.8322620	-2.4207046
C	-1.1397788	-3.7080806	-3.1649006
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C	-3.1736632	-5.1033146	-3.4481450
C	-2.7166759	-4.0181587	-1.2695377
C	-3.9663777	-4.5286205	-0.8066777
C	-1.8449468	-3.2194208	-0.4409927
C	-0.7456989	-2.6167292	-1.0623067
O	-1.9170974	-0.6429586	0.7454781
O	0.0794510	-1.7779202	-0.3147474
P	-0.4681997	-0.2943266	0.0832319
O	0.5303256	0.2404544	1.1222382
O	-0.7770005	0.6017272	-1.1255936
C	-2.5595034	-6.3004613	3.7680258
C	-2.2470262	-6.5574638	2.4066543
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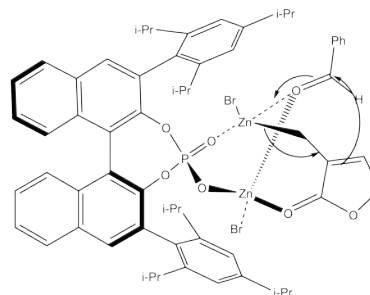
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TS1-8-j; COSMO

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C	-4.7732129	-5.3024823	-1.6299944
C	-4.3688080	-5.6075900	-2.9571462
H	-4.2942098	-4.2930048	0.2155070
H	-5.7365190	-5.6774804	-1.2519039
H	-5.0123837	-6.2292535	-3.5980762
H	-2.8624263	-5.3109134	-4.4840252
C	-0.6733250	0.1391591	4.2008062
C	-1.8918003	-0.0976144	3.4955430
C	-0.3924288	1.4451173	4.6343821
C	-2.7772540	0.9800024	3.2297058
C	-2.4491434	2.2681070	3.6977191
C	-1.2610616	2.5262097	4.4011422
H	0.5552690	1.6383554	5.1619181
C	-4.0897567	0.7843599	2.4735305
H	-3.1473331	3.0937432	3.4942245
C	-4.1826103	1.6865445	1.2292172
H	-4.1918247	2.7627167	1.5013377
H	-5.1166507	1.4806130	0.6672730
H	-3.3302888	1.5111717	0.5434006
C	-5.2984516	0.9840387	3.4072009
H	-4.1236156	-0.2668391	2.1216760
H	-5.3395625	2.0224543	3.7978656
H	-5.2497337	0.2994434	4.2783328
H	-6.2489314	0.7891931	2.8685228
C	-0.8969946	3.9050141	4.9429670
C	-1.5694473	5.0719396	4.2081958
H	-1.1724135	6.0397249	4.5760908
H	-2.6663397	5.0859009	4.3787043
H	-1.3980233	5.0238869	3.1140534
C	-1.1832680	3.9745389	6.4569081
H	0.2037691	4.0094759	4.8087854
H	-0.8570567	4.9473315	6.8801651
H	-0.6591819	3.1668730	7.0061785
H	-2.2706389	3.8625928	6.6516545
C	0.3314310	-0.9719996	4.5137086
C	1.7777248	-0.6192770	4.1258664
H	2.4536617	-1.4686354	4.3535542
H	2.1621523	0.2649326	4.6741141
H	1.8585873	-0.4099577	3.0433893
C	0.2467902	-1.3680945	6.0011038
H	0.0494550	-1.8614756	3.9153359
H	0.9305269	-2.2131354	6.2245559
H	-0.7803378	-1.6727176	6.2866992
H	0.5338709	-0.5170681	6.6540030
H	3.6974304	1.2686762	-4.8651786
H	4.2196333	-4.1180813	-2.4061467
H	-1.7893418	-1.2725929	-6.4986485
C	4.1405447	0.4447056	-4.2637881
H	3.2214768	-3.6550675	0.6124994
H	5.6271983	1.8241311	-3.4355618
H	-2.1756440	0.7892039	-5.0240795
C	2.9851341	-0.4390417	-3.8127400
C	3.2315277	-4.4919539	-2.0649323
C	4.8814307	1.0844784	-3.0784032
H	5.4226491	0.3286640	-2.4730050
C	3.1647313	-1.4426439	-2.8446243
C	-0.7869633	-1.4051941	-6.0410574
H	4.5808700	-0.7521830	-6.0588158
C	1.7038848	-0.2899111	-4.3668534
C	5.1069262	-0.3322604	-5.1775804
H	5.9229926	0.3255944	-5.5429040
H	1.5527035	0.4824436	-5.1383395
C	3.1050977	-2.8409902	-0.1323933
H	3.4122460	-5.3224281	-1.3511585
H	2.7051260	-4.9054247	-2.9492544
C	2.1099098	-2.2637072	-2.4122854
C	-1.1520118	0.6616159	-4.6162660
C	0.6053494	-1.0737554	-3.9620218
H	-0.5451067	-2.4874834	-6.0494989

H	-0.0463557	-0.8967793	-6.6938236
C	2.4118598	-3.3685359	-1.4002990
C	0.8099107	-2.0703117	-2.9648715
C	-0.7535939	-0.8221123	-4.6149654
H	2.5196166	-2.0276201	0.3368396
H	-1.1458637	1.0808996	-3.5933073
H	4.1170216	-2.4404774	-0.3465753
H	4.1793466	1.6019348	-2.3967902
H	-0.4757231	1.2815075	-5.2413194
H	5.5739565	-1.1778803	-4.6300182
H	1.4488499	-3.8206290	-1.0875581
H	-1.5188827	-1.3556582	-4.0164034
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H	3.2789303	3.6287475	-0.3742252

TS1-8-j

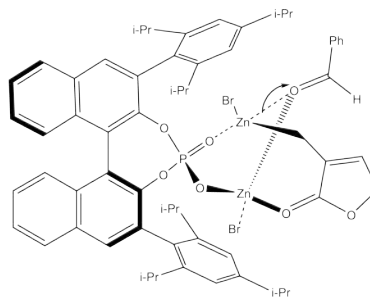


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Br	-1.3728583	3.9804171	-2.6879273
H	-1.4286549	4.1443118	0.3046643
Zn	-0.3828695	2.5252015	-1.1537511
C	1.3388797	5.1675848	0.0107811
C	2.4561698	5.7509818	0.8354409
C	0.6441700	4.2763552	0.8632351
C	-0.5850059	3.6174673	0.7803488
C	1.6954877	3.8538821	1.8355277
O	2.6741412	4.7781260	1.8902965
O	1.7748910	2.7813724	2.4407782
H	2.1881272	6.7253155	1.3016200
H	-0.8263062	2.8893503	1.5738589
H	0.8709700	5.7185525	-0.8184785
C	2.1410491	3.8382866	-4.8093694
C	1.9207778	3.3790219	-3.5052537
C	2.5606913	4.0026400	-2.4109124
C	3.4433992	5.0807817	-2.6582037
C	3.6570797	5.5412815	-3.9613511
C	3.0002763	4.9240065	-5.0419166
H	1.6348420	3.3401452	-5.6500899
H	1.2816028	2.5016371	-3.3382858
C	2.3862385	3.4923398	-1.0374229
H	3.9810707	5.5504214	-1.8196874
H	4.3476199	6.3791825	-4.1406208
H	3.1698034	5.2846962	-6.0678631
O	1.6701621	2.4069212	-0.8266534
C	-2.0482719	-1.7495359	1.5845134
C	-2.0658400	-3.0316067	1.0240468
C	-2.2102976	-4.1517758	1.9268198
C	-2.0772205	-5.5104561	1.5092175
C	-2.4624160	-3.8943330	3.3258206
C	-2.6536792	-4.9941206	4.2151548
C	-2.4426281	-2.5562817	3.8136355

H	-2.5822953	-2.3815767	4.8913971	H	5.6339437	1.8235353	-3.4415096
C	-2.1736909	-1.4771150	2.9809954	H	-2.1774352	0.7918668	-5.0242183
C	-0.3583237	-2.8279066	-2.4177506	C	2.9844359	-0.4339659	-3.8078931
C	-1.1379776	-3.7047383	-3.1628269	C	3.2312759	-4.4826656	-2.0541740
H	-0.8555982	-3.9265466	-4.2031632	C	4.8868268	1.0869956	-3.0809824
C	-2.3280168	-4.2861673	-2.6357261	H	5.4275651	0.3326886	-2.4735462
C	-3.1687121	-5.1040587	-3.4489058	C	3.1629717	-1.4355339	-2.8379588
C	-2.7167163	-4.0185858	-1.2705479	C	-0.7842775	-1.4023546	-6.0378613
C	-3.9653802	-4.5324487	-0.8094654	H	4.5746463	-0.7586244	-6.0544525
C	-1.8479982	-3.2183313	-0.4406972	C	1.7035156	-0.2853631	-4.3622270
C	-0.7487011	-2.6135041	-1.0598462	C	5.1035554	-0.3368118	-5.1760379
O	-1.9251216	-0.6419621	0.7469876	H	5.9214687	0.3166597	-5.5449430
O	0.0733686	-1.7738823	-0.3113490	H	1.5526681	0.4859023	-5.1348971
P	-0.4769512	-0.2899278	0.0840051	C	3.1011606	-2.8293850	-0.1233557
O	0.5190898	0.2465182	1.1244400	H	3.4127115	-5.3123312	-1.3397226
O	-0.7846454	0.6011993	-1.1278616	H	2.7065099	-4.8972199	-2.9387432
C	-2.5593508	-6.3018839	3.7657382	C	2.1083641	-2.2563617	-2.4055989
C	-2.2486660	-6.5573545	2.4042909	C	-1.1543241	0.6648721	-4.6154176
H	-2.8579355	-4.7798552	5.2759910	C	0.6048107	-1.0686451	-3.9577743
H	-2.7025837	-7.1402496	4.4642428	H	-0.5401720	-2.4840672	-6.0458196
H	-1.8258632	-5.7277084	0.4625802	H	-0.0429895	-0.8945084	-6.6901016
H	-2.1355667	-7.5947497	2.0542876	C	2.4102254	-3.3592530	-1.3915019
C	-4.7689665	-5.3081662	-1.6334783	C	0.8091066	-2.0644044	-2.9600394
C	-4.3626382	-5.6116215	-2.9597948	C	-0.7536733	-0.8180960	-4.6122882
H	-4.2935981	-4.2977579	0.2127076	H	2.5144661	-2.0162737	0.3445137
H	-5.7314856	-5.6859142	-1.2562693	H	-1.1520042	1.0855640	-3.5932452
H	-5.0037740	-6.2346018	-3.6018024	H	4.1129632	-2.4273843	-0.3346151
H	-2.8558796	-5.3100435	-4.4846180	H	4.1889441	1.6080280	-2.3981151
C	-0.6705756	0.1342033	4.1984908	H	-0.4789731	1.2861288	-5.2401521
C	-1.8918680	-0.1000054	3.4976793	H	5.5685883	-1.1824840	-4.6272216
C	-0.3860187	1.4394764	4.6307047	H	1.4471770	-3.8119291	-1.0795753
C	-2.7766453	0.9787090	3.2356972	H	-1.5192147	-1.3517155	-4.0141166
C	-2.4448681	2.2658601	3.7029684	H	4.1602557	-1.5810995	-2.3950067
C	-1.2538074	2.5216145	4.4016090	H	3.2662924	3.6176200	-0.3698296
H	0.5648716	1.6312632	5.1529321				
C	-4.0927821	0.7842846	2.4855980				
H	-3.1431675	3.0923544	3.5033349				
C	-4.1908701	1.6850648	1.2409133				
H	-4.1982302	2.7616831	1.5114820				
H	-5.1276800	1.4801742	0.6834204				
H	-3.3430958	1.5075055	0.5503712				
C	-5.2963295	0.9847997	3.4254685				
H	-4.1286230	-0.2670812	2.1344107				
H	-5.3350209	2.0229510	3.8168131				
H	-5.2431928	0.3009955	4.2967125				
H	-6.2502074	0.7908102	2.8925971				
C	-0.8854143	3.8989488	4.9441613				
C	-1.5565847	5.0682666	4.2120767				
H	-1.1578841	6.0353768	4.5800704				
H	-2.6529210	5.0849541	4.3853756				
H	-1.3884668	5.0209105	3.1174338				
C	-1.1682450	3.9675720	6.4585900				
H	0.2152699	4.0009376	4.8070102				
H	-0.8393294	4.9387154	6.8835628				
H	-0.6458138	3.1575283	7.0054885				
H	-2.2551328	3.8569080	6.6556735				
C	0.3335494	-0.9784926	4.5080226				
C	1.7791020	-0.6294084	4.1145851				
H	2.4545748	-1.4795582	4.3400523				
H	2.1690944	0.2543624	4.6593609				
H	1.8575154	-0.4216578	3.0317919				
C	0.2532187	-1.3729867	5.9960054				
H	0.0474049	-1.8679874	3.9116651				
H	0.9358281	-2.2190844	6.2185186				
H	-0.7734138	-1.6746860	6.2861361				
H	0.5437579	-0.5222732	6.6475704				
H	3.6998315	1.2694530	-4.8656834				
H	4.2191744	-4.1087316	-2.3954475				
H	-1.7856951	-1.2714577	-6.4979433				
C	4.1414990	0.4457172	-4.2625808				
H	3.2173672	-3.6418996	0.6231231				

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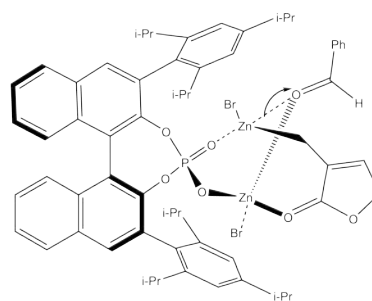


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H	1.9313901	6.1220841	1.1186878
Br	-2.3822538	4.3629694	-0.4271883
H	-1.6128396	3.1750805	3.0614624
Zn	-1.3065197	2.5499229	0.6268935
C	0.3691691	5.1680936	2.3151355
C	1.7701523	5.6367945	2.1086581
C	0.3558020	3.8041408	2.4516012
C	-0.7126649	2.8077668	2.5331769
C	1.7681005	3.3838790	2.3487881
O	2.5799443	4.4429374	2.1452611
O	2.2242733	2.2319514	2.4179671
H	2.1512427	6.3301746	2.8915237
H	-0.3606170	1.8561612	2.9707554
H	-0.5046579	5.8322796	2.2904203

C	0.5884218	6.0847711	-2.3572570	C	0.8677122	1.2825952	7.6844288
C	0.9842849	4.8985589	-1.7358497	H	1.7652671	2.0628137	5.8854052
C	2.3617614	4.6108030	-1.5848613	H	1.2199445	2.1069481	8.3391561
C	3.3368013	5.5188106	-2.0634201	H	1.5752755	0.4353155	7.7853381
C	2.9335387	6.7054388	-2.6853008	H	-0.1182397	0.9411415	8.0637445
C	1.5613960	6.9850524	-2.8332022	C	2.1991454	-2.3875771	3.7113408
H	-0.4855391	6.3008106	-2.4623100	C	3.3910230	-1.7018054	3.0310272
H	0.2274758	4.1930189	-1.3622113	H	4.2042601	-2.4301409	2.8350573
C	2.7908344	3.3777431	-0.9385917	H	3.8273121	-0.8845220	3.6406498
H	4.4059336	5.2806509	-1.9455135	H	3.0945279	-1.2799574	2.0526453
H	3.6849565	7.4157833	-3.0611187	C	2.6458339	-3.1690873	4.9632009
H	1.2472575	7.9179795	-3.3268330	H	1.8035320	-3.1254295	2.9861737
O	1.9968750	2.5684102	-0.4234146	H	3.4172553	-3.9231505	4.7027414
C	-0.9590500	-2.4737456	1.3925351	H	1.7951643	-3.6967481	5.4409450
C	-1.1420575	-3.4453884	0.4023820	H	3.0812021	-2.4890847	5.7252094
C	-0.8665520	-4.8215817	0.7492439	H	0.9974027	3.3300664	-6.0462079
C	-0.8325346	-5.8736524	-0.2150966	H	2.9735656	-2.1893638	-5.4441789
C	-0.5787318	-5.1528521	2.1243367	H	-4.5035285	0.6593225	-4.9750425
C	-0.3452802	-6.5144796	2.4823311	C	1.7417639	2.5282531	-5.8440266
C	-0.4770852	-4.1129479	3.0910204	H	3.5131302	-2.5684012	-2.3188512
H	-0.2357145	-4.3766022	4.1323165	H	3.3315232	3.9993482	-5.4739663
C	-0.6016039	-2.7731119	2.7447884	H	-3.8877288	2.2154042	-2.9905882
C	-1.1488219	-1.7536362	-3.0574168	C	0.9984738	1.4124233	-5.1204056
C	-2.1500919	-2.4781681	-3.6954979	C	2.2836840	-2.7940377	-4.8190410
H	-2.3482039	-2.2904827	-4.7612353	C	2.8485203	3.1386167	-4.9660138
C	-2.9640761	-3.4183863	-3.0031880	H	3.6425011	2.3961632	-4.7400776
C	-4.0540496	-4.0715620	-3.6532473	C	1.6658633	0.2620402	-4.6680098
C	-2.7072725	-3.6928918	-1.6104144	C	-3.4258889	0.5132245	-5.1950440
C	-3.6022641	-4.5624844	-0.9175694	H	1.4848834	1.6569844	-7.8458283
C	-1.5778280	-3.0606256	-0.9710784	C	-0.3783446	1.5016037	-4.8773364
C	-0.8890492	-2.0741793	-1.6884115	C	2.2936517	2.0545605	-7.2005674
O	-1.1827886	-1.1359829	1.0764936	H	2.7911215	2.8861312	-7.7418264
O	0.1677667	-1.4078598	-1.0801493	H	-0.9152449	2.4020642	-5.2158544
P	-0.1139317	-0.3292398	0.1191534	C	2.9901925	-1.6500022	-2.6563848
O	1.2493722	-0.1920882	0.8047467	H	2.8238076	-3.7157816	-4.5184107
O	-0.8661660	0.9087697	-0.3803815	H	1.4265141	-3.0899061	-5.4572584
C	-0.3526522	-7.5158935	1.5240693	C	1.0049541	-0.7781322	-3.9920166
C	-0.5810569	-7.1854848	0.1622063	C	-2.8397628	2.1230980	-3.3357247
H	-0.1383981	-6.7503597	3.5381309	C	-1.0924024	0.4983266	-4.1949399
H	-0.1630678	-8.5609934	1.8125491	H	-3.2980239	-0.5039878	-5.6160553
H	-0.9975777	-5.6343371	-1.2742864	H	-3.1412636	1.2365770	-5.9879763
H	-0.5525832	-7.9751224	-0.6040361	C	1.8121844	-2.0087106	-3.5805586
C	-4.6660076	-5.1655749	-1.5737251	C	-0.3955608	-0.6642159	-3.7565578
C	-4.8872275	-4.9335656	-2.9572477	C	-2.5782984	0.7298469	-3.9272846
H	-3.4479134	-4.7444370	0.1549543	H	2.6453473	-1.1079391	-1.7544878
H	-5.3470976	-5.8245213	-1.0138650	H	-2.1964738	2.3087496	-2.4548449
H	-5.7293061	-5.4241012	-3.4686921	H	3.7404651	-1.0161353	-3.1737382
H	-4.2309999	-3.8604394	-4.7196141	H	2.4395722	3.4975359	-4.0005007
C	1.0633353	-1.4297701	4.0748899	H	-2.6590740	2.9316765	-4.0746413
C	-0.2909331	-1.6616249	3.6954912	H	3.0425923	1.2459531	-7.0675904
C	1.3518647	-0.3037087	4.8648688	H	1.1425469	-2.6838963	-3.0118122
C	-1.3196697	-0.8054994	4.1694191	H	-2.9040160	-0.0090619	-3.1671131
C	-0.9763876	0.2899517	4.9851088	H	2.7434332	0.1667040	-4.8652376
C	0.3566637	0.5759271	5.3248712	H	3.8902376	3.1607440	-0.8998290
H	2.4000428	-0.1003682	5.1405340				
C	-2.7921413	-1.0846569	3.8701827				
H	-1.7808682	0.9434562	5.3553436				
C	-3.4955775	0.0863370	3.1661399				
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H	-4.5465609	-0.1686174	2.9222475				
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C	-3.5353042	-1.4965326	5.1554260				
H	-2.8339088	-1.9535301	3.1815053				
H	-3.5453694	-0.6712422	5.8977378				
H	-3.0518949	-2.3715817	5.6351520				
H	-4.5896811	-1.7623027	4.9338780				
C	0.7510967	1.7471851	6.2187572				
C	-0.1721380	2.9676030	6.1041189				
H	0.2316245	3.8148176	6.6950956				
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TS1-8-o

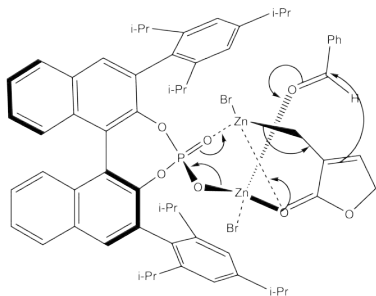


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H	-0.6650778	5.4823545	2.6606033	C	-3.7135800	-2.0095644	2.0761034
Br	-3.7586459	3.0081042	-0.1847429	H	-4.1180248	-1.4001166	2.9106532
H	-3.1855421	1.1861757	3.0795231	H	-4.5776117	-2.4147233	1.5106726
Zn	-2.3024244	1.3783856	0.7014908	H	-3.1508211	-1.3348936	1.4006576
C	-1.9409005	3.8096789	3.2579611	C	-3.5948070	-4.1433418	3.4606200
C	-0.7759218	4.7186457	3.4643890	H	-2.4651843	-3.7115730	1.6922275
C	-1.4963366	2.5239763	3.0899181	H	-3.9892899	-3.6525670	4.3749888
C	-2.1450494	1.2680556	2.7125662	H	-2.9494102	-4.9845156	3.7849669
C	-0.0262090	2.5980153	3.2029751	H	-4.4586847	-4.5650377	2.9061632
O	0.3867599	3.8646349	3.4156350	C	-0.8219308	-0.4242409	6.4091862
O	0.7854428	1.6638705	3.1101451	C	-2.1010434	0.4233549	6.4236232
H	-0.7657008	5.2515885	4.4414618	H	-2.1013374	1.1075387	7.2963530
H	-1.5496536	0.3869099	3.0142582	H	-3.0107382	-0.2073469	6.5086292
H	-2.9795212	4.1586768	3.1894141	H	-2.1981264	1.0341937	5.5045545
C	-1.3601446	6.0562823	-0.9951327	C	-0.7225378	-1.2923636	7.6797578
C	-0.6839808	4.9181886	-0.5504758	H	0.0437540	0.2758939	6.4138662
C	0.6756798	5.0142816	-0.1669380	H	-0.7715798	-0.6682538	8.5963946
C	1.3505766	6.2568382	-0.2404259	H	0.2244439	-1.8680145	7.7039968
C	0.6675168	7.3928499	-0.6880028	H	-1.5579966	-2.0225844	7.7170898
C	-0.6848998	7.2903460	-1.0663687	C	2.3060984	-2.8669542	3.2958251
H	-2.4185613	5.9710833	-1.2842946	C	3.2118131	-1.6487375	3.0595851
H	-1.2080097	3.9521579	-0.4957289	H	4.2594758	-1.9645984	2.8795362
C	1.3990456	3.8360989	0.2887329	H	3.2232461	-0.9472977	3.9187819
H	2.4108603	6.3169492	0.0525510	H	2.8873492	-1.0922897	2.1608844
H	1.1854697	8.3616137	-0.7484778	C	2.8878212	-3.7936539	4.3815278
H	-1.2186827	8.1853267	-1.4225126	H	2.2942634	-3.4391360	2.3474593
O	0.8649418	2.7197192	0.4306299	H	3.9070699	-4.1337418	4.1043558
C	-0.2895989	-3.2977321	0.3887669	H	2.2545824	-4.6916077	4.5328907
C	0.0217410	-3.9708299	-0.7978108	H	2.9602622	-3.2727211	5.3592435
C	0.7231898	-5.2308075	-0.6927478	H	0.4367379	4.6152877	-5.0463566
C	1.2634836	-5.9159173	-1.8227105	H	4.1849908	0.0966810	-5.1312666
C	0.9190097	-5.8158254	0.6121298	H	-3.7887519	0.1675110	-5.8438624
C	1.5706636	-7.0809200	0.7212548	C	1.3837366	4.0712039	-4.8342336
C	0.5122029	-5.0979686	1.7721685	H	4.3713168	-0.9696607	-2.1266334
H	0.6905558	-5.5434954	2.7630472	H	2.2590404	5.8344574	-3.8592999
C	-0.0311230	-3.8211069	1.6936675	H	-4.1043528	1.1156587	-3.4454570
C	-0.1086370	-1.4949896	-3.7414659	C	1.0008007	2.6313813	-4.5139807
C	-0.6676828	-2.2962934	-4.7307357	C	3.6824590	-0.8477818	-4.8349726
H	-0.7621858	-1.8976225	-5.7518814	C	2.0547994	4.7661307	-3.6378880
C	-1.1748137	-3.5967610	-4.4526067	H	3.0230652	4.2872258	-3.3806971
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C	-1.0442697	-4.1427878	-3.1233771	C	-2.7178752	0.4576429	-5.8163544
C	-1.6555225	-5.4031995	-2.8495492	H	1.7552245	3.6907780	-6.9682330
C	-0.3291969	-3.3851750	-2.1230924	C	-0.3361719	2.2106744	-4.5702497
C	0.0453780	-2.0744394	-2.4443083	C	2.2607704	4.1526808	-6.0965683
O	-0.9417677	-2.0699204	0.3212689	H	2.4951953	5.2073135	-6.3511902
O	0.6775678	-1.2902636	-1.4887636	H	-1.1121997	2.9532092	-4.8171596
P	-0.1255960	-0.7351818	-0.1745980	C	3.5996340	-0.2107959	-2.3699953
O	0.9894497	-0.3638679	0.8065268	H	4.4737967	-1.5969676	-4.6248047
O	-1.2049977	0.2930949	-0.5383848	H	3.0952231	-1.2018857	-5.7065314
C	2.0527104	-7.7350058	-0.4017049	C	1.6487445	0.3326549	-3.9127519
C	1.9120385	-7.1347540	-1.6807245	C	-3.0620551	1.4869436	-3.5237110
H	1.7010235	-7.5181319	1.7237105	C	-0.7214958	0.8809198	-4.3128938
H	2.5605893	-8.7063956	-0.3026269	H	-2.1497864	-0.2743799	-6.4246942
H	1.1727907	-5.4613145	-2.8184022	H	-2.6229403	1.4449336	-6.3155542
H	2.3262563	-7.6361479	-2.5687213	C	2.7830112	-0.6430048	-3.6010540
C	-2.3181863	-6.1092303	-3.8438319	C	0.2860949	-0.0741980	-3.9965149
C	-2.4004293	-5.5936604	-5.1645355	C	-2.2076804	0.5264999	-4.3644638
H	-1.6060065	-5.8113014	-1.8305535	H	2.9556332	-0.0909840	-1.4780936
H	-2.7885872	-7.0749430	-3.6036360	H	-2.6652593	1.5861546	-2.4963243
H	-2.9209522	-6.1667643	-5.9468333	H	4.1271008	0.7510028	-2.5378133
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C	0.8632798	-2.4900943	3.6375370	H	-3.1120841	2.5043753	-3.9643089
C	-0.2602949	-2.9765992	2.9068182	H	3.2244021	3.6217040	-5.9492163
C	0.6324558	-1.6480225	4.7388067	H	2.3332573	-1.6289415	-3.3685031
C	-1.5759836	-2.6304903	3.3156491	H	-2.3257453	-0.4812719	-3.9179399
C	-1.7478715	-1.8103015	4.4469078	H	3.0310431	1.9805144	-4.1204368
C	-0.6580428	-1.2932986	5.1665355	H	2.4882173	3.9511539	0.5291309
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TS2-8-o; COSMO



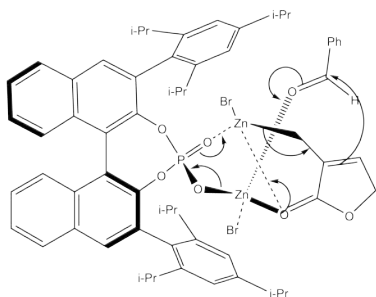
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C	4.2083424	3.8545399	1.3449332
C	1.9862508	4.8557911	1.6891731
C	2.6151962	6.1329546	1.7982959
C	0.5696049	4.7302206	1.7140720
H	-0.0397018	5.6382337	1.8393619
C	-0.0698099	3.5105250	1.5188726
C	3.4770713	-0.9401259	0.0439620
C	4.5603079	-1.1618974	0.8878949
H	5.2145147	-2.0264469	0.7032179
C	4.8175727	-0.3419729	2.0225034
C	5.8683961	-0.6547400	2.9368490
C	3.9744723	0.7992526	2.2807803
C	4.1817928	1.5353509	3.4857171
C	2.9441288	1.1323843	1.3275775
C	2.7002947	0.2349981	0.2833144
O	0.1100259	1.1157448	1.3221491
O	1.6648565	0.5135969	-0.6143633
P	0.1409160	0.2606020	-0.0777308
O	-0.7636983	0.9025975	-1.1471741
O	-0.0847032	-1.2080095	0.2921628
C	3.9906995	6.2620211	1.6821695
C	4.7884718	5.1123886	1.4358065
H	1.9801712	7.0184021	1.9591453
H	4.4638213	7.2526526	1.7616152
H	4.8402344	2.9788291	1.1439219
H	5.8767857	5.2192259	1.3098114
C	5.1980843	1.1920841	4.3667541
C	6.0611007	0.0989834	4.0848252
H	3.5158030	2.3773285	3.7201843
H	5.3316151	1.7684122	5.2949578
H	6.8686008	-0.1579657	4.7872725
H	6.5115215	-1.5224515	2.7212917
C	-2.1337440	3.9075381	0.1423387
C	-1.5553784	3.4318551	1.3523781
C	-3.5356689	3.8775844	0.0124944
C	-2.3792847	2.9210714	2.3941739
C	-3.7733442	2.9189278	2.2109751
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C	-1.7622343	2.4859479	3.7244331
H	-4.4116640	2.5370910	3.0206845
C	-2.5851701	1.4481097	4.5000440
H	-3.5329211	1.8762701	4.8895708
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H	-2.8260117	0.5740375	3.8668560
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H	-2.4325546	4.2352099	4.8642774
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H	-0.9911425	3.4184274	5.5579210
C	-5.8898868	3.4369216	0.8510573
C	-6.4284317	2.0770707	0.3695124
H	-7.5199202	2.1327122	0.1739098

H	-6.2540009	1.2950609	1.1370725
H	-5.9205671	1.7555739	-0.5615848
C	-6.6389248	3.9160475	2.1047274
H	-6.0900483	4.1728856	0.0408767
H	-7.7208541	4.0357293	1.8902341
H	-6.2490940	4.8893203	2.4657354
H	-6.5506496	3.1874952	2.9376739
C	-1.2916940	4.5198764	-0.9800269
C	-1.6170620	3.9622529	-2.3740045
H	-0.9515051	4.4216398	-3.1337457
H	-2.6629281	4.1674299	-2.6798988
H	-1.4646167	2.8679199	-2.4096222
C	-1.4223028	6.0561748	-0.9720957
H	-0.2303586	4.2724046	-0.7762783
H	-0.7679833	6.5118195	-1.7441849
H	-1.1449253	6.4888270	0.0098882
H	-2.4671652	6.3639628	-1.1872439
H	1.5205226	-5.6501886	-3.6053253
H	4.8880339	-0.9033966	-4.5224765
H	3.6552794	-4.8581339	2.2577157
C	1.8125780	-4.7117351	-4.1266541
H	3.0081727	1.6203979	-3.9451699
H	0.1745983	-4.9174072	-5.5739026
H	1.0885717	-4.5445775	2.1684715
C	2.2909390	-3.7421045	-3.0535295
C	5.0028852	-0.3094293	-3.5915755
C	0.5602617	-4.1749228	-4.8447309
H	0.7872819	-3.2423907	-5.4027363
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H	3.8166157	-5.4797764	-4.6111429
C	2.2815539	-4.1032725	-1.6971429
C	2.9287310	-5.0612388	-5.1268014
H	2.5758800	-5.8078777	-5.8681257
H	1.9547991	-5.1200498	-1.4295480
C	2.6295344	0.6064205	-3.7006300
H	5.4082312	0.6845506	-3.8735295
H	5.7559589	-0.8209065	-2.9580646
C	3.1383476	-1.5251578	-2.4015662
C	1.2290902	-4.4275087	1.0758296
C	2.6501305	-3.2131153	-0.6710503
H	4.7041105	-4.0408580	1.0557504
H	3.7669466	-5.4857054	0.5796205
C	3.6591794	-0.1614639	-2.8525635
C	3.0927515	-1.9066070	-1.0307131
C	2.5395135	-3.6780814	0.7826712
H	1.6720494	0.7198307	-3.1560246
H	0.3508206	-3.8816590	0.6740394
H	2.4248416	0.0903363	-4.6620442
H	-0.2492751	-3.9487009	-4.1221060
H	1.2134262	-5.4410821	0.6243460
H	3.2593139	-4.1633097	-5.6900117
H	3.8573764	0.4454417	-1.9464623
H	2.5394736	-2.7748929	1.4266602
H	2.7572951	-2.1417413	-4.4388396
Zn	-2.4267379	0.3029665	-1.9066915
Br	-4.1887605	1.2140454	-3.0826401
C	-1.9685628	-6.6519283	-2.1203414
C	-3.1702170	-2.5326483	-1.9603431
C	-1.0877901	-5.6817395	-1.6156050
C	-3.6289692	-4.9295840	-2.5394656
C	-2.7479824	-3.9506698	-2.0243618
C	-3.2404474	-6.2724420	-2.5910756
C	-1.4659298	-4.3313443	-1.5715125
O	-2.2715476	-1.6268403	-1.7591721
H	-1.6614600	-7.7084579	-2.1560242
H	-4.6240005	-4.6266819	-2.9052468
H	-0.0916482	-5.9802143	-1.2597412
H	-3.9263369	-7.0293499	-3.0011930
H	-0.7773645	-3.5492251	-1.2180577
Br	0.1984324	-2.1332867	3.9116165

Zn	-0.9164463	-2.0081924	1.8721079
H	-5.2380238	-0.8387944	-1.3565104
H	-2.6532645	-4.4647452	1.2699140
C	-4.4273764	-2.6166512	-0.2610675
C	-5.1420761	-1.2824798	-0.3434568
H	-4.9675423	-3.5423191	-0.5011725
C	-3.5439839	-2.5261298	0.8420632
C	-2.6959043	-3.3997195	1.5381394
C	-3.4165121	-1.0702901	1.1261704
O	-4.3050266	-0.3655454	0.4184942
O	-2.5513205	-0.5366355	1.8269280
H	-6.1494449	-1.3001523	0.1254341
H	-2.5725978	-3.1993595	2.6238869
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TS2-8-o



Energy(Hartree)= -11969.99557971
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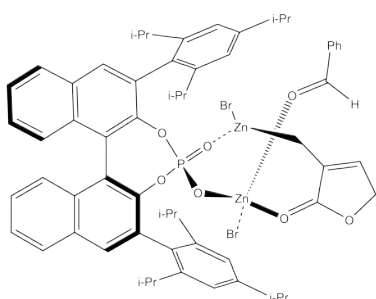
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C	4.2056720	3.8718642	1.3416533
C	1.9808057	4.8519310	1.7225819
C	2.6014744	6.1320924	1.8373349
C	0.5655897	4.7156720	1.7564194
H	-0.0504944	5.6177840	1.8904080
C	-0.0669891	3.4939529	1.5531264
C	3.4898892	-0.9303546	0.0313703
C	4.5924872	-1.1401630	0.8524665
H	5.2502199	-1.9988147	0.6536693
C	4.8649844	-0.3174735	1.9811731
C	5.9373542	-0.6183693	2.8735628
C	4.0137974	0.8132441	2.2579866
C	4.2351241	1.5480491	3.4609993
C	2.9629582	1.1385553	1.3240485
C	2.7090403	0.2394238	0.2832928
O	0.1287604	1.1007121	1.3545290
O	1.6606982	0.5103946	-0.6016324
P	0.1430160	0.2570002	-0.0510467
O	-0.7700672	0.9126169	-1.1047370
O	-0.0832558	-1.2142278	0.3121604
C	3.9739059	6.2731388	1.7066466
C	4.7768731	5.1328533	1.4384118
H	1.9613634	7.0109139	2.0133854
H	4.4401163	7.2666093	1.7904978
H	4.8410614	3.0028249	1.1241133
H	5.8625887	5.2492768	1.2997414
C	5.2728700	1.2157545	4.3202973
C	6.1439540	0.1352560	4.0184869
H	3.5626416	2.3802816	3.7104021
H	5.4166394	1.7910842	5.2474669
H	6.9683299	-0.1132714	4.7040240
H	6.5858044	-1.4783479	2.6436583
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C	-1.5511492	3.4100792	1.3755716
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C	-3.7755911	2.8905353	2.2115253
C	-4.3676439	3.3844464	1.0338670
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C	-1.7767526	2.4475068	3.7386316
H	-4.4197778	2.5055974	3.0150288
C	-2.6011696	1.3981126	4.4968146
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H	-2.4654397	4.1840060	4.8873005
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C	-1.2687215	4.5096190	-0.9501965
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H	-0.9142199	4.4330499	-3.1026608
H	-2.6297280	4.1839062	-2.6654747
H	-1.4410530	2.8756332	-2.4016900
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H	-0.2091866	4.2569046	-0.7436132
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H	-1.1219486	6.4682961	0.0606047
H	-2.4384489	6.3587418	-1.1425378
H	1.4572342	-5.6598346	-3.5476931
H	4.8319616	-0.9249851	-4.5450715
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C	1.7535987	-4.7302724	-4.0827021
H	2.9481367	1.6036132	-3.9678109
H	0.1058287	-4.9466723	-5.5172955
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C	2.2461425	-3.7514279	-3.0244186
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H	0.7317456	-3.2744772	-5.3777784
C	2.6773076	-2.4589923	-3.3679237
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H	5.3543594	0.6706315	-3.9176578
H	5.7136477	-0.8249670	-2.9905693
C	3.1052939	-1.5307205	-2.4032973
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H	4.7395249	-3.9985807	1.0520687
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H	-0.3021607	-3.9500302	-4.0805034
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Zn	-2.4255274	0.3437637	-1.8931907
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C	-1.9465638	-6.6309294	-2.0528854
C	-3.1192838	-2.5043347	-2.0248881
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Br	0.0604195	-2.1964858	3.9525856
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C	-3.5865529	-2.5029421	0.7816438
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H	-6.1514157	-1.2249682	-0.0027925
H	-2.6356851	-3.1695092	2.5814728
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P	-0.0060562	0.4202762	0.1529153
O	-0.8630275	1.1398329	-0.8988250
O	-0.4358662	-0.9594855	0.6561385
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H	2.8193763	6.9542363	1.6495384
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H	5.0994831	2.5254502	1.0616298
H	6.4268109	4.6167183	1.0467866
C	5.3074918	0.7782218	4.3414502
C	5.9480472	-0.4688779	4.1110714
H	3.8454541	2.2093604	3.6585834
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H	-7.0700564	1.8172705	0.9194390
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C	-0.9441765	4.6420601	-1.0109026
C	-1.3067639	4.0703126	-2.3897647
H	-0.6384244	4.5003614	-3.1639672
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C	-1.0540026	6.1807447	-1.0179364
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H	-0.4113758	6.6191584	-1.8096575
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H	-2.1002910	6.4972779	-1.2132449
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H	4.7030478	-1.3579989	-4.3550335
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C	1.4010093	-4.9091159	-4.0629349
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H	0.1919445	-5.0319263	-5.8867649
H	-0.0608085	-4.2292076	2.1523876
C	1.7904748	-3.9237364	-2.9675235
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C	0.5228368	-4.2697298	-5.1514417
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H	3.2603684	-6.0745268	-3.8943445
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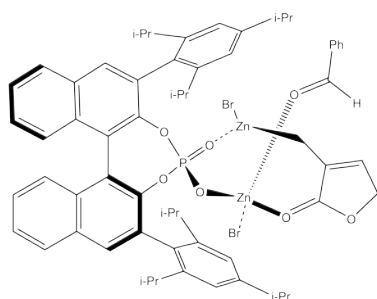


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C	4.5954009	3.4901476	1.2108839
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C	3.3270730	5.9832370	1.5372683
C	1.1100595	4.8683455	1.6005772
H	0.6305023	5.8565755	1.6695803
C	0.3193450	3.7295822	1.5229098
C	3.1187485	-1.2341655	0.1769017
C	4.1626795	-1.6067461	1.0163492
H	4.6559475	-2.5782554	0.8612014
C	4.5867209	-0.7891552	2.1013828
C	5.5885180	-1.2368599	3.0138799
C	3.9704164	0.4984763	2.3075533
C	4.3444099	1.2505826	3.4607135
C	2.9708585	0.9508243	1.3729150
C	2.5410384	0.0542982	0.3879570
O	0.1844754	1.3305042	1.5145994
O	1.5113496	0.4362596	-0.4743326

C	2.5979313	0.3752698	-3.5593119
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H	5.5311893	-1.3991961	-2.7671156
C	2.8280522	-1.8005056	-2.2741395
C	0.1624383	-4.1257641	1.0686764
C	1.9582758	-3.3551374	-0.5730025
H	3.6316424	-4.5703882	1.3060867
H	2.4180665	-5.7933096	0.8222233
C	3.5214042	-0.5075763	-2.6999909
C	2.6194437	-2.1389846	-0.9073473
C	1.6391774	-3.7360805	0.8712599
H	1.6545626	0.5967840	-3.0230657
H	-0.5124171	-3.3568218	0.6421437
H	2.3451482	-0.1162469	-4.5223848
H	-0.3805068	-3.7989540	-4.7156205
H	-0.0887324	-5.0988267	0.5952794
H	3.2957583	-4.8188734	-5.1700565
H	3.7643283	0.0667250	-1.7837800
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H	2.5794265	-2.4311504	-4.3267417
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C	-1.9268170	-3.9373091	-2.2790890
O	-2.2244040	-1.1224912	-2.0985880
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H	-1.3498904	-3.4123747	-1.5028795
Br	1.1609643	-1.4191320	3.8939592
Zn	-0.7811338	-1.4538845	2.5896937
H	-4.2251165	-3.9448889	-0.6618491
H	-2.8543303	-2.4262203	3.8271912
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C	-3.4897945	-2.1711687	1.7955672
C	-2.7400597	-1.7303537	2.9743018
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O	-4.3980415	-1.9058085	-0.3352972
O	-3.2923085	-0.1173567	0.4883586
H	-5.7758049	-3.4060216	0.0705044
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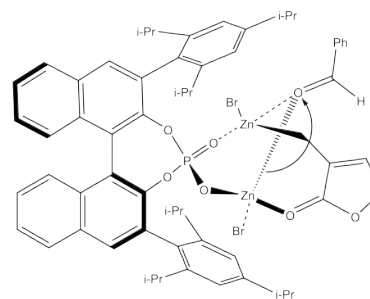


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C	3.3212383	5.9727890	1.5415168

C	1.1063709	4.8541278	1.5996037
H	0.6235705	5.8414388	1.6589561
C	0.3177903	3.7137861	1.5261225
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C	4.1689401	-1.6133491	1.0114777
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C	5.5980645	-1.2487570	3.0073634
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O	0.1898844	1.3131020	1.5291824
O	1.5119152	0.4294939	-0.4672646
P	-0.0058835	0.4174076	0.1585515
O	-0.8534236	1.1590319	-0.8853866
O	-0.4473333	-0.9641576	0.6477682
C	4.6982513	5.9136556	1.3920613
C	5.3350074	4.6566938	1.2171531
H	2.8110014	6.9430034	1.6486598
H	5.2959196	6.8379279	1.3909478
H	5.1010166	2.5178816	1.0833114
H	6.4245363	4.6115974	1.0671446
C	5.3154503	0.7594867	4.3429702
C	5.9576554	-0.4849523	4.1066532
H	3.8482433	2.1897911	3.6687597
H	5.5779685	1.3492948	5.2344320
H	6.7250878	-0.8485594	4.8068521
H	6.0671798	-2.2291119	2.8287333
C	-1.7601657	4.0500625	0.1375877
C	-1.1723410	3.7210767	1.3910905
C	-3.1522980	3.8876878	-0.0119856
C	-1.9843091	3.2801099	2.4703208
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C	-3.9734881	3.4197781	1.0305882
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C	-1.3879354	3.0400093	3.8559572
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H	-1.2040580	1.4976325	5.4002351
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H	-7.3311015	4.2423272	1.5306082
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H	-0.4424017	6.6286565	-1.7976753
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H	3.0578297	1.3424206	-3.7985856
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C	1.7899185	-3.9292674	-2.9667628
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H	1.0719731	-3.4988169	-5.7133616
C	2.3910325	-2.6964037	-3.2717132
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H	3.2681818	-6.0728131	-3.8902103
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C	2.8151261	-1.7997154	-2.2749933
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C	1.9723184	-3.3665677	-0.5718970
H	3.6614369	-4.5860604	1.2897613
H	2.4470707	-5.8103240	0.8152737
C	3.4987346	-0.5024233	-2.7029780
C	2.6206066	-2.1439809	-0.9076853
C	1.6650189	-3.7536249	0.8731835
H	1.6245631	0.5914551	-3.0241361
H	-0.4894296	-3.3775730	0.6616203
H	2.3178541	-0.1157294	-4.5242165
H	-0.3822701	-3.8145896	-4.7186055
H	-0.0625037	-5.1190730	0.6061440
H	3.2992086	-4.8197830	-5.1665286
H	3.7404414	0.0733063	-1.7875064
H	1.8388686	-2.8597091	1.5050993
H	2.5532999	-2.4245794	-4.3269658
Zn	-2.7398395	0.8467756	-1.2765857
Br	-4.3724154	1.6420658	-2.7231088
C	-2.6323810	-5.9032111	-3.3676399
C	-2.8625812	-1.6652750	-2.9602627
C	-1.8585056	-5.2510317	-2.3876494
C	-3.5216339	-3.7720270	-4.1144439
C	-2.7454834	-3.1150969	-3.1336943
C	-3.4572713	-5.1660184	-4.2359522
C	-1.8997400	-3.8586868	-2.2753251
O	-2.1980808	-1.0450220	-2.1220568
H	-2.5891523	-6.9997768	-3.4564870
H	-4.1757603	-3.1805299	-4.7748797
H	-1.2138140	-5.8349265	-1.7144131
H	-4.0540184	-5.6831061	-5.0020871
H	-1.2915787	-3.3203307	-1.5323809
Br	1.1671311	-1.4565697	3.8881121
Zn	-0.7665819	-1.4538189	2.5941241
H	-4.1960904	-3.9197853	-0.6891019
H	-2.8638764	-2.3926556	3.8194346
C	-4.0535193	-3.3408132	1.4261116
C	-4.6491841	-3.2343719	0.0627128
H	-4.0957990	-4.2541553	2.0344165
C	-3.4780009	-2.1501559	1.7795686
C	-2.7371049	-1.7078986	2.9596254
C	-3.6774914	-1.2588988	0.6144519
O	-4.3735021	-1.8837154	-0.3589211
O	-3.2848412	-0.0913059	0.4799978
H	-5.7519556	-3.3826519	0.0356917
H	-3.0499191	-0.6842780	3.2520670
H	-3.6144771	-1.1198731	-3.5902223



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C	3.263476	3.370925	1.611587
C	4.672579	3.502272	1.426007
C	2.487397	4.573119	1.804971
C	3.156014	5.831492	1.876510
C	1.067786	4.492702	1.882400
H	0.490696	5.417112	2.036357
C	0.390812	3.288146	1.736859
C	3.719441	-1.333623	0.250842
C	4.793102	-1.610570	1.088100
H	5.375080	-2.530880	0.928077
C	5.124177	-0.770488	2.189852
C	6.167815	-1.127032	3.095500
C	4.366524	0.436492	2.426789
C	4.654454	1.192760	3.602290
C	3.329962	0.805125	1.491565
C	3.018786	-0.109457	0.479419
O	0.502265	0.899172	1.561646
O	1.981533	0.190477	-0.398378
P	0.443432	0.064133	0.149136
O	-0.366707	0.875639	-0.882964
O	0.033863	-1.352963	0.516243
C	4.530925	5.919202	1.724480
C	5.289821	4.743973	1.480862
H	2.550748	6.737277	2.039040
H	5.032680	6.897314	1.775439
H	5.271328	2.602657	1.228789
H	6.377262	4.817283	1.327790
C	5.664038	0.807132	4.473536
C	6.440431	-0.352902	4.212675
H	4.054406	2.086570	3.822109
H	5.859384	1.403245	5.377901
H	7.243412	-0.644983	4.906386
H	6.742158	-2.045461	2.896334
C	-1.821865	3.693950	0.570775
C	-1.107890	3.222030	1.709635
C	-3.228037	3.650265	0.585799
C	-1.823072	2.700096	2.821680
C	-3.230539	2.698992	2.791937
C	-3.957276	3.167266	1.685532
H	-3.786061	4.004356	-0.296318
C	-1.109707	2.153003	4.056215
H	-3.773114	2.299772	3.662723
C	-1.413835	0.660794	4.283926
H	-2.491037	0.485755	4.487016
H	-0.846223	0.276378	5.156003
H	-1.128736	0.055222	3.401732
C	-1.429869	2.998204	5.302451
H	-0.018272	2.240468	3.880664
H	-2.508151	2.949781	5.561844
H	-1.171913	4.064524	5.140662
H	-0.858603	2.634599	6.181259
C	-5.481699	3.203872	1.662182
C	-6.145129	1.971937	2.294743
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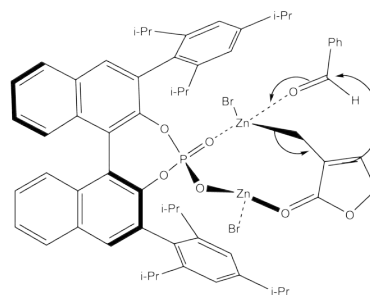
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H	-5.780991	1.035265	1.830587
C	-5.996521	4.502303	2.313726
H	-5.778993	3.228930	0.589304
H	-7.101876	4.573642	2.241016
H	-5.558613	5.398730	1.830931
H	-5.722576	4.532881	3.389028
C	-1.110067	4.254635	-0.660709
C	-1.695543	3.728415	-1.980413
H	-1.023496	3.931019	-2.837252
H	-2.688805	4.160234	-2.216867
H	-1.863603	2.634435	-1.905577
C	-1.137053	5.795274	-0.666484
H	-0.052668	3.923549	-0.614212
H	-0.589783	6.200773	-1.542402
H	-0.679011	6.216724	0.248978
H	-2.182995	6.164456	-0.715992
H	1.462860	-5.941505	-3.362287
H	5.152286	-1.568009	-4.288431
H	3.413991	-5.290069	2.482777
C	1.560635	-4.939020	-3.834854
H	3.591800	1.184631	-3.783978
H	-0.363072	-5.119374	-4.901694
H	0.936171	-4.548142	2.462465
C	2.193051	-4.022432	-2.793558
C	5.331151	-0.972381	-3.368778
C	0.139141	-4.451949	-4.170229
H	0.167297	-3.428673	-4.602078
C	2.795709	-2.802630	-3.145597
C	3.509016	-5.017333	1.411206
H	3.437134	-5.432830	-4.866594
C	2.127011	-4.350713	-1.430175
C	2.406453	-5.102960	-5.105891
H	1.951072	-5.853979	-5.783512
H	1.645636	-5.298172	-1.138651
C	3.089607	0.230190	-3.523112
H	5.862626	-0.044539	-3.666263
H	6.005948	-1.562207	-2.715642
C	3.321449	-1.923986	-2.181712
C	1.056326	-4.398997	1.370707
C	2.627745	-3.505904	-0.422370
H	4.552603	-4.688704	1.231340
H	3.343313	-5.938391	0.813691
C	4.008001	-0.642886	-2.651214
C	3.236661	-2.277041	-0.806431
C	2.480740	-3.933206	1.037332
H	2.146720	0.470972	-2.995511
H	0.308030	-3.651909	1.057217
H	2.820863	-0.271408	-4.475742
H	-0.488867	-4.420487	-3.258145
H	0.798192	-5.360855	0.881493
H	2.479219	-4.153082	-5.675335
H	4.270398	-0.049037	-1.751887
H	2.683352	-3.042894	1.666285
H	2.861550	-2.519210	-4.207488
Zn	-1.432241	0.654525	-2.436011
Br	-0.845049	0.410538	-4.643164
H	-6.539041	-1.962648	-1.452617
Br	-2.506951	-3.773822	2.067955
Zn	-1.929388	-1.819651	0.915297
C	-5.481690	-1.024171	0.238072
C	-6.274271	-0.970853	-1.020727
C	-4.263323	-0.413070	0.051980
C	-3.134158	-0.178875	0.939391
C	-4.258501	-0.012500	-1.370561
O	-5.419617	-0.310039	-1.973988
O	-3.369327	0.540176	-2.048098
H	-7.212840	-0.376792	-0.937353
C	-5.085905	-4.678591	-2.979526
C	-4.125910	-3.913186	-2.310990
C	-3.154859	-3.213659	-3.065649

C	-3.154431	-3.272280	-4.475788
C	-4.113244	-4.047953	-5.136306
C	-5.072967	-4.751725	-4.387755
H	-5.840456	-5.240076	-2.407887
H	-4.083406	-3.857906	-1.210323
C	-2.104479	-2.449120	-2.394199
H	-2.393699	-2.704404	-5.034766
H	-4.108457	-4.112661	-6.234401
H	-5.819304	-5.371517	-4.907923
O	-2.038501	-2.291869	-1.174553
H	-5.843620	-1.481951	1.167989
H	-1.330492	-1.983214	-3.061467
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H	-2.561173	0.721341	0.650707

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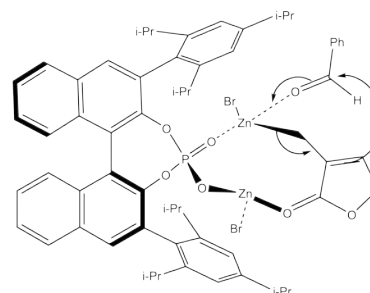


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C	4.6216366	3.7187189	1.0442979
C	2.4812601	4.9001963	1.3412111
C	3.2126203	6.1173633	1.4846844
C	1.0568078	4.8886756	1.3795022
H	0.5220616	5.8286736	1.5852894
C	0.3322251	3.7267813	1.1496782
C	3.4943811	-1.1056248	-0.1299473
C	4.4808704	-1.4042260	0.8035993
H	5.0310747	-2.3521994	0.7305959
C	4.7697710	-0.5447369	1.9036153
C	5.7130821	-0.9310431	2.9027327
C	4.0595010	0.7020587	2.0518604
C	4.2708316	1.4637634	3.2388614
C	3.1453762	1.1024581	1.0091955
C	2.8800730	0.1857136	-0.0073824
O	0.2956672	1.3811473	0.7086251
O	1.9926370	0.5658186	-1.0099097
P	0.3887934	0.5982717	-0.7341376
O	-0.1151091	1.4546962	-1.9180578
O	-0.2814821	-0.7572250	-0.5021428
C	4.5971939	6.1316286	1.4051929
C	5.3029921	4.9219433	1.1678047
H	2.6511952	7.0509702	1.6470395
H	5.1488681	7.0781843	1.5109248
H	5.1802134	2.7922019	0.8523402
H	6.3997549	4.9378827	1.0757833
C	5.1782116	1.0483782	4.2044945
C	5.9215212	-0.1489812	4.0292645
H	3.6942412	2.3859080	3.3941099
H	5.3161408	1.6493572	5.1163531
H	6.6448328	-0.4642400	4.7967393
H	6.2575469	-1.8794729	2.7714377
C	-1.9369729	4.0346842	0.0567613
C	-1.1652119	3.6771372	1.1941888
C	-3.3388104	3.9627699	0.1422651

C	-1.8054938	3.2179412	2.3784471	H	2.7521854	-3.0452106	1.3769421
C	-3.2112724	3.1396368	2.4016425	H	1.8384502	-2.0150368	-4.3989053
C	-3.9982953	3.5055520	1.2960283	Zn	-1.7801235	1.2309442	-2.8506798
H	-3.9509556	4.2440237	-0.7297619	Br	-2.3118184	0.8244188	-5.0316552
C	-0.9917102	2.8557276	3.6211312	H	-4.2202840	-3.1288580	-2.1036014
H	-3.7031138	2.7721555	3.3130261	Br	0.6896592	-1.1402366	3.0698705
C	-1.6022107	1.7281706	4.4650678	Zn	-0.8536448	-1.4121725	1.3389496
H	-2.5587897	2.0288027	4.9415449	C	-3.9728440	-2.3755464	-0.0316117
H	-0.9039652	1.4470599	5.2784958	C	-4.5090871	-2.2945471	-1.4329840
H	-1.7760694	0.8173816	3.8598888	C	-3.4572981	-1.0932609	0.2969083
C	-0.7468722	4.1129160	4.4797675	C	-2.8961462	-0.5785573	1.4755646
H	-0.0023159	2.4891194	3.2762507	C	-3.3644845	-0.3776409	-0.9934586
H	-1.7085253	4.5281733	4.8481277	O	-3.9299298	-1.0769353	-1.9790552
H	-0.2347102	4.9080772	3.9021148	O	-2.8433682	0.7327661	-1.2049884
H	-0.1172639	3.8709462	5.3609180	H	-5.6139948	-2.1849430	-1.4803146
C	-5.5136092	3.3345437	1.2736117	C	-3.5512144	-6.9436367	0.6574283
C	-5.8782719	1.9962059	0.5969160	C	-3.0231805	-5.6578972	0.8248080
H	-6.9786493	1.8760347	0.5156887	C	-2.7355906	-4.8559502	-0.3017503
H	-5.4796670	1.1428303	1.1850270	C	-2.9658815	-5.3728726	-1.5955745
H	-5.4452414	1.9302417	-0.4215521	C	-3.4937584	-6.6631553	-1.7604001
C	-6.1802512	3.4536677	2.6502473	C	-3.7923388	-7.4485599	-0.6348753
H	-5.9161525	4.1498326	0.6312608	H	-3.7719437	-7.5641994	1.5396470
H	-7.2842858	3.4379742	2.5486851	H	-2.8114879	-5.2533669	1.8261339
H	-5.8951496	4.3940788	3.1637636	C	-2.1580338	-3.4954018	-0.1267468
H	-5.9037344	2.6077608	3.3137512	H	-2.7036443	-4.7701263	-2.4794636
C	-1.2675517	4.4539906	-1.2512906	H	-3.6623874	-7.0601712	-2.7730851
C	-2.0516317	3.9970547	-2.4950725	H	-4.2044076	-8.4612601	-0.7631196
H	-1.3958938	3.9030110	-3.3838776	O	-1.5519540	-3.2165647	0.9729373
H	-2.8699611	4.6932420	-2.7723078	H	-4.4459128	-3.0335734	0.7096861
H	-2.5931654	3.0395211	-2.2976398	H	-1.8045476	-3.0104886	-1.0689809
C	-1.0210016	5.9726248	-1.3231966	H	-3.1969807	-1.0214721	2.4384498
H	-0.2818022	3.9465036	-1.2819532	H	-2.6357816	0.4949762	1.4844196
H	-0.5351709	6.2488171	-2.2819334				
H	-0.3648286	6.3148108	-0.5005003				
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H	-0.3906171	-4.8564155	-3.1919407				
H	4.6183003	-1.8427201	-4.6182303				
H	4.0847431	-5.1488772	1.5621071				
C	0.0790181	-4.0384339	-3.7821428				
H	3.6431804	1.2320808	-4.3343926				
H	-1.8528298	-3.4710108	-4.6764626				
H	1.6364742	-4.9872696	2.3009043				
C	1.1509480	-3.4188910	-2.8964682				
C	4.9304133	-1.2043026	-3.7650417				
C	-1.0161793	-3.0056858	-4.1140329				
H	-0.6213224	-2.1750550	-4.7346271				
C	1.9361517	-2.3465832	-3.3535524				
C	3.7846450	-4.7723156	0.5619615				
H	1.4264775	-5.4290051	-4.8221844				
C	1.3700900	-3.8810263	-1.5886904				
C	0.6598227	-4.6647904	-5.0615933				
H	-0.1371215	-5.1509189	-5.6618451				
H	0.8071011	-4.7615076	-1.2420801				
C	2.9752962	0.3956276	-4.0430598				
H	5.6215726	-0.4277289	-4.1543153				
H	5.4935711	-1.8439940	-3.0554765				
C	2.8162692	-1.6576785	-2.5043958				
C	1.3759013	-4.6762574	1.2690177				
C	2.2550173	-3.2422583	-0.6980348				
H	4.6520086	-4.2483093	0.1133574				
H	3.5704654	-5.6499196	-0.0837084				
C	3.7056045	-0.5587252	-3.0849543				
C	2.9153693	-2.0510569	-1.1368358				
C	2.5343382	-3.8703027	0.6666648				
H	2.0701792	0.8249879	-3.5711327				
H	0.4417299	-4.0886121	1.3189296				
H	2.6675278	-0.1130035	-4.9804660				
H	-1.4332141	-2.5421322	-3.1961455				
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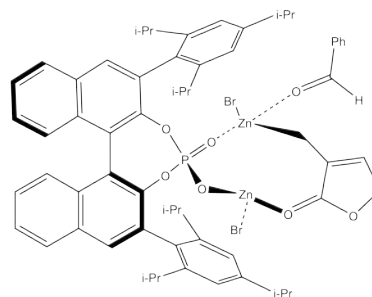


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C	4.6205119	3.7252653	1.0491287
C	2.4790173	4.9045263	1.3425170
C	3.2094265	6.1212516	1.4896445
C	1.0547959	4.8908715	1.3781701
H	0.5173390	5.8290114	1.5858152
C	0.3317881	3.7288804	1.1449663
C	3.4935541	-1.1032434	-0.1258297
C	4.4782088	-1.4010355	0.8096657
H	5.0250448	-2.3510866	0.7396523
C	4.7683320	-0.5398868	1.9075739
C	5.7098983	-0.9252226	2.9079647
C	4.0597738	0.7079731	2.0530501
C	4.2709391	1.4709972	3.2389234
C	3.1474147	1.1077045	1.0085398
C	2.8827767	0.1900755	-0.0072902
O	0.2969758	1.3852556	0.7001513
O	1.9984301	0.5705620	-1.0125862
P	0.3950420	0.6018985	-0.7416658

O	-0.1109490	1.4566209	-1.9265324	H	5.6204196	-0.4524008	-4.1555952
O	-0.2779319	-0.7534096	-0.5137601	H	5.4843177	-1.8638601	-3.0516125
C	4.5936255	6.1367397	1.4139019	C	2.8108460	-1.6593228	-2.4974132
C	5.3004505	4.9283163	1.1766684	C	1.3837467	-4.6776321	1.2852736
H	2.6469792	7.0542713	1.6519127	C	2.2497432	-3.2394841	-0.6870302
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H	5.1789839	2.7986606	0.8580018	H	3.5697027	-5.6458771	-0.0835808
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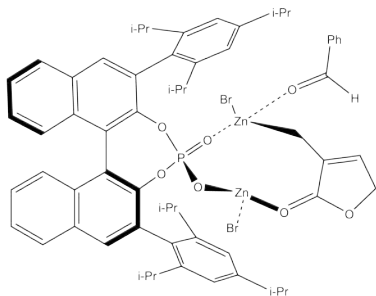


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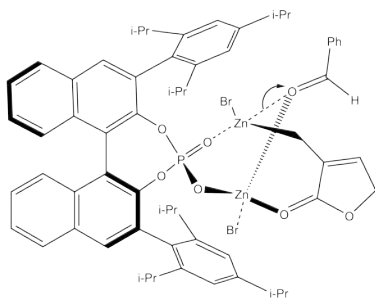
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H	1.0909128	-5.3903208	1.1303526
H	2.2451182	-4.4745837	-5.6033848
H	4.1215087	-0.0545540	-2.0800445
H	2.5536114	-2.7173894	1.6220969
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Zn	-1.7877999	0.0321613	-2.3683877
Br	-1.3110095	-0.6468507	-4.5053355
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Br	-0.9828848	-2.3312208	3.9600912
Zn	-1.5985880	-1.5600216	1.8476367
C	-5.3187691	-1.3471643	1.2445419
C	-6.1499536	-1.8880948	0.1354211
C	-4.1820532	-0.7587692	0.7405068
C	-3.0223081	-0.1509948	1.3768256
C	-4.3044399	-0.9127914	-0.7251886
O	-5.4373508	-1.5440453	-1.0683847
O	-3.5335718	-0.5533888	-1.6374863
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C	-2.9949888	-3.7911539	-2.8968977
C	-3.9074745	-4.4460339	-3.7332797
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H	-5.5745004	-5.8358629	-3.8404896
O	-2.2479618	-3.2320015	0.6033703
H	-5.5863830	-1.4397080	2.3053594
H	-1.3286999	-2.6563591	-1.1270411
H	-3.2724696	0.2936501	2.3581470
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7.2.4.7 to 15p-ma

TS1-8-p; woelfling data



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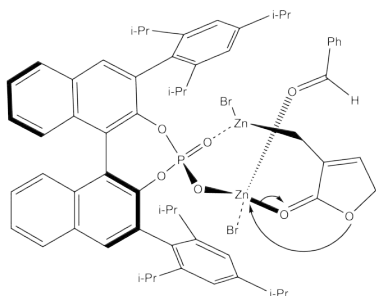
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C	4.886514	-0.330772	2.141090
C	5.897665	-0.587131	3.114922
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C	4.371728	1.769808	3.318400
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P	0.277348	0.301744	-0.203507
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H	4.762408	7.267162	1.095979
H	5.034440	2.951187	0.771911
H	6.120141	5.179136	0.737941
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C	6.132553	0.301353	4.152395
H	3.767905	2.681411	3.423865
H	5.513797	2.170413	5.102299
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C	2.687188	-3.040111	-2.956706
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H	4.429133	-4.355743	1.672529
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TS2-8-p; woelfling data



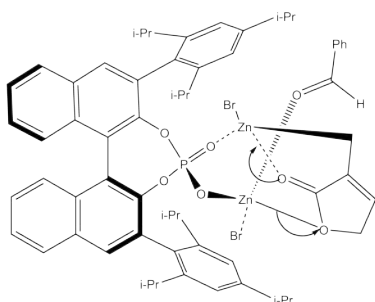
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H	0.1165080	-5.1266296	0.4148119
H	4.7640617	-5.6595984	-3.3220141
H	3.9946279	0.2657839	-1.3061816
H	1.3508856	-2.5399163	1.5706076
H	3.6548180	-2.4751203	-3.8511279
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H	-0.719120	1.093170	5.565752
H	-1.611031	0.486245	4.144939
C	-1.195225	3.833759	5.131269
H	-0.272470	2.562507	3.672170
H	-2.168262	3.983776	5.644854
H	-0.936654	4.781732	4.616564
H	-0.427117	3.643299	5.909686
C	-6.116105	2.885386	2.628167
C	-6.435972	1.379040	2.686361
H	-7.517092	1.205727	2.869473
H	-5.868052	0.884704	3.501923
H	-6.156422	0.877994	1.738442
C	-6.584340	3.611289	3.900183
H	-6.680960	3.313944	1.770412
H	-7.677315	3.487520	4.046137
H	-6.363559	4.696598	3.849565
H	-6.084394	3.209463	4.805854
C	-2.437162	4.084470	-0.658427
C	-3.254402	3.365869	-1.744005
H	-2.824776	3.554054	-2.752140
H	-4.306366	3.713376	-1.807495
H	-3.354440	2.275597	-1.509469
C	-2.524077	5.608847	-0.853298
H	-1.379180	3.781637	-0.796113
H	-2.208634	5.899624	-1.877160
H	-1.872870	6.140822	-0.132578
H	-3.562155	5.969965	-0.697483
H	2.413272	-6.067698	-3.516845
H	5.535005	-1.136127	-4.000142

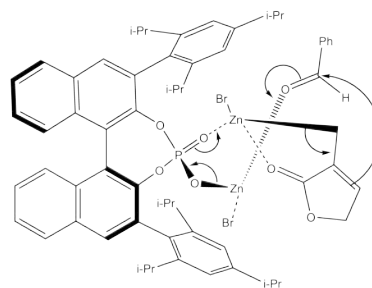
TS3-8-p; woelfling data



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C	2.448028	3.643681	1.182755
C	3.853078	3.773880	0.972022

H	1.900796	-4.693948	2.716244
C	3.331804	-5.454813	-3.670682
H	3.388782	1.135412	-3.889145
H	3.323278	-5.947445	-5.800436
H	-0.259371	-4.347316	1.448756
C	3.220983	-4.276382	-2.706332
C	5.432988	-0.551092	-3.062337
C	3.361877	-5.050144	-5.149996
H	4.292779	-4.503234	-5.406939
C	3.576474	-2.965300	-3.056499
C	2.474061	-4.594747	1.772387
H	4.464673	-6.701198	-2.257341
C	2.685846	-4.486921	-1.419242
C	4.528199	-6.354167	-3.307971
H	4.566923	-7.248526	-3.964078
H	2.354288	-5.502373	-1.141992
C	3.036555	0.120025	-3.612370
H	5.803264	0.473463	-3.271230
H	6.100904	-1.011260	-2.306270
C	3.487435	-1.895217	-2.141728
C	0.310467	-4.267758	0.500908
C	2.486559	-3.439075	-0.504417
H	3.468758	-4.174195	2.020788
H	2.630620	-5.612476	1.355648
C	3.975878	-0.512713	-2.568202
C	2.963387	-2.140852	-0.846388
C	1.712027	-3.695680	0.787333
H	2.007616	0.215498	-3.213841
H	-0.260676	-3.606843	-0.181318
H	2.995608	-0.486527	-4.541493
H	2.503980	-4.398263	-5.413506
H	0.349219	-5.277332	0.039718
H	5.482803	-5.800430	-3.421490
H	3.956778	0.140467	-1.672229
H	1.549086	-2.718200	1.286158
H	3.959161	-2.759348	-4.066740
Zn	-1.931900	1.340616	-2.862096
Br	-2.058548	1.915309	-5.082579
C	-0.499432	-5.140699	-4.073772
C	-2.656869	-1.512905	-3.655053
C	-0.091781	-4.188489	-3.122394
C	-2.358862	-3.732274	-4.721784
C	-1.943122	-2.768787	-3.770388
C	-1.637112	-4.920328	-4.870708
C	-0.805034	-3.002583	-2.960931
O	-2.361175	-0.645611	-2.815122
H	0.085458	-6.066133	-4.193249
H	-3.248174	-3.535229	-5.340597
H	0.797662	-4.361717	-2.507010
H	-1.950174	-5.675311	-5.606335
H	-0.503219	-2.249398	-2.215862
Br	-0.601290	-1.968005	3.252786
Zn	-1.933666	-1.881614	1.324490
H	-5.077240	-0.436369	-2.932105
H	-3.677223	-3.772693	0.438547
C	-5.084257	-1.967296	-1.334443
C	-5.430549	-0.618145	-1.891672
H	-5.443826	-2.910530	-1.769447
C	-4.325905	-1.816512	-0.212895
C	-3.689061	-2.714581	0.761338
C	-4.099153	-0.352028	-0.055294
O	-4.771709	0.332463	-1.037462
O	-3.389308	0.209578	0.763943
H	-6.525382	-0.413899	-1.882039
H	-4.235168	-2.657944	1.731130
H	-3.493242	-1.331944	-4.379845



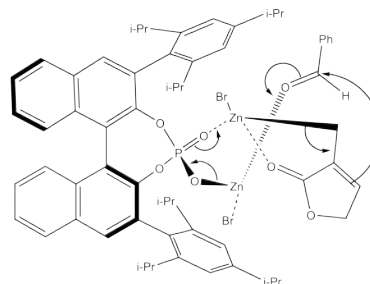
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C	1.8756084	2.1381780	1.6755873
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C	3.9503738	3.5617884	1.7960295
C	1.7209354	4.6118536	1.8528846
C	2.3604764	5.8815446	1.9818679
C	0.3028395	4.5034123	1.7776354
H	-0.3058425	5.4152328	1.8773212
C	-0.3352227	3.2843711	1.5758891
C	3.2939296	-1.2568532	0.5770142
C	4.1780351	-1.5256309	1.6165694
H	4.8164834	-2.4198990	1.5578980
C	4.2735583	-0.6902850	2.7657301
C	5.1285790	-1.0303823	3.8570446
C	3.4799057	0.5125114	2.8408488
C	3.5395327	1.2907561	4.0358445
C	2.6382637	0.8592197	1.7226916
C	2.5323020	-0.0537256	0.6705436
O	-0.1512291	0.8915043	1.3246926
O	1.6671954	0.2483967	-0.3856357
P	0.0637678	0.1011800	-0.0937026
O	-0.6464717	0.8344530	-1.2341294
O	-0.3089935	-1.3657052	0.1465566
C	3.7432157	5.9834395	2.0121552
C	4.5416426	4.8129767	1.9047637
H	1.7307063	6.7829851	2.0439506
H	4.2241539	6.9690802	2.1052836
H	4.5800897	2.6657525	1.7049706
H	5.6390465	4.8985010	1.9024355
C	4.3684385	0.9228139	5.0868415
C	5.1811775	-0.2389396	4.9945793
H	2.9088065	2.1863043	4.1247205
H	4.3909134	1.5339816	6.0020194
H	5.8390958	-0.5161838	5.8322644
H	5.7363613	-1.9458563	3.7827453
C	-2.5181879	3.4781366	0.2989743
C	-1.8292923	3.1884013	1.5078865
C	-3.9242068	3.4424339	0.3007258
C	-2.5535118	2.8319206	2.6763889
C	-3.9588059	2.7999857	2.6195103
C	-4.6659946	3.1090023	1.4467095
H	-4.4715657	3.6644120	-0.6292242
C	-1.8500778	2.4583048	3.9796922
H	-4.5158655	2.5169344	3.5262844
C	-1.9816848	0.9511647	4.2675099
H	-3.0448629	0.6553085	4.3866095
H	-1.4475068	0.6802732	5.2017372
H	-1.5597215	0.3431955	3.4456452
C	-2.3362522	3.3092399	5.1660952
H	-0.7693148	2.6752898	3.8521067
H	-3.4045668	3.1182645	5.3995226
H	-2.2252049	4.3934647	4.9595111
H	-1.7526877	3.0713294	6.0793487
C	-6.1895397	3.1155325	1.4081921
C	-6.8161135	1.8652799	2.0464685
H	-7.9180585	1.8704449	1.9162537

TS4-8-p; COSMO

H	-6.6167059	1.8187236	3.1372457	Zn	-1.7680075	-2.1572973	1.1944870
H	-6.4132829	0.9399369	1.5898961	H	-5.3388670	0.4069440	-2.2459888
C	-6.7418988	4.4031051	2.0500067	H	-3.3923571	-4.0236693	-0.5326179
H	-6.4801797	3.1245370	0.3339581	C	-4.8387053	-1.6760542	-1.6376032
H	-7.8490817	4.4432035	1.9789627	C	-5.4592127	-0.3118646	-1.4110285
H	-6.3307539	5.3073638	1.5574178	H	-5.3995596	-2.4651137	-2.1579650
H	-6.4682531	4.4536199	3.1250190	C	-4.0877805	-1.9650280	-0.4785430
C	-1.7647351	3.8156809	-0.9870900	C	-3.4311264	-3.0929503	0.0520606
C	-2.4183727	3.1934618	-2.2344478	C	-3.9474601	-0.6710178	0.2510009
H	-1.7060881	3.1931719	-3.0891519	O	-4.7356332	0.2603432	-0.2882708
H	-3.3077536	3.7601504	-2.5803407	O	-3.1701497	-0.4512901	1.1861643
H	-2.7836096	2.1671694	-2.0187500	H	-6.5334509	-0.3755707	-1.1339986
C	-1.5984396	5.3349656	-1.1751393	H	-3.6097501	-3.2653577	1.1370807
H	-0.7528977	3.3710472	-0.8957657	H	-4.4917184	-1.2917963	-3.9353933
H	-1.0468640	5.5587591	-2.1119149				
H	-1.0385890	5.7899232	-0.3350779				
H	-2.5884016	5.8345033	-1.2317719				
H	2.5507318	-5.7677156	-3.7249165				
H	6.0180857	-1.0010373	-3.3348699				
H	2.3890420	-5.1766428	2.5635876				
C	3.1618289	-4.8869600	-4.0250033				
H	4.0156848	1.4755569	-3.2228072				
H	2.4551198	-5.0270332	-6.0950980				
H	0.0872569	-4.8138012	1.5334779				
C	3.1573178	-3.9264268	-2.8420037				
C	5.8395616	-0.4667828	-2.3782301				
C	2.5157662	-4.2758247	-5.2807403				
H	3.1069111	-3.4191581	-5.6657919				
C	3.6796957	-2.6268736	-2.9532018				
C	2.8752569	-4.8682345	1.6151725				
H	5.0373054	-5.8719582	-3.4273942				
C	2.6322928	-4.3160230	-1.5980017				
C	4.5872720	-5.3913262	-4.3194048				
H	4.5848111	-6.1307295	-5.1471476				
H	2.2027421	-5.3266183	-1.5037009				
C	3.5870341	0.4555255	-3.1379285				
H	6.2954630	0.5410709	-2.4673304				
H	6.3768415	-1.0181574	-1.5797373				
C	3.7120123	-1.7370249	-1.8648103				
C	0.5949144	-4.6201113	0.5678770				
C	2.6098943	-3.4560722	-0.4817679				
H	3.8377530	-4.3825132	1.8690279				
H	3.1067307	-5.7864073	1.0349326				
C	4.3353122	-0.3568811	-2.0664771				
C	3.1878649	-2.1615859	-0.6113147				
C	1.9502123	-3.9330173	0.8134247				
H	2.5121688	0.5556048	-2.8920382				
H	-0.0743512	-3.9843721	-0.0465643				
H	3.6579397	-0.0193463	-4.1385665				
H	1.4913191	-3.9069371	-5.0727747				
H	0.7057550	-5.5918591	0.0430222				
H	5.2490037	-4.5512831	-4.6183683				
H	4.2486015	0.2005904	-1.1123094				
H	1.7473491	-3.0361970	1.4350888				
H	4.0852896	-2.2913618	-3.9207612				
Zn	-1.2948317	0.6515865	-3.0475783				
Br	-0.0298028	1.0494547	-4.9222905				
C	-0.9980658	-4.6481421	-3.6287988				
C	-3.5754369	-1.2277532	-3.3041898				
C	-0.6027208	-3.5484867	-2.8494134				
C	-3.1040046	-3.5405777	-4.1356172				
C	-2.7053827	-2.4225014	-3.3685934				
C	-2.2543666	-4.6470682	-4.2636358				
C	-1.4603900	-2.4516204	-2.7064943				
O	-3.1183177	-0.0367853	-3.1057896				
H	-0.3250626	-5.5125083	-3.7387965				
H	-4.0775570	-3.5262804	-4.6521270				
H	0.3735955	-3.5439891	-2.3445756				
H	-2.5651530	-5.5090307	-4.8734234				
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Br	-1.3197445	-2.9178369	3.3571025				

TS4-8-p

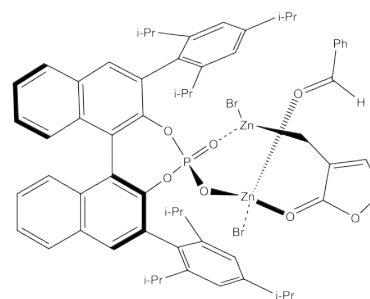


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number of imaginary frequencies: 2

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C	2.5232553	3.4154342	1.8023615
C	3.9432414	3.5605264	1.8217643
C	1.7127697	4.6070304	1.8744087
C	2.3502511	5.8758491	2.0161426
C	0.2957348	4.4966542	1.7906429
H	-0.3165012	5.4057802	1.8934540
C	-0.3400106	3.2785894	1.5772425
C	3.2994105	-1.2524008	0.5710734
C	4.1832714	-1.5219711	1.6103518
H	4.8227621	-2.4151771	1.5479457
C	4.2749658	-0.6919885	2.7632492
C	5.1285866	-1.0340138	3.8543859
C	3.4768996	0.5073037	2.8429658
C	3.5312822	1.2792261	4.0419434
C	2.6367976	0.8571996	1.7246540
C	2.5355292	-0.0509943	0.6679693
O	-0.1533724	0.8880779	1.3145362
O	1.6731504	0.2539079	-0.3892252
P	0.0699400	0.0998416	-0.1033435
O	-0.6394022	0.8291629	-1.2470289
O	-0.2985619	-1.3688308	0.1344272
C	3.7320663	5.9794512	2.0549868
C	4.5320410	4.8111796	1.9433104
H	1.7188904	6.7759711	2.0810011
H	4.2110153	6.9650047	2.1580792
H	4.5735871	2.6654058	1.7277629
H	5.6292962	4.8978174	1.9477545
C	4.3595048	0.9091311	5.0920797
C	5.1763498	-0.2486277	4.9956069
H	2.8965801	2.1715601	4.1332407
H	4.3775102	1.5154836	6.0104797
H	5.8331994	-0.5282819	5.8332506
H	5.7387930	-1.9475820	3.7769658
C	-2.5142092	3.4828803	0.2885591
C	-1.8336593	3.1849742	1.4999938

C	-3.9201395	3.4571820	0.2838401	H	4.2390028	0.2115151	-1.1239397
C	-2.5652402	2.8279239	2.6634848	H	1.7751832	-3.0450931	1.4426967
C	-3.9701173	2.8045299	2.5989516	H	4.0574496	-2.2742711	-3.9351372
C	-4.6693851	3.1243843	1.4247321	Zn	-1.2593485	0.6454163	-3.0686853
H	-4.4614878	3.6883542	-0.6474862	Br	-0.0336313	1.0466754	-4.9558184
C	-1.8704647	2.4480046	3.9695880	C	-1.0239212	-4.6983168	-3.5985973
H	-4.5329846	2.5211458	3.5019490	C	-3.5489457	-1.2402348	-3.3034944
C	-2.0087092	0.9412180	4.2553977	C	-0.6115387	-3.5978232	-2.8297969
H	-3.0729004	0.6468014	4.3675001	C	-3.1128939	-3.5655501	-4.1132154
H	-1.4811786	0.6668077	5.1920330	C	-2.6972225	-2.4461674	-3.3570947
H	-1.5831008	0.3317671	3.4368608	C	-2.2804609	-4.6852067	-4.2321818
C	-2.3593471	3.2998999	5.1541193	C	-1.4518831	-2.4867158	-2.6961302
H	-0.7882970	2.6615336	3.8478971	O	-3.0882631	-0.0560817	-3.1064913
H	-3.4292885	3.1128216	5.3827800	H	-0.3621398	-5.5720804	-3.7018868
H	-2.2441754	4.3838974	4.9494480	H	-4.0863227	-3.5408281	-4.6299804
H	-1.7819275	3.0588535	6.0703081	H	0.3658883	-3.6022628	-2.3271543
C	-6.1926771	3.1444550	1.3800921	H	-2.6042141	-5.5476939	-4.8344115
C	-6.8329905	1.8938115	2.0037320	H	-1.1445726	-1.6656466	-2.0330789
H	-7.9344132	1.9086566	1.8699464	Br	-1.2829232	-2.9410628	3.3686785
H	-6.6385802	1.8347723	3.0946335	Zn	-1.7241723	-2.1607880	1.2260696
H	-6.4349083	0.9689850	1.5420787	H	-5.2846044	0.4054628	-2.2273508
C	-6.7367618	4.4307851	2.0308719	H	-3.3905872	-4.0319490	-0.4882849
H	-6.4789721	3.1658508	0.3045845	C	-4.8271646	-1.6796588	-1.5976173
H	-7.8432087	4.4822095	1.9561700	C	-5.4242778	-0.3036347	-1.3858290
H	-6.3145995	5.3353077	1.5487892	H	-5.3919130	-2.4655039	-2.1182554
H	-6.4665265	4.4697801	3.1069993	C	-4.0703637	-1.9677297	-0.4437002
C	-1.7521955	3.8198327	-0.9928047	C	-3.4184359	-3.0992795	0.0889387
C	-2.4025233	3.2055652	-2.2459046	C	-3.9126592	-0.6693060	0.2752370
H	-1.6869159	3.2044922	-3.0976635	O	-4.6978009	0.2666395	-0.2672404
H	-3.2880848	3.7780333	-2.5925365	O	-3.1294844	-0.4474048	1.2023108
H	-2.7703888	2.1789080	-2.0374059	H	-6.5022290	-0.3414104	-1.1150540
C	-1.5753257	5.3385010	-1.1749688	H	-3.5696993	-3.2561590	1.1793602
H	-0.7435732	3.3685438	-0.8979949	H	-4.4774387	-1.3034092	-3.9190048
H	-1.0184718	5.5627341	-2.1084397				
H	-1.0155109	5.7866121	-0.3314637				
H	-2.5615145	5.8451310	-1.2328455				
H	2.5486806	-5.7617306	-3.7294333				
H	5.9980592	-0.9856082	-3.3571056				
H	2.4340104	-5.1846416	2.5572788				
C	3.1479976	-4.8746717	-4.0358621				
H	3.9921509	1.4887714	-3.2319439				
H	2.4157251	-5.0159962	-6.0978693				
H	0.1226669	-4.8261956	1.5497512				
C	3.1500413	-3.9168353	-2.8506527				
C	5.8234355	-0.4524619	-2.3992321				
C	2.4793163	-4.2672287	-5.2814696				
H	3.0562357	-3.4036250	-5.6721380				
C	3.6634968	-2.6143232	-2.9644125				
C	2.9112573	-4.8726973	1.6057508				
H	5.0394866	-5.8434442	-3.4640504				
C	2.6405789	-4.3117742	-1.6022930				
C	4.5735789	-5.3662947	-4.3494800				
H	4.5681863	-6.1040263	-5.1786605				
H	2.2202826	-5.3259942	-1.5043631				
C	3.5657036	0.4681756	-3.1454446				
H	6.2779415	0.5557540	-2.4904404				
H	6.3659862	-1.0042456	-1.6048205				
C	3.7025041	-1.7265980	-1.8748491				
C	0.6217051	-4.6296951	0.5803590				
C	2.6225658	-3.4541228	-0.4844993				
H	3.8744163	-4.3851451	1.8529847				
H	3.1415668	-5.7882691	1.0210648				
C	4.3207821	-0.3446063	-2.0793061				
C	3.1916086	-2.1560318	-0.6176275				
C	1.9764903	-3.9380076	0.8150589				
H	2.4924545	0.5690771	-2.8940745				
H	-0.0553610	-3.9951942	-0.0267948				
H	3.6303894	-0.0037377	-4.1477856				
H	1.4542917	-3.9080596	-5.0602821				
H	0.7309441	-5.6001113	0.0523805				
H	5.2243287	-4.5201350	-4.6545719				

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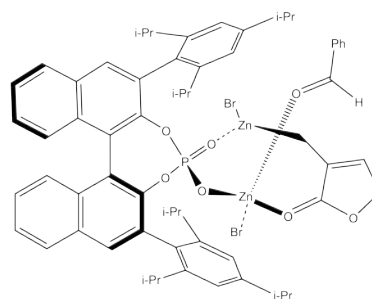


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C	2.0685856	4.6934128	2.3356472
C	2.8227534	5.8820151	2.5730259
C	0.6601465	4.7492887	2.1235848
H	0.1566382	5.7273939	2.1583481
C	-0.0764057	3.6126417	1.8175076
C	3.0379815	-1.2204723	0.7166912
C	3.9042935	-1.6453259	1.7178515
H	4.4401924	-2.5986984	1.5951832
C	4.0885176	-0.9059015	2.9199885
C	4.9009613	-1.4109863	3.9789550
C	3.4161151	0.3588875	3.0894677
C	3.5404773	1.0287321	4.3429366
C	2.6097062	0.8700999	2.0100439
C	2.4007244	0.0439525	0.8997215
O	-0.1565244	1.2178176	1.6292928
O	1.5506313	0.4785502	-0.1188908
P	-0.0592677	0.4069359	0.1970245

O	-0.7095947	1.1957974	-0.9486478	H	5.9743406	0.4753661	-2.4902871
O	-0.5498537	-1.0085930	0.5080472	H	5.9902309	-1.1338062	-1.6937032
C	4.2041813	5.8411373	2.6895441	C	3.2544964	-1.6064750	-1.7768189
C	4.8871693	4.6027668	2.5563773	C	0.0296147	-4.1910867	0.7875723
H	2.2831037	6.8395163	2.6451752	C	2.1019975	-3.2913354	-0.3985951
H	4.7732079	6.7665221	2.8670333	H	3.3891259	-4.6310716	1.6885107
H	4.7248888	2.4774746	2.2341025	H	2.3227678	-5.8229739	0.8857448
H	5.9859023	4.5748048	2.6175815	C	3.9825754	-0.2765854	-1.9642933
C	4.3217602	0.5010115	5.3614880	C	2.7854070	-2.0466952	-0.5070312
C	5.0213758	-0.7216478	5.1761526	C	1.5075444	-3.7794282	0.9210360
H	2.9921846	1.9672499	4.5042033	H	2.1860800	0.8239485	-2.5732269
H	4.3924386	1.0305056	6.3239775	H	-0.5614938	-3.3953264	0.2916123
H	5.6425079	-1.1274144	5.9893076	H	3.1774064	0.2323287	-3.9517234
H	5.4160378	-2.3735064	3.8325456	H	0.6726364	-3.4579497	-4.9621643
C	-1.8487938	4.0427871	0.0768326	H	-0.1012575	-5.1266165	0.2031678
C	-1.5116807	3.6234259	1.3943381	H	4.3852182	-4.4110796	-4.7047127
C	-3.1822469	3.8918007	-0.3532891	H	4.0241296	0.2312851	-0.9800982
C	-2.5113987	3.1009622	2.2582867	H	1.5320687	-2.9304770	1.6331938
C	-3.8262256	2.9700093	1.7790592	H	3.4411268	-2.0891004	-3.8755454
C	-4.1836698	3.3482439	0.4717528	Zn	-2.4559933	0.8231331	-1.7400813
H	-3.4570710	4.2050041	-1.3720467	Br	-3.7675295	1.7790537	-3.4091141
C	-2.1921338	2.7454908	3.7091886	C	-1.7162110	-5.7023487	-4.3279995
H	-4.5987717	2.5637131	2.4518290	C	-2.1512935	-1.5275509	-3.5953774
C	-2.5892952	1.3104844	4.0808196	C	-1.2245797	-5.1484111	-3.1288596
H	-3.6840046	1.1453161	3.9999588	C	-2.4545053	-3.5103935	-5.0653617
H	-2.2884212	1.0738926	5.1215046	C	-1.9614720	-2.9516498	-3.8641076
H	-2.0804237	0.5839025	3.4197083	C	-2.3238182	-4.8854320	-5.2985943
C	-2.8285575	3.7736888	4.6641130	C	-1.3326405	-3.7748470	-2.8977345
H	-1.0926773	2.8208514	3.8379634	O	-1.7349438	-0.9859413	-2.5612101
H	-3.9364396	3.7556034	4.5919133	H	-1.6215244	-6.7844129	-4.5075451
H	-2.4940572	4.8036371	4.4248879	H	-2.9412802	-2.8588728	-5.8084558
H	-2.5538415	3.5568995	5.7173182	H	-0.7487851	-5.7967386	-2.3781241
C	-5.6179698	3.2199419	-0.0286512	H	-2.7004646	-5.3261301	-6.2336165
C	-6.1073118	1.7613053	-0.0362864	H	-0.9397561	-3.3110461	-1.9805381
H	-7.1556986	1.7037716	-0.3960618	Br	0.3904297	-1.7066354	3.9535909
H	-6.0735385	1.3149642	0.9798180	Zn	-1.2568466	-1.6538074	2.2930625
H	-5.4803371	1.1385736	-0.7030413	H	-3.8921328	-3.9347481	-1.7603958
C	-6.5689618	4.1281280	0.7726746	H	-3.5159582	-2.7291438	3.0089343
H	-5.6200442	3.5711684	-1.0833321	C	-4.1868704	-3.5073205	0.3726597
H	-7.5976025	4.0865827	0.3578461	C	-4.5060057	-3.3129122	-1.0704110
H	-6.2313813	5.1842113	0.7519044	H	-4.3189690	-4.4643509	0.8951447
H	-6.6241346	3.8144397	1.8364674	C	-3.7278523	-2.3362849	0.9121745
C	-0.8255353	4.7017540	-0.8489897	C	-3.2466141	-1.9727749	2.2472964
C	-0.8828794	4.2170363	-2.3056836	C	-3.7196601	-1.3684202	-0.2058531
H	-0.0844374	4.7090269	-2.8984911	O	-4.1936481	-1.9290206	-1.3357971
H	-1.8495864	4.4525263	-2.7954465	O	-3.3367166	-0.1873745	-0.1822309
H	-0.7276267	3.1235322	-2.3651352	H	-5.5758029	-3.4791103	-1.3255916
C	-0.9751903	6.2356358	-0.7819285	H	-3.6533764	-0.9852057	2.5492731
H	0.1831994	4.4466300	-0.4646466	H	-2.7277106	-0.9276584	-4.3470036
H	-0.1979519	6.7357425	-1.3966033				
H	-0.8879061	6.6135767	0.2565363				
H	-1.9685047	6.5492624	-1.1665184				
H	1.6347236	-5.4333551	-3.7309922				
H	5.4908882	-0.9846779	-3.4076528				
H	1.9157149	-5.2116683	2.5257823				
C	2.3044827	-4.5958242	-4.0265911				
H	3.7284173	1.6403009	-2.9940420				
H	1.5038213	-4.6025107	-6.0664356				
H	-0.4044261	-4.3775406	1.7935158				
C	2.4355471	-3.6865133	-2.8105825				
C	5.4395028	-0.4939910	-2.4130408				
C	1.6571475	-3.8900163	-5.2297930				
H	2.2957285	-3.0659876	-5.6106655				
C	3.0660634	-2.4335795	-2.8985919				
C	2.3310422	-4.9236636	1.5378986				
H	4.1152907	-5.7529759	-3.5509688				
C	1.9607789	-4.0884949	-1.5509167				
C	3.6685846	-5.2042145	-4.4045423				
H	3.5685776	-5.9097258	-5.2557457				
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C	3.2221959	0.6550474	-2.9259320				

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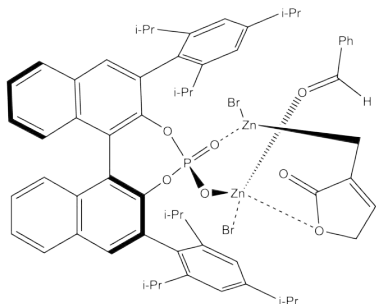


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C	4.0505572	3.4613752	2.2242230
C	1.9185305	4.6952578	2.2807617
C	2.6497321	5.8717810	2.6218742
C	0.5025601	4.7236616	2.1234298

H	-0.0388234	5.6592233	2.3317363	H	2.0493130	-4.8343661	-6.1875719
C	-0.2076981	3.6061090	1.7057343	H	-0.6067925	-4.1608095	1.6223436
C	3.0250720	-1.2267233	0.5990031	C	2.4889111	-3.8042873	-2.8566273
C	3.7772241	-1.6419342	1.6914476	C	5.6782262	-0.8082445	-2.3612986
H	4.2858676	-2.6170403	1.6520494	C	2.2884035	-4.0938800	-5.3971881
C	3.8676323	-0.8688168	2.8830225	H	3.2531369	-3.6210454	-5.6755932
C	4.5638890	-1.3616451	4.0266510	C	3.1990971	-2.5975648	-2.9580762
C	3.2059551	0.4111232	2.9573288	C	2.0939472	-4.8646042	1.5138164
C	3.2151497	1.1030536	4.2046517	H	3.5281391	-6.3459663	-3.0116648
C	2.5250568	0.9100352	1.7866271	C	1.9279888	-4.1267309	-1.6079145
C	2.4237840	0.0646385	0.6810866	C	3.5032592	-5.8124845	-3.9829981
O	-0.2154534	1.3093092	1.0482346	H	3.3906488	-6.5665254	-4.7900731
O	1.7290791	0.5149549	-0.4402297	H	1.3579807	-5.0654632	-1.5138948
P	0.0956798	0.5165907	-0.3874246	C	3.5985870	0.4547885	-3.1205269
O	-0.2985998	1.3376547	-1.6230448	H	6.2853686	0.1168622	-2.4455485
O	-0.5514772	-0.8415244	-0.1089908	H	6.1218007	-1.4395141	-1.5648217
C	4.0296668	5.8418582	2.7535101	C	3.3812849	-1.7390733	-1.8574130
C	4.7337720	4.6272044	2.5402799	C	-0.1243489	-4.0201483	0.6334104
H	2.0935451	6.8111453	2.7679262	C	2.0568450	-3.2951313	-0.4807168
H	4.5814574	6.7587298	3.0110374	H	3.1599370	-4.6299683	1.7055560
H	4.6058812	2.5282146	2.0549976	H	2.0645370	-5.7829621	0.8892279
H	5.8313102	4.6099541	2.6216088	C	4.2082148	-0.4694889	-2.0511023
C	3.8840617	0.5862547	5.3050183	C	2.8196080	-2.0968779	-0.6015468
C	4.5798273	-0.6480314	5.2146796	C	1.3682481	-3.6960483	0.8235212
H	2.6669573	2.0503309	4.2962546	H	2.5503512	0.7116458	-2.8726983
H	3.8654577	1.1346789	6.2591550	H	-0.6381674	-3.1849760	0.1182766
H	5.1118666	-1.0447150	6.0927473	H	3.6130298	-0.0168695	-4.1255101
H	5.0717571	-2.3360344	3.9513764	H	1.5081490	-3.3070774	-5.4188551
C	-2.3237715	3.9867893	0.3638444	H	-0.2818734	-4.9530468	0.0503122
C	-1.7001537	3.5842920	1.5738211	H	4.4866426	-5.3144525	-4.1144451
C	-3.7256465	3.9189612	0.2768794	H	4.2042035	0.0885154	-1.0934307
C	-2.4791192	3.0966977	2.6593761	H	1.4047400	-2.8258721	1.5088200
C	-3.8787159	3.0464715	2.5172105	H	3.6437233	-2.3125171	-3.9236282
C	-4.5226323	3.4493659	1.3345560	Zn	-1.6682430	0.8059967	-2.9205222
H	-4.2224795	4.2215568	-0.6580392	Br	-2.1436138	1.5478399	-5.0570508
C	-1.8204718	2.6590326	3.9689100	C	-1.4773329	-6.1167732	-4.2556041
H	-4.4807376	2.6617847	3.3525963	C	-1.3042862	-1.8590781	-4.1861235
C	-2.5434809	1.5035365	4.6760585	C	-1.2906001	-5.4441642	-3.0316222
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H	-1.9390462	1.1443063	5.5324293	C	-1.3294726	-3.3205374	-4.2135192
H	-2.6888554	0.6387418	3.9990224	C	-1.5830833	-5.3969880	-5.4593390
C	-1.6555370	3.8618425	4.9183975	C	-1.2075694	-4.0493758	-3.0062927
H	-0.8025873	2.2886022	3.7223444	O	-1.1442639	-1.2191443	-3.1368728
H	-2.6461597	4.2827031	5.1906551	H	-1.5363042	-7.2160731	-4.2708417
H	-1.0622352	4.6720212	4.4506229	H	-1.6038852	-3.4192802	-6.3723681
H	-1.1421565	3.5583645	5.8542952	H	-1.1964727	-6.0163132	-2.0960844
C	-6.0263061	3.2971777	1.1318926	H	-1.7230189	-5.9306604	-6.4111255
C	-6.3397125	1.9080091	0.5382666	H	-1.0379712	-3.4961344	-2.0711130
H	-7.4187406	1.8090531	0.2969158	Br	-0.0686937	-1.3489020	3.5379959
H	-6.0728123	1.1064243	1.2583185	Zn	-1.4792964	-0.7626218	1.7809423
H	-5.7564574	1.7275328	-0.3873983	H	-3.7545386	-3.6523856	-1.7683330
C	-6.8560824	3.5589830	2.3963423	H	-4.0220631	-0.8042818	2.2922082
H	-6.3216791	4.0553649	0.3725201	C	-4.3330993	-2.4882830	0.0003606
H	-7.9399360	3.5423291	2.1618040	C	-4.3884053	-2.7898059	-1.4594160
H	-6.6157459	4.5433261	2.8461939	H	-4.6543731	-3.1969371	0.7755267
H	-6.6813218	2.7821186	3.1698062	C	-3.8055850	-1.2401786	0.2014641
C	-1.4981466	4.4712622	-0.8259492	C	-3.4435022	-0.4887973	1.4032900
C	-2.1310408	4.1181719	-2.1788366	C	-3.5257895	-0.7161186	-1.1552276
H	-1.3965620	4.2167871	-3.0017601	O	-3.8657267	-1.6120096	-2.1037706
H	-2.9914755	4.7742120	-2.4261445	O	-3.0519870	0.3894631	-1.4578912
H	-2.5139036	3.0785975	-2.1868467	H	-5.4133780	-2.9672995	-1.8558004
C	-1.2232901	5.9852648	-0.7459783	H	-3.5479939	0.6041778	1.2507986
H	-0.5218225	3.9441877	-0.7752799	H	-1.4715801	-1.3094041	-5.1500027
H	-0.6162714	6.3197717	-1.6126045				
H	-0.6749637	6.2573254	0.1763127				
H	-2.1759257	6.5553402	-0.7546153				
H	1.4076698	-5.3282623	-3.8748753				
H	5.7747503	-1.3604888	-3.3195097				
H	1.6173840	-5.0972702	2.4883833				
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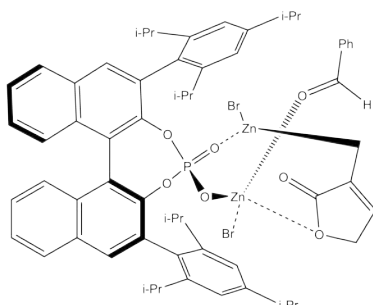
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C	4.1360144	3.5499023	1.4082714
C	2.0358788	4.7803183	1.8039934
C	2.7937859	5.9892085	1.8395631
C	0.6180258	4.7928200	1.9569764
H	0.1158981	5.7488546	2.1687377
C	-0.1407996	3.6355569	1.8421028
C	2.8837279	-1.2533794	0.4672236
C	3.8799559	-1.5691322	1.3844927
H	4.4169324	-2.5246952	1.2842440
C	4.2107764	-0.7046131	2.4658504
C	5.1735040	-1.0856553	3.4486172
C	3.5408356	0.5676723	2.5870108
C	3.8249155	1.3718342	3.7325719
C	2.5924957	0.9585947	1.5711251
C	2.2520956	0.0198123	0.5899956
O	-0.1998862	1.2483222	1.4989375
O	1.3128087	0.3487559	-0.3778092
P	-0.2744903	0.5593771	0.0147207
O	-0.7566963	1.6084766	-1.0111407
O	-0.9981698	-0.7728325	0.1538487
C	4.1694514	5.9759355	1.6607509
C	4.8414707	4.7456169	1.4309169
H	2.2595733	6.9388439	2.0004469
H	4.7398754	6.9170136	1.6841110
H	4.6656798	2.6047591	1.2225080
H	5.9296254	4.7396456	1.2648437
C	4.7519459	0.9639194	4.6819585
C	5.4459758	-0.2670443	4.5342700
H	3.2889087	2.3212116	3.8680853
H	4.9451769	1.5981791	5.5605658
H	6.1844552	-0.5754540	5.2899248
H	5.6845172	-2.0546872	3.3348036
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int2-8-p



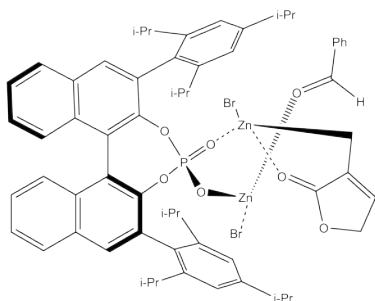
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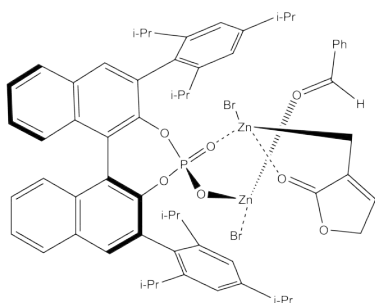
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H	-0.1990916	-5.2660907	-0.9039323
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H	1.0600626	-3.1091745	0.9107769
H	4.6392666	-2.7942632	-3.7383943
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Br	-1.4262010	1.6342739	-5.4429056
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C	-2.9341257	-1.5377019	-2.9669583
C	0.4684624	-2.7312751	-4.1289760
C	-2.1081094	-3.7404901	-3.6169906
C	-1.8344252	-2.3616635	-3.4318934
C	-1.1079214	-4.6022283	-4.0755821
C	-0.5306320	-1.8658088	-3.6886271
O	-2.9624664	-0.2993387	-2.8076505
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H	-3.1175074	-4.1240317	-3.3991496
H	1.4890384	-2.3559772	-4.2936137
H	-1.3219716	-5.6706037	-4.2247700
H	-0.2849198	-0.8082046	-3.5217918
Br	-0.4863342	-1.8882894	2.9223062
Zn	-1.9839980	-1.7534389	1.1005391
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H	-3.9092014	-3.5044755	0.2363932
C	-5.5999075	-1.4199282	-0.8818420
C	-5.8656477	0.0032734	-1.2697316
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C	-4.1721256	-0.0490477	0.2466438
O	-4.9495009	0.7934444	-0.4878615
O	-3.2337848	0.3411030	0.9320634
H	-6.9043669	0.3365486	-1.0496863
H	-4.2047877	-2.6299527	1.7719502
H	-3.8749303	-2.0884379	-2.7257179

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C	3.6056855	-1.9314928	1.5296468
H	4.1465230	-2.8903026	1.5188634
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O	-0.3875229	0.9998871	0.8794218
O	1.4712140	0.0683221	-0.6791221
P	-0.1571145	0.2739893	-0.5688393
O	-0.4241395	1.2574438	-1.7343957
O	-0.9528187	-1.0265195	-0.5341116
C	4.0089611	5.5529996	2.0087298
C	4.6738904	4.3046998	1.8794422
H	2.0993306	6.5735855	2.0269629
H	4.5937505	6.4733537	2.1585725
H	4.4724206	2.1733584	1.5931423
H	5.7731311	4.2644318	1.9199419
C	3.6751645	0.4621625	5.0368322
C	4.3466140	-0.7891400	5.0234093
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H	4.8616591	-1.1458175	5.9283373
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C	-2.6176656	3.8221781	0.4056829
C	-1.8308889	3.3745835	1.4931455
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H	-7.9324520	2.5064914	2.0919416
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H	0.8975429	-5.2143283	2.0920737
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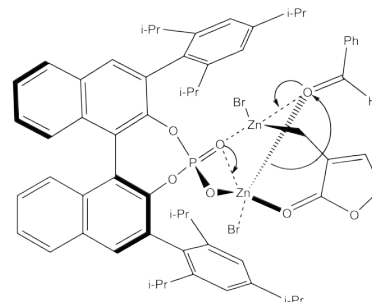
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C	3.9496353	3.1347624	1.6977780
C	1.8506483	4.4287346	1.7379659
C	2.6251706	5.6099990	1.9367730
C	0.4272100	4.4740751	1.6755501

H	4.1366404	-5.8344803	-5.9490136
H	-0.9714350	-4.3942954	0.5441947
C	3.3213127	-4.3733634	-2.8505542
C	5.9593946	-0.9196986	-2.2142285
C	4.0269819	-4.9830008	-5.2474306
H	4.9967021	-4.4437798	-5.2401149
C	3.9389003	-3.1121458	-2.9005792
C	1.6298293	-5.0846089	1.2692591
H	4.4691212	-6.7989564	-2.2833585
C	2.4170719	-4.6172300	-1.8003971
C	4.7556502	-6.3911333	-3.2731503
H	4.9672063	-7.2431399	-3.9523626
H	1.8836187	-5.5823362	-1.7717442
C	3.7932757	0.0462477	-3.1479701
H	6.4379037	0.0811387	-2.2205143
H	6.4167279	-1.5139400	-1.3975039
C	3.7423116	-2.1418570	-1.8979383
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H	2.6072323	-4.8322886	1.7272388
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C	4.4386938	-0.7888203	-2.0246538
C	2.8940228	-2.4510445	-0.8007488
C	1.1569933	-3.9791227	0.3113144
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H	-0.5647141	-3.4969834	-0.9567909
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H	4.2794241	-0.2389149	-1.0749452
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Zn	-1.6622345	1.2964385	-3.1871404
Br	-1.4342134	1.8067129	-5.4096758
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C	-2.8558053	-1.4963520	-2.9746863
C	0.5625314	-2.5824627	-4.1967021
C	-1.9624636	-3.6762608	-3.6153732
C	-1.7356563	-2.2867941	-3.4518068
C	-0.9437026	-4.5065802	-4.0890605
C	-0.4567754	-1.7480807	-3.7428620
O	-2.9306790	-0.2588845	-2.8374127
H	1.1232547	-4.6067745	-4.7454091
H	-2.9514458	-4.0929514	-3.3665338
H	1.5651347	-2.1732139	-4.3870678
H	-1.1222973	-5.5837449	-4.2212252
H	-0.2457985	-0.6798786	-3.5962457
Br	-0.5237466	-1.8493101	2.9291486
Zn	-2.0110261	-1.7233408	1.1149705
H	-5.6073406	0.2154192	-2.4439595
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C	-5.5883565	-1.3964796	-0.9514271
C	-5.8422585	0.0207314	-1.3730834
H	-6.1442148	-2.2532079	-1.3586022
C	-4.6053142	-1.4225711	-0.0085332
C	-3.8675090	-2.4590585	0.7344626
C	-4.1877988	-0.0050900	0.1877114
O	-4.9474228	0.8243335	-0.5841090
O	-3.2648020	0.3966108	0.8829989
H	-6.8864051	0.3582410	-1.1845309
H	-4.2481497	-2.5176568	1.7798824
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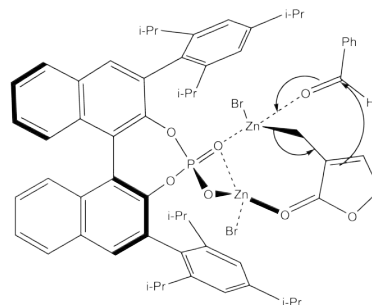
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C	2.457644	4.828449	1.047348
C	3.105819	6.098880	0.997694
C	1.053037	4.723985	1.265964
H	0.474730	5.643275	1.445181
C	0.392950	3.500558	1.242917
C	3.750621	-1.098787	-0.341151
C	4.861056	-1.323187	0.464237
H	5.465339	-2.228639	0.304013
C	5.217724	-0.439494	1.523995
C	6.307377	-0.738970	2.395318
C	4.448210	0.761812	1.749564
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C	3.363722	1.070709	0.850479
C	3.030986	0.115546	-0.113639
O	0.545543	1.109041	1.105086
O	1.933576	0.369166	-0.934743
P	0.460703	0.187298	-0.251800
O	-0.483753	0.859299	-1.275663
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C	4.461647	6.199520	0.725417
C	5.222973	5.026084	0.480016
H	2.500789	7.003531	1.166873
H	4.946507	7.186581	0.683802
H	5.225065	2.872948	0.343300
H	6.292378	5.108538	0.232956
C	5.824221	1.239254	3.719342
C	6.610798	0.083605	3.469379
H	4.162751	2.462996	3.087126
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C	-1.094459	3.386018	1.435421
C	-3.373277	3.567904	0.594277
C	-1.612321	3.012090	2.708049
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H	-4.070274	3.782702	-0.231359
C	-0.685628	2.694909	3.881751
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C	-0.686196	1.195490	4.233753
H	-1.683017	0.860157	4.587894
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H	-0.409799	0.570988	3.363342
C	-1.003097	3.560536	5.113956
H	0.345254	2.955726	3.564810
H	-2.001116	3.322860	5.537953
H	-0.992171	4.640949	4.864542
H	-0.256525	3.383372	5.915125
C	-5.425103	3.201627	2.047810
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7.2.4.8 to 15b-ma

TS1-8-b; woelfling data

H	-5.552780	1.508330	3.452661	Br	-0.981638	-3.093602	3.344680
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C	-5.889446	4.284056	3.037690	C	-5.122369	-1.438159	1.397198
H	-5.875273	3.438963	1.058162	C	-6.125863	-1.490548	0.298282
H	-6.997498	4.299566	3.104025	C	-4.029069	-0.705854	0.997117
H	-5.546388	5.292280	2.732463	C	-2.804214	-0.293831	1.657188
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C	-1.488759	4.140569	-1.000988	O	-5.517284	-0.781365	-0.800446
C	-2.247526	3.531796	-2.189992	O	-3.592390	0.273807	-1.213730
H	-1.767431	3.815383	-3.147714	H	-7.080380	-0.971117	0.544990
H	-3.304937	3.862551	-2.237416	H	-5.288996	-1.869590	2.393003
H	-2.257657	2.426393	-2.127647	H	-2.425828	-2.801727	-2.297549
C	-1.554573	5.679619	-1.079214	H	-2.924516	-0.226835	2.753796
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H	3.655251	-5.021927	1.912904				
C	1.598769	-4.751425	-4.392661				
H	3.467280	1.418856	-4.333826				
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H	1.098208	-4.526536	1.854877				
C	2.246799	-3.836283	-3.361984				
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C	0.280269	-4.136380	-4.899248				
H	0.461329	-3.174471	-5.422262				
C	2.813626	-2.601390	-3.720160				
C	3.727627	-4.744549	0.840861				
H	3.480421	-5.566477	-5.182435				
C	2.232508	-4.175449	-2.001951				
C	2.541388	-5.108322	-5.553204				
H	2.058043	-5.827013	-6.247059				
H	1.791633	-5.140954	-1.708308				
C	2.999127	0.449175	-4.065449				
H	5.773397	0.234782	-4.330837				
H	5.982994	-1.297477	-3.416516				
C	3.334880	-1.713408	-2.763000				
C	1.232707	-4.392856	0.764354				
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H	4.736326	-4.321046	0.663438				
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C	3.975249	-0.413376	-3.245827				
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H	2.075683	0.656970	-3.490544				
H	0.411272	-3.741953	0.412107				
H	2.707559	-0.050457	-5.012788				
H	-0.410313	-3.918406	-4.059559				
H	1.113732	-5.387414	0.286134				
H	2.815845	-4.211300	-6.146330				
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H	2.845052	-2.311621	-4.782614				
C	-5.158585	-5.701057	0.051496				
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H	-5.468489	-6.158894	1.003022				
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H	-6.557619	-6.873009	-1.135386				
O	-2.063583	-2.739056	-0.295407				
Zn	-1.922133	0.094019	-2.244694				
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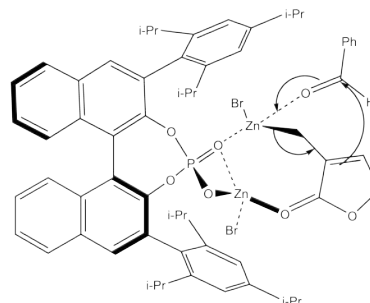


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C	2.0501584	4.9558708	0.8826748
C	2.7146828	6.2184933	0.9188291
C	0.6329762	4.8656814	0.9998456
H	0.0535072	5.7818753	1.1916721
C	-0.0334472	3.6520712	0.8871363
C	3.5273937	-0.9100033	-0.4997790
C	4.5349779	-1.1402128	0.4272714
H	5.2085004	-1.9995497	0.2904297
C	4.7160269	-0.2966696	1.5622090
C	5.6891199	-0.6042163	2.5592407
C	3.9004329	0.8839771	1.7173836
C	4.0631942	1.6719929	2.8946894
C	2.9238192	1.1947920	0.7018928
C	2.7189368	0.2471057	-0.2982143
O	0.0601405	1.2782477	0.5632241
O	1.7061061	0.4646132	-1.2421892
P	0.1501473	0.3823285	-0.7970945
O	-0.6462226	0.8769905	-2.0255683
O	-0.4118875	-1.0111952	-0.3779642
C	4.0916337	6.3041478	0.7777531
C	4.8574659	5.1232938	0.5857999
H	2.1072978	7.1278733	1.0495124
H	4.5909435	7.2847272	0.8009037
H	4.8479454	2.9744539	0.4065176
H	5.9470600	5.1947922	0.4473311
C	5.0054590	1.3335081	3.8561039
C	5.8360422	0.1943842	3.6836143
H	3.4162595	2.5471415	3.0472511
H	5.1031945	1.9488985	4.7634766
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C	-1.9871864	3.2798380	2.4142065	H	1.9082546	-2.6261358	0.3583510
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C	-5.7800664	2.8530564	1.7327412	Zn	-1.9153136	-0.6597773	-2.1091146
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H	-7.2497491	1.2793304	1.2803008	H	-5.4320173	-3.4523721	-0.0511686
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H	-6.3066316	3.5923134	1.0874895	C	-5.3210315	-2.4734991	0.4580929
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H	0.2802661	-4.4165971	0.5726407				
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TS2-8-b

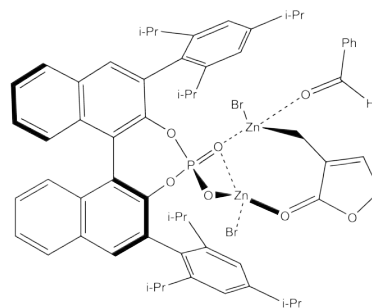


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H	0.0473368	5.7793457	1.1891392
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C	4.5406744	-1.1332119	0.4280007
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H	3.4209798	2.5536621	3.0451755	H	2.7307696	1.2619525	-3.4370198
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H	-2.4435026	4.0882553	5.1204865	H	-5.1924180	-7.3209848	-0.6222799
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C	-1.8132071	5.3740113	-1.6362891	H	-2.5349430	-0.6905640	3.1445737
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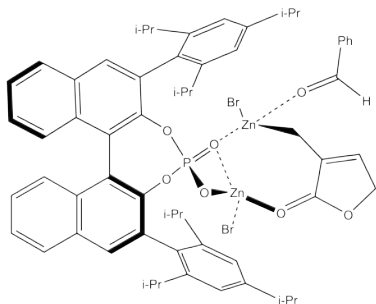


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C	2.7621901	0.1315218	-0.2056640	C	3.7576064	-4.3876475	-6.1435139
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C	-0.9521699	3.2463794	3.6571068	C	-3.4355806	-4.7301435	0.4395746
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H	-6.2423779	3.7969632	1.1707629	C	-5.7983573	-2.1052487	0.7619236
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int1-8-b



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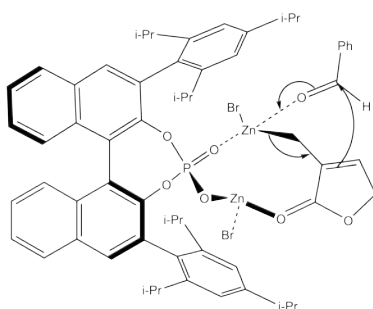
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H	2.1710952	7.0372058	0.9868145
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H	3.4148495	2.4690346	3.1344948
H	5.0872861	1.8957789	4.8752687
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H	-4.9851163	-2.1369124	2.9055149
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TS-8-l; woelfling data



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C	4.492723	-0.214169	2.980529
C	5.500648	-0.458038	3.960478
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C	4.880417	1.577220	5.129363
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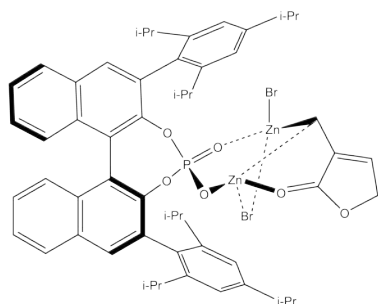
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Br	-2.447806	1.993256	-3.407417
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C	-2.7886189	4.7067149	89.8090118
C	-2.2956337	2.7011749	87.9086266
C	-2.9472511	3.8990889	87.5509619
C	-3.2146047	4.9136561	88.4834813
H	-2.9713216	5.5010539	90.5506195
C	-2.0690899	1.6489699	86.8250639
H	-3.2558566	4.0315980	86.5037729
C	-1.2258901	2.1977280	85.6595238
H	-1.7558773	3.0085094	85.1170960
H	-1.0095466	1.3949372	84.9249360
H	-0.2584899	2.5966217	86.0224865
C	-3.4072599	1.0656538	86.3334412
H	-1.5011921	0.8113159	87.2764749
H	-4.0361048	1.8428162	85.8506093
H	-3.9902379	0.6345621	87.1725712
H	-3.2337147	0.2631365	85.5870059
C	-3.9839285	6.1839561	88.1303621
C	-4.0133349	6.5085217	86.6317325
H	-4.4842589	7.4978886	86.4595420
H	-4.6102128	5.7638930	86.0651936
H	-2.9953090	6.5301220	86.1936155
C	-5.4165234	6.1119602	88.6986816
H	-3.4707886	7.0239784	88.6523926
H	-5.9678185	7.0560246	88.5080681
H	-5.4118291	5.9311806	89.7920173
H	-5.9803017	5.2824999	88.2227631
C	-1.7813925	3.3748550	91.7037721
C	-1.0219857	4.5824958	92.2782148
H	-0.7798509	4.4069670	93.3461754
H	-1.6073788	5.5224693	92.2213796
H	-0.0645450	4.7352326	91.7455782
C	-3.0452369	3.0891825	92.5403549

7.3 Complexes 13

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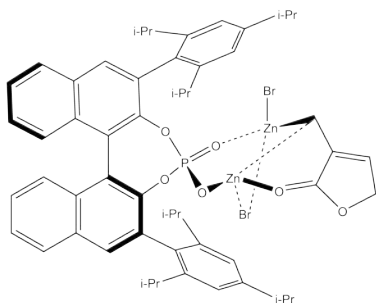


Energy (Hartree)= -11625.10064996

Zn	1.0115538	5.6711736	89.4376570
Br	3.3295690	6.4730539	89.5533698
H	-0.8891327	10.2812114	87.4934327
Br	3.3767881	6.4631744	85.3417603
H	0.4892130	5.6893725	86.3352500
Zn	2.5361342	5.5456524	87.3041254
C	-0.7984686	8.2181062	86.7344107
C	-1.4157972	9.3041488	87.5537813
C	-0.3944529	7.2103413	87.5579080
C	0.2426013	5.8911447	87.3975971
C	-0.6875894	7.6770712	88.9255463
O	-1.3213416	8.8503802	88.9286449
O	-0.3602323	7.0966077	89.9843908
H	-2.4885013	9.4770378	87.3167412

H	-1.1077309	2.4997883	91.7956948	H	-2.3834961	9.5415187	87.2941746
H	-2.7813904	2.9070731	93.6026329	H	-0.4753925	5.1098365	87.6274308
H	-3.5963456	2.2027017	92.1674873	H	-0.5615921	8.3214986	85.6686837
H	-3.7444077	3.9510681	92.5065788	C	0.1019021	0.9273518	89.2343831
H	7.3007357	5.6650536	86.1265168	C	0.8568084	-0.1720894	89.6630000
H	7.8580258	2.5030782	91.0800544	C	0.2805063	-1.0284950	90.6706786
H	5.2143102	0.3143672	83.9125936	C	1.0153198	-2.0711826	91.3109541
C	7.3270334	5.5451909	87.2317960	C	-1.0858893	-0.8049430	91.0802476
H	5.0527800	2.7401082	92.5931277	C	-1.6735487	-1.6735275	92.0484461
H	7.1950090	7.7065848	87.5765446	C	-1.8082556	0.3044891	90.5549733
H	3.2362111	1.9134474	83.9300234	H	-2.8432036	0.4686745	90.8909354
C	6.5687520	4.2619882	87.5491654	C	-1.2249641	1.2149868	89.6810223
C	7.1428951	1.6538287	91.0874879	C	4.4071137	0.5904970	88.4054207
C	6.6429233	6.7807039	87.8413596	C	4.8120245	-0.6556221	87.9420027
H	6.6036135	6.7154056	88.9489372	H	5.8065251	-0.7578696	87.4815284
C	6.4652062	3.7746130	88.8645683	C	3.9432728	-1.7844917	87.9589667
C	5.6830153	0.8854904	84.7409795	C	4.3515728	-3.0316836	87.3979319
H	9.3025214	4.5737769	87.1969136	C	2.5993224	-1.6470284	88.4707674
C	5.9507252	3.5233090	86.5276141	C	1.7048862	-2.7483006	88.3126156
C	8.8035101	5.4509589	87.6567846	C	2.2117452	-0.3966590	89.0816031
H	9.3591708	6.3625734	87.3536433	C	3.1281839	0.6598298	89.0377375
H	6.0019187	3.9102553	85.4977004	O	0.6522526	1.8043587	88.3009757
C	5.1371054	3.1480974	91.5645158	O	2.7921908	1.8690578	89.6459846
H	7.1034265	1.2550771	92.1226550	P	1.7582647	2.8723761	88.8793508
H	7.5555851	0.8625107	90.4289944	O	1.1596288	3.7690713	89.9842064
C	5.7867993	2.5813776	89.1691886	O	2.3561176	3.5554877	87.6429367
C	3.7340618	2.5085246	84.7236327	C	-0.9407456	-2.6987718	92.6259236
C	5.2578474	2.3231345	86.7741196	C	0.4199585	-2.8852079	92.2642531
H	6.2894382	0.1796445	85.3439338	H	-2.7206009	-1.4993344	92.3424153
H	6.3809888	1.6231407	84.2920446	H	-1.4045708	-3.3564386	93.3767214
C	5.7449173	2.0985124	90.6173921	H	2.0711387	-2.2200069	91.0456329
C	5.1911724	1.8386463	88.1133895	H	1.0103583	-3.6783613	92.7477392
C	4.6124296	1.5929849	85.5942529	C	2.1286735	-3.9417872	87.7444321
H	4.1267718	3.4525053	91.2288618	C	3.4681595	-4.0954133	87.2996980
H	2.9542821	3.0035959	85.3320851	H	0.6619929	-2.6436047	88.6410182
H	5.7646753	4.0618126	91.6202703	H	1.4163259	-4.7734610	87.6326935
H	5.6040107	6.8801740	87.4696380	H	3.7955291	-5.0492979	86.8589183
H	4.3217030	3.3042277	84.2219350	H	5.3830647	-3.1239687	87.0231492
H	8.9009909	5.3537452	88.7586061	C	-2.1563091	3.5063841	90.2225332
H	5.0920622	1.2022547	90.6550847	C	-1.9069649	2.4810206	89.2594400
H	3.9445576	0.8101067	86.0062638	C	-2.7849149	4.6090983	89.7984935
H	6.9314390	4.3421770	89.6856821	C	-2.2759578	2.6863100	87.9022004

13d-ma



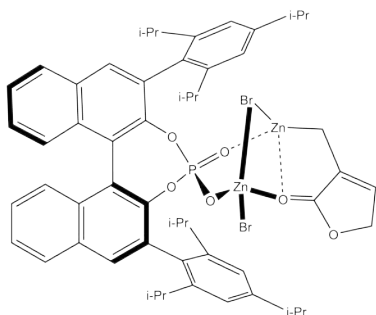
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Zn	1.0053004	5.6538401	89.4309026
Br	3.3277909	6.4430925	89.6414624
H	-0.7814333	10.3173914	87.5558929
Br	3.4218278	6.4700514	85.4036419
H	0.6206820	5.7311981	86.3858893
Zn	2.6784274	5.5138500	87.3751821
C	-0.6897894	8.2653967	86.7579296
C	-1.3243099	9.3467330	87.5741505
C	-0.3428008	7.2327768	87.5765501
C	0.2781057	5.9083536	87.4247087
C	-0.6778170	7.6828223	88.9441344
O	-1.2964769	8.8683400	88.9408094
O	-0.3890916	7.0855985	90.0002194

H	-2.3834961	9.5415187	87.2941746
H	-0.4753925	5.1098365	87.6274308
H	-0.5615921	8.3214986	85.6686837
C	0.1019021	0.9273518	89.2343831
C	0.8568084	-0.1720894	89.6630000
C	0.2805063	-1.0284950	90.6706786
C	1.0153198	-2.0711826	91.3109541
C	-1.0858893	-0.8049430	91.0802476
C	-1.6735487	-1.6735275	92.0484461
C	-1.8082556	0.3044891	90.5549733
H	-2.8432036	0.4686745	90.8909354
C	-1.2249641	1.2149868	89.6810223
C	4.4071137	0.5904970	88.4054207
C	4.8120245	-0.6556221	87.9420027
H	5.8065251	-0.7578696	87.4815284
C	3.9432728	-1.7844917	87.9589667
C	4.3515728	-3.0316836	87.3979319
C	2.5993224	-1.6470284	88.4707674
C	1.7048862	-2.7483006	88.3126156
C	2.2117452	-0.3966590	89.0816031
C	3.1281839	0.6598298	89.0377375
O	0.6522526	1.8043587	88.3009757
O	2.7921908	1.8690578	89.6459846
P	1.7582647	2.8723761	88.8793508
O	1.1596288	3.7690713	89.9842064
O	2.3561176	3.5554877	87.6429367
C	-0.9407456	-2.6987718	92.6259236
C	0.4199585	-2.8852079	92.2642531
H	-2.7206009	-1.4993344	92.3424153
H	-1.4045708	-3.3564386	93.3767214
H	2.0711387	-2.2200069	91.0456329
H	1.0103583	-3.6783613	92.7477392
C	2.1286735	-3.9417872	87.7444321
C	3.4681595	-4.0954133	87.2996980
H	0.6619929	-2.6436047	88.6410182
H	1.4163259	-4.7734610	87.6326935
H	3.7955291	-5.0492979	86.8589183
H	5.3830647	-3.1239687	87.0231492
C	-2.1563091	3.5063841	90.2225332
C	-1.9069649	2.4810206	89.2594400
C	-2.7849149	4.6090983	89.7984935
C	-2.2759578	2.6863100	87.9022004
C	-2.9161238	3.8878530	87.5375589
C	-3.1897004	4.9026595	88.4676991
H	-2.9720365	5.4856913	90.5385447
C	-2.0405506	1.6338743	86.8207235
H	-3.2097778	4.0231548	86.4863993
C	-1.1847593	2.1796393	85.6631880
H	-1.7082753	2.9885879	85.1117756
H	-0.9597839	1.3754647	84.9329025
H	-0.2213014	2.5796905	86.0347680
C	-3.3752676	1.0529795	86.3173741
H	-1.4787189	0.7954540	87.2781907
H	-3.9990861	1.8310673	85.8296550
H	-3.9666602	0.6231142	87.1509942
H	-3.1975097	0.2505368	85.5719307
C	-3.9457287	6.1783711	88.1056828
C	-3.9261885	6.5211921	86.6107517
H	-4.3907655	7.5130478	86.4344812
H	-4.5060839	5.7855091	86.0157405
H	-2.8943927	6.5457873	86.2064642
C	-5.3955483	6.1015514	88.6271347
H	-3.4475359	7.0117198	88.6525465
H	-5.9416568	7.0477109	88.4315512
H	-5.4252085	5.9060894	89.7174146
H	-5.9441428	5.2779074	88.1245655
C	-1.8111565	3.3519301	91.7051958
C	-1.0458215	4.5510026	92.2898364
H	-0.8281207	4.3765418	93.3632222
H	-1.6150823	5.4998329	92.2180963
H	-0.0761121	4.6856266	91.7756121

C	-3.0896564	3.0782807	92.5230559	Zn	2.6500220	4.9054746	86.3618272
H	-1.1479686	2.4699672	91.8060565	Br	0.3393130	5.9118937	86.4035398
H	-2.8437423	2.8917877	93.5888250	C	-0.1146959	0.8224577	88.9447067
H	-3.6450870	2.1984776	92.1407949	C	0.6564896	-0.2570848	89.3898679
H	-3.7803420	3.9465537	92.4811698	C	0.0833974	-1.1225981	90.3966371
H	7.1006934	5.7507750	86.1051120	C	0.8223707	-2.1512101	91.0560050
H	7.8781855	2.5534595	91.0301229	C	-1.2921950	-0.9200285	90.7883327
H	5.1482945	0.3180583	83.9282571	C	-1.8859421	-1.8021177	91.7410213
C	7.2241986	5.5889067	87.1981914	C	-2.0085072	0.2066053	90.2917430
H	5.1068317	2.7413196	92.6088127	H	-3.0291906	0.3906312	90.6607911
H	7.1814468	7.7361835	87.6297729	C	-1.4206093	1.1303971	89.4358475
H	3.1442513	1.8834087	83.9657055	C	4.3270315	0.5579745	88.5840327
C	6.4791531	4.3027209	87.5343700	C	4.8123211	-0.6993919	88.2395579
C	7.1765167	1.6934277	91.0508609	H	5.8826917	-0.8193221	88.0127240
C	6.6285933	6.8151804	87.9084591	C	3.9538640	-1.8275172	88.1042100
H	6.6803535	6.7135961	89.0127181	C	4.4547872	-3.0828880	87.6438020
C	6.4116974	3.8124186	88.8509626	C	2.5448630	-1.6909600	88.3870024
C	5.6173662	0.8998811	84.7488417	C	1.6921744	-2.8045704	88.1211650
H	9.1646120	4.5793040	86.9468748	C	2.0517247	-0.4327567	88.8944571
C	5.8584471	3.5505140	86.5241748	C	2.9410163	0.6504221	88.9237604
C	8.7303133	5.4460063	87.4850943	O	0.3972351	1.6544313	87.9515208
H	9.2804867	6.3580031	87.1731266	O	2.4880600	1.8937085	89.3523871
H	5.8823985	3.9390180	85.4941329	P	1.5294222	2.7685253	88.3496456
C	5.1577569	3.1531540	91.5796369	O	0.9803275	3.8945584	89.2313967
H	7.1678977	1.2903065	92.0849815	O	2.2246289	3.1067446	87.0204508
H	7.5867028	0.9118979	90.3795501	C	-1.1497980	-2.8201828	92.3279812
C	5.7646449	2.6051189	89.1675699	C	0.2217420	-2.9789636	91.9952945
C	3.6416607	2.4895321	84.7510237	H	-2.9396712	-1.6411275	92.0181112
C	5.1969245	2.3355407	86.7825921	H	-1.6179004	-3.4888673	93.0663913
H	6.2441198	0.2069168	85.3457486	H	1.8871773	-2.2828103	90.8216483
H	6.2972802	1.6474062	84.2891071	H	0.8178118	-3.7607489	92.4904654
C	5.7614343	2.1179051	90.6148199	C	2.2072121	-4.0051421	87.6514322
C	5.1649411	1.8506353	88.1230160	C	3.6021999	-4.1548816	87.4268961
C	4.5462431	1.5921198	85.6138067	H	0.6103427	-2.7000959	88.2834717
H	4.1334175	3.4387848	91.2716961	H	1.5271838	-4.8460822	87.4465457
H	2.8600615	2.9732024	85.3661898	H	4.0001195	-5.1148447	87.0640925
H	5.7681940	4.0789603	91.6233920	H	5.5340904	-3.1764284	87.4449857
H	5.5667638	6.9567321	87.6274372	C	-2.0596538	3.4173998	90.2396249
H	4.2073160	3.2943429	84.2391217	C	-2.0212664	2.4753139	89.1696819
H	8.9198968	5.2959346	88.5687770	C	-2.5784577	4.7012246	89.9851337
H	5.1235997	1.2112150	90.6626438	C	-2.4738049	2.8493176	87.8753576
H	3.8969739	0.7993296	86.0365911	C	-2.9862994	4.1444108	87.6794213
H	6.8833265	4.3884745	89.6629551	C	-3.0579474	5.0864899	88.7217793

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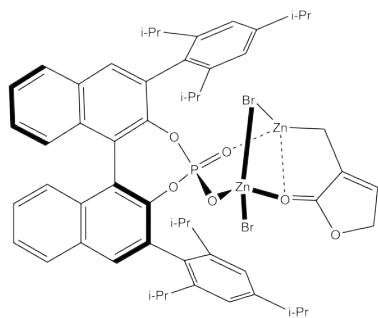


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Zn	0.6727321	5.7989401	88.8812118	C	-1.5736702	3.0930642	91.6544127
Br	-0.0305957	7.5080770	90.2704416	C	-0.5617240	4.1167370	92.1975605
C	4.9066865	8.2906214	86.9844831	H	-0.2111666	3.8063872	93.2037734
C	4.3460666	7.0489026	86.9397103	H	-0.9963881	5.1323303	92.2934401
C	3.5957387	6.9173377	88.2089142	H	0.3191138	4.1916442	91.5320679
O	3.7578798	7.9850141	88.9960125	C	-2.7690017	2.9351859	92.6141832
C	4.5717867	8.9456463	88.2840587				
O	2.8478861	5.9684383	88.5157940				
C	4.3029319	5.9482769	85.9469337				
H	5.4631780	9.1789086	88.9067868				
H	3.9725307	9.8766146	88.1824268				

H	-1.0483767	2.1182646	91.6176938	H	3.9265517	9.8755948	88.1801636
H	-2.4243391	2.6460599	93.6288618	Zn	2.6271678	4.9133759	86.3871293
H	-3.4799574	2.1613693	92.2597553	Br	0.3222982	5.8808400	86.3866880
H	-3.3327401	3.8872439	92.7066719	C	-0.1117934	0.8146995	88.9351249
H	7.3253176	5.9021524	87.2953580	C	0.6562884	-0.2661360	89.3825209
H	6.8209711	2.5150801	92.1456927	C	0.0797482	-1.1297782	90.3887710
H	6.5715485	0.1741123	84.5663567	C	0.8140926	-2.1617511	91.0475174
C	7.5979364	5.4274771	88.2656468	C	-1.2947810	-0.9215490	90.7807975
H	3.6610922	2.8643369	92.7151088	C	-1.8913581	-1.8018601	91.7325978
H	7.8928935	7.4031217	89.1494655	C	-2.0057093	0.2086874	90.2853335
H	4.6694010	1.7622093	83.9595469	H	-3.0244946	0.3996863	90.6560546
C	6.7396065	4.1715882	88.3846840	C	-1.4153655	1.1294062	89.4282892
C	6.1073296	1.6837718	91.9655708	C	4.3275951	0.5528732	88.5870883
C	7.3492954	6.4621891	89.3711969	C	4.8157028	-0.7034596	88.2437980
H	7.7100092	6.1039145	90.3577637	H	5.8868544	-0.8200796	88.0187271
C	6.1879509	3.7379507	89.5998291	C	3.9598940	-1.8330760	88.1068469
C	6.7637770	0.7629653	85.4870644	C	4.4629026	-3.0877734	87.6483421
H	9.2920966	4.3463627	87.3615118	C	2.5501749	-1.6983794	88.3861573
C	6.5012084	3.3813821	87.2450798	C	1.7000067	-2.8131900	88.1186819
C	9.0920061	5.0536424	88.1912581	C	2.0532978	-0.4412651	88.8919814
H	9.7216974	5.9542073	88.0355625	C	2.9407902	0.6433275	88.9241060
H	6.9324435	3.7019815	86.2818495	O	0.4025994	1.6431108	87.9408649
C	4.1017775	3.2419926	91.7695966	O	2.4858719	1.8858886	89.3510065
H	5.7448689	1.3309582	92.9533948	P	1.5302565	2.7587838	88.3424365
H	6.6698811	0.8548394	91.4895473	O	0.9771061	3.8854149	89.2204424
C	5.4224965	2.5602074	89.7016031	O	2.2369334	3.0995814	87.0197582
C	4.8955236	2.3607863	84.8656386	C	-1.1603020	-2.8236870	92.3181091
C	5.7185961	2.2134747	87.2802804	C	0.2098707	-2.9879980	91.9851906
H	7.1693776	0.0743995	86.2557924	H	-2.9442083	-1.6361066	92.0101336
H	7.5578455	1.5035133	85.2547740	H	-1.6315242	-3.4910133	93.0556757
C	4.9280955	2.1387072	91.0841018	H	1.8781965	-2.2970093	90.8125381
C	5.1779486	1.7882696	88.5318041	H	0.8026564	-3.7729867	92.4791189
C	5.4781104	1.4609475	85.9693982	C	2.2177413	-4.0129630	87.6512633
H	3.2749319	3.5864787	91.1188650	C	3.6128840	-4.1608271	87.4300506
H	3.9530625	2.8342546	85.2026411	H	0.6180141	-2.7089529	88.2792970
H	4.7271470	4.1222608	92.0273019	H	1.5392921	-4.8548637	87.4454273
H	6.2723121	6.7021607	89.4794913	H	4.0132034	-5.1202455	87.0686119
H	5.5978783	3.1653033	84.5637889	H	5.5427850	-3.1796951	87.4518984
H	9.4175554	4.5658825	89.1339232	C	-2.0310970	3.4227540	90.2315008
H	4.2662364	1.2594079	90.9585929	C	-2.0072277	2.4783270	89.1633620
H	4.7230347	0.6745721	86.1652183	C	-2.5355934	4.7118099	89.9755882
H	6.3593142	4.3279898	90.5119614	C	-2.4607220	2.8541536	87.8701920
H	4.4491417	6.3057810	84.9105597	C	-2.9599855	4.1541093	87.6734084
H	5.1049958	5.2134813	86.1778003	C	-3.0167581	5.0995469	88.7133561
H	5.5185942	8.7727046	86.2096319	H	-2.5547165	5.4509507	90.7911782
				C	-2.4666816	1.8675453	86.7046839
				H	-3.3243114	4.4350487	86.6724497
				C	-1.6913820	2.3955764	85.4854192
				H	-2.1645413	3.3049948	85.0605340
				H	-1.6627901	1.6297746	84.6827535
				H	-0.6487783	2.6525153	85.7546209
				C	-3.9081126	1.4722151	86.3322320
				H	-1.9557638	0.9436211	87.0455609
				H	-4.4871461	2.3501511	85.9765369
				H	-4.4465614	1.0480134	87.2038736
				H	-3.9134168	0.7144136	85.5212791
				C	-3.6377712	6.4772385	88.5139308
				C	-2.9656631	7.2869596	87.3945743
				H	-3.4535234	8.2775556	87.2848135
				H	-3.0320101	6.7710097	86.4139721
				H	-1.8951953	7.4590020	87.6198696
				C	-5.1565136	6.3543442	88.2866258
				H	-3.4790057	7.0359430	89.4617795
				H	-5.6283514	7.3563453	88.2143966
				H	-5.6457889	5.8006183	89.1133223
				H	-5.3767059	5.8103901	87.3438654
				C	-1.5464319	3.0963204	91.6462583
				C	-0.5254476	4.1113290	92.1889210
				H	-0.1840371	3.8032227	93.1988159
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				H	0.3611586	4.1710095	91.5296727

13d-mi

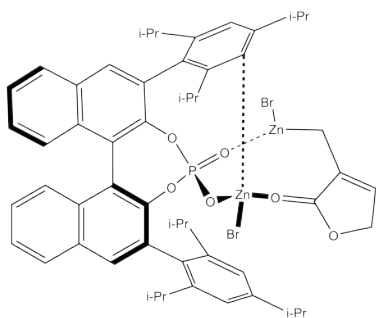


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Br	-0.0514144	7.5220044	90.2339835
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C	4.3258602	7.0500567	86.9336186
C	3.5783147	6.9138403	88.2081726
O	3.7397094	7.9846443	88.9940369
C	4.5365125	8.9503542	88.2760716
O	2.8351121	5.9648627	88.5127142
C	4.2870126	5.9423841	85.9515303
H	5.4311456	9.1927098	88.8916569

C	-2.7439305	2.9513117	92.6053727
H	-1.0306130	2.1163379	91.6114058
H	-2.4034809	2.6592107	93.6205187
H	-3.4633539	2.1854700	92.2508978
H	-3.2982308	3.9087918	92.6968387
H	7.3225815	5.8998572	87.2994963
H	6.8142861	2.5099465	92.1501997
H	6.5802998	0.1844381	84.5665256
C	7.5865935	5.4300280	88.2747020
H	3.6495571	2.8532415	92.7177233
H	7.8701786	7.4108350	89.1521374
H	4.6635555	1.7593831	83.9662520
C	6.7293330	4.1731711	88.3917313
C	6.1012730	1.6785483	91.9684947
C	7.3248277	6.4703112	89.3721726
H	7.6765032	6.1182017	90.3640856
C	6.1776052	3.7375961	89.6058037
C	6.7691698	0.7742189	85.4872694
H	9.2911337	4.3459084	87.3951798
C	6.4947043	3.3829201	87.2517873
C	9.0817691	5.0582453	88.2180325
H	9.7134449	5.9578283	88.0644179
H	6.9261593	3.7050214	86.2890208
C	4.0923175	3.2335464	91.7744499
H	5.7397512	1.3238291	92.9558692
H	6.6653237	0.8515847	91.4912528
C	5.4163575	2.5572971	89.7063792
C	4.8838364	2.3567312	84.8745242
C	5.7162033	2.2123824	87.2856198
H	7.1834031	0.0888469	86.2541417
H	7.5571032	1.5207932	85.2537004
C	4.9215373	2.1333693	91.0878674
C	5.1758299	1.7850343	88.5361462
C	5.4789436	1.4600590	85.9740782
H	3.2660521	3.5791230	91.1238133
H	3.9358909	2.8149695	85.2162107
H	4.7148272	4.1144196	92.0368324
H	6.2464185	6.7084163	89.4691812
H	5.5755337	3.1710574	84.5739411
H	9.3975404	4.5748536	89.1660152
H	4.2614373	1.2531380	90.9600862
H	4.7312325	0.6670086	86.1707009
H	6.3451253	4.3277548	90.5185764
H	4.4473111	6.2842698	84.9124138
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13j-ma; COSMO



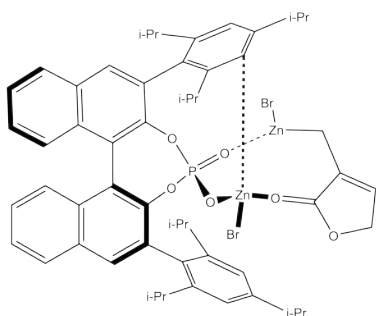
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H	3.3743472	6.6396805	86.5363238
Br	0.9550399	0.3763036	85.0691777
H	-0.8976536	4.4238358	84.5807698
Zn	0.8671441	2.6943410	85.3073544
C	2.0123103	6.2004523	84.8897520
C	2.4040836	6.9739023	86.1024146
C	0.8844081	5.4705745	85.1502213

C	0.2002420	4.3919308	84.4307255
C	0.5126753	5.8165308	86.5362109
O	1.3757133	6.6860170	87.0732592
O	-0.4627871	5.3866853	87.1865857
H	2.4498491	8.0762820	85.9683323
H	0.4342671	4.3729482	83.3495140
H	2.6043586	6.1917951	83.9648943
C	-0.2004085	0.9202660	89.2444542
C	0.6646709	-0.1342165	89.5471001
C	0.2689414	-1.0395598	90.6015185
C	1.1322783	-2.0562600	91.1103425
C	-1.0413398	-0.8999339	91.1956718
C	-1.4509872	-1.8199122	92.2072575
C	-1.8812830	0.1874270	90.8133667
H	-2.8585694	0.3041642	91.3063712
C	-1.4583032	1.1312295	89.8886627
C	4.1024214	0.8021295	88.1027759
C	4.5213239	-0.4203781	87.5916214
H	5.5230615	-0.5011226	87.1440213
C	3.6713664	-1.5623240	87.5762430
C	4.0824403	-2.7758733	86.9474501
C	2.3541985	-1.4802749	88.1583503
C	1.4813987	-2.5995317	88.0131457
C	1.9586356	-0.2604325	88.8188541
C	2.8178401	0.8408430	88.7271205
O	0.1293526	1.8156880	88.2390406
O	2.4305176	2.0550463	89.3018188
P	1.3220785	2.9335565	88.4725010
O	0.8974422	4.0432145	89.4481279
O	1.7660845	3.3115998	87.0598266
C	-0.5979621	-2.8186574	92.6525493
C	0.7101681	-2.9231596	92.1092814
H	-2.4570638	-1.7086845	92.6415049
H	-0.9248304	-3.5175588	93.4374388
H	2.1497209	-2.1450529	90.7058278
H	1.3986509	-3.6948545	92.4862046
C	1.9027683	-3.7580842	87.3753513
C	3.2198291	-3.8573659	86.8523985
H	0.4546328	-2.5321219	88.3982160
H	1.2064521	-4.6036952	87.2667428
H	3.5451218	-4.7840687	86.3554525
H	5.0952390	-2.8275471	86.5176974
C	-2.0664203	3.4831781	90.5301070
C	-2.1572841	2.4194142	89.5918118
C	-2.5475380	4.7642852	90.1458568
C	-2.7582435	2.6329747	88.3193251
C	-3.2513231	3.9095582	87.9943703
C	-3.1548499	4.9946623	88.8813638
H	-2.5608040	5.5776521	90.8894987
C	-2.9005106	1.4821847	87.3290990
H	-3.7085632	4.0677497	87.0085863
C	-2.7418835	1.9071879	85.8638598
H	-3.5915578	2.5246592	85.5054166
H	-2.6775542	1.0147392	85.2108254
H	-1.8109714	2.4903926	85.7183225
C	-4.2370166	0.7517250	87.5685497
H	-2.0881965	0.7584286	87.5417721
H	-5.0968365	1.4305150	87.3886855
H	-4.3109723	0.3783770	88.6100217
H	-4.3346794	-0.1159286	86.8844163
C	-3.7257542	6.3706628	88.5679386
C	-3.6915757	6.7295139	87.0766012
H	-3.9935651	7.7861209	86.9324236
H	-4.3938831	6.1062631	86.4844083
H	-2.6753870	6.5964686	86.6559712
C	-5.1515387	6.4864701	89.1442311
H	-3.0835510	7.1030063	89.1071954
H	-5.5543331	7.5074707	88.9838022
H	-5.1693605	6.2782472	90.2329850
H	-5.8355745	5.7655401	88.6492333
C	-1.5338712	3.2797126	91.9461758

C	-0.5681640	4.3737832	92.4269751	C	0.9185065	5.4741667	85.1750320
H	-0.2241291	4.1416547	93.4551250	C	0.2157181	4.4199742	84.4408496
H	-1.0345714	5.3795987	92.4568618	C	0.5399670	5.8142372	86.5621249
H	0.3278942	4.4290016	91.7781398	O	1.4249469	6.6480829	87.1209988
C	-2.7254144	3.1259869	92.9144878	O	-0.4554121	5.4095208	87.1954708
H	-0.9713207	2.3250783	91.9532283	H	2.5777747	8.0081499	86.0631467
H	-2.3653592	2.9006123	93.9390854	H	0.4542290	4.4038864	83.3606794
H	-3.4073856	2.3100243	92.6014021	H	2.6743922	6.1540799	84.0211396
H	-3.3213483	4.0615857	92.9611713	C	-0.2063959	0.9167743	89.2411044
H	7.2212348	6.0183205	86.5348848	C	0.6592281	-0.1370383	89.5448113
H	7.4096570	2.3856265	91.1711612	C	0.2620999	-1.0444245	90.5968044
H	5.1029694	0.7860613	83.7419474	C	1.1247532	-2.0616526	91.1050753
C	7.1477200	5.7922076	87.6217787	C	-1.0491355	-0.9068821	91.1888673
H	4.5016927	2.5101415	92.5030338	C	-1.4593421	-1.8291912	92.1974326
H	6.8920463	7.9133001	88.1421438	C	-1.8883612	0.1806526	90.8066010
H	3.2517709	2.6047737	83.7283587	H	-2.8658911	0.2981812	91.2992672
C	6.3907221	4.4758746	87.7480349	C	-1.4656332	1.1260210	89.8834684
C	6.6914258	1.5479364	91.0477261	C	4.0971007	0.8088524	88.1077674
C	6.3698709	6.9444806	88.2845152	C	4.5218079	-0.4137665	87.6021979
H	6.2588091	6.7772644	89.3762412	H	5.5250479	-0.4906414	87.1574369
C	6.1967804	3.8614234	88.9976157	C	3.6762998	-1.5585928	87.5859794
C	5.5616693	1.2568691	84.6360404	C	4.0926914	-2.7719533	86.9613920
H	9.1480530	4.8803509	87.6807528	C	2.3563517	-1.4787369	88.1616124
C	5.8368099	3.8514212	86.6187371	C	1.4867376	-2.5997095	88.0128957
C	8.5806968	5.6954563	88.1736450	C	1.9553765	-0.2595336	88.8200673
H	9.1306861	6.6456150	88.0121861	C	2.8113645	0.8445159	88.7299883
H	5.9800479	4.3255155	85.6341386	O	0.1243354	1.8127545	88.2377055
C	4.6616452	3.0119785	91.5262699	O	2.4211806	2.0575569	89.3038150
H	6.5786678	1.0532978	92.0348638	P	1.3117051	2.9355488	88.4755097
H	7.1446935	0.8177524	90.3467076	O	0.8794134	4.0393359	89.4530986
C	5.4711218	2.6655282	89.1389674	O	1.7554902	3.3187263	87.0638996
C	3.8516352	3.1055269	84.5174472	C	-0.6073114	-2.8284497	92.6417607
C	5.0971741	2.6559786	86.7026082	C	0.7011962	-2.9310393	92.1005896
H	6.0177444	0.4528750	85.2459961	H	-2.4662145	-1.7192969	92.6302072
H	6.3829695	1.9206886	84.2920058	H	-0.9355327	-3.5293021	93.4242715
C	5.3302138	2.0488214	90.5292852	H	2.1424388	-2.1485215	90.7011097
C	4.9169898	2.0529398	87.9805254	H	1.3893399	-3.7034865	92.4764162
C	4.5084324	2.0541054	85.4279964	C	1.9140664	-3.7578399	87.3792868
H	3.6778496	3.3516437	91.1475987	C	3.2334883	-3.8551591	86.8637145
H	3.1974495	3.7855566	85.1000612	H	0.4577553	-2.5326662	88.3916640
H	5.2895515	3.9079669	91.7139337	H	1.2196348	-4.6043991	87.2671526
H	5.3492146	7.0383770	87.8598055	H	3.5631867	-4.7813921	86.3690182
H	4.5970187	3.7428788	83.9968404	H	5.1072383	-2.8213355	86.5356564
H	8.5807711	5.4934636	89.2651501	C	-2.0834316	3.4731050	90.5338333
H	4.6738073	1.1595973	90.4404723	C	-2.1648742	2.4143837	89.5890522
H	3.7064328	1.3496946	85.7291653	C	-2.5641526	4.7543707	90.1537081
H	6.6223733	4.3308660	89.8991708	C	-2.7541410	2.6345881	88.3120183
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				H	-2.5744844	5.5668090	90.8982541
				C	-2.8843971	1.4891213	87.3132609
				H	-3.6898581	4.0775275	87.0010838
				C	-2.7555103	1.9278314	85.8492555
				H	-3.6294246	2.5181878	85.5028760
				H	-2.6659944	1.0424756	85.1898946
				H	-1.8463636	2.5429790	85.6970627
				C	-4.1995516	0.7248712	87.5639096
				H	-2.0522053	0.7829142	87.5067602
				H	-5.0779195	1.3846539	87.4043650
				H	-4.2493829	0.3386495	88.6019740
				H	-4.2876445	-0.1378608	86.8723350
				C	-3.7250669	6.3709041	88.5749723
				C	-3.6948255	6.7305938	87.0839757
				H	-3.9894939	7.7894176	86.9411837
				H	-4.4041600	6.1137350	86.4931886
				H	-2.6812257	6.5914358	86.6593566
				C	-5.1477870	6.4943800	89.1565743
				H	-3.0760776	7.0999165	89.1109524
				H	-5.5467462	7.5173671	88.9992222
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13j-ma

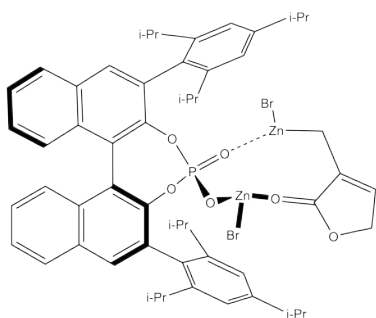


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H	3.4246856	6.5149611	86.6128407
Br	0.9266918	0.3921391	85.0621158
H	-0.8817928	4.4712707	84.5865925
Zn	0.8492767	2.6995952	85.3089846
C	2.0709902	6.1730754	84.9383082
C	2.4785210	6.9060892	86.1720541

C	-1.5559966	3.2666416	91.9518715	O	3.4767375	6.4835811	88.3510380
C	-0.5696047	4.3455129	92.4260700	C	3.2692925	6.0966454	85.3488584
H	-0.2357183	4.1189038	93.4588631	H	-0.1568053	8.2569642	87.4688078
H	-1.0117188	5.3625979	92.4403042	H	-0.5525389	6.5093961	87.6196667
H	0.3308442	4.3733951	91.7817584	Zn	2.8928477	4.1145100	85.4120766
C	-2.7497157	3.1379920	92.9206060	Br	1.5578871	2.6105276	84.2337456
H	-1.0108776	2.3020814	91.9641645	H	4.2871182	6.2982089	85.7342774
H	-2.3952739	2.9113471	93.9469201	H	3.1596009	6.4600840	84.3102206
H	-3.4457355	2.3324665	92.6108762	H	0.3729229	6.9612649	85.0963895
H	-3.3307262	4.0830516	92.9636016	C	0.3905627	1.5146701	88.9077935
H	7.1494198	6.0532685	86.5074026	C	0.9490515	0.2553709	89.1705344
H	7.3905486	2.4308749	91.1619795	C	0.2492964	-0.6098959	90.0938710
H	5.1254471	0.7561232	83.7536141	C	0.8031063	-1.8324802	90.5829890
C	7.1200299	5.8087067	87.5927026	C	-1.0471251	-0.2106939	90.5869767
H	4.4802745	2.5562281	92.4977865	C	-1.7568626	-1.0725893	91.4764054
H	6.9184652	7.9240643	88.1574841	C	-1.5850429	1.0509636	90.2063130
C	3.2535843	2.5525300	83.7134315	H	-2.5825714	1.3361695	90.5743689
C	6.3582488	4.4959771	87.7282222	C	-0.8765339	1.9415075	89.4089279
C	6.6735967	1.5910718	91.0464527	C	4.7123345	0.3357343	88.3775970
C	6.3907090	6.9597837	88.3094012	C	4.9027079	-0.9311363	87.8368587
H	6.3295436	6.7789879	89.4026603	H	5.9208228	-1.2749287	87.5984763
C	6.1645465	3.8915062	88.9822831	C	3.8059774	-1.7966928	87.5456360
C	5.5742957	1.2422095	84.6443062	C	4.0132723	-3.0505416	86.8953307
H	9.1081492	4.8708243	87.5417941	C	2.4589857	-1.3960817	87.8812542
C	5.8138717	3.8565810	86.6029829	C	1.3803175	-2.2434881	87.4909397
C	8.5749382	5.6813582	88.0778238	C	2.2599872	-0.1512949	88.5826470
H	9.1316455	6.6276430	87.9163490	C	3.3700575	0.6780002	88.7465114
H	5.9596692	4.3206983	85.6138956	O	1.0535184	2.4101252	88.0695882
C	4.6397639	3.0525810	91.5182719	O	3.1831885	1.8984991	89.3831518
H	6.5648202	1.1035934	92.0375268	P	2.4468833	3.1090275	88.5693988
H	7.1275351	0.8573802	90.3498600	O	2.1887271	4.1645173	89.6703060
C	5.4487164	2.6913333	89.1323070	O	3.2053371	3.5687634	87.3353872
C	3.8446897	3.0690185	84.4985115	C	-1.2023253	-2.2692764	91.9037598
C	5.0841592	2.6556989	86.6948633	C	0.0966726	-2.6395170	91.4643918
H	6.0375021	0.4505070	85.2646034	H	-2.7511043	-0.7573016	91.8301201
H	6.3901685	1.9112867	84.2977956	H	-1.7563291	-2.9225100	92.5949635
C	5.3101940	2.0849274	90.5272523	H	1.8112244	-2.1310183	90.2658870
C	4.9040028	2.0636024	87.9777003	H	0.5522865	-3.5723214	91.8303232
C	4.5082817	2.0350090	85.4232690	C	1.6157867	-3.4464943	86.8387827
H	3.6557011	3.3894262	91.1383906	C	2.9429099	-3.8632804	86.5512182
H	3.1799312	3.7465677	85.0720301	H	0.3494289	-1.9274781	87.7048857
H	5.2656385	3.9507015	91.7022214	H	0.7667133	-4.0792786	86.5384694
H	5.3515830	7.0740455	87.9382729	H	3.1184428	-4.8230236	86.0417873
H	4.5855908	3.7098215	83.9752229	H	5.0446881	-3.3529640	86.6547299
H	8.6184981	5.4504902	89.1626361	C	-1.3755448	4.3624432	89.9783597
H	4.6563242	1.1932639	90.4450712	C	-1.4540961	3.2809324	89.0572718
H	3.7109446	1.3257373	85.7254521	C	-2.0419673	5.5617885	89.6642977
H	6.5838254	4.3717757	89.8810425	C	-2.1260547	3.4452951	87.8156364
				C	-2.7680453	4.6695668	87.5466815
				C	-2.7579339	5.7344908	88.4647654
				H	-1.9948547	6.4032449	90.3740388
				C	-2.2053660	2.3033297	86.8039100
				H	-3.2957244	4.7879170	86.5897267
				C	-2.1308797	2.7749427	85.3444900
				H	-3.0312665	3.3507701	85.0437892
				H	-2.0624924	1.9006068	84.6662331
				H	-1.2321673	3.3982887	85.1671014
				C	-3.4667429	1.4524185	87.0511313
				H	-1.3238880	1.6505362	86.9724694
				H	-4.3843022	2.0609397	86.9070796
				H	-3.4888983	1.0461600	88.0822633
				H	-3.5089892	0.5970397	86.3454066
				C	-3.5152355	7.0354018	88.2152758
				C	-3.6006111	7.4369454	86.7355858
				H	-4.0544131	8.4432388	86.6320929
				H	-4.2335124	6.7341561	86.1550908
				H	-2.6022959	7.4618020	86.2520561
				C	-4.9210389	6.9582387	88.8445636
				H	-2.9571723	7.8359401	88.7519681
				H	-5.4639558	7.9191237	88.7277067
				H	-4.8657051	6.7213203	89.9259658

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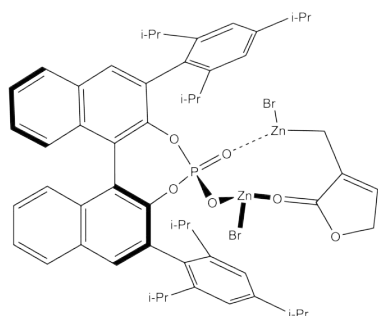
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C	0.9115704	6.9497564	86.0537385
C	2.2294733	6.6151840	86.2481193
C	2.4297516	6.7085228	87.7052752
O	1.3066671	7.0701087	88.3388570
C	0.2560082	7.2301840	87.3589398

H	-5.5220394	6.1626068	88.3563139
C	-0.5890435	4.2509063	91.2843108
C	0.1749793	5.5418358	91.6327052
H	0.9361059	5.3427411	92.4144252
H	-0.4980729	6.3321053	92.0260477
H	0.6872027	5.9573640	90.7420874
C	-1.4956476	3.8339160	92.4582992
H	0.1690370	3.4546696	91.1374203
H	-0.9083830	3.7519788	93.3963428
H	-1.9810329	2.8554224	92.2758922
H	-2.2975301	4.5844569	92.6214443
H	8.6962955	5.1928222	88.1157424
H	7.4782445	1.2478893	92.0954960
H	7.4469322	0.9471500	84.2214464
C	7.9221696	5.1625131	88.9151960
H	4.4053131	1.5998072	92.9668545
H	7.3471695	7.2574851	88.5494228
H	4.9479178	1.5095042	84.2483611
C	7.2620989	3.7916917	88.8340322
C	6.6998783	0.5235348	91.7759436
C	6.8791489	6.2520195	88.5907850
H	6.0975851	6.2795793	89.3784583
C	6.7205472	3.1436185	89.9565406
C	7.5441741	1.5271641	85.1616316
H	9.3313188	4.6545491	90.5285868
C	7.1243224	3.1591962	87.5856022
C	8.6116794	5.4525904	90.2551559
H	9.1644840	6.4125429	90.2052094
H	7.5875768	3.6351139	86.7070056
C	4.8039454	2.1822217	92.1109514
H	6.3690249	-0.0385585	92.6740951
H	7.1748272	-0.1930814	91.0753886
C	5.9843622	1.9499800	89.8420739
C	5.0463785	1.9420698	85.2644134
C	6.3976419	1.9681107	87.4122429
H	8.4393442	1.1598567	85.7031182
H	7.7328792	2.5816505	84.8715429
C	5.5100672	1.2490370	91.1149855
C	5.7612583	1.3893983	88.5515194
C	6.2687308	1.3764886	86.0057327
H	3.9569415	2.7110746	91.6333404
H	4.1095564	1.7268896	85.8117812
H	5.4894888	2.9487979	92.5266182
H	6.3706644	6.0604190	87.6249449
H	5.1520541	3.0468052	85.1487443
H	7.8731221	5.5468018	91.0784036
H	4.7822106	0.4649889	90.8223130
H	6.0874042	0.2897138	86.1142305
H	6.8624038	3.5819405	90.9549316

C	0.2931709	6.9768142	87.4964923
O	3.6540374	6.2925130	87.8477867
C	2.7612119	5.4794610	85.0293336
H	-0.1041709	8.0152879	87.5305409
H	-0.4226058	6.3247038	88.0468185
Zn	2.5735031	3.5065579	85.4301459
Br	1.4873600	1.5723235	84.7389612
H	3.8341575	5.7408980	85.1125357
H	2.3882960	5.6915002	84.0098981
H	-0.1195014	6.3430117	85.3462856
C	0.3896237	1.5686132	88.9167709
C	0.9311023	0.2922100	89.1374636
C	0.1664737	-0.6214963	89.9598358
C	0.6873731	-1.8697352	90.4193937
C	-1.1653065	-0.2546556	90.3776992
C	-1.9351963	-1.1681094	91.1581226
C	-1.6772194	1.0285213	90.0372900
H	-2.6967935	1.2991078	90.3526833
C	-0.9108527	1.9623197	89.3525117
C	4.7363116	0.3714828	88.5303872
C	4.9415102	-0.8992682	87.9947447
H	5.9667620	-1.2468525	87.8029892
C	3.8551808	-1.7435399	87.6242764
C	4.0866519	-2.9831610	86.9558073
C	2.4949553	-1.3277242	87.8738924
C	1.4332083	-2.1338701	87.3702648
C	2.2705248	-0.1072778	88.6095044
C	3.3796008	0.6992806	88.8607061
O	1.0747834	2.5289407	88.1827624
O	3.1610307	1.9047258	89.5206391
P	2.5371898	3.1157493	88.6269338
O	2.4064784	4.2850612	89.6317260
O	3.2964644	3.3995711	87.3377273
C	-1.4092551	-2.3872165	91.5550334
C	-0.0789166	-2.7279435	91.1953745
H	-2.9546642	-0.8741640	91.4536147
H	-2.0107014	-3.0806747	92.1621832
H	1.7183359	-2.1476706	90.1640864
H	0.3541408	-3.6793677	91.5399452
C	1.6943327	-3.3200936	86.6987030
C	3.0302768	-3.7602868	86.5053085
H	0.3968244	-1.7959661	87.5095525
H	0.8588828	-3.9203448	86.3075422
H	3.2253576	-4.7076503	85.9801529
H	5.1272391	-3.2997144	86.7820622
C	-1.3922219	4.3366625	90.0771513
C	-1.4617522	3.3302461	89.0757649
C	-2.0875414	5.5435038	89.8673981
C	-2.1190895	3.5913069	87.8443276
C	-2.7990342	4.8141220	87.6842160
C	-2.8225868	5.7930773	88.6934170
H	-2.0550666	6.3231622	90.6453568
C	-2.1230362	2.5644923	86.7144556
H	-3.3309988	5.0002425	86.7393502
C	-1.8553113	3.1985547	85.3405740
H	-2.6838064	3.8615424	85.0136598
H	-1.7297536	2.4112758	84.5715135
H	-0.9152071	3.7860324	85.3523837
C	-3.4295843	1.7493558	86.7181207
H	-1.2886673	1.8573810	86.9010418
H	-4.3085288	2.4059723	86.5463841
H	-3.5792530	1.2325965	87.6876147
H	-3.4158941	0.9802853	85.9186940
C	-3.6352484	7.0760125	88.5560760
C	-3.5734546	7.7030181	87.1546131
H	-4.1007169	8.6784044	87.1393924
H	-4.0610261	7.0593790	86.3935106
H	-2.5290288	7.8777446	86.8244637
C	-5.0954834	6.8263343	88.9828990
H	-3.1999177	7.8084960	89.2722692
H	-5.6890886	7.7634126	88.9473536

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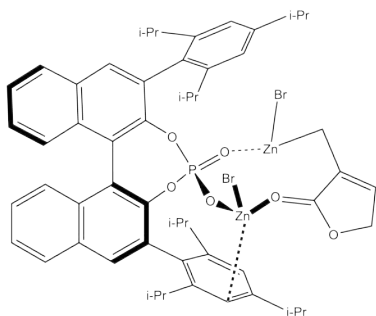


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Zn	3.7568345	5.6781159	89.7684787
Br	4.7543614	6.5939998	91.5968856
C	0.6308895	6.4757978	86.1373514
C	1.9614754	6.1432607	86.0683832
C	2.4964419	6.4594643	87.4081502
O	1.5444014	6.9586702	88.2131469

H	-5.1488226	6.4214926	90.0131608	O	2.0583405	6.8486667	88.0799609
H	-5.5787162	6.0888663	88.3083602	C	0.7213949	6.9679591	87.5611970
C	-0.5823649	4.1322661	91.3567279	O	3.9665844	5.8097230	87.5103005
C	0.2230127	5.3823979	91.7522910	C	2.5710389	5.0032607	84.8900861
H	0.9573513	5.1342167	92.5449787	H	0.4438624	8.0444335	87.5572181
H	-0.4281967	6.1889186	92.1492841	H	0.0372475	6.4387869	88.2648395
H	0.7865273	5.7845565	90.8886751	Zn	2.3579407	3.0666142	85.4021241
C	-1.4756479	3.6618588	92.5199112	Br	1.3884320	1.0033678	84.8815277
H	0.1522029	3.3260002	91.1498168	H	3.6603233	5.1698663	84.7674263
H	-0.8732786	3.5037553	93.4381255	H	2.0498631	5.2006390	83.9341525
H	-1.9886634	2.7092238	92.2820332	H	-0.0938380	6.2455953	85.5563398
H	-2.2550397	4.4186642	92.7491078	C	0.2872823	1.4097126	88.9031441
H	8.8816411	5.0770144	88.1268251	C	0.8474891	0.1371001	89.1162501
H	7.4310740	1.5505776	92.2271806	C	0.0539066	-0.8062481	89.8796576
H	7.5941821	0.7914839	84.3946615	C	0.5730038	-2.0539937	90.3439079
C	8.0251194	5.1915737	88.8293103	C	-1.3060168	-0.4738647	90.2358555
H	4.3481225	1.9763725	93.0515487	C	-2.1004973	-1.4227703	90.9470733
H	7.6639305	7.2481479	88.1317253	C	-1.8195244	0.8179002	89.9265283
H	5.0623492	1.1427628	84.3965074	H	-2.8498001	1.0704657	90.2211389
C	7.2942160	3.8536935	88.8298843	C	-1.0284561	1.7795981	89.3167253
C	6.6507978	0.8101430	91.9530440	C	4.6658241	0.4164132	88.6389195
C	7.1106115	6.2945991	88.2576730	C	4.9715400	-0.8442697	88.1348987
H	6.2699755	6.4943598	88.9541240	H	6.0184348	-1.1325635	87.9598255
C	6.6917517	3.3048900	89.9733861	C	3.9486516	-1.7670243	87.7574939
C	7.6416016	1.4478732	85.2870843	C	4.2833208	-2.9972442	87.1143936
H	9.2238756	4.8108677	90.6350484	C	2.5546071	-1.4322679	87.9431076
C	7.1928789	3.1259983	87.6309516	C	1.5676682	-2.2978230	87.3893291
C	8.5858971	5.6044223	90.1961757	C	2.2275313	-0.2256109	88.6632246
H	9.1988623	6.5233395	90.1003428	C	3.2837234	0.6324599	88.9609377
H	7.7032598	3.5238636	86.7406476	O	0.9455665	2.4185281	88.2114509
C	4.7628222	2.4977545	92.1647523	O	2.9734400	1.8201590	89.6038099
H	6.3126589	0.3114277	92.8851589	P	2.4348355	2.9813143	88.5867798
H	7.1262729	0.0462639	91.3051200	O	2.4431383	4.2597969	89.4459894
C	5.9563820	2.1033403	89.9241418	O	3.1999884	3.0344279	87.2679233
C	5.1211595	1.6551412	85.3779256	C	-1.5742436	-2.6429245	91.3425941
C	6.4594839	1.9338780	87.5176520	C	-0.2177855	-2.9471133	91.0543179
H	8.5692449	1.2061309	85.8441420	H	-3.1398305	-1.1542625	91.1935644
H	7.7319911	2.4889046	84.9132495	H	-2.1953892	-3.3631891	91.8964791
C	5.4671812	1.4939971	91.2379702	H	1.6232482	-2.3058715	90.1473702
C	5.7756171	1.4416745	88.6751480	H	0.2161954	-3.8968547	91.4026488
C	6.3860148	1.2465589	86.1496027	C	1.9290223	-3.4709856	86.7408655
H	3.9266450	3.0062131	91.6475309	C	3.2959910	-3.8371902	86.6205411
H	4.2064959	1.3945499	85.9413958	H	0.5083974	-2.0173388	87.4712602
H	5.4538498	3.2800810	92.5401554	H	1.1497011	-4.1190089	86.3117307
H	6.6765367	6.0082540	87.2792329	H	3.5703023	-4.7757690	86.1152698
H	5.1246385	2.7531807	85.1921638	H	5.3475052	-3.2537932	86.9920072
H	7.7712503	5.8317835	90.9146891	C	-1.3512003	4.1194492	90.1934666
H	4.7381993	0.6945405	90.9952285	C	-1.4951106	3.1917345	89.1247289
H	6.3025964	0.1572296	86.3267099	C	-1.8541666	5.4226431	90.0244140
H	6.8061059	3.8130020	90.9413920	C	-2.0524485	3.6067716	87.8889054
				C	-2.5540965	4.9183882	87.7745182
				C	-2.4824334	5.8386160	88.8343770
				H	-1.7546987	6.1466998	90.8493932
				C	-2.1160113	2.6674499	86.6879498
				H	-3.0090604	5.2262767	86.8211869
				C	-1.5297783	3.3128386	85.4215955
				H	-2.1331347	4.1777548	85.0740922
				H	-1.4804725	2.5757394	84.5958839
				H	-0.4934319	3.6638450	85.6038146
				C	-3.5496243	2.1566399	86.4562693
				H	-1.4835124	1.7848605	86.9156698
				H	-4.2416460	2.9946355	86.2276537
				H	-3.9384827	1.6349903	87.3545669
				H	-3.5827375	1.4458987	85.6048166
				C	-3.0884609	7.2361724	88.7493975
				C	-3.0776172	7.8428213	87.3391035
				H	-3.4280855	8.8943274	87.3667998
				H	-3.7526235	7.2939492	86.6500419
				H	-2.0634006	7.8355175	86.8903306
				C	-4.5175588	7.2272024	89.3294572
				H	-2.4697586	7.8909091	89.4037216

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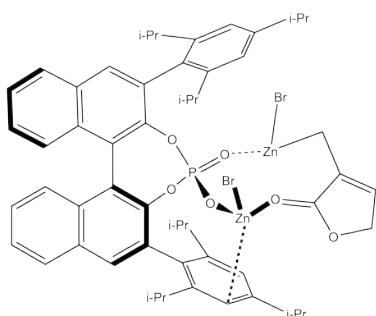


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Br	4.5555618	6.7233250	91.2203053
C	0.7782082	6.3277553	86.2187954
C	2.0298367	5.8174067	85.9917786
C	2.8000580	6.1409588	87.2138186

H	-4.9524569	8.2483024	89.3354473	C	2.7795330	6.1605283	87.2393942
H	-4.5280121	6.8407742	90.3682941	O	2.0286360	6.8547904	88.1097144
H	-5.1795599	6.5752409	88.7216530	C	0.6895354	6.9537095	87.5959432
C	-0.6767543	3.7232969	91.5066688	O	3.9492097	5.8443144	87.5358138
C	0.3034075	4.7885984	92.0266385	C	2.5603383	5.0227422	84.9152828
H	0.8554080	4.3994263	92.9068600	H	0.3926883	8.0254705	87.6014149
H	-0.2191723	5.7114478	92.3541086	H	0.0155779	6.4087167	88.2974694
H	1.0482237	5.0587022	91.2535108	Zn	2.3410268	3.0828573	85.4278822
C	-1.7282416	3.3622087	92.5733573	Br	1.3771247	1.0277069	84.9091155
H	-0.0823502	2.8066896	91.3061644	H	3.6495661	5.1924990	84.7991318
H	-1.2388752	3.0415351	93.5163195	H	2.0433447	5.2199301	83.9571817
H	-2.3883066	2.5391270	92.2334736	H	-0.1200365	6.2270741	85.5902434
H	-2.3719065	4.2374721	92.8030594	C	0.2993036	1.4289959	88.9100788
H	8.5745253	5.2173621	87.9928391	C	0.8564658	0.1548057	89.1207100
H	7.2401201	2.2406385	92.1644975	C	0.0599440	-0.7897489	89.8793388
H	7.6583791	0.7962337	84.5793595	C	0.5766198	-2.0390438	90.3412135
C	7.6993134	5.4681835	88.6329706	C	-1.3005989	-0.4577687	90.2320775
H	4.1705627	2.3084770	93.0843938	C	-2.0970120	-1.4078434	90.9384745
H	7.6630167	7.4763049	87.7680257	C	-1.8122146	0.8339571	89.9214408
H	5.1265946	0.7883866	84.4621187	H	-2.8441286	1.0871138	90.2098766
C	6.8751394	4.1813388	88.6718348	C	-1.0191891	1.7967683	89.3163239
C	6.5642782	1.3826282	91.9665136	C	4.6760548	0.4142237	88.6410873
C	6.9645313	6.6319899	87.9386049	C	4.9721525	-0.8486606	88.1373159
H	6.1349498	7.0113054	88.5706104	H	6.0178676	-1.1426568	87.9637632
C	6.2246004	3.7034106	89.8384538	C	3.9442003	-1.7640819	87.7575666
C	7.5793749	1.5451870	85.3928451	C	4.2691014	-2.9956482	87.1131277
H	8.7796824	5.0741470	90.5112371	C	2.5530391	-1.4187641	87.9425858
C	6.8561500	3.3438183	87.5435740	C	1.5599316	-2.2748255	87.3856961
C	8.2346282	5.8973143	90.0061513	C	2.2345031	-0.2114905	88.6656345
H	8.9339168	6.7497392	89.8909103	C	3.2957418	0.6401778	88.9635981
H	7.3819014	3.6901700	86.6420571	O	0.9614721	2.4403565	88.2271437
C	4.4704085	2.8125576	92.1434811	O	2.9938018	1.8281830	89.6109967
H	6.3236708	0.9082828	92.9401290	P	2.4536128	2.9962662	88.6041119
H	7.1210559	0.6467410	91.3518105	O	2.4532865	4.2687020	89.4734794
C	5.6425573	2.4046342	89.8889672	O	3.2143360	3.0640357	87.2839478
C	5.0549423	1.4019040	85.3827505	C	-1.5731303	-2.6290120	91.3319833
C	6.2450901	2.0779217	87.5260287	C	-0.2167471	-2.9332777	91.0463906
H	8.5078317	1.4944510	85.9969492	H	-3.1368162	-1.1391920	91.1827309
H	7.5403353	2.5424129	84.9074370	H	-2.1964150	-3.3501862	91.8821342
C	5.2708232	1.8436274	91.2598623	H	1.6270636	-2.2905195	90.1457819
C	5.5795364	1.6088116	88.7088900	H	0.2156130	-3.8843791	91.3927993
C	6.3263479	1.2573306	86.2350812	C	1.9126170	-3.4492795	86.7357432
H	3.5499239	3.1578841	91.6342851	C	3.2760957	-3.8264965	86.6168483
H	4.1552584	1.0743946	85.9345056	H	0.5034376	-1.9841568	87.4658315
H	5.0578970	3.7097432	92.4278050	H	1.1286062	-4.0890601	86.3031120
H	6.5337019	6.3271131	86.9653512	H	3.5436075	-4.7659974	86.1098171
H	4.9182279	2.4622843	85.0746283	H	5.3313188	-3.2604021	86.9909652
H	7.4137018	6.2341610	90.6722330	C	-1.3599181	4.1381574	90.1833004
H	4.6530715	0.9377097	91.1018337	C	-1.4930111	3.2055132	89.1178833
H	6.3885830	0.1925723	86.5270727	C	-1.8802235	5.4339219	90.0102080
H	6.3638967	4.2449680	90.7864579	C	-2.0550510	3.6091270	87.8804412
				C	-2.5734838	4.9136952	87.7623839
				C	-2.5145823	5.8375341	88.8195391
				H	-1.7896914	6.1612856	90.8333129
				C	-2.1079219	2.6639838	86.6835058
				H	-3.0333984	5.2118236	86.8082939
				C	-1.5407456	3.3129594	85.4105904
				H	-2.1638163	4.1622203	85.0584821
				H	-1.4767223	2.5713321	84.5902803
				H	-0.5109912	3.6857217	85.5862590
				C	-3.5329531	2.1256354	86.4628811
				H	-1.4575088	1.7942958	86.9100731
				H	-4.2427272	2.9490603	86.2359620
				H	-3.9063708	1.6001848	87.3652723
				H	-3.5577994	1.4111151	85.6145551
				C	-3.1415427	7.2255307	88.7307563
				C	-3.1205242	7.8370921	87.3226154
				H	-3.4875334	8.8830186	87.3468907
				H	-3.7774790	7.2805094	86.6225069
				H	-2.1002839	7.8458364	86.8875763
				C	-4.5777815	7.1926201	89.2913319

13j-mod-mi



Energy (Hartree)= -11625.08021221

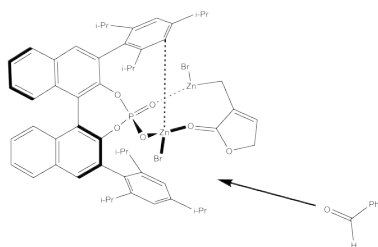
Zn	4.1936107	5.2759319	89.5045774
Br	4.6443728	6.7033508	91.2712383
C	0.7535222	6.3236383	86.2484759
C	2.0114123	5.8303200	86.0166054

H	-2.5418605	7.8882542	89.3949780	Zn	0.7457337	0.6744614	2.4559060
H	-5.0300727	8.2061214	89.2951398	Br	2.1157674	2.4478117	3.1053432
H	-4.5958263	6.8016092	90.3281030	H	-1.9211287	4.5722224	0.0055792
H	-5.2208113	6.5314954	88.6735243	Br	-4.5142642	1.0025709	-2.1538973
C	-0.6792422	3.7548294	91.4969212	H	-4.9927774	0.8570844	1.3329843
C	0.2852575	4.8353144	92.0143183	Zn	-3.2139984	0.1217995	-0.3904645
H	0.8457642	4.4561256	92.8932378	C	-3.5169297	3.3625350	0.8956769
H	-0.2499616	5.7502706	92.3434550	C	-2.3031975	4.2277424	0.9923273
H	1.0250400	5.1173114	91.2408984	C	-3.2243236	2.1136422	1.3790855
C	-1.7248496	3.3803298	92.5646207	C	-3.8912099	0.8107865	1.3970076
H	-0.0717863	2.8465391	91.2977096	C	-1.8103389	2.1762094	1.7798926
H	-1.2305850	3.0702177	93.5083797	O	-1.2797798	3.3852721	1.5795546
H	-2.3715888	2.5457315	92.2278118	O	-1.1670541	1.2145754	2.2334773
H	-2.3825502	4.2455177	92.7922015	H	-2.4172765	5.1229574	1.6419383
H	8.6006197	5.2016106	87.9724996	H	-3.5438628	0.1826866	2.2363706
H	7.2737579	2.2039390	92.1684750	H	-4.4625852	3.6940135	0.4475548
H	7.6430681	0.7773614	84.5635583	C	0.1555856	-3.6470867	1.0009248
C	7.7351482	5.4458683	88.6287669	C	0.6938609	-4.4843367	0.0227180
H	4.2070809	2.2971938	93.0904004	C	1.5803285	-5.5457932	0.4551788
H	7.6754214	7.4591391	87.7736790	C	2.3365377	-6.3500318	-0.4503063
H	5.1065416	0.8074584	84.4583818	C	1.7393825	-5.7930900	1.8690939
C	6.9134274	4.1577179	88.6743448	C	2.5595905	-6.8763957	2.3063421
C	6.5900546	1.3527610	91.9684161	C	1.1449892	-4.9037400	2.8095380
C	6.9839379	6.6111064	87.9547247	H	1.3267402	-5.0658703	3.8832642
H	6.1680428	6.9864647	88.6065543	C	0.4190026	-3.7943964	2.3988757
C	6.2721102	3.6795714	89.8430102	C	0.7123320	-2.7683130	-3.4067775
C	7.5766332	1.5227076	85.3814866	C	0.4842548	-3.8640337	-4.2334862
H	8.8457932	5.0444559	90.4873668	H	0.5799691	-3.7386917	-5.3231964
C	6.8834869	3.3234152	87.5438371	C	0.0758822	-5.1264153	-3.7199188
C	8.2918365	5.8694334	89.9951539	C	-0.2950316	-6.1987744	-4.5861260
H	8.9883287	6.7233797	89.8740582	C	0.0164237	-5.3185518	-2.2927144
H	7.4054743	3.6696757	86.6399049	C	-0.4681808	-6.5667684	-1.7981812
C	4.5091750	2.8003445	92.1496536	C	0.4229847	-4.2420222	-1.4201863
H	6.3468808	0.8776377	92.9410616	C	0.6322290	-2.9761261	-1.9915035
H	7.1408544	0.6144138	91.3514293	O	-0.7249759	-2.6388000	0.6225840
C	5.6774332	2.3892441	89.8928015	O	0.9086691	-1.8768904	-1.1868850
C	5.0502502	1.4145116	85.3842814	P	-0.1441246	-1.2636216	-0.0808490
C	6.2623401	2.0630118	87.5249276	O	0.7779771	-0.4761123	0.8607503
H	8.5075848	1.4587126	85.9803837	O	-1.3643871	-0.5880336	-0.7102577
H	7.5482540	2.5221462	84.8998579	C	3.2428674	-7.6664633	1.3945244
C	5.3013542	1.8276360	91.2628364	C	3.1450263	-7.3823717	0.0067789
C	5.6009419	1.5972481	88.7105555	H	2.6556969	-7.0581774	3.3883764
C	6.3239167	1.2481804	86.2286837	H	3.8772022	-8.4953467	1.7436674
C	3.5897208	3.1526994	91.6436689	H	2.2845415	-6.1421182	-1.5270478
H	4.1495370	1.0927876	85.9376693	H	3.7195810	-7.9817310	-0.7158263
H	5.1012441	3.6942010	92.4344815	C	-0.8447910	-7.5827592	-2.6660715
H	6.5331956	6.3109581	86.9889768	C	-0.7445909	-7.4061061	-4.0723794
H	4.9235201	2.4790621	85.0870558	H	-0.5578656	-6.7138636	-0.7125206
H	7.4811707	6.2026285	90.6752443	H	-1.2304419	-8.5304224	-2.2601082
H	4.6755549	0.9275240	91.1018867	H	-1.0394221	-8.2214550	-4.7503543
H	6.3723467	0.1807172	86.5138347	H	-0.2357972	-6.0397008	-5.6743189
H	6.4007919	4.2299590	90.7868810	C	1.0532288	-1.8107794	3.8002101
				C	0.0328015	-2.6751721	3.3073623
				C	0.6607947	-0.6279275	4.4802331
				C	-1.3325734	-2.3986157	3.5776761
				C	-1.6729542	-1.2375120	4.2994264
				C	-0.7038094	-0.3290701	4.7487718
				H	1.4376634	0.0087995	4.9357990
				C	-2.4236783	-3.3749188	3.1489683
				H	-2.7340251	-1.0359334	4.5037814
				C	-3.5561331	-2.7124307	2.3503174
				H	-4.1438643	-2.0033583	2.9688817
				H	-4.2602700	-3.4819430	1.9740862
				H	-3.1562288	-2.1581526	1.4788834
				C	-2.9621362	-4.1351427	4.3766451
				H	-1.9500629	-4.1263563	2.4855256
				H	-3.4489092	-3.4441422	5.0962584
				H	-2.1473530	-4.6630519	4.9123442
				H	-3.7154598	-4.8884060	4.0671296
				C	-1.0440516	0.9266685	5.5410482
				C	-2.4983098	1.3886401	5.3908120

7.4 Agglomeration to Complexes 13

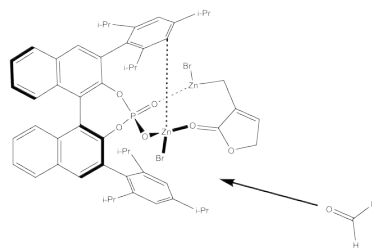
7.4.1 Pathways starting from 13j-ma

TS-7-d-ma; COSMO



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H	-3.2045957	0.6845869	5.8785368
H	-2.7936608	1.4817407	4.3278321
C	-0.6843602	0.7306967	7.0286415
H	-0.3829509	1.7293887	5.1404613
H	-0.8655451	1.6647321	7.5985501
H	0.3793310	0.4502903	7.1633789
H	-1.3069983	-0.0713204	7.4776523
C	2.5384126	-2.1564642	3.7012613
C	3.4143944	-1.0412025	3.1138325
H	4.4667304	-1.3846267	3.0475819
H	3.4077450	-0.1165821	3.7255475
H	3.0887457	-0.7775078	2.0863126
C	3.0473854	-2.6018023	5.0878171
H	2.6322407	-3.0236350	3.0205810
H	4.1020070	-2.9391732	5.0235873
H	2.4428609	-3.4369603	5.4968054
H	3.0024564	-1.7674084	5.8186553
H	0.7467112	3.0187759	-5.7871450
H	4.9621940	-0.9062793	-4.4275329
H	-2.5140551	-1.9855794	-6.8178546
C	1.7094406	2.6653539	-5.3564296
H	4.7265452	-1.3195243	-1.2647604
H	2.1488052	4.6523302	-4.5367107
H	-3.4490697	-1.1016648	-4.5636287
C	1.4795733	1.2338557	-4.8885285
C	4.5161742	-1.8313361	-4.0055186
C	2.0672319	3.6018160	-4.1888839
H	3.0411307	3.3277641	-3.7319103
C	2.4620000	0.5301932	-4.1671983
C	-1.5473479	-1.4856484	-6.6008261
H	2.4829716	2.0891416	-7.3331590
C	0.2793485	0.5676659	-5.1777706
C	2.7672655	2.7291700	-6.4735045
H	2.8912187	3.7684741	-6.8430011
H	-0.4944718	1.1014208	-5.7537904
C	3.9416231	-0.7283413	-1.7804983
H	5.3307768	-2.4095302	-3.5216702
H	4.1252509	-2.4303215	-4.8533969
C	2.2526724	-0.7773611	-3.6980436
C	-2.4694225	-0.6112701	-4.3902533
C	0.0192041	-0.7461067	-4.7413780
H	-0.7397402	-2.0740636	-7.0837008
H	-1.5722500	-0.4890163	-7.0888827
C	3.3997607	-1.5018519	-2.9945960
C	1.0051016	-1.4127679	-3.9620381
C	-1.3318152	-1.3702660	-5.0821380
H	3.1344845	-0.5173226	-1.0518184
H	-2.3044471	-0.5667550	-3.2974135
H	4.4010891	0.2368887	-2.0794983
H	1.2996480	3.5615378	-3.3898430
H	-2.5554634	0.4361916	-4.7451418
H	3.7561131	2.3814051	-6.1073178
H	3.0133365	-2.4712623	-2.6200671
H	-1.3475469	-2.3989040	-4.6737116
H	3.4283148	1.0175214	-3.9604660
C	-0.4122251	12.0313469	-0.5590679
C	0.3456341	10.8753538	-0.3453092
C	1.7276028	10.8733210	-0.6384092
C	2.3407409	12.0379794	-1.1458850
C	1.5795864	13.1963648	-1.3603586
C	0.2046400	13.1918556	-1.0670091
H	-1.4893179	12.0363957	-0.3316254
H	-0.1038053	9.9513014	0.0500547
C	2.5315908	9.6456151	-0.4135203
H	3.4199166	12.0282441	-1.3718103
H	2.0556071	14.1061015	-1.7569614
H	-0.3938876	14.1006793	-1.2352083
O	2.0856274	8.5916635	0.0159892
H	3.6270357	9.7514968	-0.6758262



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number of imaginary frequencies: 6

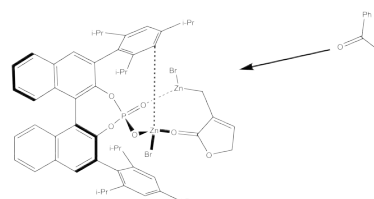
Zn	0.7562891	0.6845488	2.4455502
Br	2.1141176	2.4436229	3.1121336
H	-1.9199999	4.5716206	0.0059057
Br	-4.5157237	0.9963190	-2.1490658
H	-4.9920361	0.8544909	1.3308191
Zn	-3.2128470	0.1438699	-0.4021592
C	-3.5189409	3.3617938	0.8965309
C	-2.3028119	4.2255991	0.9923555
C	-3.2266059	2.1129349	1.3815315
C	-3.8909978	0.8113077	1.3998960
C	-1.8110544	2.1750994	1.7808941
O	-1.2803886	3.3848664	1.5783453
O	-1.1672943	1.2145072	2.2327622
H	-2.4146176	5.1218127	1.6421665
H	-3.5412838	0.1817151	2.2368062
H	-4.4640537	3.6892321	0.4447318
C	0.1556021	-3.6468721	1.0005720
C	0.6941299	-4.4845776	0.0225069
C	1.5805045	-5.5458888	0.4554782
C	2.3365890	-6.3503259	-0.4496734
C	1.7396198	-5.7933064	1.8692331
C	2.5596238	-6.8764098	2.3058207
C	1.1449596	-4.9039066	2.8090085
H	1.3268436	-5.0648343	3.8829483
C	0.4192851	-3.7944272	2.3987448
C	0.7129127	-2.7680174	-3.4069284
C	0.4846521	-3.8642190	-4.2327855
H	0.5800031	-3.7374214	-5.3223517
C	0.0760578	-5.1265352	-3.7198345
C	-0.2952124	-6.1988993	-4.5851614
C	0.0169671	-5.3188765	-2.2928313
C	-0.4678608	-6.5668587	-1.7986792
C	0.4235351	-4.2423777	-1.4204893
C	0.6321624	-2.9761830	-1.9916243
O	-0.7242708	-2.6394432	0.6241377
O	0.9068472	-1.8772297	-1.1867316
P	-0.1461104	-1.2630412	-0.0815046
O	0.7760198	-0.4752365	0.8594422
O	-1.3699679	-0.5901039	-0.7043730
C	3.2427127	-7.6663854	1.3946328
C	3.1446445	-7.3824176	0.0074554
H	2.6556975	-7.0579501	3.3879279
H	3.8769551	-8.4951644	1.7440551
H	2.2833298	-6.1419469	-1.5261814
H	3.7189837	-7.9818208	-0.7151951
C	-0.8446409	-7.5825029	-2.6662515
C	-0.7446894	-7.4059127	-4.0719629
H	-0.5570278	-6.7130628	-0.7129409
H	-1.2306739	-8.5298908	-2.2601379
H	-1.0399261	-8.2209138	-4.7500962
H	-0.2365507	-6.0394195	-5.6732961
C	1.0527673	-1.8114797	3.8024081
C	0.0328451	-2.6756708	3.3078548
C	0.6602722	-0.6311669	4.4849418
C	-1.3323630	-2.3988316	3.5775018
C	-1.6725380	-1.2380677	4.2992270

TS-7-d-ma

C	-0.7035294	-0.3305320	4.7503160
H	1.4368759	0.0109567	4.9329911
C	-2.4236984	-3.3749411	3.1485598
H	-2.7337598	-1.0354404	4.5018260
C	-3.5560906	-2.7127264	2.3499653
H	-4.1444976	-2.0036124	2.9679043
H	-4.2608342	-3.4814285	1.9733147
H	-3.1557343	-2.1584977	1.4789937
C	-2.9618349	-4.1355856	4.3758348
H	-1.9495822	-4.1256525	2.4846305
H	-3.4482446	-3.4452082	5.0962520
H	-2.1471372	-4.6629874	4.9119036
H	-3.7154855	-4.8891100	4.0678257
C	-1.0436797	0.9264526	5.5408676
C	-2.4978842	1.3886334	5.3901200
H	-2.6377229	2.3755588	5.8741668
H	-3.2049605	0.6853656	5.8780940
H	-2.7939800	1.4819495	4.3274511
C	-0.6852897	0.7311100	7.0285632
H	-0.3820944	1.7283517	5.1390802
H	-0.8661190	1.6643763	7.5997822
H	0.3780326	0.4502222	7.1639654
H	-1.3074336	-0.0713499	7.4774681
C	2.5383026	-2.1561587	3.7017575
C	3.4145734	-1.0407001	3.1150579
H	4.4669929	-1.3840452	3.0488637
H	3.4082601	-0.1145409	3.7244348
H	3.0905258	-0.7764740	2.0874235
C	3.0472240	-2.6023748	5.0877886
H	2.6314217	-3.0231371	3.0205901
H	4.1019406	-2.9396798	5.0251706
H	2.4423087	-3.4370736	5.4972029
H	3.0020519	-1.7686818	5.8193246
H	0.7462975	3.0182527	-5.7863630
H	4.9621948	-0.9069149	-4.4288539
H	-2.5140870	-1.9855121	-6.8177029
C	1.7094126	2.6648253	-5.3560993
H	4.7274875	-1.3196018	-1.2654277
H	2.1489129	4.6523589	-4.5360147
H	-3.4495292	-1.1007524	-4.5623408
C	1.4796601	1.2331433	-4.8886875
C	4.5162439	-1.8315933	-4.0062248
C	2.0670371	3.6016019	-4.1890131
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C	2.4618838	0.5297493	-4.1677471
C	-1.5471524	-1.4863487	-6.6003777
H	2.4827125	2.0891495	-7.3329849
C	0.2799532	0.5670089	-5.1776473
C	2.7664150	2.7295426	-6.4736851
H	2.8910004	3.7687584	-6.8432477
H	-0.4946886	1.1008284	-5.7522946
C	3.9420682	-0.7289795	-1.7810062
H	5.3314413	-2.4095697	-3.5231307
H	4.1253300	-2.4297424	-4.8544614
C	2.2529851	-0.7774183	-3.6985959
C	-2.4695678	-0.6110386	-4.3903666
C	0.0195546	-0.7465437	-4.7419357
H	-0.7394909	-2.0738819	-7.0842231
H	-1.5719293	-0.4902498	-7.0892389
C	3.4001310	-1.5018800	-2.9952565
C	1.0056266	-1.4127411	-3.9626888
C	-1.3318601	-1.3701741	-5.0817984
H	3.1356344	-0.5165906	-1.0522186
H	-2.3047635	-0.5660993	-3.2977455
H	4.4013241	0.2365271	-2.0790037
H	1.3005670	3.5606592	-3.3893636
H	-2.5566824	0.4364428	-4.7443480
H	3.7553709	2.3814579	-6.1084690
H	3.0137307	-2.4715138	-2.6210188
H	-1.3477816	-2.3988479	-4.6732181
H	3.4278148	1.0173089	-3.9601570

C	-0.4113515	12.0315519	-0.5592879
C	0.3467773	10.8760713	-0.3455953
C	1.7279680	10.8742785	-0.6386051
C	2.3394789	12.0386251	-1.1457951
C	1.5786285	13.1967725	-1.3603983
C	0.2043243	13.1920241	-1.0670973
H	-1.4884799	12.0363952	-0.3317902
H	-0.0985267	9.9499870	0.0497174
C	2.5309092	9.6432258	-0.4124183
H	3.4188228	12.0282569	-1.3715509
H	2.0544937	14.1065405	-1.7570883
H	-0.3944331	14.1006650	-1.2352896
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H	3.6282515	9.7502999	-0.6753310

TS-7-d-mi; COSMO



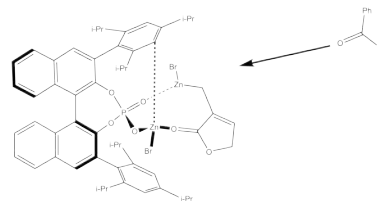
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Br	-2.4413180	1.6004209	2.4540807
H	0.0409569	4.8315682	1.2041700
Zn	-0.7972464	2.3516425	0.9803326
C	2.1915969	4.1236648	2.9440578
C	3.3520556	3.3132923	3.4156003
C	1.6664336	3.5645742	1.8103634
C	0.5211047	3.8685398	0.9477859
C	2.4781898	2.3564521	1.5725574
O	3.4587701	2.2230715	2.4692795
O	2.2749158	1.5151947	0.6750590
H	3.2193491	2.8620355	4.4233736
H	0.8144943	3.8644035	-0.1216636
H	1.8356011	5.0235631	3.4633695
C	-1.0179882	-2.4075991	-2.1135333
C	-1.4261190	-2.2175604	-3.4377784
C	-1.3721419	-3.3589147	-4.3253183
C	-1.5879731	-3.2623536	-5.7332217
C	-1.0549905	-4.6571373	-3.7767873
C	-1.0645781	-5.7996947	-4.6323877
C	-0.6565442	-4.7699397	-2.4130820
H	-0.3512986	-5.7554292	-2.0289119
C	-0.5581958	-3.6569792	-1.5889966
C	-1.3067570	1.5633655	-4.1535654
C	-2.4065740	1.7099066	-4.9923296
H	-2.6152548	2.6950511	-5.4381790
C	-3.3179767	0.6420340	-5.2300273
C	-4.5065494	0.8452201	-5.9946695
C	-3.0711537	-0.6506194	-4.6371796
C	-4.0753077	-1.6560560	-4.7733917
C	-1.8427999	-0.8654721	-3.9074844
C	-1.0366561	0.2522917	-3.6479205
O	-1.0826552	-1.3408583	-1.2234314
O	0.1325889	0.0995260	-2.9103895
P	0.0476659	-0.1538692	-1.2893430
O	1.4491393	-0.7129803	-0.9561869
O	-0.5147907	1.0175248	-0.5126897
C	-1.3262109	-5.6748126	-5.9885638
C	-1.5665588	-4.3899243	-6.5434355
H	-0.8381882	-6.7843516	-4.1938494

H	-1.3255107	-6.5634948	-6.6379224
H	-1.7661627	-2.2761602	-6.1824988
H	-1.7326567	-4.2838865	-7.6263785
C	-5.2334438	-1.4191521	-5.5013326
C	-5.4452701	-0.1657121	-6.1356032
H	-3.9300779	-2.6273665	-4.2808475
H	-5.9964410	-2.2084083	-5.5813217
H	-6.3625337	0.0069569	-6.7188771
H	-4.6737007	1.8329619	-6.4524797
C	1.5685817	-3.7569239	-0.2596418
C	0.1460592	-3.6511291	-0.2696994
C	2.2464868	-3.5459696	0.9549592
C	-0.5580983	-3.3846814	0.9330521
C	0.1684359	-3.1870955	2.1234060
C	1.5719987	-3.2480256	2.1581020
H	3.3449945	-3.6228758	0.9742292
C	-2.0836547	-3.3578740	0.9712308
H	-0.3886153	-2.9765710	3.0480046
C	-2.6448771	-2.0790684	1.6103418
H	-2.3779215	-1.9965916	2.6842626
H	-3.7525759	-2.0680464	1.5491044
H	-2.2688799	-1.1691107	1.1060479
C	-2.6193897	-4.6232496	1.6700348
H	-2.4427220	-3.3914544	-0.0784759
H	-2.2972171	-4.6591950	2.7320702
H	-2.2529869	-5.5462854	1.1758880
H	-3.7289589	-4.6398224	1.6540173
C	2.3814360	-3.0672782	3.4387543
C	1.6407796	-2.3085802	4.5467199
H	2.3217309	-2.1104876	5.3989830
H	0.7836075	-2.8921939	4.9436650
H	1.2469807	-1.3350948	4.1888187
C	2.8903766	-4.4309644	3.9492286
H	3.2762913	-2.4671988	3.1562177
H	3.5464113	-4.3024391	4.8350961
H	3.4703843	-4.9655364	3.1703277
C	2.0403625	-5.0826770	4.2422698
C	2.3751572	-4.1164072	-1.5086374
C	3.5706820	-3.1871983	-1.7705514
H	4.0934347	-3.4906550	-2.7007374
H	4.3164216	-3.2066100	-0.9503309
H	3.2320301	-2.1404092	-1.9042577
C	2.8250232	-5.5892870	-1.4377120
H	1.7029242	-4.0193791	-2.3835521
H	3.3545768	-5.8851305	-2.3671504
H	1.9620213	-6.2722737	-1.3013641
H	3.5164009	-5.7532338	-0.5845736
H	1.2853857	6.5334150	-1.3495853
H	2.6544022	3.3223382	-6.1408124
H	-4.3721641	4.9604786	-2.8092178
C	1.9251895	6.0020060	-2.0883946
H	3.2581375	0.3964544	-4.9762594
H	3.7219355	6.3587048	-0.8852984
H	-3.8937940	3.5477066	-0.7686237
C	1.0886675	4.8583849	-2.6500857
C	1.9305195	2.4919046	-6.2792308
C	3.1790715	5.5077232	-1.3457889
H	3.8858773	4.9977646	-2.0328324
C	1.6576937	3.8693158	-3.4712890
C	-3.2830043	5.0111264	-3.0142849
H	1.3917629	7.3988871	-3.7036731
C	-0.2885556	4.7741341	-2.3884348
C	2.2957611	7.0077690	-3.1948436
H	2.8579687	7.8688333	-2.7773156
H	-0.7495925	5.5459693	-1.7501331
C	2.8374012	1.1706424	-4.3020565
H	2.3829906	1.7632911	-6.9835719
H	1.0229378	2.9141581	-6.7565829
C	0.9036175	2.8077998	-3.9999282
C	-2.8152055	3.4970364	-1.0215075
C	-1.0945034	3.7330182	-2.8896432

H	-3.1448177	5.1510215	-4.1060960
H	-2.8906274	5.9183665	-2.5095123
C	1.5924304	1.8160819	-4.9359678
C	-0.4855334	2.7263017	-3.6955906
C	-2.5812552	3.7319593	-2.5235945
H	2.5861441	0.6850833	-3.3390320
H	-2.4753416	2.4799926	-0.7378614
H	3.6386247	1.9165131	-4.1177268
H	2.9161734	4.7935872	-0.5402583
H	-2.2966494	4.2530334	-0.3938339
H	2.9350511	6.5287680	-3.9661345
H	0.8747228	1.0011942	-5.1578356
H	-3.0616453	2.8818987	-3.0437473
H	2.7306165	3.9263097	-3.7140027
C	-3.6451898	0.4834836	11.9221010
C	-3.2926365	0.7474695	10.5943154
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C	-1.7225395	-1.1247900	10.6428059
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H	-4.3977079	1.1071827	12.4287353
H	-3.7489754	1.5731073	10.0265533
C	-1.9461976	0.2236259	8.5402429
H	-0.9712608	-1.7479188	10.1298929
H	-1.6022108	-2.2184145	12.5192179
H	-3.3137969	-0.7876674	13.6583501
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TS-7-d-mi

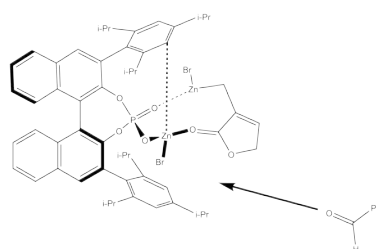


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H	4.3403050	3.8687729	3.4026841
Br	-2.5135601	1.5553569	2.3975863
H	0.0304452	4.7918029	1.2229897
Zn	-0.8148835	2.3101968	1.0177201
C	2.2067535	4.1244116	2.9457082
C	3.3721201	3.3200292	3.4201260
C	1.6654788	3.5415164	1.8312954
C	0.5125406	3.8270287	0.9769539
C	2.4778494	2.3278693	1.6044925
O	3.4701227	2.2146947	2.4951588
O	2.2697997	1.4729629	0.7255489
H	3.2496845	2.8871773	4.4380828
H	0.7945551	3.8040474	-0.0956149
H	1.8597539	5.0375670	3.4475560
C	-1.0191826	-2.3987690	-2.1156342
C	-1.4307620	-2.2147358	-3.4398028
C	-1.3800747	-3.3596377	-4.3228835
C	-1.5943103	-3.2672039	-5.7310867
C	-1.0654236	-4.6564797	-3.7704016
C	-1.0740305	-5.8006504	-4.6230054
C	-0.6676138	-4.7643584	-2.4065145
H	-0.3656466	-5.7486317	-2.0167218
C	-0.5628915	-3.6482199	-1.5882015
C	-1.3054332	1.5631984	-4.1610780
C	-2.4078299	1.7117339	-4.9956761
H	-2.6169092	2.6986641	-5.4373551

C	-3.3205473	0.6453431	-5.2333200	H	3.8805155	4.9812220	-2.0102673
C	-4.5094109	0.8492395	-5.9964513	C	1.6596608	3.8640271	-3.4693207
C	-3.0739032	-0.6477578	-4.6417974	C	-3.2798298	5.0019873	-3.0263929
C	-4.0785174	-1.6523647	-4.7788138	H	1.3988739	7.3865816	-3.7029953
C	-1.8447565	-0.8640094	-3.9140602	C	-0.2859500	4.7642343	-2.3829178
C	-1.0345331	0.2514063	-3.6580748	C	2.3007987	6.9967143	-3.1899452
O	-1.0742732	-1.3289722	-1.2296692	H	2.8629003	7.8587165	-2.7742991
O	0.1381168	0.0964242	-2.9275592	H	-0.7470836	5.5333944	-1.7414626
P	0.0629829	-0.1482055	-1.3036810	C	2.8378287	1.1656532	-4.3098666
O	1.4650538	-0.7144392	-0.9807557	H	2.3853180	1.7692209	-6.9893684
O	-0.4771121	1.0335989	-0.5283339	H	1.0260137	2.9200199	-6.7584685
C	-1.3316523	-5.6795071	-5.9797270	C	0.9058350	2.8050660	-4.0026137
C	-1.5712536	-4.3966034	-6.5379725	C	-2.8145636	3.4996918	-1.0229962
H	-0.8480767	-6.7839975	-4.1813266	C	-1.0923752	3.7268745	-2.8899177
H	-1.3278341	-6.5697612	-6.6268342	H	-3.1437617	5.1327449	-4.1195615
H	-1.7717387	-2.2818307	-6.1822745	H	-2.8834384	5.9132625	-2.5322074
H	-1.7347897	-4.2931761	-7.6214984	C	1.5943633	1.8158081	-4.9416740
C	-5.2357970	-1.4148270	-5.5071248	C	-0.4836038	2.7241016	-3.7002643
C	-5.4477526	-0.1610211	-6.1392855	C	-2.5792708	3.7262760	-2.5254424
H	-3.9325921	-2.6239562	-4.2873247	H	2.5853836	0.6733781	-3.3508034
H	-5.9983115	-2.2043108	-5.5888451	H	-2.4585558	2.4916716	-0.7291703
H	-6.3647407	0.0125605	-6.7226434	H	3.6397640	1.9091693	-4.1192507
H	-4.6766724	1.8378357	-6.4523557	H	2.9031828	4.7949654	-0.5204718
C	1.5674585	-3.7375326	-0.2659219	H	-2.3110711	4.2671530	-0.3972665
C	0.1449593	-3.6378772	-0.2714522	H	2.9408407	6.5153203	-3.9588803
C	2.2470473	-3.5232400	0.9470718	H	0.8755773	1.0027003	-5.1663786
C	-0.5580500	-3.3712977	0.9315733	H	-3.0579093	2.8722801	-3.0408514
C	0.1703019	-3.1661503	2.1196021	H	2.7326112	3.9216738	-3.7118719
C	1.5738665	-3.2259786	2.1518355	C	-3.6485868	0.4836191	11.9260586
H	3.3453023	-3.6010561	0.9655762	C	-3.3001105	0.7419640	10.5964493
C	-2.0836576	-3.3544641	0.9709701	C	-2.3338695	-0.0607569	9.9513608
H	-0.3858955	-2.9525812	3.0440195	C	-1.7239365	-1.1219650	10.6506310
C	-2.6545169	-2.0760850	1.6006752	C	-2.0735764	-1.3800738	11.9839541
H	-2.3840121	-1.9776914	2.6722311	C	-3.0352365	-0.5770356	12.6204409
H	-3.7623507	-2.0755531	1.5453980	H	-4.4016625	1.1077985	12.4313025
H	-2.2935001	-1.1669370	1.0848730	H	-3.7586515	1.5619502	10.0223574
C	-2.6078959	-4.6203180	1.6773210	C	-1.9619401	0.2210213	8.5384211
H	-2.4427793	-3.3976941	-0.0784812	H	-0.9709987	-1.7450681	10.1397888
H	-2.2759541	-4.6530877	2.7362796	H	-1.5978285	-2.2082209	12.5311265
H	-2.2425723	-5.5433373	1.1825873	H	-3.3109137	-0.7785112	13.6673684
H	-3.7173947	-4.6408619	1.6722597	O	-2.4307617	1.1226529	7.8654128
C	2.3887225	-3.0489341	3.4294218	H	-1.1814239	-0.4832096	8.1132326
C	1.6526332	-2.2997831	4.5463165				
H	2.3369525	-2.1118259	5.3982612				
H	0.7950630	-2.8841748	4.9411598				
H	1.2604665	-1.3217217	4.1996071				
C	2.9085060	-4.4124596	3.9287178				
H	3.2790364	-2.4432727	3.1451527				
H	3.5742139	-4.2846501	4.8074301				
H	3.4826810	-4.9410926	3.1417579				
H	2.0657068	-5.0704315	4.2279764				
C	2.3720031	-4.0984457	-1.5161170				
C	3.5733094	-3.1767242	-1.7794191				
H	4.1035809	-3.4954335	-2.7002090				
H	4.3129367	-3.1862181	-0.9534738				
H	3.2403198	-2.1309947	-1.9329738				
C	2.8144276	-5.5734706	-1.4447214				
H	1.6995254	-3.9978334	-2.3906108				
H	3.3413479	-5.8734412	-2.3742806				
H	1.9487385	-6.2522035	-1.3055795				
H	3.5057771	-5.7401494	-0.5922991				
H	1.2821043	6.5282403	-1.3480348				
H	2.6570146	3.3254149	-6.1423654				
H	-4.3685339	4.9574484	-2.8178028				
C	1.9252020	5.9943213	-2.0823930				
H	3.2597048	0.3956995	-4.9880857				
H	3.7198413	6.3525740	-0.8754168				
H	-3.8943059	3.5320427	-0.7727569				
C	1.0905171	4.8499441	-2.6447415				
C	1.9330346	2.4955022	-6.2825710				
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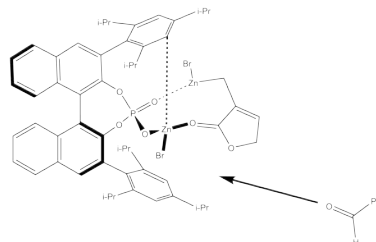


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Br	4.6462080	-1.1780497	1.3897986
H	1.6991851	2.9929973	1.9441972
Br	-4.3308079	-0.6091440	1.7173899
H	-0.9946845	-0.5718963	4.6307912
Zn	-2.2119989	0.0197935	2.4592027
C	0.4828343	2.3451963	3.6428841
C	1.7737566	2.4314443	2.9026979
C	0.0713835	1.0416603	3.7112966
C	-1.1768480	0.4098361	4.1488068
C	1.1284062	0.2674611	3.0304218
O	2.1046874	1.0642534	2.5801662
O	1.1725558	-0.9680066	2.8525997
H	2.6196836	2.8607495	3.4825174
H	-1.7747911	1.0546925	4.8202291

H	-0.0551255	3.2249850	4.0207412	H	2.8125257	-6.1850926	-2.1663683
C	-1.4803839	-3.3304109	-0.3913366	H	1.7953178	-6.7368861	-0.7943568
C	-2.3593970	-3.1767873	-1.4664801	H	3.4739994	-6.1907273	-0.4983871
C	-2.5499142	-4.3100083	-2.3422871	H	0.3409453	6.0021120	-1.3361074
C	-3.2998986	-4.2318100	-3.5546738	H	-0.3903567	2.3118146	-5.8822691
C	-1.9348730	-5.5733183	-2.0038671	H	-4.9919658	3.3847502	0.6530138
C	-2.1575010	-6.7060681	-2.8435154	C	0.6135311	5.3930657	-2.2263539
C	-1.0644073	-5.6577955	-0.8778212	H	0.8478427	-0.4738250	-4.9492713
H	-0.5692071	-6.6159493	-0.6584210	H	2.7142289	6.0184489	-2.1119318
C	-0.7830243	-4.5430009	-0.1010616	H	-3.0734138	2.6804526	2.2395374
C	-2.7585715	0.5947644	-2.0736192	C	-0.2363327	4.1296426	-2.1718146
C	-4.1216164	0.6822339	-2.3326774	C	-1.0539540	1.4687321	-5.5968102
H	-4.5525779	1.6551717	-2.6126956	C	2.1179230	5.0827138	-2.1339321
C	-4.9896572	-0.4374942	-2.1979159	H	2.4625126	4.4892741	-3.0065441
C	-6.4005865	-0.2987502	-2.3613256	C	-0.0975586	3.1129146	-3.1333168
C	-4.4433889	-1.7251048	-1.8465143	C	-4.2592184	3.5412980	-0.1656467
C	-5.3495367	-2.8004722	-1.6059257	H	-0.7897756	6.4844215	-3.5221880
C	-3.0150111	-1.8603039	-1.7038135	C	-1.1943681	3.9470955	-1.1617430
C	-2.2364655	-0.6983565	-1.7663286	C	0.2886332	6.2304301	-3.4773805
O	-1.2714507	-2.2752890	0.4843193	H	0.8675015	7.1774053	-3.4834707
O	-0.8580949	-0.7926605	-1.5505889	H	-1.3037176	4.7299691	-0.3935135
P	-0.3837102	-0.9625617	0.0107940	C	0.7425476	0.3313283	-4.1927138
O	1.1185519	-1.2788477	-0.0687808	H	-0.9550176	0.6857089	-6.3770987
O	-0.8598715	0.1716446	0.9172586	H	-2.0981166	1.8421534	-5.6146842
C	-2.9224328	-6.6018299	-3.9955975	C	-0.8900283	1.9513943	-3.1162568
C	-3.4819956	-5.3481111	-4.3597070	C	-2.3790329	2.9806796	1.4249003
H	-1.6921648	-7.6649147	-2.5656210	C	-2.0114120	2.8023190	-1.0933674
H	-3.0812161	-7.4819601	-4.6371220	H	-4.7644690	3.3024483	-1.1220855
H	-3.7326837	-3.2676976	-3.8543391	H	-3.9937519	4.6195680	-0.1883350
H	-4.0615279	-5.2578616	-5.2911501	C	-0.6857542	0.9059897	-4.2115372
C	-6.7190693	-2.6282532	-1.7513845	C	-1.8701851	1.8003626	-2.0955773
C	-7.2517169	-1.3724400	-2.1483129	C	-3.0093422	2.6699998	0.0552163
H	-4.9533303	-3.7726832	-1.2817732	H	0.9829579	-0.0958504	-3.1996959
H	-7.3983917	-3.4702292	-1.5481800	H	-1.4164877	2.4465503	1.5532240
H	-8.3391764	-1.2497832	-2.2665258	H	1.4985496	1.1095216	-4.4282245
H	-6.8023048	0.6883293	-2.6394438	H	2.3556571	4.5015912	-1.2198324
C	1.6382453	-4.3567281	0.5411037	H	-2.1773567	4.0636714	1.5635062
C	0.2815274	-4.4820222	0.9481757	H	0.5413975	5.6763645	-4.4056919
C	2.6218323	-4.1217388	1.5393104	H	-1.3805441	0.0652866	-4.0127153
C	-0.0640273	-4.4086316	2.3255204	H	-3.3408549	1.6124659	0.0901547
C	0.9470607	-4.2033777	3.2823086	H	0.6530029	3.2282077	-3.9319992
C	2.2964111	-4.0524533	2.9205088	C	4.5463176	10.3601429	1.3665068
H	3.6852105	-4.1059664	1.2524479	C	4.9985214	9.0399557	1.4621824
C	-1.5083539	-4.5799072	2.7816362	C	6.3819633	8.7742412	1.5695089
H	0.6708109	-4.1525644	4.3462918	C	7.3044976	9.8413994	1.5791412
C	-1.9738285	-3.4460648	3.7062073	C	6.8497663	11.1647061	1.4841653
H	-1.4409022	-3.4507426	4.6796766	C	5.4718314	11.4225845	1.3781129
H	-3.0589774	-3.5326101	3.9138696	H	3.4691582	10.5711250	1.2823260
H	-1.8047490	-2.4616930	3.2296665	H	4.3027967	8.1865724	1.4564983
C	-1.7017596	-5.9642274	3.4299986	C	6.8646887	7.3743564	1.6745556
H	-2.1491329	-4.5484303	1.8770995	H	8.3824650	9.6251682	1.6625542
H	-1.0792477	-6.0699057	4.3432582	H	7.5678733	11.9988194	1.4925137
H	-1.4191491	-6.7786483	2.7324845	H	5.1136276	12.4611539	1.3034483
H	-2.7614573	-6.1125634	3.7223488	O	6.1427029	6.3879212	1.6864623
C	3.3999594	-3.8989438	3.9587529	H	7.9894929	7.2751173	1.7469204
C	3.1716349	-2.7118700	4.9083498				
H	3.9925052	-2.6537842	5.6515334				
H	2.2168383	-2.8042208	5.4661377				
H	3.1506569	-1.7571317	4.3479538				
C	3.5835293	-5.2197598	4.7304213				
H	4.3373243	-3.6946108	3.3976270				
H	4.4378892	-5.1425158	5.4335722				
H	3.7783696	-6.0676964	4.0431331				
H	2.6780934	-5.4661210	5.3237931				
C	2.0740531	-4.5470672	-0.9098557				
C	3.1317998	-3.5449664	-1.3972349				
H	3.3770387	-3.7506530	-2.4587302				
H	4.0799604	-3.6058021	-0.8250733				
H	2.7572038	-2.5046819	-1.3359221				
C	2.5623257	-5.9984628	-1.1020294				
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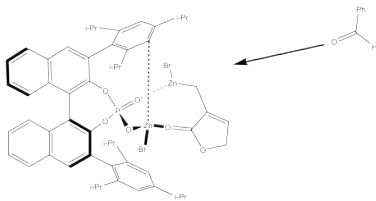


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number of imaginary frequencies: 5

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Br	4.6720759	-1.2180246	1.4127007

H	1.6973043	3.0036291	1.9532763	H	3.1552448	-1.7523229	4.3386721
Br	-4.3284844	-0.5917797	1.7242816	C	3.5857430	-5.2129070	4.7301647
H	-0.9783444	-0.5866992	4.6139617	H	4.3356750	-3.6872495	3.3935111
Zn	-2.2120938	0.0166222	2.4569850	H	4.4394290	-5.1342677	5.4340036
C	0.4844538	2.3468812	3.6532312	H	3.7816467	-6.0622480	4.0450156
C	1.7750939	2.4397626	2.9105282	H	2.6806832	-5.4610579	5.3233946
C	0.0754381	1.0421313	3.7140038	C	2.0734112	-4.5553677	-0.9100008
C	-1.1670594	0.4007618	4.1467545	C	3.1316264	-3.5535239	-1.3973568
C	1.1363601	0.2737982	3.0293611	H	3.3798397	-3.7608367	-2.4578951
O	2.1105783	1.0769021	2.5833736	H	4.0789198	-3.6095557	-0.8233960
O	1.1858864	-0.9590394	2.8476769	H	2.7564788	-2.5133199	-1.3401653
H	2.6218715	2.8697657	3.4896763	C	2.5595379	-6.0068906	-1.1045518
H	-1.7676389	1.0320341	4.8283839	H	1.1750090	-4.4138029	-1.5436746
H	-0.0574930	3.2219653	4.0360481	H	2.8102580	-6.1937666	-2.1687479
C	-1.4834377	-3.3306498	-0.3887247	H	1.7915826	-6.7448429	-0.7981077
C	-2.3629470	-3.1773714	-1.4636890	H	3.4704155	-6.2025801	-0.5009099
C	-2.5537908	-4.3103462	-2.3397277	H	0.3368404	6.0054671	-1.3406232
C	-3.3059306	-4.2325114	-3.5505576	H	-0.3769944	2.3048366	-5.8740048
C	-1.9367480	-5.5730528	-2.0036145	H	-4.9948563	3.3926712	0.6459994
C	-2.1583379	-6.7044228	-2.8445558	C	0.6077569	5.3971879	-2.2322628
C	-1.0656364	-5.6567985	-0.4785226	H	0.8600027	-0.4813894	-4.9369643
H	-0.5680542	-6.6140690	-0.6603271	H	2.7050300	6.0387710	-2.1348347
C	-0.7844859	-4.5430674	-0.1004087	H	-3.0811202	2.6831135	2.2346782
C	-2.7547170	0.5940690	-2.0710669	C	-0.2346984	4.1291963	-2.1713788
C	-4.1173623	0.6834640	-2.3306922	C	-1.0405681	1.4618414	-5.5884923
H	-4.5449877	1.6580103	-2.6100595	C	2.1148894	5.0990509	-2.1503613
C	-4.9880191	-0.4338023	-2.1965710	H	2.4582899	4.5063455	-3.0237045
C	-6.3981678	-0.2927633	-2.3603959	C	-0.0891451	3.1080231	-3.1263708
C	-4.4444824	-1.7223084	-1.8448937	C	-4.2591640	3.5507242	-0.1694418
C	-5.3528159	-2.7957972	-1.6054450	H	-0.8144374	6.4748723	-3.5182597
C	-3.0164906	-1.8600317	-1.7011532	C	-1.1971033	3.9497535	-1.1655402
C	-2.2351476	-0.6997942	-1.7630776	C	0.2663647	6.2309713	-3.4812579
O	-1.2744688	-2.2761139	0.4866347	H	0.8371613	7.1827375	-3.4944675
O	-0.8571971	-0.7962926	-1.5473991	H	-1.3134058	4.7371740	-0.4028492
P	-0.3796624	-0.9669860	0.0129411	C	0.7539788	0.3244891	-4.1813550
O	1.1194680	-1.2945448	-0.0695327	H	-0.9410448	0.6791441	-6.3689738
O	-0.8469829	0.1688494	0.9219219	H	-2.0841578	1.8362366	-5.6075595
C	-2.9246057	-6.6005391	-3.9950869	C	-0.8809939	1.9466244	-3.1093306
C	-3.4873195	-5.3480053	-4.3561340	C	-2.3832604	2.9810532	1.4223356
H	-1.6903873	-7.6625712	-2.5685448	C	-2.0120258	2.8040279	-1.0948674
H	-3.0820359	-7.4801837	-4.6375458	H	-4.7624052	3.3165246	-1.1279386
H	-3.7413867	-3.2687251	-3.8469137	H	-3.9912117	4.6284063	-0.1892641
H	-4.0690213	-5.2577189	-5.2861537	C	-0.6738569	0.8997355	-4.2026203
C	-6.7214001	-2.6208785	-1.7524762	C	-1.8654537	1.7986979	-2.0925990
C	-7.2512392	-1.3644099	-2.1488227	C	-3.0129615	2.6746637	0.0513891
H	-4.9581021	-3.7682028	-1.2804988	H	0.9943728	-0.1013852	-3.1880066
H	-7.4023550	-3.4614305	-1.5493647	H	-1.4239281	2.4410485	1.5512422
H	-8.3383538	-1.2391443	-2.2666528	H	1.5112261	1.1013729	-4.4168368
H	-6.7976610	0.6956190	-2.6367998	H	2.3647411	4.5207024	-1.2380209
C	1.6381153	-4.3650173	0.5415159	H	-2.1758763	4.0630547	1.5619086
C	0.2806112	-4.4833806	0.9480251	H	0.5151891	5.6772806	-4.4106927
C	2.6213302	-4.1329882	1.5389391	H	-1.3693006	0.0594624	-4.0043519
C	-0.0657087	-4.4032139	2.3246167	H	-3.3493266	1.6186745	0.0871137
C	0.9456351	-4.1949290	3.2799210	H	0.6655342	3.2201093	-3.9215081
C	2.2957730	-4.0515932	2.9181361	C	4.5435239	10.3542128	1.3619969
H	3.6843947	-4.1119818	1.2518831	C	4.9972108	9.0344250	1.4504793
C	-1.5103916	-4.5764449	2.7802304	C	6.3794632	8.7697624	1.5651201
H	0.6689444	-4.1357369	4.3433966	C	7.2992050	9.8378724	1.5887481
C	-1.9803028	-3.4498600	3.7106988	C	6.8434736	11.1610700	1.5011025
H	-1.4429922	-3.4524982	4.6819054	C	5.4664811	11.4177891	1.3881072
H	-3.0636839	-3.5444777	3.9234231	H	3.4665875	10.5641447	1.2721339
H	-1.8236956	-2.4628178	3.2360036	H	4.3065610	8.1771042	1.4333995
C	-1.7015098	-5.9654170	3.4191291	C	6.8584247	7.3657575	1.6644175
H	-2.1512280	-4.5401916	1.8759275	H	8.3769806	9.6221386	1.6776550
H	-1.0791384	-6.0765479	4.3318240	H	7.5600783	11.9962916	1.5206989
H	-1.4156255	-6.7744272	2.7168118	H	5.1071692	12.4563552	1.3193089
H	-2.7607692	-6.1197297	3.7099234	O	6.1344870	6.3840531	1.6671823
C	3.3996221	-3.8942441	3.9558786	H	7.9845911	7.2643684	1.7421074
C	3.1724334	-2.7048209	4.9024825				
H	3.9933301	-2.6451812	5.6454851				
H	2.2177121	-2.7932120	5.4612157				

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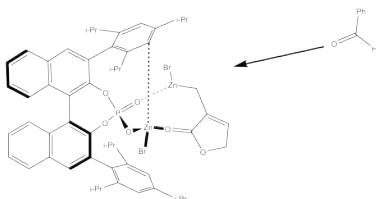
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Br	4.3836381	0.4623954	-2.5267977
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C	1.9441705	4.2588528	0.2650446
C	2.6505784	2.9749926	0.1038383
O	3.9483131	3.1426645	-0.1554446
C	4.2091270	4.5606986	-0.2420062
O	2.1372694	1.8320316	0.1457861
C	0.4882044	4.3423658	0.5543686
H	4.6055295	4.7645443	-1.2606861
H	5.0033311	4.8157225	0.4925324
Zn	-0.5335811	2.6189688	0.6132374
Br	-2.0092025	2.0259695	2.3564835
H	0.0135385	5.0834241	-0.1234466
H	0.3452258	4.7469452	1.5815026
H	2.7489372	6.2970698	0.0208480
C	-1.5432171	-2.5665492	-0.5230389
C	-2.3986025	-2.8492930	-1.5956496
C	-2.5459236	-4.2275269	-2.0011755
C	-3.2541892	-4.6183854	-3.1780462
C	-1.9189221	-5.2593623	-1.2112493
C	-2.0854861	-6.6264524	-1.5866255
C	-1.1165987	-4.8971849	-0.0921745
H	-0.6553681	-5.6958372	0.5081671
C	-0.8745619	-3.5711333	0.2455473
C	-2.8210808	0.3612433	-3.6590415
C	-4.1699372	0.2998883	-3.9921392
H	-4.5985547	1.0647520	-4.6583580
C	-5.0333679	-0.6967095	-3.4480908
C	-6.4361108	-0.6812710	-3.7132858
C	-4.4959028	-1.7124227	-2.5729566
C	-5.4019837	-2.6243368	-1.9540741
C	-3.0734548	-1.7464709	-2.3372426
C	-2.3054600	-0.6954605	-2.8424777
O	-1.3552650	-1.2363089	-0.1343913
O	-0.9385204	-0.6927765	-2.5854851
P	-0.4203030	-0.2851364	-1.0846363
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O	-0.6857188	1.1771174	-0.7726481
C	-2.8097671	-6.9728727	-2.7173297
C	-3.3832420	-5.9559268	-3.5264802
H	-1.6113053	-7.4023578	-0.9652330
H	-2.9265762	-8.0304204	-2.9989926
H	-3.6940327	-3.8450513	-3.8221862
H	-3.9306726	-6.2284379	-4.4417633
C	-6.7642984	-2.5672282	-2.2154273
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H	-5.0091504	-3.3725974	-1.2512607
H	-7.4448017	-3.2741883	-1.7167381
H	-8.3675468	-1.5681155	-3.3195915
H	-6.8344007	0.0908133	-4.3903682
C	1.4385754	-3.2717681	1.2512568
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H	3.3332521	-2.9421790	2.2534787
C	-2.0701420	-2.7626551	2.8037534
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H	-2.2637377	-1.5683667	4.6493166
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H	-2.2926080	-0.6045595	3.1331789
C	-2.4857425	-4.0987837	3.4514139
H	-2.5441460	-2.7258252	1.8015824
H	-2.0290819	-4.2037352	4.4582242
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C	2.6138356	-2.0779317	4.7163375
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H	2.8156389	-0.7113776	6.4094116
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H	1.7072668	-0.1149168	5.1264184
C	3.0077867	-3.3580196	5.4818872
H	3.5441014	-1.6630787	4.2669528
H	3.7303605	-3.1322037	6.2937342
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C	2.1060745	-3.8245632	-0.0084821
C	3.3713852	-3.0620944	-0.4298190
H	3.7323615	-3.4174150	-1.4158278
H	4.2039529	-3.1886087	0.2920982
H	3.1783518	-1.9758906	-0.5273454
C	2.4453974	-5.3185073	0.1776058
H	1.3758785	-3.7361126	-0.8392687
H	2.8935743	-5.7429691	-0.7447294
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H	0.0003877	0.8604604	-7.4356243
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C	1.2292640	4.5152855	-4.2363180
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C	2.4612276	3.9524888	-3.5042872
H	2.8917019	3.0779752	-4.0335927
C	0.2524243	2.2463163	-4.8538168
C	-4.0902552	4.3610116	-3.3454089
H	0.7012683	5.4119790	-6.1728982
C	-1.1005370	3.7426075	-3.5425125
C	1.5840586	4.9817524	-5.6585395
H	2.3804667	5.7542879	-5.6349360
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H	-0.6280965	-0.8142971	-7.5714727
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C	-0.4988668	-0.0729670	-5.5072093
C	-1.9035063	1.4901902	-4.0021402
C	-3.3969118	3.1590413	-2.6767241
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C	3.3934360	4.6941438	10.2743266
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C	6.6511532	2.7268954	8.2924496
H	6.7766059	4.1948965	10.5708028
H	4.8692043	5.3505117	11.7339844
H	2.5573031	5.1995163	10.7822533
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TS-7-j-mi



Energy (Hartree) = -11969.96576458
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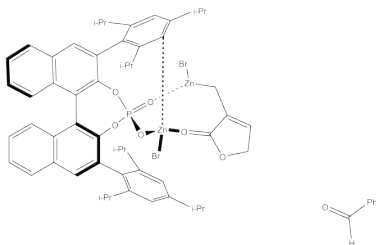
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C	1.9417477	4.2556759	0.2641148
C	2.6536334	2.9695056	0.1091722
O	3.9537113	3.1432464	-0.1461846
C	4.2091935	4.5583101	-0.2403660
O	2.1481258	1.8269070	0.1523644
C	0.4859071	4.3368870	0.5478944
H	4.6044810	4.7567226	-1.2610292
H	5.0038435	4.8190711	0.4924808
Zn	-0.5573546	2.6200076	0.6251438
Br	-2.0075051	2.0255885	2.3620895
H	0.0155851	5.0838333	-0.1266845
H	0.3402354	4.7381141	1.5762744
H	2.7416157	6.2935490	0.0178114
C	-1.5435923	-2.5643132	-0.5231921
C	-2.3987583	-2.8482029	-1.5957390
C	-2.5458176	-4.2263902	-2.0013896
C	-3.2543446	-4.6173689	-3.1777828
C	-1.9185938	-5.2580347	-1.2118740
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H	-0.6539828	-5.6922746	0.5075916
C	-0.8741918	-3.5689960	0.2450222
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C	-4.1700514	0.2997075	-3.9921852
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C	-5.0336081	-0.6963478	-3.4481663
C	-6.4360306	-0.6815169	-3.7122996
C	-4.4958895	-1.7117287	-2.5732062
C	-5.4014956	-2.6234746	-1.9540286
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C	-2.3054471	-0.6951722	-2.8432330
O	-1.3565951	-1.2339249	-0.1347531
O	-0.9389774	-0.6919889	-2.5860021
P	-0.4224584	-0.2834012	-1.0840378
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O	-0.6737901	1.1824241	-0.7793314
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C	-3.3835848	-5.9545231	-3.5259055
H	-1.6110797	-7.4004437	-0.9664134
H	-2.9268428	-8.0286782	-2.9989084
H	-3.6944576	-3.8434379	-3.8208617

H	-3.9313841	-6.2268612	-4.4409730
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C	-0.5559832	-2.7426186	2.6001739
C	0.2891142	-2.3687475	3.6609824
C	1.6883325	-2.4273046	3.5549037
H	3.3334588	-2.9440085	2.2541824
C	-2.0695759	-2.7616213	2.8034579
H	-0.1676612	-2.0220274	4.5986547
C	-2.6060574	-1.5604180	3.5917502
H	-2.2637207	-1.5651578	4.6478390
H	-3.7148401	-1.5830352	3.6128344
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C	-2.4845322	-4.0977294	3.4516533
H	-2.5436054	-2.7251105	1.8013147
H	-2.0277663	-4.2026987	4.4582796
H	-2.1575753	-4.9652107	2.8427290
H	-3.5866946	-4.1549499	3.5691361
C	2.6139032	-2.0794772	4.7165411
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H	2.8156459	-0.7125627	6.4096543
H	1.1824966	-1.4113912	6.2490958
H	1.7054044	-0.1174629	5.1274131
C	3.0088283	-3.3592821	5.4816992
H	3.5438142	-1.6633105	4.2673483
H	3.7314013	-3.1339163	6.2936138
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C	2.4606242	3.9518314	-3.5041421
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H	2.3808425	5.7545920	-5.6356953
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H	1.9567764	4.1395495	-6.2771425
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P	1.3130175	2.9457119	88.5194607
O	0.7899099	3.9737460	89.5358602
O	1.9135133	3.4361530	87.2024920
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H	-1.5105683	-3.8749655	92.6215884
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H	0.9001898	-4.0121900	91.9107351
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H	3.7547551	2.9753115	83.9972545
C	6.4449924	4.4643932	88.4721993
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agg-7-d-ma; COSMO



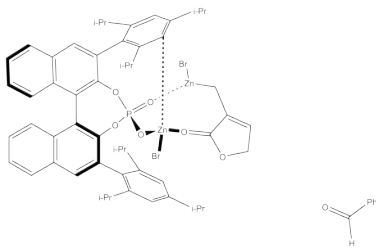
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Br	1.3141890	0.6900711	84.8936367
H	1.0072230	4.8297110	83.4753460
Zn	1.2095059	2.9816019	85.3148697
C	2.4167435	6.4917290	85.3354089
C	2.6750049	7.1518077	86.6469204
C	1.2618209	5.7607256	85.4040592
C	0.6546904	4.7590854	84.5218204
C	0.7396740	5.9921736	86.7650487
O	1.5425632	6.7975948	87.4687006
O	-0.3054635	5.5236705	87.2632237
H	2.7424633	8.2607891	86.6162402
H	-0.4529718	4.7966250	84.5522046
H	3.1091189	6.5532367	84.4852576
C	-0.2983142	0.8975009	88.9405128
C	0.5213683	-0.1935125	89.2409171
C	0.0049615	-1.1812862	90.1605762
C	0.7987633	-2.2549141	90.6657129
C	-1.3611638	-1.0712037	90.6200636
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H	-3.1709892	0.1488001	90.6394119
C	-1.6182132	1.0722989	89.4599191
C	4.1042239	0.8117050	88.2724069
C	4.5712745	-0.3686016	87.7066002
H	5.6165085	-0.4248129	87.3678500
C	3.7224497	-1.4921702	87.4977561

C	6.1053674	3.7576988	89.6393189
C	5.9490754	1.5300053	85.0317546
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C	6.0179862	3.9392569	87.2419615
C	8.5839745	5.6105143	89.2305025
H	9.1543082	6.5622603	89.2091524
H	6.2774508	4.4851614	86.3203662
C	4.2913902	2.7404394	91.9056484
H	6.1190827	0.7110707	92.4650795
H	6.8694334	0.5988648	90.8375390
C	5.3590052	2.5667493	89.6028026
C	4.2658264	3.4009620	84.8863883
C	5.2631866	2.7543415	87.1469785
H	6.3346084	0.6722732	85.6167435
H	6.8043118	2.2116517	84.8384732
C	5.0577568	1.8457002	90.9153086
C	4.9344625	2.0559965	88.3444348
C	4.8165313	2.2682952	85.7694700
H	3.3601900	3.1280000	91.4482401
H	3.5538972	4.0369019	85.4511475
H	4.9035542	3.6066686	92.2333598
H	5.4177420	7.0269479	88.6730033
H	5.0648457	4.0719149	84.5065874
H	8.4627187	5.3198345	90.2949306
H	4.4068808	0.9784217	90.6842741
H	3.9846201	1.5502205	85.9197077
H	6.4293925	4.1480056	90.6174639
C	6.1105733	18.4629305	86.3190562
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C	6.7305783	17.0682384	88.2154339
C	7.1621600	18.2130295	88.9174985
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H	5.6999341	18.5691909	85.3032240
H	5.8750881	16.2884421	86.3866323
C	6.8315079	15.7297049	88.8487859
H	7.5720618	18.1017409	89.9350142
H	7.4059452	20.3737038	88.8684776
H	6.4705541	20.5967323	86.5556435
O	6.4860627	14.6815226	88.3232586
H	7.2666983	15.7423730	89.8932177

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C	0.7965485	-2.2328822	90.7230815
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C	-1.8860838	-2.0317876	91.5522167
C	-2.1445790	0.0783362	90.2723280
H	-3.1672811	0.1786642	90.6674465
C	-1.6169705	1.0784638	89.4686000
C	4.0993946	0.7895107	88.2707477
C	4.5630841	-0.4016833	87.7259574
H	5.6071441	-0.4646572	87.3850760
C	3.7127375	-1.5274470	87.5380942
C	4.1808719	-2.7008600	86.8750092
C	2.3399246	-1.4651334	87.9756414
C	1.4797038	-2.5571936	87.6555974
C	1.8834663	-0.2886062	88.6743054
C	2.7550189	0.8040098	88.7548339
O	0.1455741	1.8506705	88.0524491
O	2.3176958	1.9799373	89.3701344
P	1.3111637	2.9337620	88.4950455
O	0.7863792	3.9717111	89.4990116
O	1.9068510	3.4089855	87.1700697
C	-1.0963880	-3.0750798	92.0102603
C	0.2609214	-3.1626645	91.6033233
H	-2.9319275	-1.9345878	91.8837991
H	-1.5129268	-3.8234141	92.7014580
H	1.8503963	-2.3093403	90.4229837
H	0.8973438	-3.9719453	91.9925799
C	1.9602816	-3.6751938	86.9888768
C	3.3260528	-3.7591562	86.6096366
H	0.4170078	-2.4984436	87.9274417
H	1.2731530	-4.4992145	86.7433736
H	3.6972102	-4.6538686	86.0870485
H	5.2343348	-2.7378797	86.5559336
C	-2.2777800	3.3838364	90.2181403
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C	-3.1543633	4.0235448	87.6047016
C	-3.1547546	5.0349772	88.5798661
H	-2.7854202	5.4543517	90.6792596
C	-2.7501061	1.6474891	86.7959856
H	-3.4880977	4.2665205	86.5873878
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H	-3.2886767	2.8145259	84.9962671
H	-2.3138941	1.3468562	84.6806140
H	-1.5356900	2.7927151	85.3764192
C	-4.0922131	0.8910877	86.8517977
H	-1.9503912	0.9146243	87.0243736
H	-4.9417874	1.5760589	86.6484982
H	-4.2560011	0.4339743	87.8485889
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C	-3.4778693	6.9060004	86.8620156
H	-3.7442183	7.9775171	86.7659321
H	-4.1267421	6.3455491	86.1565872
H	-2.4263094	6.7788809	86.5376975
C	-5.1453790	6.5502770	88.7476848
H	-3.0742468	7.1194117	88.9641620
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H	-5.2784455	6.2656632	89.8108313
H	-5.7875516	5.8823359	88.1359674
C	-1.9055779	3.0686383	91.6651455
C	-0.9638414	4.0935789	92.3165056
H	-0.7434100	3.7890372	93.3596891
H	-1.3940817	5.1150234	92.3569064
H	-0.0000990	4.1504627	91.7737661
C	-3.1963611	2.8935301	92.4916609
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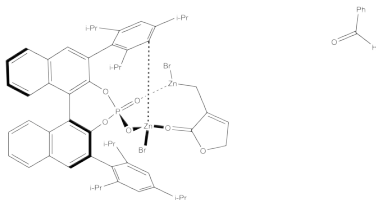


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Br	1.2733460	0.6448564	84.8890320
H	1.0208487	4.7764404	83.4387777
Zn	1.1884955	2.9309784	85.2885711
C	2.4761418	6.4011571	85.3020759
C	2.7570993	7.0382989	86.6214188
C	1.2983208	5.7071855	85.3648112
C	0.6680806	4.7195636	84.4858757
C	0.7775607	5.9550757	86.7250623
O	1.6060239	6.7315246	87.4328956
O	-0.2838545	5.5242964	87.2190996
H	2.8779433	8.1433819	86.6035420
H	-0.4382028	4.7800513	84.5169488
H	3.1733415	6.4367484	84.4545654

H	-3.8641661	2.1244388	92.0536472	C	3.5850644	5.9780852	85.0723587
H	-3.7686115	3.8436201	92.5413873	C	3.8803014	6.7085338	86.3377831
H	7.3578928	6.0785565	87.3826833	C	2.3598711	5.3748241	85.1604256
H	7.0667223	2.1329157	91.7634305	C	1.6719577	4.3787217	84.3332886
H	5.5838447	1.0250339	84.0561495	C	1.8346729	5.7600066	86.4851503
C	7.2109011	5.7585905	88.4384011	O	2.7010570	6.5320024	87.1507544
H	4.0329923	2.2148890	92.7914581	O	0.7369016	5.4384887	86.9860905
H	6.9714093	7.8322405	89.1292096	H	4.0579175	7.7998544	86.2242033
H	3.7471340	2.8533770	83.9492041	H	2.0559696	4.3350810	83.2965682
C	6.4262446	4.4530963	88.3979383	H	4.2974633	5.9053683	84.2397974
C	6.3576160	1.3161365	91.5129432	C	0.1792373	0.9797770	88.9846424
C	6.4213271	6.8689011	89.1554623	C	0.8610800	-0.1718325	89.3848266
H	6.2428356	6.6127492	90.2203996	C	0.2181049	-1.0233344	90.3590887
C	6.0939411	3.7651767	89.5778374	C	0.8744122	-2.1383135	90.9625257
C	5.9411905	1.4389311	85.0215855	C	-1.1346300	-0.7253325	90.7720472
H	9.1837325	4.7916239	88.5292636	C	-1.7864264	-1.5880443	91.7038157
C	5.9987023	3.9040404	87.1784702	C	-1.7772782	0.4556475	90.2966417
C	8.6047779	5.5715594	89.0632829	H	-2.7919946	0.6901224	90.6533122
H	9.1847623	6.5170634	89.0300065	C	-1.1211340	1.3410565	89.4538350
H	6.2539875	4.4336777	86.2461685	C	4.5550290	0.3417444	88.4540619
C	4.2998631	2.7761398	91.8721872	C	4.8908259	-0.9207301	87.9799394
H	6.1392528	0.7620039	92.4493724	H	5.9288979	-1.1225524	87.6764117
H	6.8756317	0.6254379	90.8170462	C	3.9198095	-1.9495648	87.8208827
C	5.3540772	2.5703322	89.5647908	C	4.2652404	-3.2017183	87.2294365
C	4.2563189	3.3026177	84.8273495	C	2.5537065	-1.7093318	88.2165726
C	5.2510090	2.7129712	87.1062325	C	1.5812980	-2.7131629	87.9295619
H	6.3278419	0.5972788	85.6284223	C	2.2192703	-0.4524486	88.8401148
H	6.7962461	2.1157238	84.8114477	C	3.2087463	0.5364105	88.8911786
C	5.0619857	1.8692373	90.8899952	O	0.7510405	1.8291351	88.0499246
C	4.9286548	2.0355091	88.3170297	O	2.8922093	1.7876894	89.4282317
C	4.8071929	2.1941198	85.7396076	P	2.0241934	2.7944328	88.4682507
H	3.3649671	3.1558867	91.4163110	O	1.6000079	3.9465093	89.3937978
H	3.5408826	3.9493528	85.3750167	O	2.7068501	3.1181731	87.1399000
H	4.9112633	3.6483323	92.1848608	C	-1.1290697	-2.6832058	92.2440736
H	5.4286195	7.0273380	88.6866139	C	0.2183133	-2.9471640	91.8805977
H	5.0548657	3.9662774	84.4334276	H	-2.8212728	-1.3545514	91.9999381
H	8.5306602	5.2640080	90.1272293	H	-1.6418452	-3.3366372	92.9662065
H	4.4117497	0.9971242	90.6755066	H	1.9190800	-2.3510987	90.6976265
H	3.9748420	1.4796965	85.9042519	H	0.7503110	-3.7974959	92.3339250
H	6.4199756	4.1734171	90.5479283	C	1.9448317	-3.9121147	87.3320983
C	6.0793447	18.6431732	86.4649501	C	3.3003145	-4.1692674	86.9935788
C	5.8190345	17.4723344	87.1841573	H	0.5266009	-2.5223020	88.1708985
C	6.4316643	17.2651545	88.4393983	H	1.1738365	-4.6660277	87.1109211
C	7.3030162	18.2407789	88.9653221	H	3.5776726	-5.1267341	86.5267881
C	7.5637943	19.4142153	88.2434014	H	5.3144013	-3.3753664	86.9427061
C	6.9521750	19.6137007	86.9940187	C	-1.5320424	3.7484433	90.0447178
H	5.6034086	18.8083999	85.4860539	C	-1.6148126	2.7032455	89.0848814
H	5.1425069	16.6914975	86.8035143	C	-1.8015049	5.0775430	89.6191112
C	6.1588673	16.0179637	89.2013044	C	-2.0030514	2.9870909	87.7453806
H	7.7762032	18.0711341	89.9468335	C	-2.2939643	4.3131314	87.3770568
H	8.2440776	20.1768415	88.6523162	C	-2.1956016	5.3788078	88.2868764
H	7.1570105	20.5338480	86.4250622	H	-1.8223364	5.8867189	90.3671663
O	5.4304259	15.1163785	88.8218176	C	-2.1378589	1.8631576	86.7237598
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agg-7-d-mi; COSMO



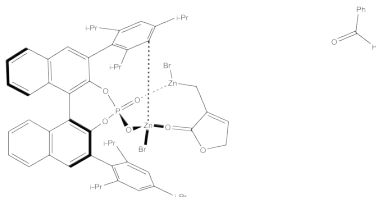
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Br	1.8675383	0.3028419	84.9984020
H	0.5743750	4.5337257	84.3245248
Zn	2.0096139	2.6151059	85.2650142

C	3.5850644	5.9780852	85.0723587
C	3.8803014	6.7085338	86.3377831
C	2.3598711	5.3748241	85.1604256
C	1.6719577	4.3787217	84.3332886
C	1.8346729	5.7600066	86.4851503
O	2.7010570	6.5320024	87.1507544
O	0.7369016	5.4384887	86.9860905
H	4.0579175	7.7998544	86.2242033
H	2.0559696	4.3350810	83.2965682
H	4.2974633	5.9053683	84.2397974
C	0.1792373	0.9797770	88.9846424
C	0.8610800	-0.1718325	89.3848266
C	0.2181049	-1.0233344	90.3590887
C	0.8744122	-2.1383135	90.9625257
C	-1.1346300	-0.7253325	90.7720472
C	-1.7864264	-1.5880443	91.7038157
C	-1.7772782	0.4556475	90.2966417
H	-2.7919946	0.6901224	90.6533122
C	-1.1211340	1.3410565	89.4538350
C	4.5550290	0.3417444	88.4540619
C	4.8908259	-0.9207301	87.9799394
H	5.9288979	-1.1225524	87.6764117
C	3.9198095	-1.9495648	87.8208827
C	4.2652404	-3.2017183	87.2294365
C	2.5537065	-1.7093318	88.2165726
C	1.5812980	-2.7131629	87.9295619
C	2.2192703	-0.4524486	88.8401148
C	3.2087463	0.5364105	88.8911786
O	0.7510405	1.8291351	88.0499246
O	2.8922093	1.7876894	89.4282317
P	2.0241934	2.7944328	88.4682507
O	1.6000079	3.9465093	89.3937978
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C	-1.1290697	-2.6832058	92.2440736
C	0.2183133	-2.9471640	91.8805977
H	-2.8212728	-1.3545514	91.9999381
H	-1.6418452	-3.3366372	92.9662065
H	1.9190800	-2.3510987	90.6976265
H	0.7503110	-3.7974959	92.3339250
C	1.9448317	-3.9121147	87.3320983
C	3.3003145	-4.1692674	86.9935788
H	0.5266009	-2.5223020	88.1708985
H	1.1738365	-4.6660277	87.1109211
H	3.5776726	-5.1267341	86.5267881
H	5.3144013	-3.3753664	86.9427061
C	-1.5320424	3.7484433	90.0447178
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C	-1.8015049	5.0775430	89.6191112
C	-2.0030514	2.9870909	87.7453806
C	-2.2939643	4.3131314	87.3770568
C	-2.1956016	5.3788078	88.2868764
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H	-2.5872643	4.5245099	86.3401683
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H	-2.4074771	2.9851353	84.8370424
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H	-1.4648497	1.0418874	87.0420667
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C	-2.5511845	6.8131636	87.9208596
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H	-4.2111974	6.8936936	89.3712064
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C	-0.2164999	4.4530659	92.1441450
H	-0.0486986	4.1822577	93.2061689
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H	0.7610939	4.3981546	91.6260720
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H	8.5258380	5.1041206	87.4798365
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H	6.1592070	0.2339879	84.2760534
C	8.2389594	4.9053106	88.5362146
H	4.5159497	1.9641208	92.9046021
H	8.1501874	7.0499640	89.0171646
H	4.5713824	2.2737503	84.0529362
C	7.3162414	3.6928424	88.5213195
C	6.7554197	0.7354752	91.7599981
C	7.4998847	6.1515856	89.0589748
H	7.1792760	6.0134713	90.1127078
C	6.8646559	3.1022410	89.7145664
C	6.5425805	0.6360438	85.2367591
H	10.0744964	3.7635768	88.9403528
C	6.8574217	3.1522273	87.3091446
C	9.5325878	4.6496163	89.3283609
H	10.2120093	5.5247140	89.2662671
H	7.2014567	3.6092640	86.3671091
C	4.8784562	2.4455326	91.9727395
H	6.4368742	0.2549602	92.7083783
H	7.2109824	-0.0437069	91.1155094
C	5.9796714	2.0097128	89.7208005
C	5.1082842	2.6876669	84.9325922
C	5.9664421	2.0630641	87.2564399
H	6.8056807	-0.2239743	85.8831320
H	7.4799198	1.1936780	85.0266184
C	5.5595135	1.4092857	91.0611493
C	5.5271338	1.4806433	88.4799916
C	5.4949540	1.5524380	85.8961242
H	4.0109275	2.9087391	91.4635974
H	4.4644984	3.4375259	85.4358810
H	5.5795700	3.2534811	92.2693570
H	6.5885083	6.3587527	88.4610303
H	5.9925628	3.2325631	84.5402564
H	9.3209780	4.4709288	90.4032517
H	4.8163035	0.6119979	90.8574598
H	4.5777843	0.9516864	86.0631251
H	7.2098205	3.5078179	90.6791249
C	-1.5819940	15.4826739	73.2315976
C	-1.4523482	14.8357683	74.4650793
C	-2.6039530	14.3913620	75.1525070
C	-3.8819282	14.6012270	74.5932964
C	-4.0104395	15.2497719	73.3565662
C	-2.8607902	15.6896147	72.6772979
H	-0.6871323	15.8304543	72.6929311
H	-0.4682553	14.6583915	74.9258356
C	-2.4723217	13.7039610	76.4613731
H	-4.7750442	14.2510916	75.1368525
H	-5.0067252	15.4141631	72.9185710
H	-2.9603311	16.1989890	71.7061651
O	-1.4123941	13.4745232	77.0255440
H	-3.4575997	13.3927324	76.9227598

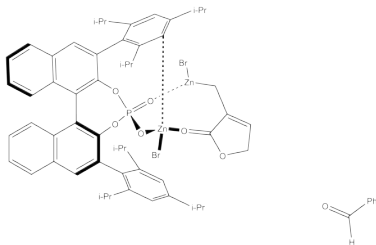
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Zn	0.4730734	5.5387876	89.0470574	H	-2.3809055	8.2593963	86.2911976
Br	0.6750520	7.6167860	90.0721779	H	-2.9249558	6.6472948	85.7570430
H	4.7951843	6.0897442	87.0066186	H	-1.1993078	6.9115249	86.1775413
Br	1.8314098	0.3184926	84.9967124	C	-3.9941979	7.1126217	88.2933180
H	0.6125218	4.5887808	84.3456660	H	-1.8797787	7.4606910	88.5563984
Zn	1.9954607	2.6182439	85.2731050	H	-4.2396560	8.1767231	88.0991193
C	3.6663543	5.9182990	85.1493140	H	-4.1917493	6.9060465	89.3643712
C	3.9765496	6.5939857	86.4426195	H	-4.6879133	6.4857408	87.6945433
C	2.4161674	5.3644517	85.2050234	C	-1.2617186	3.4668733	91.5134257
C	1.7052971	4.4046598	84.3575324	C	-0.2314672	4.4164299	92.1447266
C	1.8848069	5.7459167	86.5298173	H	-0.0803214	4.1494858	93.2103265
O	2.7736833	6.4643787	87.2258947	H	-0.5446789	5.4800674	92.1146452
O	0.7667611	5.4647308	87.0059728	H	0.7494166	4.3348065	91.6368773
H	4.2221570	7.6759616	86.3702844	C	-2.5897512	3.4837966	92.2981066
H	2.0936898	4.3619614	83.3225178	H	-0.8444475	2.4430424	91.5857153
H	4.3890272	5.8282543	84.3275379	H	-2.4176376	3.2140948	93.3601681
C	0.1729029	0.9728544	88.9805579	H	-3.3259317	2.7698638	91.8765785
C	0.8519076	-0.1789347	89.3856475	H	-3.0520423	4.4928122	92.2750850
C	0.2000552	-1.0322043	90.3524022	H	8.4129780	5.1757986	87.4293919
C	0.8507568	-2.1480296	90.9597246	H	7.5381093	1.5452504	92.0012706
C	-1.1567302	-0.7361603	90.7527109	H	6.1841926	0.1685339	84.3137956
C	-1.8169853	-1.6026823	91.6742379	C	8.1973667	4.9354925	88.4944247
C	-1.7941970	0.4462456	90.2746641	H	4.5018849	2.0243149	92.9073669
H	-2.8111803	0.6820779	90.6243641	H	8.1728602	7.0590084	89.0637461
C	-1.1313779	1.3337678	89.4394917	H	4.5695737	2.1810068	84.0394300
C	4.5505160	0.3416023	88.4754719	C	7.2712853	3.7254067	88.4944013
C	4.8932198	-0.9230921	88.0130462	C	6.7492364	0.7996185	91.7681822
H	5.9336302	-1.1217360	87.7157881	C	7.5162069	6.1662256	89.1203497
C	3.9270203	-1.9560065	87.8537363	H	7.2760124	5.9931024	90.1898794
C	4.2798339	-3.2103129	87.2724481	C	6.8262916	3.1476641	89.6960202
C	2.5569540	-1.7162186	88.2352496	C	6.5550932	0.5955466	85.2683810
C	1.5890722	-2.7222321	87.9418373	H	10.0437867	3.7616663	88.7120958
C	2.2149795	-0.4580431	88.8523758	C	6.8227586	3.1584615	87.2907444
C	3.2019336	0.5333256	88.9070626	C	9.5404947	4.6307967	89.1810327
O	0.7509730	1.8226138	88.0517540	H	10.2249069	5.5021054	89.1191024
O	2.8818115	1.7841100	89.4412682	H	7.1654323	3.6022524	86.3417858
P	2.0183364	2.7917100	88.4782785	C	4.8602297	2.4984627	91.9703206
O	1.5850734	3.9389167	89.4039766	H	6.4397569	0.3281871	92.7240266
O	2.7052311	3.1184457	87.1525786	H	7.2072359	0.0165657	91.1304681
C	-1.1653688	-2.6993616	92.2169453	C	5.9567024	2.0437449	89.7189035
C	0.1855665	-2.9605746	91.8672523	C	5.0983943	2.6205837	84.9108775
H	-2.8551069	-1.3709077	91.9601559	C	5.9478355	2.0556172	87.2540898
H	-1.6857310	-3.3560164	92.9306226	H	6.8249515	-0.2472309	85.9340187
H	1.8981978	-2.3581701	90.7044012	H	7.4874080	1.1600283	85.0546670
H	0.7134943	-3.8121408	92.3228447	C	5.5452052	1.4571765	91.0678279
C	1.9606533	-3.9230898	87.3542624	C	5.5133282	1.4885311	88.4863855
C	3.3193631	-4.1802391	87.0317848	C	5.4913116	1.5118188	85.9014168
H	0.5318051	-2.5302599	88.1700067	H	3.9896584	2.9533479	91.4593243
H	1.1927208	-4.6782493	87.1273307	H	4.4439305	3.3735693	85.3954450
H	3.6029571	-5.1391039	86.5719067	H	5.5567454	3.3131431	92.2590354
H	5.3318452	-3.3827932	86.9958536	H	6.5632633	6.4069117	88.6060273
C	-1.5492368	3.7378699	90.0384972	H	5.9791060	3.1669084	84.5118610
C	-1.6198956	2.6981777	89.0720074	H	9.3982787	4.3951150	90.2563616
C	-1.8119983	5.0686962	89.6175174	H	4.8071814	0.6522707	90.8757810
C	-1.9868839	2.9903038	87.7279468	H	4.5789171	0.9048491	86.0724852
C	-2.2673196	4.3191971	87.3638547	H	7.1657222	3.5718724	90.6546219
C	-2.1826648	5.3791740	88.2821393	C	-1.6376311	15.5137048	73.1811294
H	-1.8320101	5.8754736	90.3680630	C	-1.4876899	14.9378759	74.4467921
C	-2.1085151	1.8705815	86.6993386	C	-2.6222395	14.4798362	75.1517447
H	-2.5404842	4.5384956	86.3232962	C	-3.9036745	14.6058059	74.5777293
C	-1.7169220	2.2918691	85.2775506	C	-4.0531177	15.1831209	73.3087813
H	-2.4537957	2.9848077	84.8203810	C	-2.9200413	15.6361336	72.6118216
H	-1.6400844	1.4029889	84.6214046	H	-0.7553782	15.8715589	72.6284044
H	-0.7277599	2.7915471	85.2690344	H	-0.5015692	14.8258505	74.9235187
C	-3.5287156	1.2725749	86.7440193	C	-2.4629804	13.8645233	76.4956434
H	-1.4047102	1.0676559	86.9970331	H	-4.7840797	14.2463940	75.1361013
H	-4.2885386	2.0350143	86.4726605	H	-5.0529688	15.2815732	72.8592491
H	-3.7747319	0.8938782	87.7566459	H	-3.0358374	16.0895197	71.6150627
H	-3.6191711	0.4279642	86.0307138	O	-1.3976084	13.7111830	77.0691223
C	-2.5277176	6.8171450	87.9192285	H	-3.4375583	13.5333407	76.9707150
C	-2.2394484	7.1724361	86.4549821				

agg-7-j-ma; COSMO



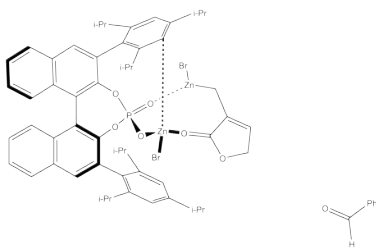
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Br	-0.3230267	7.5830224	90.2133419
H	3.3886852	6.6169541	86.5614187
Br	0.9468725	0.3796026	85.0717335
H	-0.8881240	4.4366430	84.5827338
Zn	0.8677980	2.6980452	85.3109747
C	2.0311794	6.1966064	84.9069210
C	2.4235401	6.9620915	86.1245144
C	0.8974629	5.4731625	85.1600493
C	0.2099902	4.3999966	84.4354748
C	0.5219216	5.8169727	86.5454678
O	1.3881210	6.6789356	87.0893474
O	-0.4591672	5.3909476	87.1899104
H	2.4796819	8.0645685	85.9954666
H	0.4470653	4.3821233	83.3549202
H	2.6274461	6.1871671	83.9847929
C	-0.2036357	0.9181614	89.2442343
C	0.6612111	-0.1358108	89.5495557
C	0.2616349	-1.0421671	90.6017963
C	1.1234798	-2.0585626	91.1136995
C	-1.0512743	-0.9040560	91.1905860
C	-1.4645328	-1.8249093	92.1999037
C	-1.8903455	0.1830716	90.8058607
H	-2.8695804	0.2990770	91.2951436
C	-1.4641538	1.1278827	89.8837548
C	4.1031800	0.8029799	88.1149778
C	4.5256566	-0.4202624	87.6084893
H	5.5291374	-0.5007214	87.1648114
C	3.6768079	-1.5629938	87.5913906
C	4.0912476	-2.7767142	86.9650876
C	2.3569881	-1.4810475	88.1675133
C	1.4852157	-2.6006055	88.0185187
C	1.9580593	-0.2610646	88.8259220
C	2.8168889	0.8408302	88.7360343
O	0.1288698	1.8142242	88.2404938
O	2.4272960	2.0550218	89.3089120
P	1.3200491	2.9328189	88.4772670
O	0.8923175	4.0415578	89.4525827
O	1.7667290	3.3113521	87.0655535
C	-0.6126585	-2.8232732	92.6481810
C	0.6977694	-2.9264567	92.1102595
H	-2.4724658	-1.7146365	92.6301071
H	-0.9422228	-3.5226305	93.4315350
H	2.1427628	-2.1462623	90.7136277
H	1.3852927	-3.6977930	92.4896353
C	1.9098474	-3.7592815	87.3831043
C	3.2293736	-3.8584606	86.8663999
H	0.4565755	-2.5332712	88.3985036
H	1.2141778	-4.6050080	87.2712945
H	3.5571746	-4.7851547	86.3711105
H	5.1060045	-2.8281920	86.5399298
C	-2.0744846	3.4788333	90.5259869
C	-2.1622299	2.4163356	89.5860497
C	-2.5545054	4.7603847	90.1418999
C	-2.7592031	2.6314065	88.3119129
C	-3.2509419	3.9084672	87.9869231
C	-3.1574241	4.9924516	88.8756804
H	-2.5705423	5.5727360	90.8865487

C	-2.8994382	1.4811998	87.3207060
H	-3.7050545	4.0680820	86.9999553
C	-2.7442419	1.9076753	85.8555722
H	-3.5953078	2.5245707	85.4994314
H	-2.6805190	1.0158976	85.2015950
H	-1.8140405	2.4917202	85.7084348
C	-4.2338457	0.7472096	87.5614259
H	-2.0848165	0.7594301	87.5316114
H	-5.0954977	1.4237886	87.3819311
H	-4.3061564	0.3741288	88.6031020
H	-4.3296794	-0.1210265	86.8777658
C	-3.7283164	6.3685280	88.5625172
C	-3.6842533	6.7319301	87.0724829
H	-3.9884412	7.7880151	86.9291373
H	-4.3801752	6.1082608	86.4732450
H	-2.6646344	6.6031433	86.6589202
C	-5.1584052	6.4795434	89.1290786
H	-3.0913491	7.1004473	89.1085382
H	-5.5622833	7.5001938	88.9692098
H	-5.1835758	6.2676672	90.2170059
H	-5.8373705	5.7588611	88.6267932
C	-1.5464560	3.2732696	91.9433950
C	-0.5847128	4.3682303	92.4299435
H	-0.2436258	4.1345151	93.4587236
H	-1.0534318	5.3729374	92.4604994
H	0.3134109	4.4268739	91.7842377
C	-2.7409428	3.1146965	92.9073128
H	-0.9820053	2.3197642	91.9501676
H	-2.3838464	2.8863053	93.9322667
H	-3.4208161	2.2988706	92.5893949
H	-3.3383384	4.0492928	92.9552091
H	7.1896744	6.0294459	86.5193295
H	7.4045907	2.4221885	91.1799928
H	5.0977442	0.7643617	83.7561885
C	7.1418284	5.7950498	87.6059163
H	4.4958176	2.5383802	92.5054945
H	6.9138736	7.9135831	88.1468387
H	3.2491692	2.5830215	83.7308011
C	6.3824953	4.4808876	87.7402689
C	6.6925481	1.5787588	91.0599106
C	6.3895565	6.9471973	88.2973230
H	6.3076398	6.7744705	89.3907522
C	6.1912990	3.8725061	88.9932074
C	5.5566537	1.2389702	84.6481494
H	9.1370807	4.8704174	87.6040455
C	5.8292123	3.8489498	86.6148860
C	8.5876970	5.6831327	88.1206284
H	9.1401097	6.6315295	87.9568888
H	5.9706963	4.3180372	85.6276812
C	4.6537473	3.0338581	91.5251452
H	6.5813130	1.0894319	92.0498481
H	7.1525383	0.8477171	90.3642017
C	5.4683363	2.6757842	89.1416806
C	3.8490586	3.0885108	84.5167721
C	5.0926833	2.6520854	86.7057617
H	6.0104511	0.4372058	85.2626563
H	6.3796601	1.8992809	84.3015463
C	5.3290528	2.0673965	90.5357889
C	4.9147782	2.0554177	87.9871179
C	4.5041206	2.0424884	85.4347028
H	3.6684561	3.3652522	91.1431358
H	3.1955610	3.7735195	85.0945282
H	5.2764737	3.9347505	91.7065647
H	5.3582377	7.0506674	87.9015826
H	4.5953700	3.7217114	83.9924537
H	8.6127655	5.4672304	89.2092239
H	4.6779808	1.1736918	90.4518317
H	3.7011564	1.3409307	85.7398985
H	6.6172117	4.3475542	89.8917288
C	21.6239101	28.3697317	79.9929562
C	20.5193391	28.0502637	80.7896570

C	19.9762939	29.0191263	81.6629705
C	20.5497615	30.3062748	81.7297201
C	21.6569847	30.6252165	80.9303342
C	22.1925850	29.6570282	80.0629792
H	22.0497863	27.6175915	79.3111994
H	20.0513525	27.0541444	80.7586516
C	18.8035632	28.6863301	82.5097867
H	20.1196589	31.0559649	82.4143615
H	22.1053442	31.6291428	80.9808152
H	23.0617726	29.9061971	79.4345545
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agg-7-j-ma



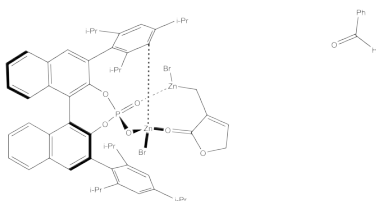
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H	3.4221923	6.5169136	86.6107450
Br	0.9289192	0.3890378	85.0629522
H	-0.8801086	4.4665703	84.5811716
Zn	0.8509916	2.6967006	85.3076034
C	2.0708835	6.1707240	84.9350201
C	2.4758908	6.9058173	86.1683335
C	0.9187627	5.4709950	85.1710026
C	0.2176044	4.4156667	84.4368973
C	0.5383006	5.8119090	86.5573463
O	1.4216474	6.6473377	87.1164074
O	-0.4573611	5.4066212	87.1899421
H	2.5736053	8.0078900	86.0580888
H	0.4574247	4.3987097	83.3570322
H	2.6756437	6.1512343	84.0187633
C	-0.2075799	0.9159502	89.2385965
C	0.6580523	-0.1372763	89.5444833
C	0.2591117	-1.0444964	90.5960523
C	1.1211766	-2.0607654	91.1072994
C	-1.0535797	-0.9075485	91.1850175
C	-1.4657137	-1.8294831	92.1931114
C	-1.8923088	0.1796577	90.8009575
H	-2.8707377	0.2971783	91.2917535
C	-1.4678073	1.1252077	89.8789299
C	4.0977247	0.8105598	88.1127664
C	4.5245788	-0.4121987	87.6093682
H	5.5286458	-0.4884965	87.1663510
C	3.6804189	-1.5579421	87.5932609
C	4.0995154	-2.7715768	86.9710410
C	2.3593836	-1.4788275	88.1664866
C	1.4914550	-2.6010929	88.0175502
C	1.9558137	-0.2591660	88.8225478
C	2.8109306	0.8456774	88.7327845
O	0.1241071	1.8114461	88.2351359
O	2.4188218	2.0589295	89.3047332
P	1.3100112	2.9355629	88.4740959
O	0.8754477	4.0395501	89.4504570
O	1.7555135	3.3182115	87.0628660
C	-0.6140591	-2.8276630	92.6404538
C	0.6958748	-2.9295214	92.1026544
H	-2.4736311	-1.7198327	92.6234869

H	-0.9436869	-3.5279844	93.4228494
H	2.1399370	-2.1473813	90.7060277
H	1.3838313	-3.7007787	92.4812421
C	1.9213569	-3.7594854	87.3861576
C	3.2418732	-3.8559781	86.8732451
H	0.4616961	-2.5349966	88.3943310
H	1.2280420	-4.6069076	87.2736488
H	3.5736230	-4.7824921	86.3804574
H	5.1149654	-2.8202614	86.5473692
C	-2.0840224	3.4723286	90.5295946
C	-2.1665190	2.4138915	89.5845807
C	-2.5668858	4.7531964	90.1509702
C	-2.7570744	2.6341998	88.3082474
C	-3.2482079	3.9122826	87.9881667
C	-3.1626252	4.9913522	88.8839013
H	-2.5771158	5.5653939	90.8957450
C	-2.8877792	1.4884879	87.3098684
H	-3.6946490	4.0775147	86.9987253
C	-2.7597520	1.9266472	85.8456463
H	-3.6331529	2.5185312	85.5005037
H	-2.6730789	1.0408512	85.1864277
H	-1.8495572	2.5399759	85.6922063
C	-4.2029820	0.7245769	87.5613700
H	-2.0555681	0.7822686	87.5034111
H	-5.0811191	1.3847374	87.4021262
H	-4.2526111	0.3384421	88.5994874
H	-4.2916735	-0.1382565	86.8700030
C	-3.7328335	6.3687970	88.5748219
C	-3.6930623	6.7353424	87.0856498
H	-3.9914653	7.7935008	86.9455695
H	-4.3949897	6.1179926	86.4866313
H	-2.6756696	6.6027059	86.6681476
C	-5.1604274	6.4825934	89.1463301
H	-3.0911008	7.0983792	89.1185406
H	-5.5642571	7.5036582	88.9887947
H	-5.1823216	6.2704427	90.2341821
H	-5.8432453	5.7628681	88.6478570
C	-1.5526132	3.2648813	91.9460387
C	-0.5754406	4.3504749	92.4238738
H	-0.2377639	4.1217289	93.4549650
H	-1.0270705	5.3632474	92.4442691
H	0.3238756	4.3900742	91.7786263
C	-2.7433695	3.1218739	92.9164481
H	-0.9988413	2.3051269	91.9531389
H	-2.3849615	2.8935166	93.9410129
H	-3.4334321	2.3121392	92.6046029
H	-3.3318552	4.0620428	92.9646929
H	7.1717796	6.0404206	86.5067208
H	7.3820379	2.4393635	91.1736918
H	5.1302583	0.7548048	83.7571644
C	7.1288865	5.8049633	87.5935459
H	4.4676006	2.5724818	92.4991762
H	6.9217219	7.9246954	88.1397262
H	3.2571885	2.5512914	83.7179132
C	6.3643537	4.4940585	87.7304793
C	6.6647080	1.5998020	91.0588297
C	6.3908394	6.9620779	88.2914085
H	6.3139451	6.7889783	89.3849317
C	6.1655949	3.8934960	88.9855790
C	5.5787338	1.2400975	84.6484940
H	9.1166034	4.8650535	87.5772943
C	5.8208536	3.8534334	86.6055566
C	8.5775296	5.6817797	88.0978235
H	9.1367937	6.6259062	87.9328102
H	5.9697854	4.3150957	85.6157794
C	4.6310624	3.0649850	91.5183995
H	6.5519190	1.1163252	92.0514132
H	7.1203762	0.8629890	90.3666911
C	5.4471480	2.6950357	89.1367689
C	3.8494614	3.0675234	84.5023031
C	5.0882159	2.6544548	86.6986123

H	6.0409723	0.4477652	85.2687555	C	3.628787	-3.239677	87.244377
H	6.3953004	1.9088435	84.3029517	C	2.114964	-1.555339	88.245770
C	5.3036176	2.0930198	90.5330874	C	1.059960	-2.509935	88.139301
C	4.9044744	2.0653124	87.9823026	C	1.920007	-0.230752	88.782783
C	4.5127114	2.0332233	85.4271067	C	2.968267	0.687964	88.653735
H	3.6487366	3.4018540	91.1341046	O	0.525445	2.076111	87.932009
H	3.1857502	3.7459079	85.0760345	O	2.783450	1.998087	89.105415
H	5.2577189	3.9628054	91.7010623	P	1.889891	2.981200	88.144662
H	5.3572616	7.0745772	87.9045732	O	1.631586	4.231796	89.001249
H	4.5907397	3.7071319	83.9780872	O	2.456327	3.146361	86.734840
H	8.6080362	5.4629558	89.1855555	C	-1.223708	-1.942878	92.651414
H	4.6491437	1.2017352	90.4517996	C	0.065902	-2.326149	92.196059
H	3.7151089	1.3242767	85.7292721	H	-2.847333	-0.525592	92.442532
H	6.5832735	4.3753718	89.8842038	H	-1.706123	-2.499813	93.469023
C	21.6268429	28.3772956	79.9858981	H	1.682764	-1.944264	90.822311
C	20.5264425	28.0453921	80.7827282	H	0.585170	-3.171492	92.672799
C	19.9784255	29.0044603	81.6624164	C	1.290329	-3.776898	87.621254
C	20.5426422	30.2943209	81.7349139	C	2.588568	-4.154726	87.185568
C	21.6459642	30.6261300	80.9358706	H	0.047114	-2.226858	88.457001
C	22.1868212	29.6673668	80.0623011	H	0.456935	-4.491334	87.539535
H	22.0566074	27.6322447	79.2987881	H	2.760772	-5.164864	86.783686
H	20.0625220	27.0474209	80.7501220	H	4.632761	-3.508515	86.879858
C	18.8083823	28.6525536	82.5092783	C	-1.433115	4.303783	89.945810
H	20.1078412	31.0366774	82.4248242	C	-1.672179	3.192485	89.092544
H	22.0873674	31.6328739	80.9914943	C	-1.658133	5.609679	89.431573
H	23.0533568	29.9263204	79.4341793	C	-2.166948	3.392848	87.773070
O	18.2553212	27.5656526	82.5148526	C	-2.406396	4.701697	87.317190
H	18.4501100	29.4963352	83.1762450	C	-2.156094	5.828368	88.118120
				H	-1.558028	6.476385	90.105011
				C	-2.469460	2.200718	86.871754
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				C	-2.172590	2.458809	85.389228
				H	-2.881715	3.180078	84.932517
				H	-2.239513	1.514011	84.814778
				H	-1.146876	2.855779	85.253203
				C	-3.924446	1.739589	87.089316
				H	-1.810244	1.368048	87.189493
				H	-4.639959	2.539436	86.805202
				H	-4.110101	1.479224	88.151135
				H	-4.145673	0.844987	86.471999
				C	-2.454928	7.249377	87.660602
				C	-2.290042	7.459899	86.149807
				H	-2.392447	8.535194	85.901640
				H	-3.064506	6.916552	85.568967
				H	-1.295709	7.115030	85.803891
				C	-3.860830	7.665460	88.138901
				H	-1.715822	7.903146	88.176243
				H	-4.065400	8.722405	87.871884
				H	-3.964412	7.563074	89.237920
				H	-4.640646	7.033875	87.663906
				C	-1.009475	4.138339	91.402870
				C	0.117230	5.082614	91.849357
				H	0.368378	4.887422	92.911509
				H	-0.159299	6.153757	91.769582
				H	1.035835	4.918476	91.252482
				C	-2.250345	4.287101	92.307818
				H	-0.630948	3.103711	91.520825
				H	-1.982689	4.095137	93.366949
				H	-3.055305	3.580334	92.022253
				H	-2.667020	5.314033	92.242396
				H	8.339678	4.774616	86.312199
				H	7.652155	1.607731	91.230496
				H	5.422574	-0.219765	83.829239
				C	8.173491	4.669568	87.407285
				H	4.761927	2.368622	92.373968
				H	8.281907	6.842318	87.728134
				H	3.934828	1.888708	83.561897
				C	7.184398	3.525875	87.595145
				C	6.799106	0.903763	91.133378
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				H	7.392994	5.957890	89.009968

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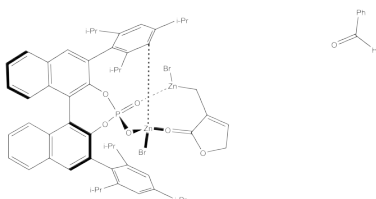


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C	2.065331	5.247609	84.609292
C	1.700126	5.775687	85.938443
O	2.680498	6.524752	86.455212
C	3.786547	6.539532	85.528122
O	0.635076	5.583256	86.561220
C	1.230774	4.246079	83.938512
H	4.660121	6.080337	86.045138
H	4.036105	7.600275	85.309309
Zn	1.539959	2.543452	84.987640
Br	1.218892	0.234143	84.942721
H	1.506227	4.088947	82.878536
H	0.151082	4.484172	84.018827
H	3.938573	5.546569	83.475904
C	-0.005110	1.346734	88.984680
C	0.640290	0.187338	89.421484
C	0.040996	-0.535751	90.519630
C	0.681883	-1.640318	91.157877
C	-1.246853	-0.113669	91.022333
C	-1.860539	-0.852217	92.078413
C	-1.858176	1.066375	90.504907
H	-2.818730	1.397892	90.928278
C	-1.231144	1.833544	89.533901
C	4.249945	0.366288	88.110042
C	4.460827	-0.951742	87.723143
H	5.449232	-1.248754	87.342025
C	3.418880	-1.921477	87.749617

C	6.825361	3.073012	88.876836	C	0.2663568	-0.8856644	90.4684025
C	5.920514	0.240607	84.707607	C	0.9812954	-1.9834290	91.0350455
H	9.969555	3.429038	87.673808	C	-1.0371551	-0.5722688	91.0081729
C	6.576830	2.909483	86.489280	C	-1.5895165	-1.4058219	92.0260160
C	9.536439	4.374816	88.057350	C	-1.7245927	0.5959001	90.5659520
H	10.256957	5.193223	87.851377	H	-2.6961930	0.8462226	91.0193599
H	6.848787	3.257905	85.479624	C	-1.1596680	1.4537529	89.6335373
C	5.052019	2.743318	91.370499	C	4.3791473	0.4119349	88.0732864
H	6.554931	0.528672	92.148968	C	4.6679476	-0.8682660	87.6165553
H	7.141334	0.043879	90.522146	H	5.6684500	-1.0799053	87.2109628
C	5.888027	2.043286	89.071326	C	3.6901072	-1.9023046	87.5995963
C	4.579734	2.344287	84.342815	C	3.9755479	-3.1757008	87.0227782
C	5.627764	1.878145	86.625712	C	2.3713922	-1.6455544	88.1240777
H	6.197551	-0.573513	85.405407	C	1.3767075	-2.6568789	87.9732753
H	6.862083	0.715770	84.359542	C	2.1006871	-0.3671115	88.7348574
C	5.576119	1.590178	90.496365	C	3.0874529	0.6220294	88.6471425
C	5.283359	1.436125	87.935479	O	0.5560157	1.8918648	88.0296709
C	4.995676	1.278350	85.371015	O	2.8285426	1.8902925	89.1735702
H	4.163717	3.216179	90.908246	P	1.8632516	2.8693201	88.2803389
H	4.034081	3.177854	84.830190	O	1.5363350	4.0483330	89.2097206
H	5.823630	3.527197	91.521181	O	2.3985998	3.1490469	86.8761648
H	6.621745	6.230188	87.420619	C	-0.8807070	-2.4862201	92.5281168
H	5.449799	2.792390	83.818460	C	0.4224040	-2.7634741	92.0376977
H	9.447011	4.281563	89.159830	H	-2.5890451	-1.1612483	92.4188665
H	4.772724	0.827998	90.441599	H	-1.3173054	-3.1172260	93.3171112
H	4.067295	0.755797	85.679837	H	1.9934932	-2.2057020	90.6708088
H	7.288400	3.539471	89.761174	H	0.9983422	-3.6014886	92.4589906
C	-4.568630	17.921449	80.882738	C	1.6800859	-3.8771590	87.3865892
C	-5.871773	17.467798	80.653112	C	2.9941248	-4.1493023	86.9223319
C	-6.597717	17.943949	79.538423	H	0.3517663	-2.4537394	88.3121935
C	-6.006496	18.875687	78.659663	H	0.8915424	-4.6363628	87.2714922
C	-4.699980	19.329605	78.891076	H	3.2243984	-5.1233037	86.4644780
C	-3.982718	18.852221	80.001983	H	4.9899041	-3.3606022	86.6356487
H	-3.999787	17.553094	81.750278	C	-1.5073048	3.8766038	90.1994225
H	-6.358805	16.741213	81.321775	C	-1.6861455	2.8077316	89.2799212
C	-7.981004	17.466484	79.290391	C	-1.8154189	5.1946198	89.7691898
H	-6.580535	19.241973	77.792457	C	-2.2014050	3.0592821	87.9769085
H	-4.237139	20.056691	78.206535	C	-2.5203462	4.3772977	87.6049904
H	-2.956823	19.207957	80.184960	C	-2.3332652	5.4648572	88.4746140
O	-8.578737	16.663978	79.992610	H	-1.7510109	6.0243914	90.4913910
H	-8.467445	17.911964	78.370896	C	-2.4394572	1.9081034	87.0049714
				H	-2.9087721	4.5653828	86.5954095
				C	-2.2093774	2.2813043	85.5352426
				H	-2.9901358	2.9653921	85.1421235
				H	-2.2113661	1.3715207	84.9035526
				H	-1.2252949	2.7724817	85.3989383
				C	-3.8468979	1.3200546	87.2282083
				H	-1.7082040	1.1112617	87.2478043
				H	-4.6307802	2.0776535	87.0185971
				H	-3.9784699	0.9763268	88.2740636
				H	-4.0186287	0.4531551	86.5579598
				C	-2.7172645	6.8921247	88.1089257
				C	-2.5942832	7.2031086	86.6117295
				H	-2.7516925	8.2857310	86.4340733
				H	-3.3543317	6.6611150	86.0106198
				H	-1.5918988	6.9299111	86.2273165
				C	-4.1326450	7.2033732	88.6357471
				H	-2.0024552	7.5524746	88.6501521
				H	-4.3983308	8.2620490	88.4386573
				H	-4.2089097	7.0295489	89.7279854
				H	-4.8891230	6.5611893	88.1376758
				C	-1.0555183	3.6505820	91.6402991
				C	0.0386921	4.6162459	92.1214868
				H	0.3101984	4.3811189	93.1705330
				H	-0.2770914	5.6791219	92.0948319
				H	0.9556689	4.5169123	91.5082684
				C	-2.2868298	3.6957539	92.5685407
				H	-0.6321695	2.6283002	91.6968643
				H	-1.9960024	3.4592227	93.6124745
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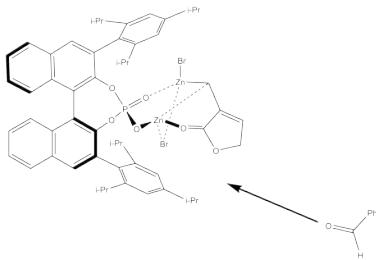
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C	1.8943333	5.3312916	84.9040619
C	1.5142563	5.7582784	86.2664609
O	2.4764629	6.4937024	86.8357533
C	3.5850213	6.5912842	85.9199850
O	0.4553432	5.4992356	86.8724447
C	1.0915909	4.3486415	84.1728276
H	4.4601871	6.1004268	86.4053665
H	3.8234901	7.6689797	85.7859929
Zn	1.4810066	2.5906353	85.1068213
Br	1.2836787	0.2841051	84.9253171
H	1.3607930	4.2714321	83.1025433
H	0.0046228	4.5375300	84.2782604
H	3.7581077	5.7558228	83.7981764
C	0.0853248	1.0740901	89.0438767
C	0.8057021	-0.0663168	89.4076752

H	8.1020664	5.1914075	86.4369529	H	-1.1078887	5.9025158	1.3253191
H	7.7438068	1.7226351	91.1984147	Br	1.5136125	2.2604950	-2.6566506
H	5.5358345	0.0935034	83.7621243	H	-2.4663552	1.9431869	-1.3624044
C	8.0073427	4.9881086	87.5270283	Zn	-0.1062689	1.2212803	-1.3690116
H	4.8288122	2.2435862	92.4232695	C	-2.0023917	4.3519637	0.0519068
H	8.0501896	7.1295271	88.0232171	C	-1.9321978	5.1560526	1.3027615
H	3.9009793	2.1006406	83.6031641	C	-1.8025303	3.0293942	0.3401845
C	7.0857970	3.7832810	87.6721246	C	-1.8163313	1.8107685	-0.4723881
C	6.9335828	0.9726893	91.0812946	C	-1.5631882	2.9858915	1.7943514
C	7.4025980	6.2427305	88.1833521	O	-1.6737956	4.1969711	2.3511158
H	7.2838767	6.1068639	89.2783626	O	-1.2971285	2.0034590	2.5204218
C	6.7778036	3.2486755	88.9350587	H	-2.8789611	5.6866740	1.5466977
C	6.0116959	0.5499777	84.6544105	H	-2.2326761	0.9662960	0.1124382
H	9.8651137	3.8130873	87.5755819	H	-2.2127083	4.7876689	-0.9339902
C	6.5050975	3.1777190	86.5463352	C	-2.7667547	-3.2213124	0.0628251
C	9.4188940	4.7000627	88.0682390	C	-2.2860394	-4.5335885	-0.0340306
H	10.0929897	5.5653297	87.8998392	C	-2.9271195	-5.5455120	0.7715194
H	6.7397986	3.5874905	85.5503482	C	-2.4170824	-6.8731226	0.8957418
C	5.0790615	2.6844676	91.4362431	C	-4.1160749	-5.1995561	1.5137475
H	6.7335313	0.5352410	92.0814230	C	-4.7816228	-6.2074162	2.2753597
H	7.3167861	0.1665025	90.4233733	C	-4.5770666	-3.8521202	1.5173521
C	5.9158854	2.1497887	89.0928923	H	-5.4751581	-3.6017081	2.1025802
C	4.5239988	2.5672803	84.3947226	C	-3.8938657	-2.8382268	0.8542087
C	5.6310246	2.0781202	86.6456084	C	-1.1779064	-4.2391832	-1.6797334
H	6.3539714	-0.2716565	85.3131686	C	1.1620214	-5.3210448	-2.5520890
H	6.9144661	1.1031813	84.3191263	H	2.0400940	-5.5104436	-3.1882693
C	5.6584921	1.6106698	90.4985963	C	0.0087567	-6.1430314	-2.7104160
C	5.3370166	1.5549835	87.9374668	C	-0.0152098	-7.1931137	-3.6772694
C	5.0258317	1.4908973	85.3716687	C	-1.1808299	-5.8677251	-1.9384197
H	4.1562813	3.1246784	91.0112229	C	-2.3633655	-6.6098004	-2.2363646
H	3.9277785	3.3383469	84.9241649	C	-1.1323618	-4.8354786	-0.9291403
H	5.8030766	3.5063682	91.6168396	C	0.0321846	-4.0659280	-0.8442491
H	6.3983323	6.4711621	87.7714252	O	-2.1392522	-2.2129407	-0.6710237
H	5.3543961	3.0971698	83.8820365	O	0.1071156	-3.0670543	0.1269343
H	9.3982969	4.5017361	89.1601302	P	-0.6950045	-1.6665722	-0.1161573
H	4.9035388	0.8026510	90.4181658	O	-0.8781870	-1.0727523	1.2982989
H	4.1384305	0.8932581	85.6644460	O	-0.0822517	-0.7926239	-1.2064831
H	7.2226499	3.7038044	89.8345160	C	-4.2787257	-7.4979041	2.3439709
C	-5.3993179	17.9531311	77.5686553	C	-3.0755936	-7.8246106	1.6625526
C	-5.2763694	18.2137475	78.9371909	H	-5.6965204	-5.9330432	2.8238240
C	-5.7335792	19.4411830	79.4647319	H	-4.7979660	-8.2642273	2.9394291
C	-6.3130257	20.4007385	78.6098625	H	-1.4829511	-7.1378927	0.3815575
C	-6.4360568	20.1385933	77.2380116	H	-2.6578537	-8.8394729	1.7465348
C	-5.9790765	18.9152207	76.7189709	C	-2.3587986	-7.6116987	-3.1976425
H	-5.0439933	16.9973677	77.1537045	C	-1.1714180	-7.9218091	-3.9127573
H	-4.8288479	17.4861296	79.6318088	H	-3.2930804	-6.3761862	-1.6997948
C	-5.6030306	19.7188279	80.9193541	H	-3.2859754	-8.1656517	-3.4099684
H	-6.6670979	21.3564020	79.0310597	H	-1.1768810	-8.7246409	-4.6656103
H	-6.8883262	20.8868566	76.5693992	H	0.9033159	-7.3996579	-4.2487542
H	-6.0749305	18.7078220	75.6418119	C	-4.0952924	-0.7437175	2.2587171
O	-5.1177792	18.9514461	81.7335656	C	-4.2707200	-1.3960499	1.0004834
H	-6.0010407	20.7326392	81.2339589	C	-4.4431046	0.6139435	2.3678601
				C	-4.7819582	-0.6652150	-0.1060109
				C	-5.1356807	0.6872191	0.0683565
				C	-4.9753357	1.3511127	1.2942323
				H	-4.2979853	1.1232895	3.3346800
				C	-4.9958277	-1.3030972	-1.4776961
				H	-5.5420574	1.2350080	-0.7943564
				C	-4.1931405	-0.5852777	-2.5784319
				H	-4.5334244	0.4627038	-2.7156110
				H	-4.3178583	-1.1038390	-3.5512227
				H	-3.1126757	-0.5716636	-2.3365305
				C	-6.4937692	-1.3780707	-1.8279310
				H	-4.6254823	-2.3467263	-1.4292592
				H	-6.9425164	-0.3661535	-1.9128712
				H	-7.0602669	-1.9332965	-1.0530007
				H	-6.6433832	-1.8935923	-2.7991480
				C	-5.3863044	2.8049048	1.5132514
				C	-5.5491645	3.6154941	0.2219815
				H	-5.7278896	4.6844902	0.4567408
				H	-6.4174607	3.2636512	-0.3731082

7.4.2 Pathways starting from 13d-ma

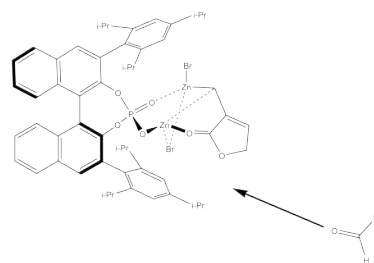
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Br	2.0928694	0.8095196	2.6243543

H	-4.6482728	3.5510208	-0.4200999
C	-6.6709685	2.8760396	2.3643568
H	-4.5709527	3.2762528	2.1097896
H	-6.9425393	3.9284014	2.5887642
H	-6.5536225	2.3389570	3.3267290
H	-7.5201407	2.4105679	1.8214543
C	-3.6018776	-1.4729918	3.5111131
C	-2.4168710	-0.7835297	4.2101040
H	-2.1728580	-1.2991323	5.1608790
H	-2.6124150	0.2816915	4.4446444
H	-1.5073579	-0.8484172	3.5774298
C	-4.7691247	-1.6708663	4.5001980
H	-3.2499188	-2.4778373	3.2052795
H	-4.4495778	-2.2739561	5.3750922
H	-5.6237930	-2.1887567	4.0201158
H	-5.1436174	-0.6961540	4.8772089
H	4.9343847	0.6882007	-2.5708029
H	5.2246596	-4.1607239	0.8282989
H	1.6525012	-3.1947004	-6.1140700
C	5.0416353	0.1592604	-1.5984557
H	2.7337268	-3.9114192	2.8214998
H	5.3390799	2.0340747	-0.4997507
H	0.0830684	-1.3553516	-5.3271474
C	4.0826629	-1.0233804	-1.6347290
C	4.3209445	-4.7918234	0.6949181
C	4.6612771	1.1548864	-0.4881112
H	4.7284181	0.6878419	0.5163605
C	3.9778833	-1.9102704	-0.5481962
C	2.2911474	-3.0314361	-5.2208670
H	6.7849263	-0.9980108	-2.2841689
C	3.2594242	-1.2510549	-2.7483500
C	6.5059507	-0.2976496	-1.4706611
H	7.1955239	0.5710898	-1.5116178
H	3.3217979	-0.5518251	-3.5967237
C	2.8236577	-3.1884529	1.9843478
H	4.2852635	-5.5139085	1.5372139
H	4.4486854	-5.3648674	-0.2460497
C	3.0749632	-2.9864457	-0.5464394
C	0.7492904	-1.1667154	-4.4597279
C	2.3342393	-2.3102830	-2.8008767
H	2.7670099	-3.9979572	-4.9571709
H	3.1023996	-2.3297667	-5.5076292
C	3.0444248	-3.9297207	0.6545918
C	2.2435588	-3.1894106	-1.6824619
C	1.4641970	-2.4657870	-4.0502457
H	1.9019329	-2.5760233	1.9547505
H	0.1365155	-0.7768962	-3.6253371
H	3.6664925	-2.5077085	2.2231472
H	3.6227440	1.5167885	-0.6222941
H	1.4590326	-0.3660828	-4.7507725
H	6.6823849	-0.8166821	-0.5050140
H	2.1903612	-4.6247548	0.5173140
H	0.6702733	-3.2039618	-3.8198396
H	4.6152502	-1.7524120	0.3361942
C	9.6585983	15.9555757	0.6886400
C	9.1995156	14.7258223	1.1720965
C	9.9776059	13.9981616	2.1001316
C	11.2160110	14.5136274	2.5368857
C	11.6747747	15.7469781	2.0518760
C	10.8959138	16.4663688	1.1286218
H	9.0552585	16.5251537	-0.0348552
H	8.2375887	14.2985979	0.8489909
C	9.4937680	12.6933098	2.6167404
H	11.8169379	13.9389488	3.2609999
H	12.6405217	16.1509188	2.3919213
H	11.2550172	17.4347876	0.7469008
O	8.4354025	12.1683324	2.3028264
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Energy (Hartree)= -11969.97924776
number of imaginary frequencies: 3

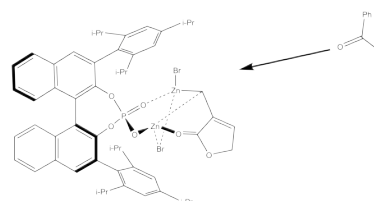
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Br	2.0925701	0.8035425	2.6717278
H	-1.1037230	5.9006275	1.3255252
Br	1.4952708	2.2677105	-2.6584528
H	-2.4799030	1.9400959	-1.3616087
Zn	-0.1035335	1.2272633	-1.3682321
C	-2.0052411	4.3519830	0.0507337
C	-1.9280960	5.1532429	1.3047889
C	-1.8072468	3.0284025	0.3356898
C	-1.8248990	1.8109877	-0.4748093
C	-1.5593901	2.9811553	1.7910973
O	-1.6666356	4.1944665	2.3495281
O	-1.2915237	1.9979289	2.5099833
H	-2.8740942	5.6842617	1.5539827
H	-2.2320818	0.9654051	0.1144364
H	-2.2184675	4.7878933	-0.9343051
C	-2.7676589	-3.2210369	0.0630962
C	-2.2860969	-4.5329070	-0.0331936
C	-2.9272589	-5.5447430	0.7721978
C	-2.4170685	-6.8720613	0.8962468
C	-4.1167798	-5.1996795	1.5135817
C	-4.7820209	-6.2081907	2.2736382
C	-4.5778479	-3.8525508	1.5172055
H	-5.4760332	-3.6014861	2.1020039
C	-3.8948089	-2.8384831	0.8547237
C	1.1784175	-4.2375846	-1.6776745
C	1.1619246	-5.3202983	-2.5488821
H	2.0407077	-5.5083284	-3.1844739
C	0.0091274	-6.1420994	-2.7082633
C	-0.0157996	-7.1916263	-3.6750745
C	-1.1802366	-5.8666655	-1.9364623
C	-2.3626959	-6.6081974	-2.2348944
C	-1.1317660	-4.8341452	-0.9274965
C	0.0322258	-4.0634553	-0.8429130
O	-2.1422094	-2.2123649	-0.6704363
O	0.1058427	-3.0626731	0.1265701
P	-0.6982939	-1.6645587	-0.1149489
O	-0.8878938	-1.0673379	1.2979300
O	-0.0898900	-0.7854057	-1.2032861
C	-4.2791862	-7.4981139	2.3420485
C	-3.0758810	-7.8238378	1.6616416
H	-5.6973701	-5.9341130	2.8214837
H	-4.7988679	-8.2646973	2.9366811
H	-1.4828107	-7.1351223	0.3816403
H	-2.6578516	-8.8385435	1.7453108
C	-2.3584199	-7.6094755	-3.1962178
C	-1.1716721	-7.9196722	-3.9111270
H	-3.2919104	-6.3737698	-1.6979765
H	-3.2859773	-8.1625357	-3.4089941
H	-1.1772725	-8.7219438	-4.6645207
H	0.9026118	-7.3978827	-4.2467996
C	-4.0966278	-0.7435569	2.2587798
C	-4.2718527	-1.3963242	1.0009111
C	-4.4443679	0.6139340	2.3672762
C	-4.7823981	-0.6655821	-0.1057974
C	-5.1367839	0.6864396	0.0684677

TS-7-d-ma

C	-4.9767708	1.3505796	1.2938280
H	-4.2983336	1.1237222	3.3337984
C	-4.9939275	-1.3028736	-1.4781441
H	-5.5436524	1.2333720	-0.7945274
C	-4.1896171	-0.5849038	-2.5774732
H	-4.5298871	0.4629787	-2.7161096
H	-4.3121467	-1.1027989	-3.5507133
H	-3.1094881	-0.5722991	-2.3347782
C	-6.4911265	-1.3785471	-1.8304456
H	-4.6227538	-2.3460983	-1.4293502
H	-6.9409830	-0.3672431	-1.9158562
H	-7.0586288	-1.9335808	-1.0564304
H	-6.6396906	-1.8937122	-2.8019117
C	-5.3874783	2.8045930	1.5126679
C	-5.5497458	3.6149920	0.2211698
H	-5.7286831	4.6844143	0.4543264
H	-6.4185757	3.2641289	-0.3735219
H	-4.6491881	3.5492365	-0.4210715
C	-6.6721292	2.8772177	2.3632025
H	-4.5711958	3.2760830	2.1082801
H	-6.9444673	3.9293805	2.5877439
H	-6.5560090	2.3396934	3.3252482
H	-7.5210088	2.4112419	1.8207597
C	-3.6030821	-1.4726202	3.5113898
C	-2.4186487	-0.7832137	4.2114632
H	-2.1766255	-1.2972834	5.1635792
H	-2.6125994	0.2826966	4.4444484
H	-1.5094725	-0.8494826	3.5794188
C	-4.7705680	-1.6718365	4.4995185
H	-3.2500821	-2.4768071	3.2045779
H	-4.4517742	-2.2747586	5.3747707
H	-5.6247741	-2.1897532	4.0190516
H	-5.1470247	-0.6980073	4.8766278
H	4.9367151	0.6859348	-2.5741274
H	5.2274479	-4.1613460	0.8270593
H	1.6482994	-3.1957355	-6.1138598
C	5.0433313	0.1579177	-1.6012445
H	2.7365950	-3.9100478	2.8214941
H	5.3362981	2.0344154	-0.5042967
H	0.0801200	-1.3552863	-5.3241098
C	4.0851549	-1.0251592	-1.6374399
C	4.3234672	-4.7919666	0.6945320
C	4.6600938	1.1542534	-0.4926190
H	4.7267272	0.6893935	0.5128870
C	3.9807855	-1.9115022	-0.5507071
C	2.2880687	-3.0326649	-5.2214688
H	6.7886270	-0.9984111	-2.2841789
C	3.2607425	-1.2525986	-2.7499288
C	6.5077133	-0.2978969	-1.4716878
H	7.1967591	0.5712357	-1.5112558
H	3.3227237	-0.5533403	-3.5982260
C	2.8267961	-3.1879796	1.9837093
H	4.2885151	-5.5137134	1.5371326
H	4.4516602	-5.3648263	-0.2462503
C	3.0774353	-2.9867851	-0.5471433
C	0.7486428	-1.1673637	-4.4584235
C	2.3351419	-2.3111459	-2.8013576
H	2.7647185	-3.9989836	-4.9587833
H	3.0995701	-2.3321353	-5.5094766
C	3.0472352	-3.9296063	0.6542588
C	2.2448082	-3.1890382	-1.6821076
C	1.4633778	-2.4666151	-4.0496207
H	1.9051219	-2.5757211	1.9551806
H	0.1376198	-0.7768599	-3.6232893
H	3.6691293	-2.5070789	2.2232622
H	3.6221237	1.5166308	-0.6289834
H	1.4567082	-0.3659560	-4.7507304
H	6.6841496	-0.8168017	-0.5060738
H	2.1930087	-4.6246992	0.5173695
H	0.6692323	-3.2044280	-3.8185194
H	4.6190651	-1.7533995	0.3329099

C	9.6593620	15.9547895	0.6891200
C	9.2012123	14.7250378	1.1726411
C	9.9791998	13.9982688	2.1002649
C	11.2162874	14.5147929	2.5362562
C	11.6745636	15.7481036	2.0515802
C	10.8957017	16.4666793	1.1286207
H	9.0557258	16.5238912	-0.0345562
H	8.2403049	14.2935278	0.8521839
C	9.4916784	12.6915688	2.6155172
H	11.8170909	13.9399073	3.2605390
H	12.6400328	16.1527146	2.3916405
H	11.2542470	17.4352648	0.7468414
O	8.4349991	12.1704380	2.3008486
H	10.1959202	12.1922914	3.3503237

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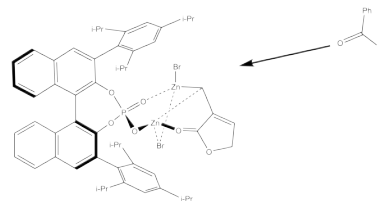


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C	2.9589051	4.6838574	-0.4197994
C	2.2291387	3.6438459	-0.9302829
C	3.0209685	2.4407683	-0.6292071
O	4.1747003	2.7279111	-0.0183419
C	4.2304608	4.1647041	0.1635508
O	2.6668950	1.2717008	-0.8610488
C	0.9195301	3.5100217	-1.5843523
H	5.1457783	4.5346165	-0.3498497
H	4.3443120	4.3652126	1.2512176
Zn	-0.3676302	2.5214368	-0.3877719
Br	-1.6815889	3.3733117	1.3532916
C	-0.9204609	-2.8559168	1.0802993
C	-1.7709136	-3.6858484	0.3401325
C	-1.7427285	-5.1035900	0.6288528
C	-2.3985682	-6.0776965	-0.1832508
C	-0.9924042	-5.5699701	1.7703056
C	-1.0068927	-6.9587552	2.1003541
C	-0.1910770	-4.6529296	2.5071347
H	0.4077121	-5.0297319	3.3504305
C	-0.0784829	-3.3177949	2.1394133
C	-2.8564840	-1.7627214	-2.8137103
C	-4.1698809	-2.1943479	-2.9535403
H	-4.7586634	-1.8564362	-3.8205453
C	-4.8015522	-3.0020216	-1.9645497
C	-6.1808579	-3.3544313	-2.0734069
C	-4.0535712	-3.4248601	-0.8043603
C	-4.7545850	-4.1095660	0.2337708
C	-2.6421540	-3.1196942	-0.7277836
C	-2.1107691	-2.2663933	-1.7029892
O	-0.9061409	-1.4862983	0.8222090
O	-0.7636071	-1.9288391	-1.6668074
P	-0.1471213	-0.9323387	-0.5180969
O	1.3457026	-1.3269215	-0.4917290
O	-0.5350440	0.5265169	-0.6900521
C	-1.6909312	-7.8718445	1.3124786
C	-2.3725572	-7.4257349	0.1489272
H	-0.4421262	-7.2929820	2.9849486
H	-1.6881477	-8.9411923	1.5731155
H	-2.9232671	-5.7536414	-1.0921209
H	-2.8809804	-8.1550310	-0.5000215

C	-6.1025184	-4.4173078	0.1084699	C	-2.2321168	-0.7304023	-3.6961572
C	-6.8202915	-4.0569405	-1.0630308	C	-3.9078938	1.0245274	-2.7792982
H	-4.2165878	-4.3876083	1.1503130	H	1.1402569	-2.2757485	-3.3939497
H	-6.6189993	-4.9404703	0.9277035	H	-2.7950911	1.7028106	-1.0239321
H	-7.8856101	-4.3172094	-1.1568140	H	1.4981980	-2.0663762	-5.1394694
H	-6.7335786	-3.0385510	-2.9721719	H	1.4960138	2.5923686	-4.6411535
C	2.3320345	-2.6707602	2.4449553	H	-3.1571928	3.0228789	-2.1916038
C	0.9569691	-2.4116980	2.7232810	H	-0.1362569	1.3110184	-7.8853821
C	3.2957787	-1.7698035	2.9329926	H	-1.1549865	-3.1172843	-3.9426952
C	0.5873187	-1.2740779	3.4902425	H	-4.2475744	0.1357364	-2.2129428
C	1.5949498	-0.4111209	3.9601215	H	0.3596528	-0.2845906	-5.8992488
C	2.9557440	-0.6361461	3.6919873	H	0.4864505	4.4894771	-1.8608589
H	4.3618298	-1.9627375	2.7261466	H	0.9954716	2.8596440	-2.4812236
C	-0.8654041	-0.9889270	3.8647160	H	2.6895258	5.7479456	-0.3962160
H	1.2990979	0.4616740	4.5620980	C	1.8896430	10.9335614	3.7380420
C	-1.3184854	0.4071688	3.4129383	C	1.9427555	9.6485339	3.1872137
H	-0.7613849	1.2155842	3.9301218	C	2.0747588	8.5224766	4.0309228
H	-2.3952242	0.5630755	3.6295514	C	2.1459390	8.6995935	5.4298462
H	-1.1767406	0.5517071	2.3265121	C	2.1081378	9.9895939	5.9794816
C	-1.0937902	-1.1954858	5.3741175	C	1.9807122	11.1051304	5.1335132
H	-1.5008139	-1.7306523	3.3391883	H	1.7805475	11.8119563	3.0835262
H	-0.4946314	-0.4782813	5.9736068	H	1.8818873	9.4833704	2.1005850
H	-0.8113511	-2.2198500	5.6919442	C	2.1734897	7.1587170	3.4509799
H	-2.1617225	-1.0361162	5.6307310	H	2.2428231	7.8182762	6.0851217
C	4.0570945	0.2434235	4.2722140	H	2.1797721	10.1301902	7.0689446
C	3.7025878	1.7367970	4.3185832	H	1.9517357	12.1184894	5.5638847
H	4.5709064	2.3303625	4.6709999	O	2.2516744	6.9090254	2.2550342
H	2.8653260	1.9400764	5.0182966	H	2.1845940	6.3290233	4.2194094
H	3.4074335	2.1155257	3.3182687				
C	4.4596574	-0.2811253	5.6661826				
H	4.9416135	0.1284792	3.6066224				
H	5.3028224	0.3038931	6.0891898				
H	4.7674749	-1.3453161	5.6188385				
H	3.6049696	-0.2123955	6.3716312				
C	2.8075839	-3.9058076	1.6763857				
C	3.7204497	-3.5728001	0.4870107				
H	4.0772868	-4.4996252	-0.0068966				
H	4.6186124	-2.9907908	0.7793572				
H	3.1664655	-2.9991256	-0.2804832				
C	3.4878408	-4.9042803	2.6335234				
H	1.9160694	-4.4089508	1.2542525				
H	3.7665117	-5.8354466	2.0979329				
H	2.8205436	-5.1790721	3.4755701				
H	4.4130236	-4.4742793	3.0711990				
H	-0.6690785	3.3735542	-5.6430380				
H	-0.5041069	-2.4528539	-6.8849456				
H	-5.9742427	1.7058536	-3.0570982				
C	-0.2350261	2.4073539	-5.9829588				
H	1.1909087	-3.6974426	-4.4795901				
H	1.7444563	3.3072802	-6.2681019				
H	-4.4391058	2.3721892	-1.1311367				
C	-0.9231274	1.3104901	-5.1804587				
C	-0.9997808	-3.0328579	-6.0783239				
C	1.2797544	2.4613295	-5.7210606				
H	1.7861617	1.5318840	-6.0549204				
C	-0.4942973	-0.0278303	-5.2523082				
C	-5.0827427	1.4652297	-3.6725167				
H	-1.6342085	2.2693117	-7.6743399				
C	-2.0314520	1.6005354	-4.3695785				
C	-0.5415582	2.2644050	-7.4858431				
H	-0.0871314	3.0944746	-8.0657393				
H	-2.3829597	2.6440045	-4.3115387				
C	0.8834953	-2.6337445	-4.4102417				
H	-0.6906323	-4.0934658	-6.1852717				
H	-2.0943221	-2.9750995	-6.2480049				
C	-1.1198808	-1.0533726	-4.5237622				
C	-3.5509669	2.0914433	-1.7333868				
C	-2.7040161	0.6107820	-3.6262477				
H	-5.3658311	0.6668414	-4.3891541				
H	-4.8277418	2.3687715	-4.2649171				
C	-0.6233566	-2.4891419	-4.6860510				

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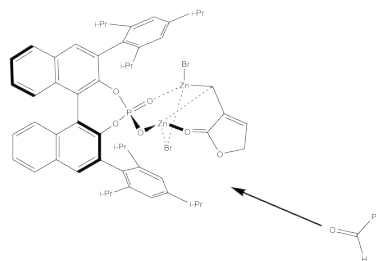


Energy (Hartree) = -11969.97519629
number of imaginary frequencies: 5

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Br	4.7087467	-1.3038040	-2.5025586
C	2.9624673	4.6854934	-0.4236234
C	2.2304446	3.6459960	-0.9326654
C	3.0206162	2.4404922	-0.6293917
O	4.1776650	2.7285418	-0.0200831
C	4.2341468	4.1634651	0.1595768
O	2.6663550	1.2728866	-0.8569566
C	0.9216461	3.5111800	-1.5832149
H	5.1502039	4.5312698	-0.3557005
H	4.3492508	4.3657645	1.2470910
Zn	-0.3694208	2.5277629	-0.3774868
Br	-1.6808187	3.3707256	1.3506826
C	-0.9204983	-2.8551729	1.0793998
C	-1.7711333	-3.6860066	0.3400828
C	-1.7427945	-5.1036448	0.6291649
C	-2.3982653	-6.0780994	-0.1825654
C	-0.9926619	-5.5699350	1.7705630
C	-1.0074099	-6.9583684	2.1002078
C	-0.1919066	-4.6523749	2.5068781
H	0.4074394	-5.0281838	3.3502749
C	-0.0788118	-3.3175123	2.1389616
C	-2.8565370	-1.7634519	-2.8139258
C	-4.1696730	-2.1954715	-2.9533435
H	-4.7578791	-1.8566445	-3.8204271
C	-4.8017177	-3.0027842	-1.9646743
C	-6.1805984	-3.3552961	-2.0727379
C	-4.0535957	-3.4254482	-0.8047236

C	-4.7547346	-4.1099119	0.2332333	H	-1.6347958	2.2688950	-7.6739556
C	-2.6422211	-3.1204129	-0.7282048	C	-2.0319132	1.5993393	-4.3697967
C	-2.1102948	-2.2669245	-1.7031415	C	-0.5423432	2.2648126	-7.4856503
O	-0.9051938	-1.4866878	0.8213476	H	-0.0880184	3.0945275	-8.0661147
O	-0.7641471	-1.9290954	-1.6672832	H	-2.3835734	2.6427389	-4.3113084
P	-0.1465625	-0.9310825	-0.5190673	C	0.8829501	-2.6340403	-4.4109323
O	1.3460433	-1.3273437	-0.4906055	H	-0.6913878	-4.0937944	-6.1859445
O	-0.5310504	0.5275721	-0.6948702	H	-2.0949786	-2.9753145	-6.2483095
C	-1.6909047	-7.8715659	1.3129168	C	-1.1205755	-1.0538597	-4.5242182
C	-2.3722173	-7.4256812	0.1498187	C	-3.5515192	2.0904925	-1.7335979
H	-0.4425066	-7.2922264	2.9848642	C	-2.7047101	0.6098950	-3.6267179
H	-1.6878505	-8.9408175	1.5738164	H	-5.3662722	0.6663746	-4.3899759
H	-2.9229143	-5.7533701	-1.0911308	H	-4.8289550	2.3672555	-4.2654214
H	-2.8804796	-8.1549896	-0.4991825	C	-0.6237299	-2.4894689	-4.6864871
C	-6.1022632	-4.4176082	0.1080286	C	-2.2326567	-0.7310322	-3.6966724
C	-6.8200151	-4.0574167	-1.0628169	C	-3.9081836	1.0237860	-2.7793692
H	-4.2158940	-4.3876357	1.1492648	H	1.1406870	-2.2765134	-3.3949663
H	-6.6185581	-4.9404915	0.9274982	H	-2.7960142	1.7035497	-1.0232315
H	-7.8853861	-4.3173372	-1.1565440	H	1.4984605	-2.0676708	-5.1401792
H	-6.7333684	-3.0391589	-2.9713902	H	1.4958901	2.5918077	-4.6415182
C	2.3316306	-2.6707951	2.4448360	H	-3.1585089	3.0226177	-2.1909714
C	0.9567776	-2.4116635	2.7231481	H	-0.1379042	1.3114470	-7.8856881
C	3.2951302	-1.7699034	2.9328087	H	-1.1552310	-3.1172488	-3.9427375
C	0.5869528	-1.2743466	3.4901560	H	-4.2475201	0.1348612	-2.2129884
C	1.5947749	-0.4116925	3.9597391	H	0.3588921	-0.2851338	-5.8990383
C	2.9552294	-0.6364982	3.6917006	H	0.4866022	4.4903924	-1.8571839
H	4.3611734	-1.9630298	2.7256837	H	0.9948300	2.8597271	-2.4793645
C	-0.8656147	-0.9882259	3.8638423	H	2.6927863	5.7493267	-0.3965808
H	1.2981597	0.4613276	4.5609077	C	1.8892528	10.9339689	3.7395679
C	-1.3180258	0.4077478	3.4117662	C	1.9405706	9.6489693	3.1893641
H	-0.7621141	1.2171270	3.9285530	C	2.0722155	8.5235835	4.0329691
H	-2.3945564	0.5648442	3.6268577	C	2.1453304	8.7020615	5.4308696
H	-1.1774511	0.5529690	2.3254929	C	2.1095516	9.9918030	5.9801944
C	-1.0942510	-1.1950065	5.3730798	C	1.9819982	11.1065493	5.1342031
H	-1.5007621	-1.7301108	3.3382426	H	1.7799467	11.8121170	3.0847612
H	-0.4956041	-0.4779543	5.9731402	H	1.8788876	9.4802504	2.1034067
H	-0.8120212	-2.2189536	5.6919486	C	2.1708295	7.1590994	3.4513645
H	-2.1619755	-1.0346544	5.6294797	H	2.2421526	7.8206438	6.0862024
C	4.0567449	0.2426367	4.2726444	H	2.1824180	10.1328144	7.0694978
C	3.7028931	1.7361452	4.3196169	H	1.9540894	12.1200958	5.5641317
H	4.5709873	2.3296204	4.6731087	O	2.2533639	6.9108076	2.2573661
H	2.8658618	1.9392771	5.0195500	H	2.1797117	6.3287888	4.2212146
H	3.4067512	2.1155859	3.3200017				
C	4.4598426	-0.2822883	5.6660542				
H	4.9412456	0.1287509	3.6065324				
H	5.3030072	0.3019442	6.0902110				
H	4.7666976	-1.3465231	5.6183146				
H	3.6051458	-0.2149392	6.3713380				
C	2.8070280	-3.9057123	1.6759555				
C	3.7195395	-3.5731773	0.4865341				
H	4.0776454	-4.4993223	-0.0074370				
H	4.6179882	-2.9908277	0.7771197				
H	3.1663479	-3.0005141	-0.2818235				
C	3.4869809	-4.9043591	2.6328115				
H	1.9151351	-4.4084163	1.2540577				
H	3.7657858	-5.8356538	2.0975923				
H	2.8204901	-5.1788303	3.4754493				
H	4.4122059	-4.4751720	3.0709916				
H	-0.6693559	3.3729767	-5.6424360				
H	-0.5057312	-2.4536327	-6.8855477				
H	-5.9746364	1.7049712	-3.0573997				
C	-0.2355514	2.4066487	-5.9829319				
H	1.1910626	-3.6974236	-4.4799653				
H	1.7444385	3.3067528	-6.2682886				
H	-4.4384497	2.3717849	-1.1302680				
C	-0.9237977	1.3097709	-5.1804499				
C	-1.0006845	-3.0333301	-6.0783862				
C	1.2791396	2.4611502	-5.7212036				
H	1.7859537	1.5320577	-6.0551454				
C	-0.4951560	-0.0282541	-5.2523044				
C	-5.0831307	1.4639067	-3.6725191				

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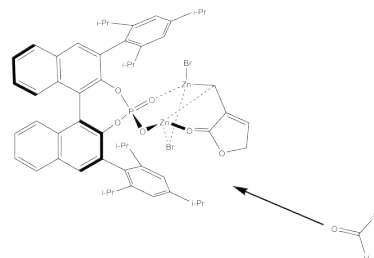


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Zn	2.1908047	0.1464833	1.2692725
Br	3.5824235	1.4883476	0.0605297
H	-0.0898621	4.1342966	4.1079242
Br	-3.5965980	2.0962936	1.0178020
H	-2.0699514	-0.4454843	3.6040648
Zn	-1.9899490	0.4188282	1.2407193
C	-1.1397997	2.2130724	4.2086829
C	-0.0548489	3.1455264	4.6173676
C	-0.5972935	1.1020527	3.6150914
C	-1.1955433	-0.0979458	3.0208661
C	0.8565793	1.3455872	3.6061841
O	1.1698692	2.4979545	4.2103635
O	1.7693817	0.6322378	3.1316543
H	0.0003591	3.3326425	5.7123609
H	-0.4647622	-0.9237277	2.9362638

H	-2.2082281	2.4233949	4.3508537	H	4.4045188	-5.3156581	2.7523226
C	-0.2921914	-4.1294403	0.0478346	H	2.8453849	-6.0394141	3.2658302
C	-0.1920790	-4.6704766	-1.2377688	H	3.6707813	-4.8584230	4.3242790
C	0.4381516	-5.9628346	-1.3792883	H	0.7319611	4.3282323	-3.9676454
C	0.7300982	-6.5525276	-2.6463349	H	3.6747513	-0.4984217	-5.7638874
C	0.8192705	-6.6873000	-0.1896531	H	-4.2003908	0.4632402	-4.7937527
C	1.3943178	-7.9879785	-0.3151362	C	1.5962458	3.6528682	-4.1525455
C	0.6571598	-6.0795001	1.0868856	H	4.1983934	-2.1497856	-3.0754135
H	0.9698767	-6.6360735	1.9836235	H	2.9574080	5.0064726	-3.0927423
C	0.1559636	-4.7905431	1.2304551	H	-3.9536490	1.1781356	-2.3122864
C	-0.4789092	-1.8170658	-3.7946971	C	1.0637586	2.2281436	-4.0691591
C	-1.2500566	-2.4176013	-4.7826897	C	3.0944081	-1.4178469	-5.5395252
H	-1.4390966	-1.8746336	-5.7205836	C	2.6512520	3.9400230	-3.0700247
C	-1.8462512	-3.6981198	-4.5978713	H	3.5649616	3.3282683	-3.2216214
C	-2.7325671	-4.2454371	-5.5737753	C	1.9262998	1.1197609	-4.1318270
C	-1.5798966	-4.4442884	-3.3911208	C	-3.1138531	0.6221766	-4.9555688
C	-2.2614806	-5.6832431	-3.1964446	H	1.3594009	3.7991194	-6.3353595
C	-0.6686448	-3.8935224	-2.4171955	C	-0.3107035	1.9817244	-3.9236952
C	-0.2196384	-2.5833619	-2.6188456	C	2.1353527	3.9654305	-5.5607882
O	-0.9061989	-2.8872842	0.2078403	H	2.4733870	5.0203113	-5.6316304
O	0.5869599	-1.9827856	-1.6513555	H	-0.9944536	2.8428663	-3.8569224
P	-0.0890874	-1.5379781	-0.2324598	C	3.5269381	-1.2670516	-3.0332977
O	1.1028511	-1.3240258	0.7192347	H	3.7882486	-2.2807846	-5.6165345
O	-1.1299808	-0.4230118	-0.3732743	H	2.3208871	-1.5264550	-6.3269910
C	1.6254316	-8.5477365	-1.5622591	C	1.4536191	-0.2013274	-4.0510622
C	1.3065098	-7.8123881	-2.7351602	C	-2.9162693	1.4631276	-2.5802884
H	1.6639883	-8.5331022	0.6031715	C	-0.8393535	0.6800306	-3.8324152
H	2.0708729	-9.5506785	-1.6460876	H	-2.7703217	-0.1125081	-5.7103895
H	0.4988728	-5.9952836	-3.5640548	H	-2.9800828	1.6347361	-5.3910706
H	1.5216699	-8.2425144	-3.7251500	C	2.4583395	-1.3491574	-4.1383080
C	-3.1339991	-6.1779689	-4.1563829	C	0.0551077	-0.4237150	-3.9104292
C	-3.3634563	-5.4621984	-5.3620993	C	-2.3426911	0.4968898	-3.6277123
H	-2.0997533	-6.2423902	-2.2641111	H	3.0611524	-1.2306935	-2.0295310
H	-3.6572111	-7.1298007	-3.9780167	H	-2.3210715	1.4510166	-1.6493077
H	-4.0536580	-5.8667407	-6.1179447	H	4.1592027	-0.3613684	-3.1395113
H	-2.9208204	-3.6686158	-6.4928411	H	2.2675249	3.7073554	-2.0564625
C	1.3159506	-3.7417391	3.2171547	H	-2.9527493	2.5091552	-2.9496416
C	0.1059385	-4.1188539	2.5661553	H	3.0019497	3.3167248	-5.8082674
C	1.2447040	-3.2125365	4.5219885	H	1.9051826	-2.2992725	-3.9910204
C	-1.1445856	-3.8976066	3.2053529	H	-2.4977410	-0.5307250	-3.2387964
C	-1.1559383	-3.3633197	4.5029787	H	3.0098147	1.2877840	-4.2378967
C	0.0237987	-3.0424688	5.1948217	C	-1.7681143	14.4838539	-1.0115087
H	2.1771918	-2.9428301	5.0452137	C	-1.3195039	13.5766805	-0.0458693
C	-2.4765251	-4.2749261	2.5610824	C	0.0077796	13.6544747	0.4320330
H	-2.1259892	-3.2149419	5.0032220	C	0.8777918	14.6471097	-0.0659348
C	-3.3780622	-3.0451101	2.3506992	C	0.4265497	15.5562509	-1.0337459
H	-3.6495221	-2.5667340	3.3148591	C	-0.8953278	15.4736663	-1.5053522
H	-4.3208605	-3.3305860	1.8410149	H	-2.8014757	14.4259934	-1.3865539
H	-2.8671218	-2.2871621	1.7242162	H	-1.9752573	12.7913714	0.3608849
C	-3.1908707	-5.3688501	3.3765878	C	0.4872340	12.6938340	1.4569080
H	-2.2649882	-4.7036117	1.5609471	H	1.9120996	14.7004171	0.3122900
H	-3.4607294	-5.0077888	4.3910394	H	1.1036951	16.3315498	-1.4234746
H	-2.5436791	-6.2608369	3.5005102	H	-1.2506855	16.1867056	-2.2654930
H	-4.1274163	-5.6878446	2.8748154	O	-0.1905943	11.8039145	1.9499902
C	-0.0421268	-2.5598711	6.6379800	H	1.5653999	12.8441735	1.7658494
C	-0.6990021	-1.1718530	6.7412206				
H	-0.7228776	-0.8196697	7.7932839				
H	-1.7446793	-1.1949976	6.3690081				
H	-0.1509695	-0.4223829	6.1356367				
C	-0.7587103	-3.5945932	7.5274665				
H	1.0041619	-2.4676433	7.0037784				
H	-0.7774650	-3.2696476	8.5879821				
H	-0.2574448	-4.5825193	7.4767346				
H	-1.8114138	-3.7409565	7.2067837				
C	2.6891136	-3.9536711	2.5741145				
C	3.5627842	-2.6873862	2.5451966				
H	4.5550797	-2.9093603	2.1028509				
H	3.7287561	-2.2507959	3.5503913				
H	3.0933124	-1.9135253	1.9035790				
C	3.4436921	-5.1064579	3.2664385				
H	2.5237839	-4.2488561	1.5185472				

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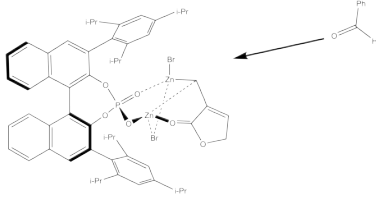


Energy (Hartree)= -11969.97104871
number of imaginary frequencies: 4

Zn 2.1897554 0.1481269 1.2549525

Br	3.5850161	1.4903174	0.0658133	H	-1.7445469	-1.1941452	6.3681020
H	-0.0895502	4.1343736	4.1073324	H	-0.1509307	-0.4239638	6.1332149
Br	-3.5939672	2.0898452	1.0152987	C	-0.7591445	-3.5953780	7.5274403
H	-2.0713685	-0.4448482	3.5979089	H	1.0030838	-2.4679550	7.0050407
Zn	-1.9925785	0.4308305	1.2441101	H	-0.7795754	-3.2717621	8.5882574
C	-1.1414514	2.2120658	4.2087957	H	-0.2574031	-4.5827547	7.4759979
C	-0.0543174	3.1446940	4.6161681	H	-1.8112255	-3.7438160	7.2061423
C	-0.5976922	1.1004356	3.6172623	C	2.6892138	-3.9532295	2.5743995
C	-1.1918841	-0.0981813	3.0219814	C	3.5637164	-2.6875379	2.5444250
C	0.8581459	1.3443024	3.6062480	H	4.5558719	-2.9103739	2.1021484
O	1.1699962	2.4990518	4.2112170	H	3.7309259	-2.2500296	3.5490499
O	1.7667820	0.6320655	3.1288419	H	3.0946320	-1.9142996	1.9025412
H	0.0011747	3.3329229	5.7116223	C	3.4434246	-5.1063162	3.2659854
H	-0.4615819	-0.9238398	2.9356468	H	2.5228260	-4.2480666	1.5188934
H	-2.2107931	2.4220497	4.3440344	H	4.4044326	-5.3159013	2.7524485
C	-0.2926936	-4.1294866	0.0482951	H	2.8452319	-6.0391173	3.2650561
C	-0.1924717	-4.6706372	-1.2373631	H	3.6700611	-4.8599706	4.3242151
C	0.4381075	-5.9628425	-1.3786454	H	0.7318694	4.3275665	-3.9676292
C	0.7300251	-6.5522937	-2.6455827	H	3.6744551	-0.4987398	-5.7645509
C	0.8192124	-6.6876076	-0.1893817	H	-4.2003062	0.4633423	-4.7935726
C	1.3939007	-7.9878337	-0.3157524	C	1.5963013	3.6522752	-4.1527764
C	0.6571097	-6.0796403	1.0867994	H	4.1986977	-2.1496437	-3.0750750
H	0.9695602	-6.6352934	1.9842050	H	2.9575894	5.0060027	-3.0926318
C	0.1562726	-4.7908041	1.2307043	H	-3.9534348	1.1788505	-2.3110970
C	-0.4783108	-1.8167182	-3.7939140	C	1.0634714	2.2276574	-4.0697901
C	-1.2491607	-2.4181618	-4.7814757	C	3.0943891	-1.4180487	-5.5396485
H	-1.4377625	-1.8736958	-5.7185719	C	2.6509180	3.9397322	-3.0701548
C	-1.8458756	-3.6982144	-4.5974264	H	3.5650534	3.3286039	-3.2211332
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C	-1.5796745	-4.4445580	-3.3909903	C	-3.1138206	0.6220865	-4.9552283
C	-2.2613681	-5.6833055	-3.1969435	H	1.3597866	3.7986232	-6.3357021
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C	-0.2200823	-2.5831780	-2.6178686	C	2.1350570	3.9654958	-5.5608630
O	-0.9069768	-2.8888013	0.2099006	H	2.4735775	5.0201901	-5.6319344
O	0.5849621	-1.9825687	-1.6489536	H	-0.9943924	2.8418028	-3.8559540
P	-0.0911465	-1.5383297	-0.2301542	C	3.5269496	-1.2671889	-3.0336171
O	1.1005602	-1.3277138	0.7240915	H	3.7886623	-2.2805730	-5.6171316
O	-1.1310051	-0.4226411	-0.3655560	H	2.3211969	-1.5258678	-6.3272716
C	1.6249757	-8.5472656	-1.5624260	C	1.4536726	-0.2013497	-4.0513951
C	1.3061020	-7.8118158	-2.7345690	C	-2.9162852	1.4627798	-2.5801383
H	1.6637119	-8.5330837	0.6024466	C	-0.8393938	0.6798707	-3.8329196
H	2.0704508	-9.5501390	-1.6462962	H	-2.7706343	-0.1119066	-5.7108852
H	0.4979883	-5.9941086	-3.5624162	H	-2.9800974	1.6342971	-5.3911633
H	1.5212651	-8.2415310	-3.7246806	C	2.4584493	-1.3491103	-4.1385374
C	-3.1335947	-6.1776300	-4.1567908	C	0.0553850	-0.4234349	-3.9104742
C	-3.3630047	-5.4618936	-5.3618291	C	-2.3426461	0.4968319	-3.6274997
H	-2.0990635	-6.2420746	-2.2645739	H	3.0620406	-1.2305891	-2.0296000
H	-3.6570289	-7.1293062	-3.9784518	H	-2.3213992	1.4519864	-1.6492370
H	-4.0533931	-5.8658482	-6.1177696	H	4.1596419	-0.3618167	-3.1385863
H	-2.9205497	-3.6682575	-6.4914303	H	2.2680564	3.7072228	-2.0564475
C	1.3160480	-3.7412805	3.2176292	H	-2.9529694	2.5090510	-2.9483355
C	0.1064076	-4.1190941	2.5665096	H	3.0014101	3.3169256	-5.8089857
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C	-1.1439759	-3.8977407	3.2055856	H	-2.4980948	-0.5307743	-3.2386118
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C	0.0239714	-3.0426777	5.1951144	C	-1.7673678	14.4843546	-1.0114625
H	2.1768171	-2.9416964	5.0453679	C	-1.3187899	13.5773356	-0.0460254
C	-2.4760789	-4.2745632	2.5613919	C	0.0078052	13.6550923	0.4316094
H	-2.1252929	-3.2160437	5.0032712	C	0.8765156	14.6473562	-0.0665540
C	-3.3774441	-3.0448726	2.3507008	C	0.4258539	15.5565047	-1.0341087
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H	-4.3201905	-3.3293341	1.8407385	H	-2.8007388	14.4264113	-1.3865566
H	-2.8672762	-2.2877649	1.7231132	H	-1.9715254	12.7906693	0.3629734
C	-3.1903501	-5.3684827	3.3766277	C	0.4854387	12.6917354	1.4580713
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H	-2.5434144	-6.2603251	3.5009240	H	-1.2507843	16.1869588	-2.2656762
H	-4.1271765	-5.6874361	2.8755245	O	-0.1921241	11.8045081	1.9491814
C	-0.0430233	-2.5602836	6.6383227	H	1.5657788	12.8433212	1.7667093
C	-0.6989906	-1.1719180	6.7405042				
H	-0.7233702	-0.8172812	7.7917010				

TS-7-j-mi; COSMO



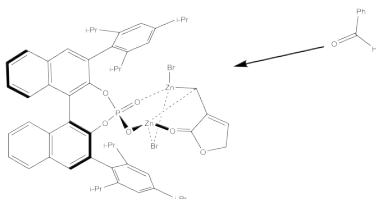
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C	0.5198142	3.3807097	2.9262610
C	0.1259189	2.5194123	4.0579421
O	-0.4788180	3.2314200	5.0228803
C	-0.4845207	4.6170814	4.6236136
O	0.3250495	1.3024947	4.1567611
C	1.1255344	2.8731427	1.6461500
H	0.0579426	5.2033365	5.3973169
H	-1.5376058	4.9755944	4.5996122
Zn	1.6453581	1.6232781	-0.0711036
Br	1.4805237	3.0294201	-1.9047473
H	2.0008617	3.5195395	1.4190150
H	0.3602203	3.1350424	0.8750107
H	0.2886204	5.5589401	2.6847207
C	-1.0499053	-2.8220776	0.2315408
C	-0.5781233	-4.1162386	-0.0252689
C	-1.3560551	-5.2179730	0.4925214
C	-0.8866492	-6.5658905	0.4841820
C	-2.6497356	-4.9498270	1.0761414
C	-3.4421927	-6.0408368	1.5454372
C	-3.0903275	-3.6040874	1.2338275
H	-4.0683537	-3.4171459	1.7034424
C	-2.2855778	-2.5252013	0.8848687
C	3.0309173	-3.5899692	-1.2666094
C	3.1201897	-4.5459324	-2.2711047
H	4.0526729	-4.6305680	-2.8507182
C	2.0038306	-5.3507506	-2.6421291
C	2.0914373	-6.2565125	-3.7419197
C	0.7375738	-5.1764300	-1.9681827
C	-0.4025747	-5.8476226	-2.5038201
C	0.6752700	-4.3083553	-0.8114155
C	1.8217966	-3.5706321	-0.4997633
O	-0.3097115	-1.7217396	-0.1982889
O	1.8173603	-2.7593029	0.6389832
P	1.0580649	-1.3228044	0.6036100
O	0.8437889	-0.8777652	2.0561985
O	1.7526010	-0.2830204	-0.3033995
C	-2.9695725	-7.3432516	1.4884230
C	-1.6723464	-7.6018760	0.9705599
H	-4.4322143	-5.8226646	1.9758745
H	-3.5876924	-8.1737590	1.8620245
H	0.1182608	-6.7785454	0.0940179
H	-1.2827737	-8.6312551	0.9598735
C	-0.2889951	-6.7038194	-3.5913302
C	0.9713948	-6.9312262	-4.2038858
H	-1.3881996	-5.6762910	-2.0512027
H	-1.1870562	-7.2046456	-3.9840561
H	1.0522816	-7.6211487	-5.0576469
H	3.0677620	-6.3893495	-4.2340725
C	-2.6234417	-0.7493472	2.6415507
C	-2.5945430	-1.1095388	1.2602846
C	-2.8191133	0.6021375	2.9798015
C	-2.7636235	-0.1073490	0.2637007
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C	-2.9875259	1.6092400	2.0135024
H	-2.8297387	0.8846990	4.0455591
C	-2.8063838	-0.4316258	-1.2290447
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C	-1.8100985	0.4115254	-2.0438890
H	-2.0701203	1.4902670	-2.0372778
H	-1.7959926	0.0849117	-3.1038354
H	-0.7795676	0.3109083	-1.6526240
C	-4.2418286	-0.2862115	-1.7707656
H	-2.5230981	-1.4955855	-1.3565050
H	-4.6006094	0.7610142	-1.6856676
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C	-3.2640602	3.0429745	2.4549064
C	-2.8445516	4.1078311	1.4328004
H	-2.9414839	5.1254863	1.8629912
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C	-4.7491641	3.2062622	2.8374580
H	-2.6714290	3.2023288	3.3837729
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C	-1.2947902	-1.4324840	4.7188141
H	-1.2021965	-2.2171427	5.4981763
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H	-0.3411207	-1.3779414	4.1613294
C	-3.7827477	-1.9338145	4.5452633
H	-2.2214102	-2.7459131	3.3166191
H	-3.6858038	-2.7186285	5.3238245
H	-4.6176272	-2.2183000	3.8720415
H	-4.0752020	-0.9910286	5.0537277
H	6.4154433	1.6981120	-1.2692919
H	6.9170453	-3.3450383	1.4143553
H	3.8056122	-1.5136355	-5.5991091
C	5.9812919	1.3424642	-0.3079942
H	4.3717286	-3.7508343	3.3279753
H	5.2616833	3.3468075	0.2736353
H	1.6370343	-0.7522853	-4.5152674
C	5.3799125	-0.0318354	-0.5817769
C	6.1080307	-4.0595158	1.1542175
C	4.8607136	2.3297358	0.0801357
H	4.3545946	1.9890283	1.0095768
C	5.3288774	-1.0472370	0.3891686
C	4.3258195	-1.3385687	-4.6348186
H	7.8979699	0.6133735	0.4858808
C	4.7796310	-0.2837255	-1.8266876
C	7.1004730	1.3399971	0.7416361
H	7.5618719	2.3454907	0.8180640
H	4.8214779	0.5024204	-2.5985291
C	4.3991880	-2.8904537	2.6280428
H	6.1561820	-4.9041327	1.8729189
H	6.3235524	-4.4552739	0.1407844
C	4.6664711	-2.2652066	0.1552237
C	2.1346890	-0.6613537	-3.5272885
C	4.0777907	-1.4699629	-2.1057500
H	5.2045002	-2.0142192	-4.5894415
H	4.7056653	-0.2958828	-4.6529428
C	4.7293304	-3.3710807	1.2066734
C	3.9989033	-2.4646839	-1.0845870
C	3.3666491	-1.5829877	-3.4567020
H	3.4169733	-2.3819459	2.6683868
H	1.3974941	-0.9180999	-2.7425967
H	5.1545644	-2.1759076	3.0138048
H	4.1177286	2.4273075	-0.7394717
H	2.4057956	0.4042062	-3.3773202
H	6.7100814	1.0844313	1.7484296
H	3.9762358	-4.1381653	0.9303767
H	2.9925739	-2.6188215	-3.5639171
H	5.8105285	-0.8878393	1.3639091
C	-4.4312286	8.9780955	-5.5618374
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H	-5.3704264	10.1759169	-7.1183193
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TS-7-j-mi



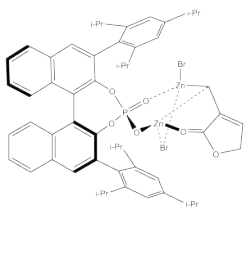
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C	0.5287188	3.3816340	2.9263911
C	0.1326682	2.5193035	4.0595623
O	-0.4691423	3.2347379	5.0268781
C	-0.4696616	4.6185560	4.6285866
O	0.3287317	1.3047922	4.1568660
C	1.1320568	2.8715929	1.6467541
H	0.0760705	5.2022195	5.4025978
H	-1.5218614	4.9807395	4.6063609
Zn	1.6563300	1.6229978	-0.0712213
Br	1.4959130	3.0334806	-1.8996564
H	2.0063582	3.5184901	1.4174297
H	0.3653586	3.1315588	0.8762423
H	0.3006725	5.5604856	2.6883133
C	-1.0507438	-2.8128740	0.2246913
C	-0.5829696	-4.1084063	-0.0325772
C	-1.3653562	-5.2077044	0.4832457
C	-0.9006568	-6.5569788	0.4734581
C	-2.6585358	-4.9359572	1.0658730
C	-3.4544888	-6.0250137	1.5327298
C	-3.0943936	-3.5889822	1.2244353
H	-4.0719264	-3.3988980	1.6937929
C	-2.2860064	-2.5125146	0.8771981
C	3.0298531	-3.5917756	-1.2661160
C	3.1180364	-4.5473565	-2.2708179
H	4.0516670	-4.6340525	-2.8482423
C	2.0004958	-5.3488726	-2.6449865
C	2.0871897	-6.2543605	-3.7446013
C	0.7334078	-5.1714311	-1.9737424
C	-0.4071894	-5.8393424	-2.5119088
C	0.6710832	-4.3039337	-0.8166929
C	1.8190977	-3.5698295	-0.5020446
O	-0.3068687	-1.7149348	-0.2030679
O	1.8154195	-2.7598016	0.6366489
P	1.0614160	-1.3211354	0.6017299
O	0.8452933	-0.8772162	2.0541227
O	1.7602832	-0.2832588	-0.3038744
C	-2.9864810	-7.3285400	1.4744385
C	-1.6900989	-7.5906846	0.9575447
H	-4.4441115	-5.8041596	1.9626839
H	-3.6077543	-8.1573990	1.8463820
H	0.1037927	-6.7721206	0.0836831

H	-1.3039728	-8.6212986	0.9457610
C	-0.2937643	-6.6952749	-3.5992000
C	0.9667648	-6.9257700	-4.2090888
H	-1.3930884	-5.6654563	-2.0609461
H	-1.1923600	-7.1935498	-3.9938361
H	1.0476126	-7.6155390	-5.0629393
H	3.0640875	-6.3897153	-4.2348879
C	-2.6189627	-0.7374275	2.6354481
C	-2.5904243	-1.0961853	1.2539241
C	-2.8109846	0.6141897	2.9746459
C	-2.7558082	-0.0926719	0.2582368
C	-2.9436216	1.2438309	0.6573242
C	-2.9763643	1.6224506	2.0093134
H	-2.8209251	0.8956904	4.0407502
C	-2.7981103	-0.4153257	-1.2348062
H	-3.0798576	2.0077301	-0.1224185
C	-1.7983420	0.4250600	-2.0484167
H	-2.0544463	1.5046633	-2.0418875
H	-1.7841367	0.0990370	-3.1083927
H	-0.7685160	0.3210442	-1.6567046
C	-4.2328063	-0.2656243	-1.7772735
H	-2.5179669	-1.4800807	-1.3625081
H	-4.5889428	0.7823873	-1.6917015
H	-4.9433834	-0.9077908	-1.2185065
H	-4.2794782	-0.5505345	-2.8487526
C	-3.2515789	3.0561800	2.4520991
C	-2.8300929	4.1222079	1.4317832
H	-2.9267326	5.1397958	1.8624503
H	-3.4703281	4.0993217	0.5261536
H	-1.7810429	3.9875379	1.0993615
C	-4.7368355	3.2209590	2.8334491
H	-2.6593155	3.2135818	3.3818477
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H	-5.0370032	2.4902618	3.6106069
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C	-2.4591873	1.7554998	3.7662599
C	-1.2933159	-1.4272978	4.7131494
H	-1.2039100	-2.2133121	5.4912830
H	-1.4292041	-0.4567690	5.2313309
H	-0.3389227	-1.3756839	4.1569194
C	-3.7830416	-1.9201076	4.5368973
H	-2.2233887	-2.7356674	3.3085406
H	-3.6892961	-2.7059368	5.3147228
H	-4.6184340	-2.2009652	3.8628584
H	-4.0731489	-0.9771601	5.0462149
H	6.4253173	1.6878557	-1.2570718
H	6.9110161	-3.3558522	1.4222660
H	3.8190697	-1.5127093	-5.5953388
C	5.9869586	1.3336186	-0.2970181
H	4.3610930	-3.7611882	3.3308078
H	5.2720980	3.3401074	0.2823957
H	1.6486464	-0.7492297	-4.5156639
C	5.3832498	-0.0392456	-0.5728137
C	6.1016554	-4.0688902	1.1598453
C	4.8681582	2.3244074	0.0876225
H	4.3587897	1.9854365	1.0160049
C	5.3281514	-1.0551234	0.3970732
C	4.3370711	-1.3398701	-4.6294831
H	7.8990564	0.5993093	0.5027261
C	4.7859095	-0.2891698	-1.8191975
H	7.1028353	1.3280909	0.7560173
C	7.5668683	2.3322177	0.8340851
H	4.8308381	0.4976198	-2.5901359
C	4.3911618	-2.8998668	2.6322860
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C	4.6647014	-2.2717340	0.1604645
C	2.1442764	-0.6600773	-3.5266044
C	4.0829737	-1.4736880	-2.1013060
H	5.2146042	-2.0167866	-4.5826926
H	4.7188544	-0.2980005	-4.6455968

C	4.7237642	-3.3788126	1.2108275
C	3.9999691	-2.4689218	-1.0811380
C	3.3746227	-1.5838409	-3.4539920
H	3.4096296	-2.3904361	2.6718333
H	1.4048081	-0.9167141	-2.7441412
H	5.1463062	-2.1869317	3.0211570
H	4.1279381	2.4247270	-0.7342029
H	2.4161367	0.4050148	-3.3750787
H	6.7083983	1.0738826	1.7614631
H	3.9702814	-4.1446360	0.9317627
H	2.9990646	-2.6189700	-3.5634139
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C	-4.4563043	8.9357109	-5.5477812
C	-4.2848656	8.7563937	-4.1714921
C	-4.9289499	9.6240099	-3.2621243
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C	-5.9156639	10.8469323	-5.1245414
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H	-3.6553770	7.9508625	-3.7628311
C	-4.7468672	9.4336184	-1.7998949
H	-6.2422570	11.3412700	-3.0269824
H	-6.5516845	11.6616623	-5.5028550
H	-5.4052492	10.1197329	-7.1084672
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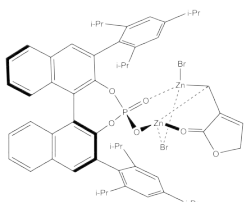
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Br	3.3754983	6.4565637	85.3437330
H	0.4921927	5.6702632	86.3278227
Zn	2.5365100	5.5375220	87.3064756
C	-0.7838920	8.2094138	86.7119130
C	-1.4022279	9.2995426	87.5251284
C	-0.3908756	7.2010021	87.5399938
C	0.2416235	5.8789125	87.3878207
C	-0.6918875	7.6710984	88.9047679
O	-1.3199779	8.8474417	88.9013785
O	-0.3753094	7.0902647	89.9667455
H	-2.4723538	9.4768168	87.2800123
H	-0.4869492	5.0783752	87.6627548
H	-0.6993490	8.2459956	85.6175260
C	0.1030894	0.9319734	89.2187463
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C	0.2899206	-1.0203013	90.6594430
C	1.0277605	-2.0609928	91.3001571
C	-1.0748286	-0.7957821	91.0745854
C	-1.6594264	-1.6617612	92.0476342
C	-1.7994457	0.3137116	90.5521992
H	-2.8322443	0.4782101	90.8944727
C	-1.2198494	1.2230807	89.6742611
C	4.4151058	0.5859198	88.3896255
C	4.8194623	-0.6635185	87.9340366
H	5.8168812	-0.7729398	87.4815992
C	3.9468234	-1.7896079	87.9517798

C	4.3557652	-3.0412274	87.3998469
C	2.6011783	-1.6464544	88.4578858
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C	2.2137040	-0.3920327	89.0607489
C	3.1317763	0.6629854	89.0116857
O	0.6478813	1.8040089	88.2767527
O	2.7960320	1.8782936	89.6090138
P	1.7577479	2.8753063	88.8385270
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O	2.3467926	3.5551085	87.5975645
C	-0.9235463	-2.6851560	92.6256174
C	0.4363807	-2.8721055	92.2591105
H	-2.7054629	-1.4870261	92.3448658
H	-1.3839681	-3.3406923	93.3804434
H	2.0828283	-2.2115749	91.0325411
H	1.0289763	-3.6633924	92.7430914
C	2.1288845	-3.9454837	87.7445178
C	3.4704107	-4.1043843	87.3057841
H	0.6608193	-2.6392389	88.6268512
H	1.4157100	-4.7769030	87.6358123
H	3.7977450	-5.0621333	86.8733197
H	5.3885775	-3.1380648	87.0298395
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C	-2.2894511	2.7015497	87.9103542
C	-2.9431114	3.9005423	87.5595915
C	-3.2153873	4.9077163	88.4986684
H	-2.9756707	5.4823333	90.5696482
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H	-3.2500429	4.0395791	86.5127289
C	-1.2108636	2.2150921	85.6617793
H	-1.7377766	3.0316633	85.1250669
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H	-0.2438170	2.6089607	86.0310147
C	-3.3952322	1.0789807	86.3178925
H	-1.4930748	0.8161325	87.2669971
H	-4.0219971	1.8607198	85.8397701
H	-3.9814855	0.6406331	87.1509458
H	-3.2191353	0.2832353	85.5648490
C	-3.9905875	6.1768486	88.1547111
C	-4.0197231	6.5140104	86.6588946
H	-4.4972675	7.5015394	86.4946313
H	-4.6104739	5.7701980	86.0849594
H	-3.0011811	6.5464124	86.2226790
C	-5.4238394	6.0914654	88.7196848
H	-3.4831224	7.0153137	88.6847391
H	-5.9804206	7.0338074	88.5361370
H	-5.4203096	5.9010890	89.8114010
H	-5.9816103	5.2627896	88.2353757
C	-1.7796897	3.3550097	91.7103572
C	-1.0140134	4.5583496	92.2861624
H	-0.7737294	4.3808826	93.3542458
H	-1.5947103	5.5013108	92.2295925
H	-0.0552896	4.7059734	91.7543592
C	-3.0438955	3.0734756	92.5477766
H	-1.1099820	2.4767115	91.7999617
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H	-3.6011305	2.1920548	92.1719167
H	-3.7378053	3.9398040	92.5191388
H	7.2426608	5.6832505	86.1048870
H	7.8648985	2.5286360	91.0554224
H	5.1993064	0.2968750	83.9213702
C	7.2900068	5.5585518	87.2088514
H	5.0709233	2.7532584	92.5939445
H	7.1661672	7.7179697	87.5660338
H	3.2100590	1.8843382	83.9398054
C	6.5397846	4.2728152	87.5347364
C	7.1542449	1.6757661	91.0723439
C	6.6182705	6.7913457	87.8366697
H	6.5988589	6.7214719	88.9444516

C	6.4451912	3.7900704	88.8525051	H	-0.5985276	8.2897228	85.6483027
C	5.6676697	0.8747919	84.7452225	C	0.1060916	0.9265844	89.2373990
H	9.2641115	4.5870524	87.1313372	C	0.8618419	-0.1722056	89.6661765
C	5.9244731	3.5246393	86.5184365	C	0.2876197	-1.0276264	90.6758287
C	8.7742618	5.4617130	87.6055083	C	1.0236054	-2.0696391	91.3158603
H	9.3246253	6.3748520	87.2972817	C	-1.0779722	-0.8037310	91.0877100
H	5.9687467	3.9078516	85.4868553	C	-1.6635936	-1.6705898	92.0586828
C	5.1439761	3.1598263	91.5639126	C	-1.8015067	0.3046137	90.5619888
H	7.1266302	1.2797380	92.1089139	H	-2.8359943	0.4688109	90.8993063
H	7.5647174	0.8847900	90.4120309	C	-1.2199940	1.2142776	89.6859299
C	5.7787344	2.5920004	89.1643005	C	4.4108122	0.5885157	88.4041183
C	3.7087882	2.4865141	84.7274870	C	4.8145289	-0.6580544	87.9407292
C	5.2420466	2.3201265	86.7726127	H	5.8083713	-0.7608229	87.4789224
H	6.2799987	0.1752905	85.3496026	C	3.9450912	-1.7863452	87.9586047
H	6.3600746	1.6140322	84.2903519	C	4.3515595	-3.0337110	87.3965710
C	5.7498237	2.1121113	90.6136637	C	2.6019488	-1.6479540	88.4721919
C	5.1848762	1.8403945	88.1139888	C	1.7064520	-2.7485191	88.3152968
C	4.5962877	1.5805344	85.5988931	C	2.2158242	-0.3972059	89.0830098
H	4.1289982	3.4575732	91.2362690	C	3.1323846	0.6590533	89.0372939
H	2.9295359	2.9806484	85.3374017	O	0.6546585	1.8023795	88.3018595
H	5.7664087	4.0774398	91.6128137	O	2.7966678	1.8692533	89.6437957
H	5.5731814	6.8932752	87.4838458	P	1.7618600	2.8712877	88.8766665
H	4.2896180	3.2825881	84.2185254	O	1.1644040	3.7702198	89.9803358
H	8.8918226	5.3576432	88.7047070	O	2.3581670	3.5519908	87.6382229
H	5.1019984	1.2124692	90.6578832	C	-0.9296062	-2.6948970	92.6362778
H	3.9346709	0.7958267	86.0174692	C	0.4301780	-2.8822501	92.2715664
H	6.9094607	4.3650428	89.6695590	H	-2.7100249	-1.4957966	92.3545140
C	10.3276257	32.6993901	82.7746847	H	-1.3916911	-3.3511272	93.3894193
C	10.0704569	31.6003769	83.6010708	H	2.0787532	-2.2191798	91.0483207
C	10.7930457	31.4388425	84.8044529	H	1.0215378	-3.6749714	92.7545983
C	11.7731047	32.3857185	85.1690356	C	2.1284342	-3.9421890	87.7462040
C	12.0300571	33.4869085	84.3395350	C	3.4670855	-4.0966548	87.2992529
C	11.3069950	33.6427746	83.1439283	H	0.6641598	-2.6430895	88.6453553
H	9.7663299	32.8289928	81.8365926	H	1.4153096	-4.7733326	87.6354993
H	9.3121491	30.8454029	83.3418024	H	3.7928769	-5.0506503	86.8575533
C	10.5221585	30.2763238	85.6867375	H	5.3823923	-3.1268381	87.0201796
H	12.3323650	32.2514488	86.1097224	C	-2.1552984	3.5032945	90.2289960
H	12.7942120	34.2267528	84.6226194	C	-1.9049340	2.4789216	89.2650596
H	11.5072304	34.5074619	82.4922350	C	-2.7938952	4.6834910	89.8079511
O	9.6936510	29.4065971	85.4600138	C	-2.2795149	2.6825320	87.9091086
H	11.1581165	30.2461024	86.6222856	C	-2.9292152	3.8799263	87.5474749
				C	-3.2068689	4.8921719	88.4791822
				H	-2.9829110	5.4770025	90.5489137
				C	-2.0396173	1.6329616	86.8257882
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				C	-1.1869408	2.1857230	85.6691553
				H	-1.7139178	2.9948289	85.1212401
				H	-0.9595872	1.3849715	84.9358162
				H	-0.2245815	2.5879553	86.0412454
				C	-3.3712082	1.0457501	86.3216193
				H	-1.4731595	0.7967422	87.2815185
				H	-3.9991611	1.8210663	85.8348108
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				H	-3.1889948	0.2452761	85.5751171
				C	-3.9769736	6.1607064	88.1217073
				C	-3.9680661	6.5048652	86.6270031
				H	-4.4457488	7.4909759	86.4535864
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				H	-2.9383098	6.5424285	86.2184636
				C	-5.4235980	6.0685484	88.6496513
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				C	-1.7999427	3.3520357	91.7096347
				C	-1.0373792	4.5559630	92.2879086
				H	-0.8120139	4.3840840	93.3601228
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				H	-0.0716587	4.6951543	91.7675350
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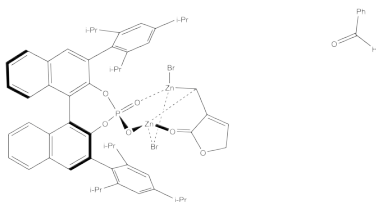


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Br	3.4140169	6.4600709	85.3875316
H	0.6111699	5.7150484	86.3743105
Zn	2.6703138	5.5110901	87.3621175
C	-0.7226595	8.2377497	86.7382302
C	-1.3648341	9.3171323	87.5510628
C	-0.3633089	7.2124853	87.5607875
C	0.2693732	5.8930063	87.4133123
C	-0.6986330	7.6660468	88.9271457
O	-1.3285399	8.8456213	88.9198959
O	-0.4013463	7.0767986	89.9852732
H	-2.4265607	9.5006345	87.2731981
H	-0.4771158	5.0889316	87.6202160

H	-2.8161286	2.8867808	93.6006493	O	-1.0330006	8.9805318	88.9460884
H	-3.6251402	2.1899844	92.1586496	C	-1.0088235	9.4859640	87.5859129
H	-3.7659693	3.9374025	92.5002966	O	-0.2258322	7.1491395	89.9996357
H	7.1067856	5.7429984	86.0934803	C	0.5148693	6.0117594	87.4173069
H	7.8787850	2.5617937	91.0292301	H	-0.4393976	10.4405628	87.5994362
H	5.1515854	0.3093273	83.9250382	H	-2.0534132	9.7131519	87.2796793
C	7.2276615	5.5847013	87.1874115	Zn	2.7872972	5.5655345	87.4845822
H	5.1051769	2.7515174	92.6027920	Br	3.8329697	6.5296780	85.6476964
H	7.1794787	7.7331899	87.6131620	C	-0.0055315	1.0162752	88.9997167
H	3.1455983	1.8722194	83.9646327	C	0.6678276	-0.1366511	89.4221370
C	6.4837231	4.2984080	87.5256971	C	-0.0074140	-1.0036865	90.3564859
C	7.1779929	1.7010826	91.0517698	C	0.6370044	-2.1074818	90.9920623
C	6.6275288	6.8118175	87.8925120	C	-1.3830017	-0.7266246	90.6968376
H	6.6759639	6.7131168	88.9972094	C	-2.0690077	-1.6014513	91.5927256
C	6.4147953	3.8115706	88.8435175	C	-2.0187333	0.4385693	90.1794450
C	5.6214260	0.8920696	84.7445471	H	-3.0631388	0.6389525	90.4620493
H	9.1706046	4.5785951	86.9431853	C	-1.3410301	1.3534144	89.3808744
C	5.8641619	3.5435399	86.5168237	C	4.3341883	0.4809053	88.4458489
C	8.7333017	5.4455518	87.4785594	C	4.7002966	-0.7630924	87.9443284
H	9.2824223	6.3580241	87.1661178	H	5.7199307	-0.9053862	87.5548936
H	5.8889367	3.9293911	85.4857557	C	3.7689012	-1.8357930	87.8361386
C	5.1567964	3.1599600	91.5722806	C	4.1436332	-3.0734052	87.2308960
H	7.1677575	1.3018885	92.0874128	C	2.4029775	-1.6456248	88.2663136
H	7.5904548	0.9174485	90.3843312	C	1.4603968	-2.6820890	87.9912670
C	5.7677492	2.6050074	89.1628239	C	2.0434975	-0.4056653	88.9132501
C	3.6436886	2.4795538	84.7486274	C	3.0152750	0.5986969	88.9810922
C	5.2021478	2.3293874	86.7778878	O	0.6446183	1.9000108	88.1390725
H	6.2494423	0.1998889	85.3410763	O	2.6980419	1.8000737	89.6154708
H	6.3002023	1.6396694	84.2832405	P	1.7663381	2.8834922	88.8249857
C	5.7631410	2.1222608	90.6116672	O	1.1423276	3.7613207	89.9332155
C	5.1690276	1.8478305	88.1195700	O	2.4757997	3.5835655	87.6607179
C	4.5509676	1.5839649	85.6105663	C	-1.4212903	-2.6838419	92.1689508
H	4.1324404	3.4431628	91.2622373	C	-0.0518434	-2.9254670	91.8772828
H	2.8625477	2.9624898	85.3649606	H	-3.1223004	-1.3866449	91.8323240
H	5.7659433	4.0867399	91.6135735	H	-1.9594680	-3.3451119	92.8651216
H	5.5662638	6.9503442	87.6077571	H	1.6978735	-2.3009872	90.7808046
H	4.2072377	3.2848868	84.2351897	H	0.4701278	-3.7651822	92.3608905
H	8.9206441	5.2980746	88.5629919	C	1.8531431	-3.8661729	87.3817592
H	5.1264343	1.2148846	90.6614539	C	3.2091812	-4.0748628	87.0139798
H	3.9033606	0.7907115	86.0349738	H	0.4051826	-2.5328564	88.2578429
H	6.8852066	4.3900850	89.6544545	H	1.1040708	-4.6458525	87.1751415
C	10.3369953	32.7119044	82.7760597	H	3.5103696	-5.0206124	86.5382640
C	10.0779166	31.6156763	83.6049890	H	5.1908553	-3.2072088	86.9172398
C	10.8003722	31.4549312	84.8076010	C	-2.1976422	3.6649176	89.9637029
C	11.7810802	32.4007638	85.1694147	C	-1.9366192	2.6673233	88.9744020
C	12.0401653	33.4995761	84.3378510	C	-2.7496802	4.8924690	89.5551370
C	11.3180364	33.6538452	83.1421614	C	-2.2154633	2.9431489	87.6081690
H	9.7759511	32.8402624	81.8376200	C	-2.7838081	4.1849739	87.2587722
H	9.3189375	30.8592654	83.3519520	C	-3.0691440	5.1736295	88.2134684
C	10.5249841	30.2892687	85.6883397	H	-2.9468348	5.6654011	90.3155301
H	12.3401675	32.2669892	86.1104549	C	-1.9571216	1.9282599	86.4965506
H	12.8057338	34.2387011	84.6190777	C	-3.0096500	4.3743196	86.1992922
H	11.5206103	34.5159861	82.4878409	H	-1.0044491	2.4848050	85.4225524
O	9.6973635	29.4237240	85.4578472	H	-1.4534081	3.3449036	84.8828735
H	11.1612109	30.2572945	86.6261327	H	-0.7723032	1.7052954	84.6680598

agg-7-d-mi; COSMO



Energy (Hartree)=-11970.00885505

Zn	1.1141666	5.6782732	89.5002523
Br	3.4535717	6.3447228	89.8310856
C	-0.3790387	8.4033912	86.7718712
C	-0.0767696	7.3513496	87.5833337
C	-0.4495081	7.7814832	88.9432007

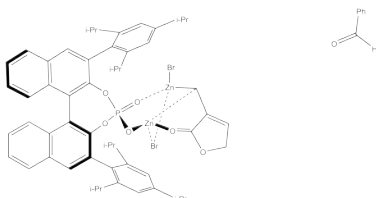
O	-1.0330006	8.9805318	88.9460884
C	-1.0088235	9.4859640	87.5859129
O	-0.2258322	7.1491395	89.9996357
C	0.5148693	6.0117594	87.4173069
H	-0.4393976	10.4405628	87.5994362
H	-2.0534132	9.7131519	87.2796793
Zn	2.7872972	5.5655345	87.4845822
Br	3.8329697	6.5296780	85.6476964
C	-0.0055315	1.0162752	88.9997167
C	0.6678276	-0.1366511	89.4221370
C	-0.0074140	-1.0036865	90.3564859
C	0.6370044	-2.1074818	90.9920623
C	-1.3830017	-0.7266246	90.6968376
C	-2.0690077	-1.6014513	91.5927256
C	-2.0187333	0.4385693	90.1794450
H	-3.0631388	0.6389525	90.4620493
C	-1.3410301	1.3534144	89.3808744
C	4.3341883	0.4809053	88.4458489
C	4.7002966	-0.7630924	87.9443284
H	5.7199307	-0.9053862	87.5548936
C	3.7689012	-1.8357930	87.8361386
C	4.1436332	-3.0734052	87.2308960
C	2.4029775	-1.6456248	88.2663136
C	1.4603968	-2.6820890	87.9912670
C	2.0434975	-0.4056653	88.9132501
C	3.0152750	0.5986969	88.9810922
O	0.6446183	1.9000108	88.1390725
O	2.6980419	1.8000737	89.6154708
P	1.7663381	2.8834922	88.8249857
O	1.1423276	3.7613207	89.9332155
O	2.4757997	3.5835655	87.6607179
C	-1.4212903	-2.6838419	92.1689508
C	-0.0518434	-2.9254670	91.8772828
H	-3.1223004	-1.3866449	91.8323240
H	-1.9594680	-3.3451119	92.8651216
H	1.6978735	-2.3009872	90.7808046
H	0.4701278	-3.7651822	92.3608905
C	1.8531431	-3.8661729	87.3817592
C	3.2091812	-4.0748628	87.0139798
H	0.4051826	-2.5328564	88.2578429
H	1.1040708	-4.6458525	87.1751415
H	3.5103696	-5.0206124	86.5382640
H	5.1908553	-3.2072088	86.9172398
C	-2.1976422	3.6649176	89.9637029
C	-1.9366192	2.6673233	88.9744020
C	-2.7496802	4.8924690	89.5551370
C	-2.2154633	2.9431489	87.6081690
C	-2.7838081	4.1849739	87.2587722
C	-3.0691440	5.1736295	88.2134684
H	-2.9468348	5.6654011	90.3155301
C	-1.9571216	1.9282599	86.4965506
C	-3.0096500	4.3743196	86.1992922
H	-1.0044491	2.4848050	85.4225524
H	-1.4534081	3.3449036	84.8828735
H	-0.7723032	1.7052954	84.6680598
H	-0.0493107	2.8179778	85.8733547
C	-3.2792931	1.4327119	85.8811989
H	-1.4635758	1.0450535	86.9485593
H	-3.8331132	2.2591380	85.3884038
H	-3.9441558	0.9963917	86.6541690
H	-3.0859037	0.6542230	85.1144455
C	-3.7471803	6.4953492	87.8625704
C	-3.6528045	6.8791841	86.3808497
H	-4.0548347	7.9002455	86.2196196
H	-4.2482378	6.1934240	85.7429286
H	-2.6066536	6.8585396	86.0152629
C	-5.2186159	6.4790758	88.3260844
H	-3.2306847	7.2856297	88.4542439
H	-5.7049624	7.4584972	88.1370397
H	-5.3022033	6.2573322	89.4086526
H	-5.7886822	5.7001603	87.7777287

C	-1.9450683	3.4366599	91.4551873
C	-1.1737534	4.5820412	92.1318714
H	-1.0068648	4.3486271	93.2030450
H	-1.7146636	5.5487417	92.0833666
H	-0.1790684	4.7153136	91.6667035
C	-3.2769974	3.1806029	92.1891910
H	-1.3209589	2.5264108	91.5551287
H	-3.0984661	2.9475920	93.2592521
H	-3.8383253	2.3350995	91.7435552
H	-3.9334946	4.0748113	92.1408232
H	7.7113121	5.4660937	86.7204183
H	7.6460251	2.0433676	91.5089850
H	5.5075154	0.4100094	84.0345711
C	7.5981892	5.3128289	87.8160651
H	4.7518778	2.3772406	92.8129005
H	7.5114826	7.4682027	88.2140345
H	3.6074235	2.0938587	83.9940948
C	6.7495236	4.0599459	87.9955638
C	6.8858816	1.2402894	91.4084380
C	6.8967199	6.5594098	88.3827626
H	6.7259883	6.4624957	89.4755049
C	6.5066194	3.5137229	89.2684696
C	5.9317014	0.9076617	84.9315784
H	9.5199364	4.2517095	87.9893843
C	6.1804502	3.4126685	86.8872678
C	9.0067459	5.1396288	88.4115968
H	9.6333145	6.0319143	88.2048260
H	6.3416120	3.8471140	85.8879305
C	4.9396465	2.8309265	91.8176326
H	6.7411086	0.7851785	92.4104791
H	7.3050327	0.4647030	90.7353667
C	5.7406111	2.3490638	89.4499937
C	4.0593343	2.6174123	84.8621224
C	5.4041462	2.2446195	87.0090925
H	6.4556212	0.1390038	85.5352604
H	6.6953433	1.6356195	84.5854601
C	5.5568825	1.7953354	90.8612282
C	5.1962382	1.6975837	88.3093812
C	4.8262684	1.6136803	85.7404583
H	3.9782166	3.2151888	91.4249987
H	3.2506784	3.1072339	85.4361553
H	5.6135510	3.6994163	91.9704647
H	5.9123756	6.7138510	87.8982174
H	4.7168556	3.4162958	84.4625020
H	8.9666747	5.0117657	89.5137849
H	4.8523439	0.9407427	90.7995179
H	4.0958665	0.8398269	86.0504105
H	6.9326415	4.0101266	90.1547749
H	-0.2617442	5.2306478	87.6019168
H	0.8315147	5.8400356	86.3682186
H	-0.2246890	8.4760729	85.6869095
C	-0.8680771	14.6941939	77.0211696
C	-1.3756594	14.1433688	78.2028352
C	-2.7622277	13.9010458	78.3284725
C	-3.6311695	14.2154727	77.2622113
C	-3.1209256	14.7674929	76.0781852
C	-1.7403156	15.0059706	75.9590388
H	0.2114811	14.8843499	76.9186116
H	-0.7214739	13.8877546	79.0509226
C	-3.3078644	13.3157069	79.5782656
H	-4.7116281	14.0226592	77.3694779
H	-3.7974664	15.0127528	75.2451355
H	-1.3377104	15.4383613	75.0296580
O	-2.6402877	13.0074223	80.5554691
H	-4.4297455	13.1664582	79.5682224

Energy (Hartree)= -11969.99390449

Zn	1.0488342	5.6191897	89.5542179
Br	3.3782814	6.2985158	89.9635386
C	-0.3679936	8.4256205	86.9153597
C	-0.1128534	7.3407451	87.6994513
C	-0.5243746	7.7331996	89.0636109
O	-1.0996545	8.9400865	89.0825812
C	-1.0176058	9.4880058	87.7442971
O	-0.3298245	7.0720109	90.1033142
C	0.4711455	6.0029963	87.5185856
H	-0.4402341	10.4362033	87.8131854
H	-2.0476119	9.7384267	87.4059262
Zn	2.8488297	5.5187342	87.6089643
Br	3.7717105	6.5453526	85.7525592
C	-0.0063466	0.9453824	89.0502684
C	0.6792253	-0.2018043	89.4699767
C	0.0070249	-1.0843018	90.3920439
C	0.6599961	-2.1852331	91.0234177
C	-1.3750859	-0.8288357	90.7225683
C	-2.0567052	-1.7214885	91.6033435
C	-2.0210432	0.3325290	90.2100453
H	-3.0697570	0.5195795	90.4861229
C	-1.3489103	1.2620925	89.4244782
C	4.3305257	0.4859826	88.4886003
C	4.7218017	-0.7502215	87.9883163
H	5.7408547	-0.8674992	87.5891534
C	3.8148783	-1.8442534	87.8891596
C	4.2157496	-3.0766070	87.2911874
C	2.4452646	-1.6808892	88.3186579
C	1.5251997	-2.7374307	88.0446700
C	2.0615208	-0.4486310	88.9673803
C	3.0150233	0.5731367	89.0384354
O	0.6357096	1.8446159	88.2005300
O	2.6809358	1.7629147	89.6847060
P	1.7358277	2.8411265	88.9045129
O	1.0926871	3.7029920	90.0119584
O	2.4389138	3.5618435	87.7476251
C	-1.4010081	-2.8019961	92.1727702
C	-0.0264201	-3.0224737	91.8915728
H	-3.1143915	-1.5219531	91.8369973
H	-1.9372596	-3.4781025	92.8558797
H	1.7253420	-2.3610643	90.8200657
H	0.5018021	-3.8611713	92.3701097
C	1.9438541	-3.9163541	87.4432398
C	3.3040055	-4.0991050	87.0795610
H	0.4668978	-2.6089148	88.3091003
H	1.2117160	-4.7130942	87.2413005
H	3.6264328	-5.0415835	86.6114110
H	5.2661979	-3.1897770	86.9801634
C	-2.2325152	3.5580722	90.0238564
C	-1.9554521	2.5733933	89.0264960
C	-2.7885838	4.7859076	89.6225081
C	-2.2243070	2.8608602	87.6607130
C	-2.7950913	4.1033004	87.3186081
C	-3.0947203	5.0799581	88.2810365
H	-2.9970606	5.5492209	90.3895249
C	-1.9540816	1.8556649	86.5429601
H	-3.0117812	4.3029109	86.2590417
C	-1.0037480	2.4252683	85.4740432
H	-1.4600930	3.2804306	84.9327269
H	-0.7587482	1.6506188	84.7187769
H	-0.0540377	2.7687094	85.9283260
C	-3.2716130	1.3528587	85.9236124
H	-1.4543292	0.9741142	86.9913194
H	-3.8334418	2.1780510	85.4379721
H	-3.9326019	0.9047214	86.6929292
H	-3.0724143	0.5826513	85.1500679
C	-3.7788709	6.4006423	87.9380628
C	-3.6468111	6.8170820	86.4677965
H	-4.0627180	7.8339766	86.3141673

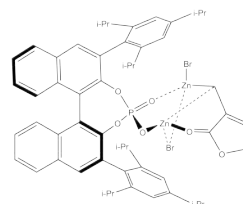
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H	-4.2113169	6.1354679	85.7982356
H	-2.5900285	6.8218291	86.1336041
C	-5.2622688	6.3540757	88.3590939
H	-3.2892380	7.1854833	88.5592768
H	-5.7602146	7.3292710	88.1780920
H	-5.3720697	6.1057854	89.4334155
H	-5.8045658	5.5783540	87.7793563
C	-1.9935712	3.3164558	91.5157774
C	-1.2269575	4.4540582	92.2113269
H	-1.0885237	4.2177491	93.2860310
H	-1.7558544	5.4268217	92.1523588
H	-0.2205863	4.5764687	91.7695064
C	-3.3330613	3.0526328	92.2329999
H	-1.3705809	2.4053447	91.6135516
H	-3.1661925	2.8037948	93.3013644
H	-3.8925795	2.2153010	91.7698133
H	-3.9880670	3.9481928	92.1916633
H	7.3541520	5.6467426	86.6440765
H	7.6849361	2.1785387	91.4332539
H	5.3620823	0.4090661	84.0613438
C	7.3982041	5.4251232	87.7327405
H	4.8214395	2.3943222	92.8357632
H	7.4024099	7.5479080	88.2732373
H	3.4168231	2.0468226	84.0497264
C	6.5872952	4.1534426	87.9511502
C	6.9533328	1.3464644	91.3633847
C	6.8000527	6.6361616	88.4666791
H	6.7744835	6.4772287	89.5650873
C	6.4138634	3.6008484	89.2328735
C	5.7951151	0.9305436	84.9402709
H	9.3142643	4.3549534	87.5556180
C	6.0099452	3.4772861	86.8643841
C	8.8756245	5.2095806	88.1094311
H	9.4773083	6.1141735	87.8827253
H	6.1170899	3.9157070	85.8600019
C	4.9565034	2.8550843	91.8353202
H	6.8613660	0.8930050	92.3723546
H	7.3796020	0.5840794	90.6801887
C	5.7043539	2.4054277	89.4426454
C	3.8808075	2.5931439	84.8969154
C	5.2895934	2.2777319	87.0147934
H	6.3555373	0.1848290	85.5396245
H	6.5302598	1.6733315	84.5657644
C	5.5866308	1.8468571	90.8589170
C	5.1498888	1.7281834	88.3229360
C	4.6932596	1.6194260	85.7686053
H	3.9662277	3.1957098	91.4761742
H	3.0766906	3.0745147	85.4842119
H	5.5951148	3.7529664	91.9675746
H	5.7650961	6.8327307	88.1251003
H	4.5073337	3.4006124	84.4663947
H	8.9865025	4.9978269	89.1937658
H	4.9152858	0.9644044	90.8172193
H	3.9896271	0.8321246	86.1058496
H	6.8499528	4.1169951	90.1030545
H	-0.3209816	5.2240934	87.6293260
H	0.8753716	5.8659577	86.4958991
H	-0.1646752	8.5322745	85.8413855
C	-1.0906988	15.1991419	76.0802918
C	-0.9416128	14.6236858	77.3462828
C	-2.0770640	14.1662243	78.0503902
C	-3.3580084	14.2923546	77.4752018
C	-3.5065916	14.8701706	76.2064802
C	-2.3727622	15.3226076	75.5103450
H	-0.2081018	15.5560290	75.5275547
H	0.0444228	14.5115926	77.8231038
C	-1.9215373	13.5521066	79.3947799
H	-4.2388603	13.9328397	78.0327867
H	-4.5061262	14.9694676	75.7565356
H	-2.4877447	15.7760715	74.5135790
O	-0.8594123	13.4019169	79.9750310

H -2.8981246 13.2184154 79.8644734

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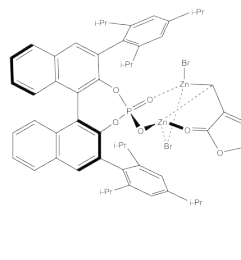


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Zn	0.8839143	5.6338212	89.1691146
Br	3.2051406	6.4299361	89.2960556
H	-1.0013672	10.2401635	87.2017295
Br	3.2694765	6.4008859	85.0827881
H	0.3833619	5.6448892	86.0697579
Zn	2.4250616	5.4926008	87.0475368
C	-0.9108297	8.1736936	86.4520818
C	-1.5295144	9.2640809	87.2646960
C	-0.5108120	7.1690617	87.2812515
C	0.1255864	5.8483671	87.1291128
C	-0.8086807	7.6418215	88.6458839
O	-1.4405363	8.8161917	88.6417597
O	-0.4868716	7.0647718	89.7081984
H	-2.6012226	9.4374149	87.0234926
H	-0.6027479	5.0453139	87.3967229
H	-0.8308798	8.2075298	85.3573134
C	-0.0164389	0.8981120	88.9946438
C	0.7455490	-0.1910156	89.4361288
C	0.1788338	-1.0336477	90.4610374
C	0.9221828	-2.0619621	91.1150633
C	-1.1868822	-0.8097206	90.8734433
C	-1.7661564	-1.6644948	91.8596128
C	-1.9177713	0.2875241	90.3334817
H	-2.9524722	0.4498032	90.6709555
C	-1.3423910	1.1873058	89.4429054
C	4.2929241	0.5534823	88.1561670
C	4.6981750	-0.7005015	87.7141393
H	5.6937087	-0.8133067	87.2584073
C	3.8280188	-1.8281354	87.7493002
C	4.2360890	-3.0848524	87.2084399
C	2.4844388	-1.6815152	88.2598515
C	1.5888140	-2.7846919	88.1206330
C	2.0976449	-0.4210627	88.8503631
C	3.0130762	0.6351833	88.7847779
O	0.5259371	1.7618078	88.0435578
O	2.6774681	1.8563681	89.3700793
P	1.6319365	2.8423529	88.5947469
O	1.0391494	3.7474040	89.6983236
O	2.2153759	3.5145250	87.3469011
C	-1.0246503	-2.6760920	92.4512691
C	0.3356904	-2.8623033	92.0859558
H	-2.8125447	-1.4906605	92.1562227
H	-1.4809744	-3.3225804	93.2163191
H	1.9777198	-2.2109590	90.8482576
H	0.9323546	-3.6440724	92.5803631
C	2.0113450	-3.9877058	87.5709069
C	3.3511646	-4.1495264	87.1279769
H	0.5458990	-2.6746432	88.4475978
H	1.2983049	-4.8205560	87.4725202
H	3.6774169	-5.1108674	86.7026786

H	5.2674404	-3.1842554	86.8349747	H	5.4612846	6.8715948	87.2599510
C	-2.2796202	3.4838008	89.9537546	H	4.1296468	3.2007954	83.9467534
C	-2.0309034	2.4445196	89.0050176	H	8.8119651	5.2737218	88.3031804
C	-2.9144820	4.6599090	89.5152503	H	5.0064218	1.2025527	90.4077861
C	-2.4064971	2.6286153	87.6464688	H	3.7702049	0.7478335	85.7908820
C	-3.0527228	3.8225998	87.2666846	H	6.7985361	4.3484425	89.3667702
C	-3.3262386	4.8504807	88.1827853	C	8.7596920	11.4328402	70.7009289
H	-3.1030705	5.4641790	90.2445478	C	7.6037998	11.1907805	71.4506784
C	-2.1727003	1.5609503	86.5796913	C	7.0684175	12.2101499	72.2694963
H	-3.3507663	3.9414295	86.2148033	C	7.7009169	13.4696967	72.3289335
C	-1.3246260	2.0924658	85.4097210	C	8.8594407	13.7110517	71.5764690
H	-1.8549019	2.8906695	84.8491831	C	9.3874070	12.6927571	70.7635565
H	-1.1006201	1.2774679	84.6910713	H	9.1800810	10.6411678	70.0618923
H	-0.3610721	2.5021929	85.7708284	H	7.0892390	10.2177775	71.4241354
C	-3.5079115	0.9690763	86.0902240	C	5.8421313	11.9588315	73.0671250
H	-1.6064781	0.7307270	87.0466862	H	7.2763827	14.2592669	72.9708792
H	-4.1347176	1.7387181	85.5929251	H	9.3539842	14.6933088	71.6213882
H	-4.0948447	0.5498371	86.9325995	H	10.2970467	12.8808836	70.1722713
H	-3.3300598	0.1559680	85.3563866	O	5.2231897	10.9048290	73.0816143
C	-4.0846843	6.1200409	87.8041490	H	5.5028590	12.8428039	73.6868297
C	-4.0980026	6.4222346	86.3007012				
H	-4.5611487	7.4116528	86.1089934				
H	-4.6939835	5.6727003	85.7397404				
H	-3.0757688	6.4313174	85.8720772				
C	-5.5224382	6.0673221	88.3612704				
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H	-6.0647383	7.0126204	88.1518332				
H	-5.5280856	5.9034392	89.4572690				
H	-6.0889290	5.2351549	87.8934103				
C	-1.9269617	3.3518445	91.4367496				
C	-1.1779699	4.5691910	92.0041665				
H	-0.9410184	4.4053634	93.0750967				
H	-1.7682351	5.5052718	91.9350161				
H	-0.2185206	4.7228613	91.4754333				
C	-3.1977666	3.0702963	92.2641770				
H	-1.2507082	2.4806990	91.5453854				
H	-2.9436676	2.9016251	93.3310661				
H	-3.7411456	2.1770924	91.8959652				
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H	7.0448435	5.6540582	85.7898936				
H	7.7624990	2.5415366	90.7761095				
H	5.0112468	0.2104089	83.6895231				
C	7.1445410	5.5178110	86.8889752				
H	4.9780315	2.7672903	92.3257667				
H	7.0669936	7.6746385	87.2690439				
H	3.0329610	1.8094049	83.7055703				
C	6.3984978	4.2358411	87.2384225				
C	7.0578885	1.6840038	90.8052599				
C	6.5209994	6.7530563	87.5598219				
H	6.5561731	6.6758481	88.6667928				
C	6.3241803	3.7648112	88.5617233				
C	5.4919939	0.7955915	84.5010299				
H	9.1002760	4.5240875	86.7022026				
C	5.7718444	3.4763051	86.2374854				
C	8.6450552	5.3972513	87.2123710				
H	9.1922045	6.3082757	86.8921153				
H	5.8006932	3.8501909	85.2020767				
C	5.0414207	3.1611814	91.2901642				
H	7.0377823	1.2993349	91.8462875				
H	7.4709792	0.8885947	90.1519541				
C	5.6634919	2.5688944	88.8939559				
C	3.5460702	2.4206410	84.4768435				
C	5.0956488	2.2729308	86.5121021				
H	6.1049554	0.0996367	85.1086545				
H	6.1850985	1.5237265	84.0295180				
C	5.6482839	2.1057104	90.3489907				
C	5.0572649	1.8063702	87.8588448				
C	4.4339925	1.5212891	85.3547793				
H	4.0223924	3.4480800	90.9655881				
H	2.7783412	2.9339166	85.0853771				
H	5.6578292	4.0835915	91.3228432				

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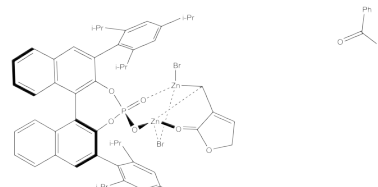


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Br	3.2859030	6.3914084	85.0930205
H	0.4873659	5.6595700	86.0894128
Zn	2.5471782	5.4590908	87.0773072
C	-0.8282882	8.1951155	86.4320344
C	-1.4635906	9.2852789	87.2357898
C	-0.4771895	7.1738207	87.2629877
C	0.1465851	5.8490243	87.1266566
C	-0.8104593	7.6403588	88.6254308
O	-1.4317849	8.8243934	88.6083809
O	-0.5183881	7.0571681	89.6884206
H	-2.5237956	9.4740823	86.9556079
H	-0.6046559	5.0513929	87.3409746
H	-0.7024958	8.2376141	85.3418823
C	-0.0155838	0.8909232	89.0001750
C	0.7426441	-0.2013100	89.4411549
C	0.1703409	-1.0460814	90.4608387
C	0.9087607	-2.0789904	91.1127091
C	-1.1956744	-0.8202840	90.8704613
C	-1.7793503	-1.6777110	91.8509354
C	-1.9215977	0.2808021	90.3326561
H	-2.9561890	0.4470659	90.6687023
C	-1.3421476	1.1813382	89.4459416
C	4.2885832	0.5530445	88.1664674
C	4.6952330	-0.6979609	87.7179527
H	5.6889112	-0.8038131	87.2565302
C	3.8290428	-1.8284253	87.7510913
C	4.2389101	-3.0817237	87.2050019
C	2.4859072	-1.6874564	88.2640560
C	1.5935779	-2.7925968	88.1217805
C	2.0968573	-0.4302884	88.8598143
C	3.0108604	0.6275826	88.8006505

O	0.5308533	1.7571741	88.0545892	H	9.1467736	6.3148265	86.8504445
O	2.6733868	1.8436763	89.3942442	H	5.7505196	3.8672557	85.2096631
P	1.6356795	2.8349562	88.6169818	C	5.0403399	3.1572458	91.3063097
O	1.0372861	3.7444062	89.7114988	H	7.0556564	1.3054199	91.8308573
O	2.2293228	3.5035704	87.3707299	H	7.4717309	0.9063763	90.1294663
C	-1.0430990	-2.6939659	92.4398067	C	5.6433360	2.5800758	88.9000399
C	0.3172217	-2.8821091	92.0775662	C	3.5115139	2.4038998	84.4897567
H	-2.8261475	-1.5020382	92.1449128	C	5.0712411	2.2789176	86.5198758
H	-1.5038967	-3.3430237	93.1999039	H	6.1200111	0.1344260	85.1079424
H	1.9643195	-2.2289069	90.8469632	H	6.1679273	1.5615365	84.0329892
H	0.9103641	-3.6678263	92.5697550	C	5.6442716	2.1112353	90.3533406
C	2.0188008	-3.9922542	87.5678382	C	5.0430796	1.8110925	87.8664468
C	3.3576649	-4.1485553	87.1221695	C	4.4197378	1.5193767	85.3619753
H	0.5511548	-2.6860294	88.4510420	H	4.0147129	3.4367046	90.9969943
H	1.3080490	-4.8268174	87.4681498	H	2.7301825	2.8937191	85.1003704
H	3.6861975	-5.1072000	86.6927270	H	5.6487734	4.0849078	91.3370066
H	5.2697829	-3.1764469	86.8291320	H	5.4327185	6.9111992	87.3050959
C	-2.2771832	3.4774557	89.9602166	H	4.0744027	3.2033123	83.9665140
C	-2.0277120	2.4404572	89.0097043	H	8.7914629	5.2697293	88.2602272
C	-2.9091575	4.6551863	89.5225157	H	5.0085616	1.2038364	90.4139935
C	-2.3999053	2.6277445	87.6507491	H	3.7730306	0.7306100	85.7961033
C	-3.0433655	3.8232224	87.2722446	H	6.7590996	4.3720420	89.3703341
C	-3.3171835	4.8491662	88.1900122	C	8.7595708	11.4389238	70.6951073
H	-3.0963086	5.4589436	90.2527925	C	7.6067112	11.1861265	71.4454139
C	-2.1645094	1.5622240	86.5821534	C	7.0645839	12.1983988	72.2672111
H	-3.3393802	3.9445277	86.2200514	C	7.6875044	13.4615195	72.3287674
C	-1.3123697	2.0951388	85.4159694	C	8.8434350	13.7140108	71.5764769
H	-1.8387481	2.8958953	84.8554008	C	9.3782109	12.7025017	70.7605623
H	-1.0871834	1.2822553	84.6954801	H	9.1847684	10.6523073	70.0529967
H	-0.3489907	2.5019368	85.7803590	H	7.0962340	10.2109718	71.4194176
C	-3.4990781	0.9721988	86.0890956	C	5.8388672	11.9303969	73.0647212
H	-1.5998776	0.7308453	87.0489265	H	7.2563858	14.2459033	72.9729415
H	-4.1255783	1.7427367	85.5929037	H	9.3307457	14.6997695	71.6239339
H	-4.0877629	0.5516889	86.9293845	H	10.2858739	12.8992071	70.1690256
H	-3.3212115	0.1607716	85.3534815	O	5.2327269	10.8722591	73.0744971
C	-4.0767402	6.1185337	87.8133881	H	5.4913219	12.8110057	73.6884135
C	-4.0611499	6.4422901	86.3141718				
H	-4.5281747	7.4308473	86.1262455				
H	-4.6407654	5.6978678	85.7298611				
H	-3.0302975	6.4638511	85.9073195				
C	-5.5252757	6.0452750	88.3389182				
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H	-5.5521930	5.8637019	89.4316748				
H	-6.0731311	5.2140781	87.8481126				
C	-1.9285997	3.3425519	91.4439862				
C	-1.1646662	4.5505731	92.0117867				
H	-0.9442108	4.3901341	93.0868134				
H	-1.7362349	5.4971298	91.9293313				
H	-0.1964324	4.6808650	91.4936986				
C	-3.2047782	3.0765400	92.2679547				
H	-1.2632623	2.4633763	91.5546020				
H	-2.9562338	2.9041327	93.3354874				
H	-3.7590568	2.1907593	91.8980437				
H	-3.8974423	3.9427203	92.2164957				
H	6.9659740	5.6893278	85.7949686				
H	7.7609112	2.5566951	90.7585896				
H	5.0210228	0.2254070	83.6914322				
C	7.0922189	5.5416656	86.8897244				
H	4.9925530	2.7583564	92.3407245				
H	7.0456494	7.6941561	87.2939738				
H	3.0137487	1.7868845	83.7132054				
C	6.3507490	4.2582418	87.2438656				
C	7.0612154	1.6954401	90.7917046				
C	6.4954425	6.7755790	87.5856313				
H	6.5498058	6.6881918	88.6909853				
C	6.2870814	3.7846431	88.5667478				
C	5.4905743	0.8184840	84.5036220				
H	9.0342658	4.5331699	86.6469706				
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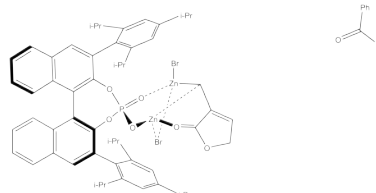


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C	-0.2092264	7.2448052	86.7158471
C	-0.5891519	7.8485724	88.0060655
O	-1.1396478	9.0533559	87.8515826
C	-1.0818312	9.3869132	86.4405330
O	-0.3968168	7.3458347	89.1356870
C	0.3498880	5.8819519	86.7279736
H	-0.4857660	10.3207093	86.3482364
H	-2.1151398	9.6034657	86.0909878
Zn	2.6138513	5.4228681	86.8641131
Br	3.6597321	6.1359898	84.9154743
H	0.6634664	5.5648022	85.7124849
H	-0.4436690	5.1493173	87.0119467
H	-0.2966370	8.1311744	84.6937159
C	-0.1938829	1.1103964	88.9520725
C	0.4747296	0.0272723	89.5365479
C	-0.2122091	-0.7033530	90.5739604
C	0.4232640	-1.7098505	91.3619014
C	-1.5917251	-0.3837492	90.8570440
C	-2.2897596	-1.1299531	91.8544219

C	-2.2202943	0.7002634	90.1790627	H	4.6302641	3.0225896	92.5171873
H	-3.2671366	0.9381473	90.4208451	H	7.3283424	7.4165783	87.2903633
C	-1.5326248	1.4970322	89.2702646	H	3.2752752	1.4401268	83.8703519
C	4.1417425	0.5112521	88.4897040	C	6.4729031	4.0215369	87.4506252
C	4.5171570	-0.7904555	88.1788288	C	6.7588600	1.7377516	91.2413177
H	5.5370216	-0.9821178	87.8118417	C	6.7158736	6.5479419	87.6101791
C	3.5922977	-1.8730487	88.2322514	H	6.6877693	6.5469553	88.7199963
C	3.9775751	-3.1855817	87.8232727	C	6.2819304	3.6623379	88.7970850
C	2.2227597	-1.6281209	88.6220774	C	5.6272777	0.4129961	84.9266188
C	1.2870399	-2.6992294	88.4970534	H	9.2077455	4.1343017	87.0453305
C	1.8548511	-0.3087518	89.0812727	C	5.8890995	3.2069422	86.4673492
C	2.8239314	0.6981284	89.0077998	C	8.7757183	5.0620497	87.4726111
O	0.4632394	1.8673075	87.9825836	H	9.3885016	5.9200482	87.1257816
O	2.5056615	1.9758839	89.4687974	H	6.0099614	3.4939676	85.4110633
P	1.5752639	2.9406586	88.5358856	C	4.7843785	3.3300705	91.4620086
O	0.9431138	3.9560626	89.5142605	H	6.6478207	1.4379954	92.3042966
O	2.2870617	3.4836147	87.2921879	H	7.1792653	0.8767488	90.6826988
C	-1.6508532	-2.1255181	92.5782787	C	5.5463706	2.5236107	89.1703129
C	-0.2779489	-2.4028657	92.3393865	C	3.7504368	2.0930437	84.6317238
H	-3.3454333	-0.8848106	92.0506483	C	5.1427956	2.0561505	86.7826003
H	-2.1988771	-2.6882377	93.3492328	H	6.1678627	-0.2514419	85.6307602
H	1.4868104	-1.9284903	91.1933849	H	6.3798500	1.0786104	84.4540629
H	0.2366995	-3.1701751	92.9374906	C	5.4060164	2.1792811	90.6513759
C	1.6900775	-3.9594358	88.0761070	C	4.9842666	1.7031453	88.1548439
C	3.0498837	-4.2139368	87.7544783	C	4.5380540	1.2376433	85.6397527
H	0.2291059	-2.5180897	88.7306355	H	3.8052780	3.6318555	91.0421563
H	0.9462413	-4.7658234	87.9851037	H	2.9581820	2.6734391	85.1404108
H	3.3595580	-5.2194017	87.4308360	H	5.4391267	4.2261346	91.4693709
H	5.0280842	-3.3592409	87.5416230	H	5.6823494	6.7018454	87.2426815
C	-2.3816185	3.8690848	89.5275700	H	4.3985601	2.8136718	84.0923355
C	-2.1171866	2.7463684	88.6839990	H	8.8776598	5.0026012	88.5768170
C	-2.9148668	5.0357812	88.9503295	H	4.7201940	1.3107024	90.7310681
C	-2.3747766	2.8391613	87.2890830	H	3.8156034	0.5225610	86.0821089
C	-2.9226008	4.0288643	86.7680224	H	6.7223829	4.2904204	89.5879229
C	-3.2100637	5.1387164	87.5779536	C	-0.5876642	4.9371613	69.8270149
H	-3.1158569	5.9041143	89.5983094	C	-0.5989563	5.3962712	71.1483436
C	-2.1175612	1.6797872	86.3285309	C	-0.7862292	6.7710139	71.4152305
H	-3.1303755	4.0781879	85.6891607	C	-0.9613866	7.6772556	70.3484264
C	-1.1557766	2.0760897	85.1931701	C	-0.9502829	7.2155710	69.0243018
H	-1.5977409	2.8517738	84.5332071	C	-0.7633325	5.8465046	68.7651326
H	-0.9216888	1.1969646	84.5582584	H	-0.4417949	3.8668715	69.6148024
H	-0.2020309	2.4669517	85.5984400	H	-0.4645454	4.7122459	72.0005507
C	-3.4417619	1.1149757	85.7804803	C	-0.7994978	7.2642377	72.8150940
H	-1.6333955	0.8634878	86.9006392	H	-1.1064725	8.7483714	70.5660836
H	-3.9875518	1.8718155	85.1788836	H	-1.0871227	7.9211949	68.1907520
H	-4.1119334	0.7920692	86.6029237	H	-0.7542479	5.4825338	67.7259359
H	-3.2527933	0.2388981	85.1262641	O	-0.6605621	6.5601605	73.8046380
C	-3.8689822	6.4072151	87.0428026	H	-0.9532233	8.3812723	72.9113208
C	-3.7305722	6.5999102	85.5275428				
H	-4.1237297	7.5924549	85.2267344				
H	-4.3105849	5.8392661	84.9648278				
H	-2.6746226	6.5327476	85.1973582				
C	-5.3529608	6.4507589	87.4627477				
H	-3.3648994	7.2652691	87.5440302				
H	-5.8307823	7.3981608	87.1377412				
H	-5.4673597	6.3668904	88.5618966				
H	-5.9099479	5.6087083	87.0011977				
C	-2.1539836	3.8399589	91.0403036				
C	-1.3789649	5.0572776	91.5721708				
H	-1.2445543	4.9729508	92.6698393				
H	-1.9002408	6.0157696	91.3750075				
H	-0.3699849	5.1097077	91.1214618				
C	-3.5001953	3.6964815	91.7789313				
H	-1.5424745	2.9452948	91.2716846				
H	-3.3412101	3.6017668	92.8730183				
H	-4.0664002	2.8071782	91.4366093				
H	-4.1431911	4.5847346	91.6044059				
H	7.2678711	5.3026586	85.9495300				
H	7.5028798	2.5608093	91.1988230				
H	5.1852300	-0.2193459	84.1286291				
C	7.3029103	5.2381634	87.0589903				

agg-7-j-mi

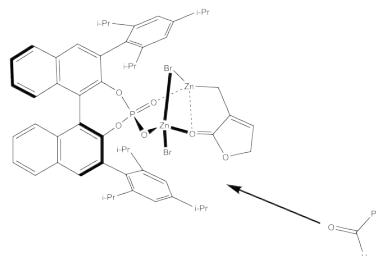


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Zn	0.9327415	5.7912564	88.7918632
Br	3.2699387	6.4930680	89.1116906
C	-0.4319689	8.2106807	85.7699180
C	-0.1958004	7.2463043	86.7032322
C	-0.6055491	7.8371563	87.9947704
O	-1.1622641	9.0427117	87.8366519
C	-1.0686794	9.3904672	86.4338518
O	-0.4240845	7.3300184	89.1197061
C	0.3683942	5.8881581	86.7197881
H	-0.4782917	10.3308710	86.3682457
H	-2.0941910	9.6031077	86.0579095
Zn	2.7405528	5.3865119	86.8924172

Br	3.6824467	6.1127743	84.9081725	H	-0.3610092	5.0942523	91.1259718
H	0.7752774	5.5999338	85.7300651	C	-3.4996412	3.7010706	91.7823969
H	-0.4359933	5.1445611	86.9356256	H	-1.5450943	2.9424981	91.2747190
H	-0.2239255	8.1579129	84.6928983	H	-3.3412068	3.6056438	92.8764610
C	-0.1921219	1.1106630	88.9557891	H	-4.0700824	2.8144070	91.4403222
C	0.4737846	0.0253935	89.5398885	H	-4.1403127	4.5911052	91.6088711
C	-0.2157626	-0.7057971	90.5747407	H	7.2479473	5.3098113	85.9464432
C	0.4176817	-1.7140275	91.3616956	H	7.5060957	2.5620368	91.1867172
C	-1.5950850	-0.3853880	90.8566083	H	5.1864203	-0.2145185	84.1292605
C	-2.2939079	-1.1322489	91.8522195	C	7.2843330	5.2464213	87.0558766
C	-2.2210040	0.6997261	90.1787268	H	4.6414654	3.0186733	92.5253050
H	-3.2678192	0.9398813	90.4184628	H	7.3190346	7.4245574	87.2862888
C	-1.5313484	1.4971698	89.2722411	H	3.2668267	1.4327756	83.8719752
C	4.1396429	0.5114575	88.4940117	C	6.4533806	4.0311560	87.4496284
C	4.5137611	-0.7893438	88.1784822	C	6.7623967	1.7389993	91.2320862
H	5.5325400	-0.9778089	87.8068287	C	6.7019527	6.5588797	87.6046997
C	3.5903755	-1.8728082	88.2312981	H	6.6695240	6.5595845	88.7143264
C	3.9746817	-3.1839958	87.8189670	C	6.2658340	3.6713835	88.7963840
C	2.2215369	-1.6294819	88.6240195	C	5.6244538	0.4203243	84.9273556
C	1.2864556	-2.7007821	88.4986206	H	9.1843768	4.1341380	87.0458026
C	1.8542708	-0.3114147	89.0868459	C	5.8708898	3.2138707	86.4676138
C	2.8232824	0.6957025	89.0171981	C	8.7568144	5.0657623	87.4685473
O	0.4675144	1.8697070	87.9903913	H	9.3732017	5.9195391	87.1180245
O	2.5048510	1.9705250	89.4844328	H	5.9886969	3.5015169	85.4113042
P	1.5804580	2.9395787	88.5518893	C	4.7871260	3.3285859	91.4697769
O	0.9475873	3.9609044	89.5210269	H	6.6591365	1.4363517	92.2949855
O	2.3001299	3.4769365	87.3085243	H	7.1801379	0.8804980	90.6680159
C	-1.6571278	-2.1291353	92.5750531	C	5.5377133	2.5286834	89.1711636
C	-0.2849317	-2.4076832	92.3369448	C	3.7369571	2.0880446	84.6342554
H	-3.3494036	-0.8858790	92.0481900	C	5.1319459	2.0588138	86.7842623
H	-2.2064114	-2.6920493	93.3449394	H	6.1705154	-0.2407237	85.6303552
H	1.4810031	-1.9327343	91.1924005	H	6.3727569	1.0906742	84.4551560
H	0.2286193	-3.1763474	92.9343145	C	5.4055264	2.1813244	90.6522628
C	1.6894559	-3.9598713	88.0754775	C	4.9783247	1.7051768	88.1568689
C	3.0481780	-4.2128374	87.7505226	C	4.5304248	1.2374271	85.6416774
H	0.2292314	-2.5200129	88.7351479	H	3.8035933	3.6284990	91.0595309
H	0.9460074	-4.7665721	87.9854310	H	2.9390576	2.6617168	85.1416611
H	3.3580503	-5.2173902	87.4246159	H	5.4389542	4.2267213	91.4752023
H	5.0245741	-3.3561012	87.5341652	H	5.6714600	6.7194129	87.2321932
C	-2.3821992	3.8680083	89.5306601	H	4.3779149	2.8151528	84.0953652
C	-2.1162890	2.7464549	88.6866236	H	8.8603627	5.0102694	88.5727223
C	-2.9178169	5.0334851	88.9539064	H	4.7210681	1.3118040	90.7337269
C	-2.3750091	2.8388178	87.2920603	H	3.8129720	0.5172759	86.0838848
C	-2.9251863	4.0275022	86.7717214	H	6.7054193	4.3011397	89.5861972
C	-3.2139333	5.1363681	87.5822150	C	-0.5890182	4.9390793	69.8243669
H	-3.1177180	5.9018269	89.6022950	C	-0.5970932	5.3959793	71.1461886
C	-2.1158853	1.6795823	86.3318929	C	-0.7834687	6.7694824	71.4158767
H	-3.1344391	4.0758111	85.6930898	C	-0.9606650	7.6764201	70.3512583
C	-1.1526234	2.0758077	85.1980427	C	-0.9538856	7.2173454	69.0265253
H	-1.5932111	2.8511316	84.5367402	C	-0.7682449	5.8492570	68.7646050
H	-0.9168922	1.1971447	84.5633116	H	-0.4424815	3.8692693	69.6100215
H	-0.1993953	2.4666722	85.6040737	H	-0.4610455	4.7140716	71.9998463
C	-3.4387808	1.1127331	85.7832545	C	-0.7936081	7.2561065	72.8205223
H	-1.6314478	0.8642738	86.9051707	H	-1.1045315	8.7473147	70.5714450
H	-3.9859447	1.8678525	85.1808560	H	-1.0927785	7.9243258	68.1944385
H	-4.1094078	0.7896867	86.6050599	H	-0.7634375	5.4870449	67.7247617
H	-3.2487019	0.2367117	85.1293959	O	-0.6530519	6.5482952	73.8036006
C	-3.8764752	6.4039781	87.0489162	H	-0.9476433	8.3748670	72.9206819
C	-3.7322241	6.6024975	85.5348462				
H	-4.1315717	7.5926969	85.2337715				
H	-4.3046557	5.8401194	84.9668286				
H	-2.6742211	6.5431546	85.2097733				
C	-5.3620678	6.4404624	87.4631111				
H	-3.3772184	7.2627114	87.5539201				
H	-5.8439012	7.3868719	87.1408172				
H	-5.4801257	6.3507721	88.5612437				
H	-5.9140988	5.5977169	86.9973679				
C	-2.1533224	3.8393266	91.0433152				
C	-1.3715897	5.0533122	91.5731126				
H	-1.2429959	4.9729515	92.6717797				
H	-1.8837559	6.0154072	91.3697026				

7.4.3 Pathways starting from 13d-mi TS-7-d-ma; COSMO



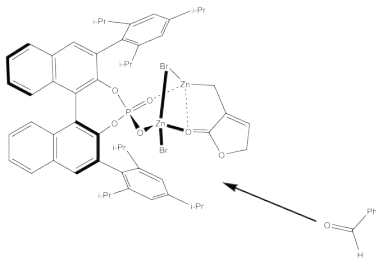
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Zn	2.4200409	0.3329882	0.9445263
Br	4.2744712	0.7066379	-0.3367154
C	1.2344552	5.1545799	1.5305136
C	0.6137904	4.0025365	1.9319216
C	1.6517178	2.9668132	1.8322030
O	2.8295180	3.4665989	1.4576963
C	2.6644575	4.8842212	1.2262201
O	1.4947014	1.7348847	2.0169066
C	-0.7658442	3.6764315	2.3311883
H	2.9503420	5.1114874	0.1764696
H	3.3739238	5.4279781	1.8878964
Zn	-1.5916174	1.9162037	1.8048467
Br	-3.6008675	1.2986502	2.8771553
C	-0.9454651	-3.3389528	1.0565531
C	-1.2041346	-4.0091452	-0.1422920
C	-0.7152096	-5.3625728	-0.2738653
C	-0.7680136	-6.0879702	-1.5021765
C	-0.1058167	-6.0008616	0.8690632
C	0.3556509	-7.3465296	0.7524670
C	0.0555748	-5.2734046	2.0845738
H	0.5064243	-5.7830604	2.9490903
C	-0.3166683	-3.9406786	2.1946385
C	-2.0169752	-1.3535356	-2.8002406
C	-3.0731620	-1.9504902	-3.4768063
H	-3.5108080	-1.4429967	-4.3505126
C	-3.6449130	-3.1796076	-3.0354289
C	-4.7872686	-3.7352767	-3.6867055
C	-3.0916270	-3.8557242	-1.8848172
C	-3.7559339	-5.0241876	-1.4044801
C	-1.9163228	-3.3088074	-1.2488528
C	-1.4568905	-2.0655255	-1.6939243
O	-1.3421567	-2.0027734	1.1841714
O	-0.3447658	-1.4927331	-1.0910357
P	-0.3958056	-0.8951443	0.4352520
O	1.0671609	-1.0195750	0.1655505
O	-1.0575955	0.4751221	0.5132837
C	0.2597078	-8.0336444	-0.4486126
C	-0.2924465	-7.3897781	-1.5877290
H	0.8054794	-7.8251144	1.6366294
H	0.6249310	-9.0691017	-0.5255339
H	-1.1829002	-5.6003858	-2.3949357
H	-0.3397037	-7.9239922	-2.5489752
C	-4.8768730	-5.5284133	-2.0502517
C	-5.3901070	-4.8902724	-3.2108867
H	-3.3760418	-5.5226935	-0.5018198
H	-5.3751036	-6.4265649	-1.6543625
H	-6.2748070	-5.3032273	-3.7190791
H	-5.1922929	-3.2154428	-4.5692374
C	1.1780336	-2.5748573	3.7306090
C	-0.1117503	-3.0791111	3.4002913
C	1.2682177	-1.5626705	4.7037378
C	-1.2580165	-2.6370574	4.1161287
C	-1.1144860	-1.6114442	5.0653681
C	0.1349411	-1.0317510	5.3452900
H	2.2539817	-1.1392021	4.9539051
C	-2.6181402	-3.3027210	3.9141224
H	-2.0126137	-1.2395360	5.5810031
C	-3.7662153	-2.3123055	3.6821236
H	-3.9553622	-1.6766827	4.5717552
H	-4.7064524	-2.8591652	3.4621306
H	-3.5466949	-1.6311467	2.8380920
C	-2.9091385	-4.2454765	5.0991852
H	-2.5485714	-3.9410466	3.0094375
H	-2.9866916	-3.6756430	6.0491068
H	-2.1048829	-4.9993113	5.2244202
H	-3.8675531	-4.7843265	4.9471382
C	0.2630570	0.1970105	6.2354640
C	-0.1193330	1.4514267	5.4221620
H	0.0215813	2.3771861	6.0188584

H	-1.1822040	1.4050363	5.1015589
H	0.4985488	1.5297273	4.5045480
C	-0.5444852	0.1043922	7.5387837
H	1.3379054	0.2886999	6.5090133
H	-0.3542678	0.9901119	8.1790674
H	-0.2787083	-0.8032524	8.1177143
H	-1.6362528	0.0740824	7.3419537
C	2.4442055	-3.1399603	3.0876460
C	3.5587151	-2.1144124	2.8471201
H	4.4277869	-2.5850735	2.3462249
H	3.9255784	-1.6442420	3.7813794
H	3.2210796	-1.2965127	2.1746085
C	2.9995078	-4.2983312	3.9441112
H	2.1595070	-3.5513599	2.0972780
H	3.8711983	-4.7763323	3.4509672
H	2.2340574	-5.0785859	4.1226116
H	3.3269638	-3.9263412	4.9375242
H	-0.5011647	4.7155293	-3.1721402
H	1.4713318	-0.1413801	-5.8246074
H	-5.7245650	1.5100736	-3.1436096
C	0.3230516	3.9685470	-3.1910618
H	2.6290805	-2.0126110	-3.5240490
H	1.4831948	5.0980194	-1.6932535
H	-5.0287403	1.6424266	-0.6878787
C	-0.3254120	2.5950981	-3.2798598
C	0.9109292	-1.0395782	-5.4895971
C	1.0740938	4.0791591	-1.8495201
H	1.9165807	3.3548723	-1.8045298
C	0.4165696	1.4493215	-3.6162749
C	-4.6623725	1.6203944	-3.4454058
H	0.6944774	4.2058329	-5.3458242
C	-1.6675544	2.4245557	-2.9066980
C	1.2318396	4.3090975	-4.3815534
H	1.5990812	5.3535331	-4.3062762
H	-2.2614694	3.3185817	-2.6543562
C	2.0691535	-1.1025748	-3.2250613
H	1.4816237	-1.9345770	-5.8139232
H	-0.0645039	-1.0426013	-6.0174549
C	-0.1325830	0.1589487	-3.5374140
C	-3.9698620	1.7519138	-0.9992098
C	-2.2661369	1.1548981	-2.8003446
H	-4.5206592	1.0883398	-4.4086391
H	-4.4748279	2.6990894	-3.6303714
C	0.7197888	-1.0367263	-3.9602072
C	-1.4785915	0.0079273	-3.0983877
C	-3.7255145	1.0689117	-2.3543795
H	1.9270873	-1.1346230	-2.1280505
H	-3.3496190	1.2896956	-0.2080980
H	2.7137060	-0.2294997	-3.4557978
H	0.3968088	3.8478362	-1.0026718
H	-3.7449273	2.8387291	-1.0287505
H	2.1238869	3.6489952	-4.4193839
H	0.1593266	-1.9594693	-3.7051562
H	-3.9761261	-0.0014088	-2.2171068
H	1.4660142	1.5584747	-3.9315156
H	-1.4584329	4.5131089	2.1123735
H	-0.7988892	3.5167476	3.4335500
H	0.7810566	6.1470916	1.4046115
C	5.9724656	9.6875109	-2.9133172
C	5.1066408	8.7821803	-2.2923452
C	4.7764847	7.5685428	-2.9382824
C	5.3199107	7.2735027	-4.2076542
C	6.1875829	8.1830727	-4.8276942
C	6.5126357	9.3879018	-4.1800817
H	6.2332422	10.6336808	-2.4150542
H	4.6686079	8.9871307	-1.3034803
C	3.8636518	6.6022153	-2.2957607
H	5.0566077	6.3247085	-4.7034024
H	6.6130585	7.9556354	-5.8167351
H	7.1943575	10.1029122	-4.6662111
O	3.3351359	6.7601517	-1.1981909

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TS-7-d-ma



Energy (Hartree)= -11969.98520766
number of imaginary frequencies: 4

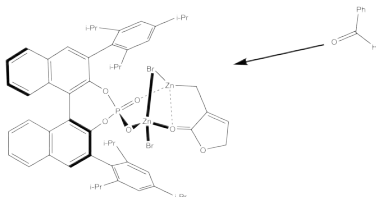
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Br	4.3356808	0.6737956	-0.2952001
C	1.3005628	5.1361689	1.5413384
C	0.6785463	3.9882908	1.9531547
C	1.7118640	2.9464777	1.8412352
O	2.8874816	3.4415011	1.4507247
C	2.7252620	4.8571856	1.2154053
O	1.5527349	1.7171703	2.0301528
C	-0.6976149	3.6658780	2.3592806
H	2.9943919	5.0775341	0.1598840
H	3.4498427	5.4008782	1.8611463
Zn	-1.5517416	1.9141665	1.8305597
Br	-3.5425206	1.3073083	2.9161432
C	-0.9310450	-3.3328971	1.0473127
C	-1.1843065	-4.0037347	-0.1523986
C	-0.6938451	-5.3567535	-0.2809155
C	-0.7393416	-6.0819513	-1.5092783
C	-0.0910922	-5.9949033	0.8653008
C	0.3713358	-7.3398336	0.7504237
C	0.0612066	-5.2677355	2.0818881
H	0.5045665	-5.7773709	2.9503053
C	-0.3109715	-3.9350718	2.1900646
C	-2.0104651	-1.3447530	-2.8033457
C	-3.0643381	-1.9443341	-3.4805728
H	-3.5064059	-1.4335526	-4.3501477
C	-3.6282034	-3.1786706	-3.0446168
C	-4.7670951	-3.7387387	-3.6970911
C	-3.0700360	-3.8563047	-1.8973958
C	-3.7272298	-5.0305715	-1.4221674
C	-1.8972192	-3.3056331	-1.2600285
C	-1.4443168	-2.0588368	-1.7017652
O	-1.3265356	-1.9973305	1.1739957
O	-0.3335257	-1.4834336	-1.1010801
P	-0.3789839	-0.8898784	0.4270439
O	1.0861372	-1.0270450	0.8992911
O	-1.0344646	0.4825652	0.5143595
C	0.2828187	-8.0267568	-0.4507426
C	-0.2629604	-7.3831668	-1.5923153
H	0.8165023	-7.8181871	1.6370775
H	0.6492044	-9.0619160	-0.5255384
H	-1.1500936	-5.5934470	-2.4033612
H	-0.3047217	-7.9171128	-2.5539100
C	-4.8448242	-5.5387678	-2.0696216
C	-5.3624633	-4.8991283	-3.2266917
H	-3.3434969	-5.5297896	-0.5217302
H	-5.3371108	-6.4416666	-1.6772703
H	-6.2448091	-5.3150800	-3.7364135
H	-5.1758316	-3.2171365	-4.5768524

C	1.1638195	-2.5749678	3.7516505
C	-0.1213907	-3.0756756	3.3997953
C	1.2410360	-1.5686841	4.7313934
C	-1.2777516	-2.6334030	4.0993423
C	-1.1465068	-1.6112516	5.0537977
C	0.0997798	-1.0377118	5.3575432
H	2.2238620	-1.1506705	5.0015293
C	-2.6359832	-3.2965028	3.8765227
H	-2.0523730	-1.2364343	5.5532069
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H	-4.7173192	-2.8531243	3.3947411
H	-3.5516700	-1.6235393	2.7886857
C	-2.9432847	-4.2399498	5.0569270
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H	-3.8998540	-4.7781179	4.8918996
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C	3.5562867	-2.1110691	2.9041629
H	4.4351502	-2.5783358	2.4173768
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H	3.2279906	-1.2938554	2.2263261
C	2.9822092	-4.2994047	3.9855165
H	2.1689061	-3.5455790	2.1290079
H	3.8609293	-4.7770472	3.5045103
H	2.2136691	-5.0792687	4.1510555
H	3.2942761	-3.9314002	4.9852445
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H	1.4617747	-0.0885014	-5.8268767
H	-5.7406208	1.4897189	-3.0998360
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C	1.1863677	4.3504880	-4.3635884
H	1.5463210	5.3974836	-4.2864528
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C	-3.9730639	1.7320927	-0.9654769
C	-2.2772985	1.1608290	-2.7833583
H	-4.5420060	1.0862783	-4.3759918
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H	-3.3450397	1.2713465	-0.1798327
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H	-3.9730161	-0.0130691	-2.1945435
H	1.4473651	1.5996648	-3.9249065
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H	5.0206344	6.2925580	-4.7575736
H	6.5617641	7.9211101	-5.8971197
H	7.1676716	10.0653378	-4.7552909
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C	-0.6752709	3.5899279	1.0530803
C	-2.4007763	4.0709311	-0.5945642
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C	-1.7404129	1.0728185	3.4994226
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C	-1.9167061	3.4412049	4.4117354
H	-0.2154485	2.5843475	3.4258422
H	-3.0263219	3.4384115	4.3739884
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H	-1.6153639	3.0851811	5.4188190
C	-4.8691514	3.6649053	-0.1457792
C	-5.6085165	2.3255594	0.0007206
H	-6.6550205	2.4179506	-0.3571455
H	-5.6487854	1.9921596	1.0585840
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C	-5.5756033	4.7914754	0.6339753
H	-4.8856832	3.9382206	-1.2235802
H	-6.6279994	4.9093997	0.3010617
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H	-5.5866868	4.5732587	1.7228484
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H	1.9010366	-4.3777709	2.6564780
C	2.8093546	-3.8018548	-2.6986477
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H	2.0662910	-3.5122466	-5.4961663
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H	3.9570394	-6.1812647	-3.4975056
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H	2.9984007	-6.4249502	-4.9973110
H	2.5027167	-5.1398865	-1.0308893
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H	6.0994770	0.4682996	-3.6997969
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C	3.7764305	-1.6114289	-2.1301601
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C	4.3322849	-0.2799699	-2.6327485
C	3.7848148	-1.9667678	-0.7517432
C	3.3058375	-3.7196458	1.1091543
H	2.3664812	0.6399248	-2.9611856
H	1.2467457	-3.1383713	1.5458730
H	3.1094830	-0.0351661	-4.4525364
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H	1.4061422	-4.8488215	1.0014169

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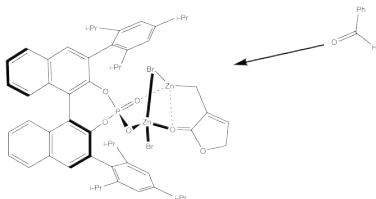


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C	3.5099681	6.1578504	1.8843337
C	1.4307572	4.8274346	1.6586940
H	0.8484220	5.7609123	1.6887595
C	0.7681860	3.6253403	1.4423629
C	4.2020949	-0.9805216	0.2907763
C	5.2835162	-1.2009663	1.1377104
H	5.9225962	-2.0828256	0.9746735
C	5.5479470	-0.3588928	2.2551340
C	6.5898449	-0.6663865	3.1818647
C	4.7173231	0.7986416	2.4852709
C	4.9259269	1.5518993	3.6798125
C	3.6951657	1.1321099	1.5211581
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O	0.8656763	1.2198104	1.4489579
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P	0.8438123	0.3373186	0.0679445
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H	2.8934274	7.0641819	1.9920092
H	5.3913160	7.2203337	1.9472884
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H	6.7623829	5.1386234	1.5918513
C	5.9319633	1.2127726	4.5742619
C	6.7849757	0.1059015	4.3171625
H	4.2685216	2.4057113	3.8949356
H	6.0650885	1.8039530	5.4931280
H	7.5856542	-0.1470759	5.0287932
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H	4.1193300	-5.0287851	-4.8585580	O	0.4418695	-1.0816887	0.4360585
H	4.5591988	0.3506410	-1.7501243	C	4.8906467	6.2427415	1.8516307
H	3.6668799	-2.8841144	1.7389516	C	5.6637117	5.0671880	1.6616313
H	3.2730978	-2.2452718	-4.1334663	H	2.8908775	7.0619423	1.9925748
Zn	-1.3685685	0.7445037	-2.2197398	H	5.3879766	7.2197828	1.9484577
Br	-3.2375624	1.5639802	-3.2343475	H	5.6670958	2.9308463	1.3962554
C	-10.6086237	-5.4380676	1.5465278	H	6.7599386	5.1389660	1.5935027
C	-9.6734327	-4.6466945	0.8714690	C	5.9316147	1.2133929	4.5734615
C	-9.6568942	-3.2481848	1.0710711	C	6.7845053	0.1069533	4.3172969
C	-10.5842260	-2.6529776	1.9518498	H	4.2682458	2.4057514	3.8920657
C	-11.5242969	-3.4470868	2.6248877	H	6.0641191	1.8049147	5.4921190
C	-11.5353917	-4.8381893	2.4219928	H	7.5847549	-0.1460804	5.0292931
H	-10.6221931	-6.5284146	1.3951715	H	7.2244404	-1.5439996	2.9872357
C	-8.6695579	-2.4061627	0.3487428	C	-1.0415290	4.0832499	-0.2351982
H	-10.5641660	-1.5610761	2.1034182	C	-0.6758171	3.5878875	1.0513950
H	-12.2510302	-2.9842003	3.3098487	C	-2.4008336	4.0712444	-0.5954391
H	-12.2723130	-5.4627225	2.9506873	C	-1.6661953	3.0645601	1.9239344
O	-7.8533174	-2.8284011	-0.4572318	C	-3.0104338	3.0745788	1.5088300
C	-2.4583342	-4.2674696	-3.0323438	C	-3.4036502	3.5839323	0.2595196
C	-1.5158064	-3.5611172	-2.3354362	C	-1.3190284	2.5369034	3.3139116
C	-1.6006806	-2.1906539	-2.8684804	H	-3.7769136	2.6802887	2.1945930
O	-2.4818863	-2.0862800	-3.8633302	C	-1.7405187	1.0700124	3.4958678
C	-3.1177379	-3.3769585	-4.0315818	H	-2.8401175	0.9422884	3.4205521
O	-0.9621509	-1.2084553	-2.4332353	H	-1.4321799	0.6946229	4.4933686
C	-0.5991713	-3.8568984	-1.2300647	H	-1.2837641	0.4127133	2.7325925
H	-2.9758024	-3.6954771	-5.0875779	C	-1.9169042	3.4377194	4.4108941
H	-4.2070355	-3.2277754	-3.8640683	H	-0.2159211	2.5821906	3.4240626
Zn	-0.9317591	-2.5615650	0.2687639	H	-3.0264508	3.4353470	4.3740920
Br	-2.6743666	-2.1451037	1.7567305	H	-1.5799252	4.4887273	4.3022932
H	0.4406768	-3.5862287	-1.5062952	H	-1.6159875	3.0803503	5.4175446
H	-0.6404516	-4.9149148	-0.9115240	C	-4.8694220	3.6694009	-0.1453151
H	-8.9365843	-5.0830241	0.1795309	C	-5.6106397	2.3311711	0.0001391
H	-2.7252696	-5.3244952	-2.9003436	H	-6.6572739	2.4252935	-0.3566362
H	-8.7256210	-1.3043005	0.5997139	H	-5.6507623	1.9959055	1.0573591
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				C	-5.5733470	4.7969269	0.6351546
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				H	-6.6257158	4.9173879	0.3031438
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				C	-0.0227002	4.6531263	-1.2269730
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				H	0.6366206	4.4824323	-3.3051695
				H	-1.1185852	4.1992294	-3.1002650
				H	0.0641328	2.9470350	-2.5985815
				C	-0.1356260	6.1883422	-1.3025783
				H	0.9909304	4.4113209	-0.8495192
				H	0.6390371	6.6096821	-1.9764951
				H	-0.0128690	6.6568738	-0.3057388
				H	-1.1286290	6.4950715	-1.6923532
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				H	5.5216969	-1.1256378	-4.2824878
				H	4.2943338	-5.1899000	2.4028922
				C	2.2607705	-4.7950286	-3.7152196
				H	3.7262601	1.4943499	-3.7624654
				H	0.9505708	-4.9026541	-5.4650569
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				C	2.8087302	-3.8000878	-2.6985624
				C	5.6648473	-0.5000302	-3.3766021
				C	1.4354388	-4.1335369	-4.8297518
				H	2.0671264	-3.5117632	-5.4974856
				C	3.2850464	-2.5326233	-3.0709487
				C	4.2656502	-4.9022512	1.3317087
				H	3.9552144	-6.1800891	-3.4957844
				C	2.8681068	-4.1439437	-1.3375513
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				H	2.9982390	-6.4247647	-4.9965426
				H	2.5017644	-5.1378112	-1.0309244
				C	3.3240954	0.4942846	-3.4998677
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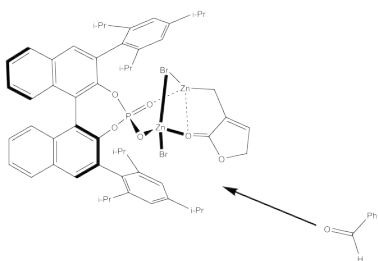


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C	5.0511430	3.8261542	1.5533307
C	2.8470820	4.8979178	1.7539143
C	3.5079106	6.1559128	1.8852334
C	1.4295689	4.8236176	1.6589853
H	0.8449482	5.7556776	1.6894378
C	0.7674658	3.6216954	1.4407106
C	4.2045565	-0.9802498	0.2900665
C	5.2850539	-1.2005503	1.1377976
H	5.9230595	-2.0831765	0.9747662
C	5.5490605	-0.3586088	2.2550894
C	6.5899501	-0.6651691	3.1824740
C	4.7181763	0.7986195	2.4846123
C	4.9261081	1.5519521	3.6789140
C	3.6968055	1.1321401	1.5200021
C	3.4344798	0.2065269	0.5010077
O	0.8662372	1.2158001	1.4435410
O	2.4167075	0.4612332	-0.4125693
P	0.8485149	0.3323235	0.0642492
O	0.0793559	1.0934607	-1.0397176

C	3.7774696	-1.6108228	-2.1302420	H	3.3309600	2.8093321	-0.8071715
C	1.8842211	-4.0430245	1.5994612	H	4.1992374	3.4141351	0.6438570
C	3.3337789	-3.2569178	-0.3498767	Zn	-0.7812931	0.9947559	2.4916919
H	5.2984753	-4.6493735	1.0157202	Br	-1.6148780	0.2009136	4.5360874
H	3.9533725	-5.7964723	0.7526968	C	-1.3757339	-4.0014745	0.4437065
C	4.3332647	-0.2794953	-2.6331210	C	-2.2202208	-4.1989817	-0.6512032
C	3.7866775	-1.9664215	-0.7521207	C	-2.2953938	-5.5304582	-1.2140335
C	3.3064486	-3.7186173	1.1088683	C	-3.0012376	-5.8299486	-2.4185676
H	2.3678066	0.6409958	-2.9613076	C	-1.6062257	-6.6126822	-0.5494565
H	1.2480123	-3.1366758	1.5487697	C	-1.7318675	-7.9410978	-1.0559233
H	3.1100184	-0.0331130	-4.4530416	C	-0.7516070	-6.3317474	0.5555918
H	0.6416889	-3.4806961	-4.4135836	H	-0.1800157	-7.1552380	1.0101425
H	1.4059639	-4.8467485	1.0022962	C	-0.5755660	-5.0370938	1.0196712
H	4.1195417	-5.0293200	-4.8560822	C	-2.8217292	-0.7997324	-2.3289552
H	4.5600555	0.3510255	-1.7504792	C	-4.1478598	-0.9326987	-2.7255969
H	3.6675340	-2.8827160	1.7381879	H	-4.6058536	-0.1446890	-3.3418059
H	3.2718631	-2.2429464	-4.1326922	C	-4.9533083	-2.0299957	-2.3076921
Zn	-1.3949349	0.7428883	-2.1770038	C	-6.3463612	-2.0860629	-2.6154256
Br	-3.2251235	1.5529625	-3.2488011	C	-4.3613495	-3.0867214	-1.5245966
C	-10.6081764	-5.4373116	1.5481877	C	-5.2135287	-4.1170573	-1.0246787
C	-9.6730684	-4.6449543	0.8748624	C	-2.9455676	-3.0439790	-1.2466279
C	-9.6584875	-3.2471426	1.0735975	C	-2.2478476	-1.8737484	-1.5796629
C	-10.5878083	-2.6539417	1.9520783	O	-1.3196163	-2.7506146	1.0482296
C	-11.5281921	-3.4485248	2.6235713	O	-0.9021707	-1.7485495	-1.2422071
C	-11.5372656	-4.8391188	2.4213349	P	-0.4938368	-1.5144222	0.3339271
H	-10.6198348	-6.5277973	1.3973988	O	1.0262489	-1.7531581	0.3543723
C	-8.6680642	-2.4070298	0.3483287	O	-1.0633977	-0.2255981	0.9114793
H	-10.5688131	-1.5618214	2.1031787	C	-2.4693180	-8.2019531	-2.2008358
H	-12.2567916	-2.9864636	3.3071344	C	-3.0886150	-7.1305834	-2.8972450
H	-12.2742895	-5.4644147	2.9489722	H	-1.2142934	-8.7554992	-0.5249101
O	-7.8567123	-2.8321653	-0.4570297	H	-2.5575213	-9.2307642	-2.5817982
C	-2.4596765	-4.2665255	-3.0268680	H	-3.4798208	-5.0151944	-2.9777848
C	-1.5126553	-3.5612258	-2.3340536	H	-3.6406506	-7.3302875	-3.8283199
C	-1.5927382	-2.1908836	-2.8749579	C	-6.5699676	-4.1294096	-1.3194568
O	-2.4758293	-2.0905648	-3.8709260	C	-7.1411659	-3.1167159	-2.1361749
C	-3.1168180	-3.3767027	-4.0300145	H	-4.7860593	-4.9010334	-0.3839595
O	-0.9535427	-1.2074072	-2.4494826	H	-7.2086617	-4.9271794	-0.9105303
C	-0.6001053	-3.8545625	-1.2277962	H	-8.2162880	-3.1423713	-2.3704916
H	-2.9773106	-3.7008714	-5.0853248	H	-6.7827058	-1.2794406	-3.2253257
H	-4.2057487	-3.2205093	-3.8630059	C	1.8118395	-4.4644877	1.5129115
Zn	-0.9471996	-2.5623102	0.2793266	C	0.4815731	-4.6087517	1.9832270
Br	-2.6675568	-2.1679766	1.7743832	C	2.7585421	-3.8461457	2.3686239
H	0.4400002	-3.5785431	-1.4969716	C	0.1237300	-4.1999794	3.2974644
H	-0.6415484	-4.9125932	-0.9088921	C	1.0817897	-3.5529244	4.0963270
H	-8.9323591	-5.0760357	0.1837991	C	2.4086401	-3.3669639	3.6590887
H	-2.7307000	-5.3214182	-2.8873296	H	3.8197400	-3.8297570	2.0747867
H	-8.7218849	-1.3033818	0.5998669	C	-1.2570903	-4.5252316	3.8560794
H	-2.6985800	4.4543679	-1.5842023	H	0.7963884	-3.2181148	5.1054524

TS-7-j-ma; COSMO



Energy (Hartree) = -11969.99664762

Zn	2.5636764	-1.4943832	1.5264064
Br	4.8838695	-1.2431614	1.3335646
C	2.0241398	3.5786263	0.7887120
C	1.3376422	2.7240842	1.6040329
C	2.1191710	1.4688208	1.5923372
O	3.2279319	1.5871068	0.8593427
C	3.2658661	2.9177068	0.2972901
O	1.7946548	0.3864679	2.1357738
C	0.0666572	2.8139839	2.3401891

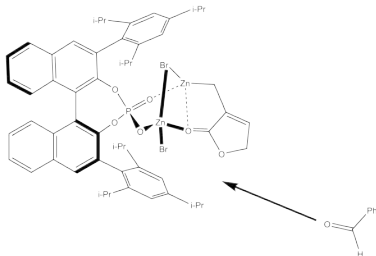
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Br	-1.6148780	0.2009136	4.5360874
C	-1.3757339	-4.0014745	0.4437065
C	-2.2202208	-4.1989817	-0.6512032
C	-2.2953938	-5.5304582	-1.2140335
C	-3.0012376	-5.8299486	-2.4185676
C	-1.6062257	-6.6126822	-0.5494565
C	-1.7318675	-7.9410978	-1.0559233
C	-0.7516070	-6.3317474	0.5555918
H	-0.1800157	-7.1552380	1.0101425
C	-0.5755660	-5.0370938	1.0196712
C	-2.8217292	-0.7997324	-2.3289552
C	-4.1478598	-0.9326987	-2.7255969
H	-4.6058536	-0.1446890	-3.3418059
C	-4.9533083	-2.0299957	-2.3076921
C	-6.3463612	-2.0860629	-2.6154256
C	-4.3613495	-3.0867214	-1.5245966
C	-5.2135287	-4.1170573	-1.0246787
C	-2.9455676	-3.0439790	-1.2466279
C	-2.2478476	-1.8737484	-1.5796629
O	-1.3196163	-2.7506146	1.0482296
O	-0.9021707	-1.7485495	-1.2422071
P	-0.4938368	-1.5144222	0.3339271
O	1.0262489	-1.7531581	0.3543723
O	-1.0633977	-0.2255981	0.9114793
C	-2.4693180	-8.2019531	-2.2008358
C	-3.0886150	-7.1305834	-2.8972450
H	-1.2142934	-8.7554992	-0.5249101
H	-2.5575213	-9.2307642	-2.5817982
H	-3.4798208	-5.0151944	-2.9777848
H	-3.6406506	-7.3302875	-3.8283199
C	-6.5699676	-4.1294096	-1.3194568
C	-7.1411659	-3.1167159	-2.1361749
H	-4.7860593	-4.9010334	-0.3839595
H	-7.2086617	-4.9271794	-0.9105303
H	-8.2162880	-3.1423713	-2.3704916
H	-6.7827058	-1.2794406	-3.2253257
C	1.8118395	-4.4644877	1.5129115
C	0.4815731	-4.6087517	1.9832270
C	2.7585421	-3.8461457	2.3686239
C	0.1237300	-4.1999794	3.2974644
C	1.0817897	-3.5529244	4.0963270
C	2.4086401	-3.3669639	3.6590887
H	3.8197400	-3.8297570	2.0747867
C	-1.2570903	-4.5252316	3.8560794
H	0.7963884	-3.2181148	5.1054524
C	-2.0065640	-3.2950347	4.3771666
H	-1.4900017	-2.8253430	5.2384758
H	-3.0254558	-3.5770698	4.7131031
H	-2.0990278	-2.5171902	3.5970681
C	-1.1388368	-5.6192830	4.9359865
H	-1.8527530	-4.9531066	3.0232033
H	-0.5508071	-5.2604752	5.8068054
H	-0.6425308	-6.5304301	4.5441005
H	-2.1452157	-5.9051953	5.3052484
C	3.4785055	-2.8005450	4.5846534
C	3.1250875	-1.3962336	5.0996522
H	3.9178729	-1.0212722	5.7782488
H	2.1652283	-1.3841672	5.6562307
H	3.0329624	-0.6746032	4.2616962
C	3.7576560	-3.7851809	5.7367810
H	4.4079465	-2.7099718	3.9819674
H	4.5978724	-3.4229439	6.3638512
H	4.0250749	-4.7902622	5.3518655
H	2.8700328	-3.9002602	6.3932507
C	2.2523141	-5.0084043	0.1553166
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H	3.4223828	-4.5349590	-1.6177325
H	4.1385028	-3.8765839	-0.1202422

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H	1.3370697	-5.1470811	-0.4541353
H	3.1568353	-6.8403528	-0.6413145
H	2.2190928	-7.0983020	0.8672453
H	3.8310046	-6.3233011	0.9392012
H	0.1657545	4.7015390	-2.5930722
H	-0.1128760	-0.0418332	-6.1946363
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C	0.3360637	4.0126262	-3.4506675
H	1.1734901	-2.3450136	-4.3796471
H	2.3863764	4.7500424	-3.6631740
H	-4.0265695	2.4978302	0.9545975
C	-0.4504728	2.7421475	-3.1498515
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H	2.1071774	3.1797239	-4.4637266
C	-0.1414194	1.5107821	-3.7521244
C	-4.7311943	2.4719867	-1.7692843
H	-1.3023584	4.9156608	-4.6100520
C	-1.5574642	2.7889093	-2.2857803
C	-0.2196570	4.7010272	-4.7133272
C	0.3057353	5.6584357	-4.9120925
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C	0.9451734	-1.3643348	-3.9129792
H	-0.5123994	-1.7877105	-6.2493150
H	-1.8058803	-0.5765003	-5.9579841
C	-0.8944208	0.3476857	-3.5074659
C	-3.1866569	2.5532635	0.2325857
C	-2.3480942	1.6588627	-2.0088135
H	-5.0382456	1.9178693	-2.6786962
H	-4.4709835	3.5044629	-2.0842984
C	-0.5031043	-0.9445187	-4.2231903
C	-2.0123907	0.4220514	-2.6311151
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H	1.1046503	-1.4575656	-2.8209181
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H	1.6778462	-0.6310544	-4.3103766
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H	-0.0902371	4.0485489	-5.6024479
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H	-0.5694094	3.6391188	1.9669128
H	1.7455521	4.6100255	0.5324111
C	2.9451458	15.0490692	1.0489752
C	3.3109334	13.7274932	1.3253793
C	4.6733142	13.3941977	1.4961733
C	5.6613841	14.3953282	1.3879268
C	5.2933037	15.7196248	1.1099018
C	3.9360872	16.0449598	0.9407717
H	1.8847195	15.3129445	0.9158350
H	2.5616195	12.9259438	1.4161743
C	5.0680661	11.9935215	1.7873872
H	6.7220554	14.1262950	1.5231332
H	6.0629405	16.5017817	1.0242710
H	3.6456745	17.0844452	0.7225234
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C	1.3315563	2.7322935	1.6082328
C	2.1170083	1.4768154	1.5986155
O	3.2316141	1.6012396	0.8719576
C	3.2688642	2.9303303	0.3127156
O	1.7935358	0.3940805	2.1352432
C	0.0570774	2.8162568	2.3343070
H	3.3385701	2.8232286	-0.7920561
H	4.2009168	3.4277038	0.6635428
Zn	-0.8038794	0.9971370	2.4973317
Br	-1.6343125	0.2090968	4.5271055
C	-1.3729990	-3.9972700	0.4431474
C	-2.2189421	-4.1974788	-0.6506706
C	-2.2955468	-5.5296842	-1.2116966
C	-3.0018102	-5.8302200	-2.4155938
C	-1.6071938	-6.6117444	-0.5466878
C	-1.7334678	-7.9398641	-1.0525174
C	-0.7534047	-6.3291900	0.5580264
H	-0.1817649	-7.1517341	1.0143667
C	-0.5751762	-5.0343795	1.0204146
C	-2.8211863	-0.8011801	-2.3315015
C	-4.1473839	-0.9345919	-2.7268942
H	-4.6046844	-0.1459635	-3.3427852
C	-4.9529283	-2.0310513	-2.3080549
C	-6.3458671	-2.0876354	-2.6140015
C	-4.3603081	-3.0868774	-1.5246977
C	-5.2121506	-4.1167110	-1.0238179
C	-2.9444366	-3.0439082	-1.2478328
C	-2.2459631	-1.8746878	-1.5824090
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O	-1.0519799	-0.2151785	0.8970740
C	-2.4706599	-8.2015709	-2.1967363
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H	-1.2158209	-8.7539386	-0.5210324
H	-2.5587818	-9.2306135	-2.5770029
H	-3.4803825	-5.0152720	-2.9743529
H	-3.6421342	-7.3308069	-3.8238524
C	-6.5683465	-4.1293970	-1.3176556
C	-7.1402189	-3.1174623	-2.1338126
H	-4.7832098	-4.8999162	-0.3833537
H	-7.2065384	-4.9269063	-0.9075816
H	-8.2156031	-3.1426847	-2.3667332
H	-6.7826854	-1.2808580	-3.2233418
C	1.8134614	-4.4685615	1.5139822
C	0.4826188	-4.6094684	1.9843045
C	2.7619410	-3.8564488	2.3708273
C	0.1256073	-4.2015665	3.2986372
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C	2.4137067	-3.3779855	3.6611998
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C	-2.0011937	-3.2854545	4.3758943
H	-1.4835352	-2.8148604	5.2359776
H	-3.0209080	-3.5616198	4.7137377
H	-2.0933763	-2.5077128	3.5958148
C	-1.1442913	-5.6137814	4.9372062
H	-1.8537289	-4.9460290	3.0236252
H	-0.5552980	-5.2576995	5.8084059
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H	-2.1516533	-5.8951029	5.3071614
C	3.4850763	-2.8129840	4.5858674
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TS-7-j-ma

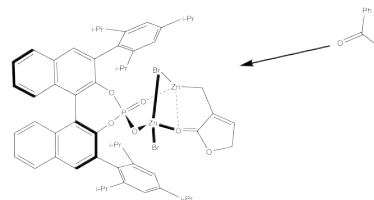


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H	4.4138545	-2.7228847	3.9819515
H	4.6039162	-3.4391694	6.3655574
H	4.0263539	-4.8041496	5.3536010
H	2.8752822	-3.9115629	6.3949861
C	2.2521421	-5.0101691	0.1544664
C	3.1791972	-4.0770248	-0.6385562
H	3.4237707	-4.5360634	-1.6180519
H	4.1390878	-3.8762220	-0.1210097
H	2.6879829	-3.1049557	-0.8407109
C	2.8955652	-6.3999593	0.3382542
H	1.3361188	-5.1463741	-0.4544845
H	3.1538389	-6.8432654	-0.6454003
H	2.2161199	-7.1010255	0.8629323
H	3.8287117	-6.3294239	0.9352519
H	0.1645160	4.6996898	-2.5940472
H	-0.1144008	-0.0428508	-6.1971964
H	-5.6118322	2.5315927	-1.0999022
C	0.3340003	4.0116909	-3.4528168
H	1.1746054	-2.3457834	-4.3809526
H	2.3851209	4.7495786	-3.6660453
H	-4.0286637	2.4955237	0.9511084
C	-0.4517594	2.7406967	-3.1521461
C	-0.7488901	-0.8316184	-5.7413067
C	1.8480680	3.7837772	-3.5716014
H	2.1056141	3.1804149	-4.4664568
C	-0.1419717	1.5096551	-3.7538329
C	-4.7328295	2.4698908	-1.7743611
H	-1.3052728	4.9145206	-4.6096050
C	-1.5591489	2.7872500	-2.2892036
C	-0.2226139	4.7014499	-4.7140319
H	0.3015720	5.6593648	-4.9134586
H	-1.8096934	3.7459589	-1.8067046
C	0.9457220	-1.3651171	-3.9147974
H	-0.5124637	-1.7884770	-6.2514690
H	-1.8060918	-0.5777633	-5.9590723
C	-0.8945776	0.3465470	-3.5096623
C	-3.1898010	2.5523434	0.2282070
C	-2.3496590	1.6574459	-2.0124997
H	-5.0392497	1.9160444	-2.6840130
H	-4.4732055	3.5020872	-2.0904400
C	-0.5024883	-0.9455751	-4.2250091
C	-2.0129072	0.4208670	-2.6341970
C	-3.5403623	1.7992142	-1.0643863
H	1.1060876	-1.4582588	-2.8230358
H	-2.2910793	2.1184606	0.7065285
H	1.6790806	-0.6326420	-4.3123207
H	2.2467901	3.2490695	-2.6854880
H	-2.9847562	3.6281156	0.0473218
H	-0.0951645	4.0495868	-5.6036241
H	-1.1642553	-1.7539933	-3.8541702
H	-3.8515228	0.7780962	-0.7654716
H	0.7165561	1.4447201	-4.4400689
H	0.2471651	2.9863717	3.4181033
H	-0.5740009	3.6483976	1.9683242
H	1.7431055	4.6214889	0.5460203
C	2.9463326	15.0494712	1.0493946
C	3.3126372	13.7284608	1.3262309
C	4.6743444	13.3956035	1.4967629
C	5.6609376	14.3967766	1.3878426
C	5.2929048	15.7206568	1.1092432
C	3.9361613	16.0455064	0.9403308
H	1.8857527	15.3129618	0.9165248
H	2.5669643	12.9237026	1.4184636
C	5.0653234	11.9915273	1.7881610
H	6.7217033	14.1275283	1.5231169
H	6.0622256	16.5030660	1.0230058
H	3.6454449	17.0847952	0.7216436
O	4.2864812	11.0583500	1.8905956

H 6.1817751 11.8393013 1.9128988

TS-7-j-mi; COSMO

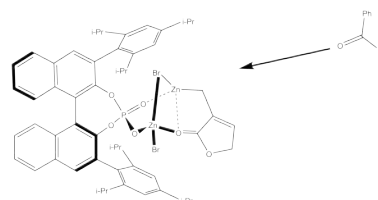


Energy (Hartree) = -11969.99218699

Zn	2.5727322	1.4037960	-0.4587100
Br	4.5126902	2.3006365	-1.2525462
C	0.4891964	5.1846506	2.6447598
C	0.1044175	4.2063235	1.7685688
C	1.3410845	3.4753481	1.4505931
O	2.4104043	3.9909451	2.0575832
C	1.9612448	5.0989879	2.8777552
O	1.3996756	2.4604331	0.7289973
C	-1.1588332	3.7765521	1.1638954
H	2.5215641	6.0062176	2.5621515
H	2.2490622	4.8696785	3.9273231
Zn	-1.4842374	1.8003833	1.3858360
Br	-2.3058189	0.4399348	3.0877729
H	-1.0694225	3.8037667	0.0576797
H	-2.0186732	4.3940624	1.4840758
H	-0.1503241	5.9440895	3.1143893
C	-0.1844865	-2.7512525	-1.7180671
C	-0.7281868	-2.7665519	-3.0086552
C	-0.2876069	-3.8085142	-3.9114151
C	-0.6150657	-3.8263853	-5.3014941
C	0.5576219	-4.8630567	-3.4034642
C	0.9588786	-5.9214137	-4.2736106
C	1.0350117	-4.7988282	-2.0635931
H	1.7053786	-5.5927745	-1.7010216
C	0.7370531	-3.7292904	-1.2287571
C	-2.0412132	0.7471921	-3.8471016
C	-3.1636396	0.4420065	-4.6088090
H	-3.7215180	1.2534468	-5.1015621
C	-3.6454329	-0.8942733	-4.7312174
C	-4.8615839	-1.1780307	-5.4232322
C	-2.9170686	-1.9782886	-4.1149243
C	-3.4834663	-3.2871699	-4.1629615
C	-1.6615547	-1.6950761	-3.4601819
C	-1.3092613	-0.3516270	-3.2923135
O	-0.5810643	-1.7634125	-0.8164848
O	-0.1349592	-0.0414173	-2.6196299
P	-0.0469659	-0.2276826	-0.9889623
O	1.4705690	-0.1328592	-0.7036590
O	-1.0035546	0.6756563	-0.2324793
C	0.5867749	-5.9279158	-5.6093342
C	-0.1896558	-4.8578833	-6.1280486
H	1.5911398	-6.7247953	-3.8638881
H	0.9090281	-6.7458299	-6.2716494
H	-1.2040029	-3.0027597	-5.7265097
H	-0.4525150	-4.8406098	-7.1968564
C	-4.6812980	-3.5257314	-4.8232745
C	-5.3697032	-2.4676967	-5.4749406
H	-2.9626569	-4.1129223	-3.6581047
H	-5.1023407	-4.5426271	-4.8372894
H	-6.3131553	-2.6704078	-6.0043989
H	-5.4005836	-0.3447545	-5.9010489
C	2.7755611	-3.1408631	0.1301533

C	1.4035681	-3.5248221	0.0949929	H	0.0945198	7.0579331	-3.6601838
C	3.3647631	-2.8756205	1.3800074	H	0.1039225	0.7837531	-5.0343530
C	0.6644358	-3.6450381	1.3018295	H	-4.1460572	1.7353812	-2.8920842
C	1.3034797	-3.3669498	2.5233366	H	1.2513967	4.0575250	-3.6208736
C	2.6508856	-2.9726285	2.5875972	C	-3.5925383	-1.4395976	9.2258969
H	4.4249825	-2.5756408	1.4194107	C	-2.3503926	-1.4006505	8.5829758
C	-0.7871185	-4.1181137	1.3100965	C	-1.2233275	-0.8818187	9.2591083
H	0.7248462	-3.4584904	3.4552061	C	-1.3549361	-0.4013801	10.5794365
C	-1.7213744	-3.1381353	2.0358402	C	-2.5999975	-0.4439637	11.2234529
H	-1.4739197	-3.0501201	3.1139866	C	-3.7171572	-0.9636333	10.5462487
H	-2.7750120	-3.4797671	1.9660708	H	-4.4733462	-1.8413041	8.7018945
H	-1.6613912	-2.1212442	1.6038000	H	-2.2206384	-1.7630100	7.5514106
C	-0.8853593	-5.5398161	1.8958761	C	0.1008382	-0.8464919	8.5882031
H	-1.1271142	-4.1803555	0.2557073	H	-0.4709474	0.0038524	11.0992667
H	-0.5587097	-5.5580070	2.9568335	H	-2.7034099	-0.0727283	12.2545966
H	-0.2468472	-6.2530986	1.3353969	H	-4.6955428	-0.9978934	11.0505869
H	-1.9312705	-5.9095042	1.8584494	O	0.3283867	-1.2727741	7.4654773
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TS-7-j-mi

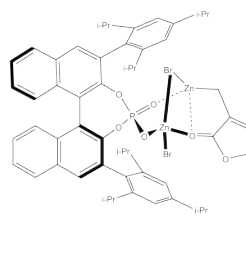


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number of imaginary frequencies: 4

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C	3.3647631	-2.8756205	1.3800074	H	0.1039225	0.7837531	-5.0343530
C	0.6644358	-3.6450381	1.3018295	H	-4.1460572	1.7353812	-2.8920842
C	1.3034797	-3.3669498	2.5233366	H	1.2513967	4.0575250	-3.6208736
C	2.6508856	-2.9726285	2.5875972	C	-3.5925383	-1.4395976	9.2258969
H	4.4249825	-2.5756408	1.4194107	C	-2.3503926	-1.4006505	8.5829758
C	-0.7871185	-4.1181137	1.3100965	C	-1.2233275	-0.8818187	9.2591083
H	0.7248462	-3.4584904	3.4552061	C	-1.3549361	-0.4013801	10.5794365
C	-1.7213744	-3.1381353	2.0358402	C	-2.5999975	-0.4439637	11.2234529
H	-1.4739197	-3.0501201	3.1139866	C	-3.7171572	-0.9636333	10.5462487
H	-2.7750120	-3.4797671	1.9660708	H	-4.4733462	-1.8413041	8.7018945
H	-1.6613912	-2.1212442	1.6038000	H	-2.2206384	-1.7630100	7.5514106
C	-0.8853593	-5.5398161	1.8958761	C	0.1008382	-0.8464919	8.5882031
H	-1.1271142	-4.1803555	0.2557073	H	-0.4709474	0.0038524	11.0992667
H	-0.5587097	-5.5580070	2.9568335	H	-2.7034099	-0.0727283	12.2545966
H	-0.2468472	-6.2530986	1.3353969	H	-4.6955428	-0.9978934	11.0505869
H	-1.9312705	-5.9095042	1.8584494	O	0.3283867	-1.2727741	7.4654773
C	3.3511260	-2.7180313	3.9175575	H	0.9223092	-0.3810273	9.2127556
C	2.4876523	-1.9479785	4.9280264				
H	3.0708524	-1.6988425	5.8376399				
H	1.6103019	-2.5331564	5.2699508				
H	2.0987615	-1.0023351	4.4993635				
C	3.8560415	-4.0485089	4.5120208				
H	4.2467213	-2.0967289	3.6912537				
H	4.4221375	-3.8775267	5.4514472				
H	4.5191933	-4.5819641	3.8008546				
H	3.0034987	-4.7207626	4.7448747				
C	3.6300231	-3.0398662	-1.1350187				
C	4.4673896	-1.7543630	-1.2133864				
H	5.0055912	-1.6998125	-2.1817581				
H	5.2306708	-1.6935399	-0.4106070				
H	3.8264135	-0.8562018	-1.1431152				
C	4.5332090	-4.2814679	-1.2762534				
H	2.9420549	-3.0254735	-2.0043838				
H	5.1125486	-4.2449400	-2.2223748				
H	3.9444661	-5.2205615	-1.2711807				
H	5.2565290	-4.3398591	-0.4358576				
H	-0.4393925	5.9061950	-0.8452561				
H	1.0247836	3.4948323	-6.1797322				
H	-5.8665967	3.4137349	-2.3890989				
C	0.0437453	5.8257154	-1.8450810	Zn	2.5909993	1.3630406	-0.3837826
H	2.5624882	0.8864673	-5.1099838	Br	4.5897278	2.2472831	-0.9973288
H	1.9007810	6.5990361	-0.9826980	C	0.4692752	5.2042964	2.6245033
H	-4.9608233	1.9015572	-0.5510169	C	0.0984695	4.2079363	1.7616581
C	-0.5272187	4.5671478	-2.4902311	C	1.3375596	3.4536720	1.5007946
C	0.5657535	2.4863183	-6.2495972	O	2.3944936	3.9764533	2.1261565
C	1.5613480	5.7549962	-1.6167923	C	1.9344136	5.1084671	2.9014194
H	2.1260611	5.8179215	-2.5702796	O	1.4076695	2.4169180	0.8149861
C	0.2272126	3.7568476	-3.3551189	C	-1.1479977	3.7722186	1.1343676
C	-4.8291680	3.7432417	-2.6032931	H	2.5144497	6.0010970	2.5775688
H	-1.4452663	7.1687032	-2.7511323	H	2.1926367	4.9046451	3.9645385
C	-1.8532392	4.1793646	-2.2258146	Zn	-1.4789317	1.7946706	1.3962923
C	-0.3451372	7.0860163	-2.6413128	Br	-2.2639409	0.4534724	3.1075192
H	0.0198382	8.0040797	-2.1353456	H	-1.0299598	3.7635109	0.0306867
H	-2.4702238	4.8235358	-1.5780675	H	-2.0132862	4.4008902	1.4154592
C	2.0119863	1.5260117	-4.3900860	H	-0.1761954	5.9814929	3.0550345
H	1.1382095	1.9035643	-7.0009163	C	-0.1891234	-2.7416768	-1.7246666
H	-0.4690209	2.6133751	-6.6278517	C	-0.7320627	-2.7615507	-3.0155364
C	-0.2787754	2.5567471	-3.8848483	C	-0.2904422	-3.8043465	-3.9164689
C	-3.9200596	2.1765366	-0.8186685	C	-0.6170066	-3.8247949	-5.3064695
C	-2.4054639	2.9776996	-2.7090602	C	0.5555878	-4.8567261	-3.4064971
H	-4.7774684	4.0487704	-3.6682496	C	0.9598755	-5.9143905	-4.2752286
H	-4.6381280	4.6454028	-1.9853976	C	1.0308754	-4.7889069	-2.0666072
C	0.5765825	1.7748850	-4.8814987	H	1.7022897	-5.5803686	-1.7007217
C	-1.5886938	2.1332364	-3.5175356	C	0.7334521	-3.7179160	-1.2335688
C	-3.8333959	2.6118342	-2.2935966	C	-2.0471434	0.7483169	-3.8624166
H	2.0153798	1.0070058	-3.4116124	C	-3.1705648	0.4400030	-4.6212602
H	-3.2767503	1.2946205	-0.6301434	H	-3.7295331	1.2507914	-5.1140021
H	2.5903046	2.4662978	-4.2800227	C	-3.6515727	-0.8966328	-4.7405062
H	1.8625292	4.8076709	-1.1242904	C	-4.8673540	-1.1849698	-5.4304244
H	-3.6083924	2.9960442	-0.1365660	C	-2.9209655	-1.9778512	-4.1226194
				C	-3.4844348	-3.2878251	-4.1677582
				C	-1.6653591	-1.6919098	-3.4699702
				C	-1.3127826	-0.3482632	-3.3060677
				O	-0.5860208	-1.7502789	-0.8273088
				O	-0.1372479	-0.0357944	-2.6367436
				P	-0.0477249	-0.2175805	-1.0049472

O	1.4726470	-0.1341115	-0.7250102	H	1.1192489	1.9011243	-7.0266705
O	-0.9898937	0.7017577	-0.2509412	H	-0.4909221	2.6004862	-6.6476106
C	0.5897164	-5.9231376	-5.6108969	C	-0.2857454	2.5575008	-3.9057613
C	-0.1888169	-4.8561245	-6.1310630	C	-3.9146293	2.1606306	-0.8309319
H	1.5941174	-6.7153657	-3.8639200	C	-2.4071079	2.9776939	-2.7211699
H	0.9153369	-6.7405932	-6.2720342	H	-4.7818938	4.0632078	-3.6575831
H	-1.2078141	-3.0028634	-5.7319961	H	-4.6364550	4.6412535	-1.9699215
H	-0.4510021	-4.8405725	-7.2000052	C	0.5684860	1.7760204	-4.9033728
C	-4.6813999	-3.5303381	-4.8270693	C	-1.5945456	2.1348046	-3.5353373
C	-5.3724584	-2.4753759	-5.4796676	C	-3.8336326	2.6103920	-2.3016982
H	-2.9601453	-4.1104786	-3.6617398	H	2.0172514	1.0263658	-3.4329999
H	-5.0996529	-4.5483448	-4.8392568	H	-3.2681365	1.2796496	-0.6507444
H	-6.3157871	-2.6810538	-6.0080967	H	2.5854880	2.4775369	-4.3210124
H	-5.4089649	-0.3539806	-5.9092664	H	1.9028593	4.7782120	-1.1955954
C	2.7794855	-3.1368807	0.1161135	H	-3.6033163	2.9744702	-0.1418546
C	1.4049337	-3.5121973	0.0870283	H	0.0485414	7.0800604	-3.6269791
C	3.3743960	-2.8734312	1.3634237	H	0.0998810	0.7819887	-5.0496558
C	0.6696814	-3.6277357	1.2962741	H	-4.1498026	1.7398281	-2.9070093
C	1.3151142	-3.3524495	2.5147792	H	1.2475582	4.0532568	-3.6414594
C	2.6649794	-2.9670839	2.5739411	C	-3.6174418	-1.4328259	9.2698951
H	4.4369553	-2.5809648	1.3986004	C	-2.3775857	-1.3822473	8.6239162
C	-0.7822916	-4.0989547	1.3102989	C	-1.2528028	-0.8592909	9.2993483
H	0.7398890	-3.4414513	3.4488730	C	-1.3853475	-0.3854176	10.6211808
C	-1.7140873	-3.1193630	2.0390463	C	-2.6278834	-0.4395709	11.2684401
H	-1.4623815	-3.0282618	3.1158192	C	-3.7424910	-0.9644467	10.5922287
H	-2.7675092	-3.4620741	1.9755325	H	-4.4967077	-1.8380471	8.7460165
H	-1.6605968	-2.1031598	1.6049868	H	-2.2450473	-1.7372863	7.5902239
C	-0.8769479	-5.5209078	1.8961357	C	0.0705481	-0.8170544	8.6232889
H	-1.1260264	-4.1617948	0.2571074	H	-0.5026577	0.0238923	11.1403477
H	-0.5467628	-5.5392517	2.9558494	H	-2.7314881	-0.0736671	12.3015066
H	-0.2391999	-6.2336555	1.3343606	H	-4.7191760	-1.0085374	11.0991457
H	-1.9224803	-5.8917927	1.8626516	O	0.2975427	-1.2422844	7.5026304
C	3.3737421	-2.7258145	3.9018664	H	0.8913504	-0.3462933	9.2481464
C	2.5194573	-1.9655051	4.9275755				
H	3.1113479	-1.7234606	5.8333849				
H	1.6463861	-2.5543342	5.2744893				
H	2.1250659	-1.0166011	4.5119620				
C	3.8812481	-4.0640175	4.4766957				
H	4.2686818	-2.1031634	3.6757310				
H	4.4534178	-3.9062257	5.4146683				
H	4.5380909	-4.5902321	3.7545655				
H	3.0294771	-4.7381266	4.7060808				
C	3.6308857	-3.0473359	-1.1522853				
C	4.4710132	-1.7649411	-1.2439007				
H	5.0133824	-1.7226447	-2.2105222				
H	5.2319515	-1.6934096	-0.4399355				
H	3.8326964	-0.8640943	-1.1872886				
C	4.5301555	-4.2923707	-1.2870429				
H	2.9409478	-3.0378893	-2.0200851				
H	5.1048122	-4.2662999	-2.2363319				
H	3.9394649	-5.2299873	-1.2700309				
H	5.2574740	-4.3464476	-0.4500550				
H	-0.3984423	5.8595122	-0.8261181				
H	0.9975508	3.4942393	-6.2109080				
H	-5.8667042	3.4152596	-2.3810891				
C	0.0583810	5.8066254	-1.8400881				
H	2.5552951	0.8896629	-5.1330445				
H	1.9328532	6.5639220	-1.0002303				
H	-4.9535857	1.8803659	-0.5620486				
C	-0.5239163	4.5604170	-2.4995001				
C	0.5464193	2.4818384	-6.2741296				
C	1.5815873	5.7376656	-1.6511642				
H	2.1225595	5.8353540	-2.6154396				
C	0.2237427	3.7543253	-3.3731936				
C	-4.8296737	3.7453759	-2.5961945				
H	-1.4588929	7.1694440	-2.6657231				
C	-1.8502213	4.1749915	-2.2332584				
C	-0.3559244	7.0845630	-2.5935323				
H	0.0256751	7.9915989	-2.0799273				
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C	2.0074851	1.5352776	-4.4167089				

agg-7-d-ma; COSMO

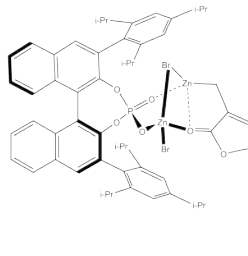


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C	4.3400690	7.0505808	86.9271836
C	3.5905034	6.9199815	88.1968645
O	3.7477334	7.9912215	88.9801874
C	4.5574028	8.9528258	88.2647826
O	2.8471679	5.9687071	88.5074477
C	4.3014689	5.9471921	85.9372649
H	5.4476671	9.1920935	88.8867811
H	3.9543311	9.8809137	88.1595421
Zn	2.6526385	4.8998807	86.3552725
Br	0.3404567	5.9057819	86.3953714
C	-0.1146943	0.8205433	88.9387370
C	0.6556192	-0.2597485	89.3835100
C	0.0817954	-1.1252413	90.3898386
C	0.8201400	-2.1543441	91.0491056
C	-1.2937384	-0.9220272	90.7813259
C	-1.8883740	-1.8046888	91.7329108
C	-2.0088425	0.2059549	90.2860172
H	-3.0290568	0.3909584	90.6558409
C	-1.4199557	1.1298149	89.4309285
C	4.3277899	0.5539921	88.5840944

C	4.8131932	-0.7034548	88.2400713	C	6.0994770	1.6780063	91.9698812
H	5.8840674	-0.8240905	88.0159863	C	7.3280593	6.4677522	89.3785414
C	3.9542654	-1.8309803	88.1021819	H	7.6822013	6.1130255	90.3687731
C	4.4554061	-3.0864488	87.6424162	C	6.1799698	3.7366073	89.6070063
C	2.5447522	-1.6939717	88.3822897	C	6.7754983	0.7588283	85.4998847
C	1.6920681	-2.8071766	88.1148912	H	9.2920826	4.3528371	87.3884646
C	2.0512038	-0.4357880	88.8892200	C	6.5008279	3.3820859	87.2529536
C	2.9409349	0.6469260	88.9204215	C	9.0839532	5.0615326	88.2150233
O	0.3977528	1.6521946	87.9456259	H	9.7122052	5.9635104	88.0617301
O	2.4876363	1.8902862	89.3481554	H	6.9338890	3.7044435	86.2911419
P	1.5309527	2.7654824	88.3438131	C	4.0919748	3.2336871	91.7726899
O	0.9826868	3.8927241	89.2244272	H	5.7359716	1.3233669	92.9566877
O	2.2277216	3.1016615	87.0149439	H	6.6638923	0.8504930	91.4935602
C	-1.1530907	-2.8238077	92.3191206	C	5.4177006	2.5566237	89.7061084
C	0.2186460	-2.9826619	91.9873130	C	4.9128101	2.3583023	84.8659790
H	-2.9420768	-1.6432985	92.0098150	C	5.7215738	2.2118452	87.2854818
H	-1.6220232	-3.4933467	93.0562137	H	7.1756968	0.0704325	86.2716007
H	1.8851541	-2.2858389	90.8156442	H	7.5717120	1.4984923	85.2721159
H	0.8141988	-3.7648870	92.4823708	C	4.9210851	2.1325924	91.0870689
C	2.2074682	-4.0079211	87.6459861	C	5.1782949	1.7847177	88.5351587
C	3.6027773	-4.1580902	87.4238514	C	5.4876724	1.4586727	85.9738868
H	0.6100316	-2.7022337	88.2755618	H	3.2668565	3.5790720	91.1202439
H	1.5275183	-4.8486729	87.4400151	H	3.9703033	2.8354144	85.1977881
H	4.0009998	-5.1180725	87.0614650	H	4.7159063	4.1138111	92.0343018
H	5.5350569	-3.1804080	87.4456649	H	6.2495711	6.7048629	89.4778758
C	-2.0499490	3.4177220	90.2385623	H	5.6189136	3.1601747	84.5659308
C	-2.0179888	2.4764721	89.1676179	H	9.4039594	4.5768873	89.1612002
C	-2.5639639	4.7038380	89.9862875	H	4.2606493	1.2525460	90.9591816
C	-2.4729817	2.8531003	87.8750180	H	4.7304734	0.6734206	86.1660797
C	-2.9811289	4.1503046	87.6814257	H	6.3470570	4.3268006	90.5198465
C	-3.0449598	5.0922218	88.7244032	H	4.4442746	6.3035019	84.9000206
H	-2.5885284	5.4403102	90.8043212	H	5.1078217	5.2172450	86.1683648
C	-2.4685657	1.8711382	86.7055316	H	5.5043242	8.7770903	86.1905680
H	-3.3453929	4.4321433	86.6806099	C	9.2140222	15.6087313	75.5982930
C	-1.6934760	2.4113703	85.4912176	C	8.9398468	14.5595222	76.4819014
H	-2.1748126	3.3175331	85.0683626	C	9.6405228	14.4671570	77.7053771
H	-1.6539712	1.6485994	84.6859979	C	10.6148686	15.4333516	78.0328500
H	-0.6549846	2.6788849	85.7667217	C	10.8886912	16.4846282	77.1460749
C	-3.9055029	1.4665338	86.3252280	C	10.1882571	16.5710886	75.9301571
H	-1.9519292	0.9494727	87.0438267	H	8.6701918	15.6843198	74.6441650
H	-4.4895916	2.3419555	85.9711943	H	8.1849608	13.7914734	76.2527828
H	-4.4437698	1.0328193	87.1925164	C	9.3539472	13.3565980	78.6471896
H	-3.9008134	0.7126405	85.5105671	H	11.1566284	15.3533060	78.9898207
C	-3.6643046	6.4705048	88.5241060	H	11.6484869	17.2394182	77.3999750
C	-2.9756935	7.2822305	87.4158377	H	10.4023988	17.3959595	75.2328686
H	-3.4533662	8.2782216	87.3088032	O	8.5305579	12.4734701	78.4559288
H	-3.0395668	6.7723382	86.4318744	H	9.9729942	13.3810426	79.5943425
H	-1.9046171	7.4396711	87.6494626				
C	-5.1802218	6.3527603	88.2764412				
H	-3.5175328	7.0250562	89.4764210				
H	-5.6475419	7.3566357	88.1999064				
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H	-5.3891982	5.8112023	87.3296658				
C	-1.5613878	3.0905140	91.6518035				
C	-0.5457595	4.1110555	92.1940878				
H	-0.1947735	3.7991411	93.1996640				
H	-0.9773477	5.1278802	92.2911113				
H	0.3343557	4.1837005	91.5274010				
C	-2.7550012	2.9345493	92.6140542				
H	-1.0385982	2.1144195	91.6127452				
H	-2.4088027	2.6438128	93.6277492				
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H	-3.3163088	3.8878613	92.7085727				
H	7.3213691	5.9023942	87.3040184				
H	6.8116744	2.5101069	92.1520958				
H	6.5883344	0.1694632	84.5784541				
C	7.5882651	5.4310533	88.2774841				
H	3.6486826	2.8535601	92.7159992				
H	7.8706778	7.4096795	89.1585641				
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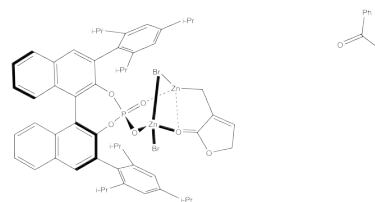


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C	4.8713198	8.2979861	86.9714136
C	4.3260577	7.0499271	86.9330697
C	3.5788369	6.9138414	88.2076945
O	3.7402035	7.9847920	88.9934110
C	4.5367354	8.9504776	88.2750023
O	2.8358318	5.9647873	88.5128309
C	4.2872911	5.9423680	85.9508069
H	5.4313952	9.1930863	88.8904483

H	3.9265973	9.8755801	88.1789280	C	-2.7439483	2.9511696	92.6055668
Zn	2.6276650	4.9131965	86.3859258	H	-1.0308333	2.1161840	91.6113221
Br	0.3224111	5.8808356	86.3874041	H	-2.4033037	2.6591041	93.6206715
C	-0.1117748	0.8148442	88.9351688	H	-3.4634005	2.1852902	92.2512287
C	0.6562544	-0.2660311	89.3825950	H	-3.2982564	3.9086418	92.6971029
C	0.0796714	-1.1297088	90.3887749	H	7.3225856	5.8998005	87.2995146
C	0.8139860	-2.1617244	91.0474895	H	6.8142101	2.5099850	92.1501820
C	-1.2949180	-0.9215668	90.7806988	H	6.5801853	0.1841844	84.5667141
C	-1.8914540	-1.8019061	91.7325134	C	7.5866261	5.4299744	88.2746959
C	-2.0058166	0.2086655	90.2852264	H	3.6496185	2.8532114	92.7178490
H	-3.0246137	0.3997005	90.6559452	H	7.8703007	7.4107401	89.1520556
C	-1.4154309	1.1294276	89.4282720	H	4.6638576	1.7593129	83.9662098
C	4.3275802	0.5529374	88.5871693	C	6.7293983	4.1730968	88.3917896
C	4.8156497	-0.7034166	88.2438599	C	6.1012265	1.6785423	91.9685504
H	5.8867836	-0.8200115	88.0187342	C	7.3248625	6.4702738	89.3721347
C	3.9598267	-1.8330030	88.1068898	H	7.6764293	6.1181433	90.3640975
C	4.4628265	-3.0876686	87.6483011	C	6.1776310	3.7375699	89.6058782
C	2.5501115	-1.6983201	88.3862265	C	6.7691240	0.7739649	85.4874295
C	1.6999594	-2.8131256	88.1187076	H	9.2911017	4.3459023	87.3950878
C	2.0532871	-0.4412040	88.8921103	C	6.4948257	3.3828177	87.2518654
C	2.9407500	0.6434056	88.9241942	C	9.0818040	5.0582636	88.2179275
O	0.4025922	1.6432899	87.9410572	H	9.7133574	5.9578839	88.0640410
O	2.4858361	1.8858585	89.3511478	H	6.9263056	3.7049080	86.2891197
P	1.5303616	2.7590797	88.3425558	C	4.0922957	3.2334920	91.7745145
O	0.9770638	3.8854907	89.2207541	H	5.7397344	1.3238364	92.9559514
O	2.2370894	3.0996822	87.0199952	H	6.6653210	0.8515938	91.4913164
C	-1.1603951	-2.8236905	92.3180541	C	5.4163328	2.5573182	89.7064358
C	0.2097786	-2.9880019	91.9851309	C	4.8840992	2.3566786	84.8744730
H	-2.9443068	-1.6361356	92.0100737	C	5.7162782	2.2123232	87.2856806
H	-1.6315835	-3.4909766	93.0557020	H	7.1833304	0.0886219	86.2543638
H	1.8780884	-2.2969511	90.8124555	H	7.5570565	1.5204923	85.2537372
H	0.8025743	-3.7730124	92.4790354	C	4.9215038	2.1333369	91.0879075
C	2.2176762	-4.0128744	87.6512283	C	5.1758474	1.7850446	88.5362116
C	3.6128193	-4.1607437	87.4299942	C	5.4789547	1.4600098	85.9741483
H	0.6179600	-2.7088906	88.2793363	H	3.2659947	3.5790276	91.1239111
H	1.5392126	-4.8547637	87.4453378	H	3.9361502	2.8150768	85.2159181
H	4.0131556	-5.1201312	87.0685082	H	4.7148308	4.1143838	92.0367720
H	5.5427090	-3.1795287	87.4518191	H	6.2464744	6.7085306	89.4690503
C	-2.0314321	3.4226463	90.2315694	H	5.5758503	3.1708899	84.5738101
C	-2.0074124	2.4782858	89.1633874	H	9.3977178	4.5750092	89.1659497
C	-2.5360705	4.7116419	89.9757196	H	4.2614197	1.9230914	90.9601002
C	-2.4608345	2.8541550	87.8701966	H	4.7311440	0.6670594	86.1708148
C	-2.9602081	4.1540606	87.6734831	H	6.3451493	4.3277794	90.5186214
C	-3.0171845	5.0993963	88.7134873	H	4.4471476	6.2846075	84.9117477
H	-2.5549870	5.4508625	90.7912380	H	5.0776046	5.2014591	86.2029232
C	-2.4665774	1.8676138	86.7046499	H	5.4736173	8.7835365	86.1912770
H	-3.3243352	4.4350720	86.6724602	C	9.2210973	15.6192631	75.6020616
C	-1.6913414	2.3957282	85.4854072	C	8.9398970	14.5677641	76.4802186
H	-2.1645500	3.3050934	85.0604861	C	9.6360473	14.4667820	77.7046794
H	-1.6626670	1.6299311	84.6827401	C	10.6119863	15.4276782	78.0391932
H	-0.6487553	2.6527318	85.7545831	C	10.8928857	16.4818085	77.1584055
C	-3.9079774	1.4721566	86.3321759	C	10.1976472	16.5759755	75.9407692
H	-1.9556172	0.9437068	87.0455002	H	8.6806708	15.7012692	74.6464639
H	-4.4870704	2.3500575	85.9765025	H	8.1832391	13.8018129	76.2498499
H	-4.4464168	1.0478740	87.2037952	C	9.3389022	13.3481507	78.6372079
H	-3.9131992	0.7144092	85.5211684	H	11.1501815	15.3412789	78.9977950
C	-3.6380292	6.4771570	88.5140485	H	11.6541211	17.2331892	77.4182078
C	-2.9657140	7.2868371	87.3947920	H	10.4181712	17.4023204	75.2472802
H	-3.4533852	8.2775289	87.2850576	O	8.5144740	12.4724829	78.4345411
H	-3.0320680	6.7709856	86.4141523	H	9.9549936	13.3640479	79.5889750
H	-1.8952334	7.4586749	87.6201495				
C	-5.1567582	6.3543838	88.2865931				
H	-3.4793023	7.0357992	89.4619410				
H	-5.6284939	7.3564245	88.2141583				
H	-5.6461616	5.8007897	89.1133065				
H	-5.3768776	5.8103262	87.3438723				
C	-1.5466090	3.0961814	91.6462736				
C	-0.5254940	4.1111135	92.1888431				
H	-0.1840355	3.8029710	93.1987145				
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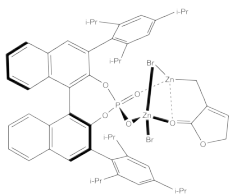


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Zn 1.2047435 5.9236478 89.0955862

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C	5.5012153	8.2648225	87.1645086	H	-5.0418973	7.7180796	88.4690066
C	4.9065956	7.0386356	87.1318057	H	-5.1229789	6.1709622	89.3789988
C	4.1592192	6.9372442	88.4054266	H	-4.8520415	6.1570805	87.6087034
O	4.3545239	8.0059058	89.1837354	C	-1.0943382	3.3220891	91.9099337
C	5.1915762	8.9380758	88.4609212	C	-0.0335158	4.3040374	92.4368547
O	3.3863951	6.0120006	88.7225214	H	0.3133296	3.9844528	93.4414490
C	4.8277630	5.9321584	86.1476047	H	-0.4226775	5.3381560	92.5309145
H	6.0926282	9.1497284	89.0772959	H	0.8430574	4.3365446	91.7623539
H	4.6186819	9.8851541	88.3561959	C	-2.2858353	3.2218226	92.8821572
Zn	3.1459511	4.9427711	86.5771149	H	-0.6122002	2.3252357	91.8740709
Br	0.8719517	6.0329351	86.6177660	H	-1.9439794	2.9244459	93.8954022
C	0.2437969	0.9815563	89.2001073	H	-3.0329389	2.4771915	92.5396107
C	0.9762195	-0.1239296	89.6470441	H	-2.8071158	4.1978768	92.9737845
C	0.3768969	-0.9612095	90.6625563	H	7.8503343	5.7791748	87.4911682
C	1.0794911	-2.0144088	91.3229444	H	7.2446772	2.4366967	92.3629065
C	-0.9870315	-0.7032112	91.0624322	H	6.8893991	0.0699579	84.7974397
C	-1.6085996	-1.5567484	92.0233930	C	8.1039997	5.3048348	88.4666743
C	-1.6619244	0.4485872	90.5656539	H	4.0999816	2.8954873	92.9418056
H	-2.6713240	0.6748962	90.9421310	H	8.4596533	7.2782658	89.3327882
C	-1.0447366	1.3438583	89.7002272	H	5.0402565	1.7171504	84.1872447
C	4.6699830	0.5513504	88.8195661	C	7.2046044	4.0788608	88.5941935
C	5.1079283	-0.7249504	88.4812848	C	6.5024293	1.6293974	92.1890865
H	6.1723481	-0.8850391	88.2512464	C	7.8857334	6.3573502	89.5619247
C	4.2084479	-1.8220998	88.3570725	H	8.2323460	5.9971639	90.5528350
C	4.6614502	-3.0981794	87.9038492	C	6.6438411	3.6692172	89.8135474
C	2.8065094	-1.6325897	88.6447067	C	7.1042116	0.6575269	85.7140006
C	1.9128917	-2.7163318	88.3901126	H	9.7650239	4.1611270	87.5782921
C	2.3613660	-0.3539267	89.1454764	C	6.9355022	3.2919007	87.4592412
C	3.2895254	0.6965074	89.1634751	C	9.5853250	4.8818333	88.4011526
O	0.7795853	1.7861033	88.1967742	H	10.2444916	5.7601032	88.2400807
O	2.8843468	1.9584799	89.5850238	H	7.3738200	3.5933751	86.4930012
P	1.9536529	2.8612878	88.5807227	C	4.5500229	3.2538706	91.9931771
O	1.4507324	4.0123519	89.4574109	H	6.1318586	1.2934395	93.1797809
O	2.6536509	3.1652226	87.2458043	H	7.0347069	0.7797957	91.7147255
C	-0.9091420	-2.6002524	92.6105412	C	5.8394162	2.5185800	89.9235786
C	0.4530303	-2.8137901	92.2699940	C	5.2873017	2.3126505	85.0899283
H	-2.6533729	-1.3530553	92.3063134	C	6.1141457	2.1510577	87.5027579
H	-1.3984736	-3.2469310	93.3548228	H	7.4898528	-0.0393007	86.4855647
H	2.1369579	-2.1883376	91.0830908	H	7.9212611	1.3702605	85.4744654
H	1.0213049	-3.6160405	92.7650996	C	5.3360226	2.1201923	91.3097364
C	2.3819716	-3.9382291	87.9272665	C	5.5640637	1.7502830	88.7581302
C	3.7696480	-4.1401232	87.6983436	C	5.8439937	1.4002066	86.1967217
H	0.8362811	-2.5713890	88.5562008	H	3.7331582	3.6234914	91.3436141
H	1.6710070	-4.7554094	87.7314744	H	4.3606856	2.8166949	85.4267179
H	4.1309293	-5.1166622	87.3414322	H	5.2058610	4.1134552	92.2448120
H	5.7357519	-3.2325890	87.7014648	H	6.8167708	6.6327324	89.6650566
C	-1.5802493	3.6590798	90.4980775	H	6.0137294	3.0933902	84.7827528
C	-1.5924433	2.7109083	89.4329004	H	9.8915802	4.3921925	89.3493162
C	-2.0458965	4.9625337	90.2412538	H	4.6443306	1.2631884	91.1904699
C	-2.0417959	3.0970503	88.1411650	H	5.0642156	0.6401098	86.3995804
C	-2.4999373	4.4120020	87.9426973	H	6.8387445	4.2572198	90.7222867
C	-2.5200276	5.3619211	88.9801548	H	4.9788033	6.2779490	85.1079514
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C	-2.0861563	2.1079802	86.9786254	H	6.1221700	8.7245345	86.3834013
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H	-1.2971477	1.8379851	84.9549156	C	-4.1665634	16.7574574	77.9110285
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H	-4.0902050	1.3552080	87.4875958	H	-5.0224819	16.4062838	78.5108570
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H	-2.8263649	8.5504882	87.5440459	H	-0.7704578	17.1607373	78.1771024
H	-2.4806253	7.0235887	86.6738809	H	-3.6250385	15.9135794	80.3733715
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agg-7-d-mi



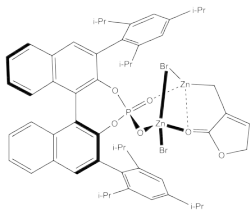
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C	4.8099810	5.9256714	86.1579375
H	6.0907968	9.1478438	89.0735775
H	4.6076557	9.8807133	88.3666764
Zn	3.1151694	4.9620600	86.6085737
Br	0.8467512	6.0112121	86.6189580
C	0.2461429	0.9787108	89.1977113
C	0.9768404	-0.1271230	89.6466345
C	0.3754426	-0.9634484	90.6614069
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C	-0.9880001	-0.7027331	91.0606397
C	-1.6106023	-1.5554275	92.0208830
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C	4.6706057	0.5517232	88.8237476
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C	2.8104093	-1.6336193	88.6470317
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O	2.8841320	1.9563397	89.5895938
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O	2.6628494	3.1663847	87.2531400
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C	3.7756658	-4.1386701	87.6981739
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H	-5.1002906	6.1654033	89.3826388
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C	7.0989148	0.6665867	85.7081703
H	9.7625444	4.1540865	87.5804705
C	6.9318557	3.2930493	87.4597948
C	9.5845460	4.8778506	88.4007454
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C	4.5532614	3.2559420	91.9973268
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C	5.8392172	2.5206656	89.9253539
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C	6.1110587	2.1521469	87.5047902
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H	7.9119980	1.3825621	85.4651757
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H	3.7360825	3.6278847	91.3497191
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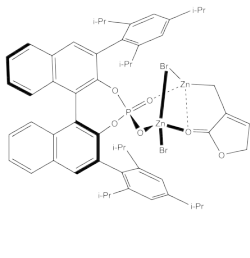
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C	-1.2961602	-0.9225234	90.7825560
C	-1.8928933	-1.8036295	91.7342077
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C	1.6964298	-2.8123467	88.1191648
C	2.0510964	-0.4397922	88.8921285
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H	-3.4792419	7.0358551	89.4618691
H	-5.6284340	7.3564416	88.2141535
H	-5.6461050	5.8008308	89.1133114
H	-5.3768681	5.8103383	87.3438578
C	-1.5465626	3.0962184	91.6462668
C	-0.5254597	4.1111573	92.1888332
H	-0.1839995	3.8030261	93.1987056
H	-0.9458609	5.1333764	92.2762965
H	0.3610698	4.1708165	91.5294913
C	-2.7439176	2.9512199	92.6055344
H	-1.0307698	2.1162248	91.6113400
H	-2.4033165	2.6591597	93.6206382
H	-3.4633904	2.1853584	92.2511791
H	-3.2982164	3.9086986	92.6970554
H	7.3226340	5.8997664	87.2995487
H	6.8142382	2.5099656	92.1501557
H	6.5801535	0.1840131	84.5667146
C	7.5866697	5.4299069	88.2747206
H	3.6496397	2.8532134	92.7178429
H	7.8703425	7.4106726	89.1520829
H	4.6637221	1.7591722	83.9662675
C	6.7294125	4.1730524	88.3917682
C	6.1012503	1.6785248	91.9685267
C	7.3249181	6.4702129	89.3721592
H	7.6765320	6.1181123	90.3641074
C	6.1776054	3.7375231	89.6058393
C	6.7690833	0.7738506	85.4874157

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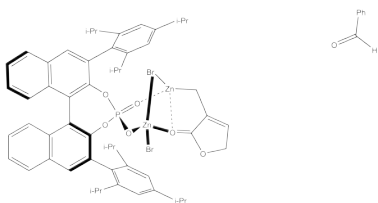


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Zn	0.6022769	5.7784818	88.8785681
Br	-0.0517826	7.5208894	90.2349731
C	4.8715591	8.2981801	86.9719507
C	4.3261127	7.0502279	86.9332752
C	3.5786982	6.9140565	88.2077756
O	3.7399210	7.9848474	88.9935643
C	4.5367643	8.9505897	88.2755143
O	2.8356456	5.9648728	88.5126014
C	4.2873978	5.9425822	85.9510183
H	5.4313490	9.1930279	88.8911292
H	3.9268197	9.8758026	88.1794337
Zn	2.6278346	4.9133688	86.3867463
Br	0.3225540	5.8806917	86.3870126
C	-0.1117856	0.8147848	88.9351193
C	0.6562556	-0.2660857	89.3825613
C	0.0796761	-1.1297175	90.3887862
C	0.8139789	-2.1617307	91.0475209
C	-1.2948880	-0.9215472	90.7807186
C	-1.8914786	-1.8018293	91.7325365
C	-2.0057911	0.2086871	90.2852377
H	-3.0245520	0.3997505	90.6559940
C	-1.4154052	1.1294262	89.4282276
C	4.3275723	0.5528458	88.5871732
C	4.8156402	-0.7035175	88.2438977
H	5.8867892	-0.8201298	88.0188101
C	3.9598209	-1.8331058	88.1069119
C	4.4627943	-3.0878003	87.6483606
C	2.5500994	-1.6984066	88.3862304

H	9.2911638	4.3457700	87.3951447	C	-1.1403834	-0.8319919	90.7841995
C	6.4948166	3.3827308	87.2518690	C	-1.7641872	-1.6888351	91.7407758
C	9.0818451	5.0581749	88.2179533	C	-1.8124755	0.3237127	90.2925541
H	9.7133991	5.9577850	88.0641125	H	-2.8213914	0.5513481	90.6697103
H	6.9263655	3.7047903	86.2891315	C	-1.1929623	1.2210689	89.4309484
C	4.0923087	3.2334933	91.7745185	C	4.5200974	0.4228671	88.5491171
H	5.7397823	1.3238271	92.9559323	C	4.9563939	-0.8525258	88.2057683
H	6.6653247	0.8515729	91.4912790	H	6.0206282	-1.0135067	87.9756551
C	5.4163166	2.5572668	89.7064269	C	4.0552381	-1.9475396	88.0762037
C	4.8839917	2.3565470	84.8745222	C	4.5068402	-3.2219330	87.6172190
C	5.7162726	2.2122463	87.2856964	C	2.6534587	-1.7573284	88.3639932
H	7.1832666	0.0885175	86.2543569	C	1.7584657	-2.8386240	88.1039769
H	7.5570526	1.5203608	85.2537894	C	2.2098637	-0.4804103	88.8702706
C	4.9214959	2.1333160	91.0879087	C	3.1397483	0.5684547	88.8930488
C	5.1758348	1.7849589	88.5362156	O	0.6323268	1.6649756	87.9289603
C	5.4789347	1.4599000	85.9741724	O	2.7364243	1.8293948	89.3192148
H	3.2659914	3.5790429	91.1239185	P	1.8074002	2.7371569	88.3178174
H	3.9360662	2.8149402	85.2160691	O	1.3054768	3.8851408	89.1990746
H	4.7148452	4.1143742	92.0367975	O	2.5083148	3.0458347	86.9844495
H	6.2465292	6.7084315	89.4691062	C	-1.0673014	-2.7367645	92.3230462
H	5.5757564	3.1707994	84.5739289	C	0.2944658	-2.9517936	91.9820422
H	9.3977367	4.5749454	89.1659850	H	-2.8086642	-1.4846377	92.0244362
H	4.2614038	1.2530675	90.9601448	H	-1.5583214	-3.3862314	93.0637348
H	4.7311304	0.6669504	86.1708578	H	1.9802484	-2.3247283	90.7986432
H	6.3451210	4.3277533	90.5185670	H	0.8607684	-3.7577861	92.4733137
H	4.4470790	6.2848747	84.9119504	C	2.2261691	-4.0588360	87.6352861
H	5.0779180	5.2018333	86.2030112	C	3.6137281	-4.2616091	87.4062041
H	5.4743841	8.7837975	86.1922618	H	0.6818875	-2.6932673	88.2698176
C	14.5430723	18.3929914	78.3571583	H	1.5143260	-4.8740626	87.4346992
C	13.3301899	18.0907685	78.9843955	H	3.9739962	-5.2365374	87.0439911
C	12.6400022	19.0912114	79.7032404	H	5.5811485	-3.3561509	87.4145289
C	13.1760079	20.3924456	79.7862226	C	-1.7221729	3.5342938	90.2382640
C	14.3925069	20.6943127	79.1579240	C	-1.7369970	2.5905614	89.1692164
C	15.0746947	19.6943279	78.4441765	C	-2.1836731	4.8402207	89.9865600
H	15.0834757	17.6160227	77.7949004	C	-2.1847755	2.9832171	87.8789303
H	12.8844392	17.0851171	78.9378983	C	-2.6389750	4.3003033	87.6856203
C	11.3511699	18.7709584	80.3711184	C	-2.6564117	5.2460419	88.7269420
H	12.6292265	21.1673694	80.3489033	H	-2.1726313	5.5784951	90.8032446
H	14.8122615	21.7097094	79.2225437	C	-2.2320536	1.9987855	86.7125950
H	16.0299746	19.9298336	77.9497888	H	-2.9981856	4.5949831	86.6867386
O	10.8135179	17.6762828	80.3581627	C	-1.4441962	2.5008118	85.4902017
H	10.8826806	19.6476819	80.9160934	H	-1.8901338	3.4246648	85.0668274
				H	-1.4432493	1.7337227	84.6881366
				H	-0.3932308	2.7252951	85.7565602
				C	-3.6884477	1.6561713	86.3455584
				H	-1.7533436	1.0565794	87.0499845
				H	-4.2361681	2.5549917	85.9921069
				H	-4.2382286	1.2504238	87.2191822
				H	-3.7236456	0.8994145	85.5343161
				C	-3.2236838	6.6468525	88.5292846
				C	-2.5207963	7.4278460	87.4081670
				H	-2.9625040	8.4405265	87.3036220
				H	-2.6172840	6.9171039	86.4273652
				H	-1.4414670	7.5462800	87.6263170
				C	-4.7464332	6.5857485	88.3033155
				H	-3.0422797	7.1984993	89.4773067
				H	-5.1766591	7.6062704	88.2296931
				H	-5.2568188	6.0547035	89.1323980
				H	-4.9887318	6.0493099	87.3615977
				C	-1.2381540	3.1900511	91.6490470
				C	-0.1753302	4.1669034	92.1813710
				H	0.1689070	3.8425234	93.1853416
				H	-0.5618097	5.2017152	92.2788060
				H	0.7024930	4.1995996	91.5084906
				C	-2.4306758	3.0889838	92.6199293
				H	-0.7586841	2.1920553	91.6094706
				H	-2.0905352	2.7859796	93.6320876
				H	-3.1798301	2.3482425	92.2735281
				H	-2.9489898	4.0662291	92.7155381
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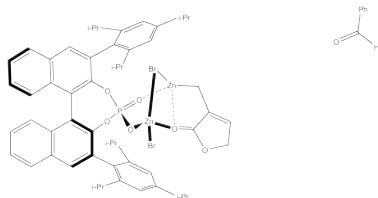


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Zn	1.0608789	5.7978075	88.8467122
Br	0.4443828	7.5467833	90.2281598
C	5.3675932	8.1392661	86.9318708
C	4.7698045	6.9146782	86.8924892
C	4.0194401	6.8096890	88.1642321
O	4.2154130	7.8747552	88.9474598
C	5.0553942	8.8085417	88.2300953
O	3.2433590	5.8853640	88.4755400
C	4.6880627	5.8133241	85.9027871
H	5.9542568	9.0187266	88.8503393
H	4.4830386	9.7561466	88.1259186
Zn	3.0023811	4.8270632	86.3250610
Br	0.7297597	5.9185878	86.3691265
C	0.0946721	0.8579169	88.9293001
C	0.8247833	-0.2506576	89.3721256
C	0.2232187	-1.0912455	90.3836507
C	0.9231917	-2.1492468	91.0391933

H	6.7389305	-0.0415612	84.5232384	O	3.2366093	5.8879525	88.4813279
C	7.9632256	5.1710642	88.2179058	C	4.6706038	5.8078105	85.9115069
H	3.9544892	2.7491963	92.6819113	H	5.9576668	9.0135945	88.8419465
H	8.3218338	7.1403165	89.0927824	H	4.4760855	9.7531449	88.1387989
H	4.8899307	1.6092816	83.9228878	Zn	2.9734074	4.8457351	86.3566281
C	7.0614125	3.9463349	88.3398215	Br	0.7076669	5.9000534	86.3714749
C	6.3543481	1.4817223	91.9235271	C	0.0974132	0.8556014	88.9271952
C	7.7462326	6.2193399	89.3175496	C	0.8260241	-0.2535285	89.3713255
H	8.0914339	5.8541892	90.3071598	C	0.2228057	-1.0933736	90.3821002
C	6.5000958	3.5321826	89.5574216	C	0.9206741	-2.1524336	91.0375630
C	6.9547922	0.5413167	85.4425321	C	-1.1402691	-0.8319723	90.7821261
H	9.6222822	4.0274806	87.3257559	C	-1.7646952	-1.6878931	91.7383165
C	6.7904193	3.1653057	87.2012385	C	-1.8100131	0.3245149	90.2898531
C	9.4436681	4.7451552	88.1514971	H	-2.8183835	0.5550069	90.6665381
H	10.1049685	5.6225490	87.9945206	C	-1.1898758	1.2209919	89.4281800
H	7.2292075	3.4701961	86.2362904	C	4.5212932	0.4224013	88.5527758
C	4.4050170	3.1108310	91.7347722	C	4.9586529	-0.8522498	88.2087432
H	5.9830269	1.1418987	92.9126026	H	6.0232504	-1.0104798	87.9780307
H	6.8849365	0.6332533	91.4452925	C	4.0590330	-1.9480862	88.0781424
C	5.6932538	2.3827567	89.6621302	C	4.5104680	-3.2216848	87.6181016
C	5.1376684	2.2000535	84.8284640	C	2.6572420	-1.7587208	88.3655514
C	5.9667419	2.0259719	87.2395828	C	1.7630825	-2.8401250	88.1044070
H	7.3410017	-0.1594205	86.2102814	C	2.2121787	-0.4827690	88.8724503
H	7.7717723	1.2550597	85.2057508	C	3.1408820	0.5670124	88.8971386
C	5.1890348	1.9788672	91.0463410	O	0.6369339	1.6620788	87.9282615
C	5.4161451	1.6205492	88.4931623	O	2.7370935	1.8269650	89.3240569
C	5.6951634	1.2818273	85.9300446	P	1.8085482	2.7348360	88.3209268
H	3.5886992	3.4845227	91.0868586	O	1.3048257	3.8820486	89.2019439
H	4.2112101	2.7020134	85.1686432	O	2.5182262	3.0481677	86.9931932
H	5.0622803	3.9682556	91.9899625	C	-1.0702025	-2.7368187	92.3204389
H	6.6776499	6.4961424	89.4209984	C	0.2906056	-2.9541149	91.9795784
H	5.8637673	2.9825107	84.5249049	H	-2.8086662	-1.4813528	92.0219332
H	9.7482220	4.2507744	89.0977454	H	-1.5625126	-3.3849417	93.0613574
H	4.4957772	1.1237325	90.9229319	H	1.9773428	-2.3288638	90.7964451
H	4.9153215	0.5209382	86.1295548	H	0.8555864	-3.7610862	92.4706484
H	6.6965151	4.1152817	90.4689896	C	2.2312780	-4.0593832	87.6351591
H	4.8418813	6.1633621	84.8649784	C	3.6183239	-4.2612357	87.4058562
H	5.4664290	5.0532147	86.1324308	H	0.6868856	-2.6940404	88.2713052
H	5.9907351	8.6008534	86.1534313	H	1.5195856	-4.8745825	87.4341674
C	-5.0121961	6.3420103	70.6951359	H	3.9791067	-5.2356747	87.0429495
C	-4.9260102	6.6810381	72.0495745	H	5.5848113	-3.3554182	87.4154003
C	-5.0808938	8.0268855	72.4506395	C	-1.7119771	3.5368355	90.2328599
C	-5.3225161	9.0255926	71.4841116	C	-1.7309279	2.5914784	89.1655002
C	-5.4085214	8.6843946	70.1265869	C	-2.1680152	4.8441860	89.9787563
C	-5.2532531	7.3434629	69.7336900	C	-2.1774563	2.9834126	87.8747113
H	-4.8920734	5.2945157	70.3785916	C	-2.6275964	4.3014249	87.6797043
H	-4.7385197	5.9233228	72.8260647	C	-2.6416967	5.2491067	88.7190529
C	-4.9898482	8.3922722	73.8865045	H	-2.1538521	5.5841480	90.7936882
H	-5.4422788	10.0732788	71.8061749	C	-2.2286464	1.9968811	86.7103027
H	-5.5966590	9.4624427	69.3711374	H	-2.9869234	4.5953721	86.6806873
H	-5.3205557	7.0742861	68.6681178	C	-1.4412853	2.4937074	85.4857285
O	-4.7836400	7.6017404	74.7957147	H	-1.8816650	3.4202785	85.0627013
H	-5.1294394	9.4959183	74.0937409	H	-1.4473208	1.7267596	84.6837121
				H	-0.3878823	2.7103786	85.7481045
				C	-3.6865540	1.6570929	86.3472318
				H	-1.7515737	1.0542697	87.0489928
				H	-4.2333991	2.5563081	85.9938353
				H	-4.2356224	1.2547409	87.2226389
				H	-3.7260181	0.8993185	85.5372046
				C	-3.2106926	6.6493911	88.5220000
				C	-2.5146539	7.4319111	87.3979586
				H	-2.9647783	8.4404091	87.2900579
				H	-2.6064694	6.9181707	86.4183169
				H	-1.4370682	7.5628928	87.6168476
				C	-4.7343338	6.5844291	88.3036359
				H	-3.0250910	7.2022525	89.4683989
				H	-5.1678556	7.6036941	88.2330292
				H	-5.2395730	6.0506400	89.1338418
				H	-4.9806305	6.0484126	87.3628405
				C	-1.2317672	3.1930219	91.6450262
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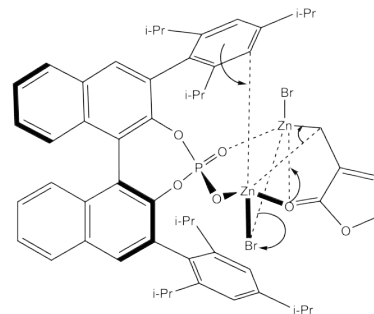
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Br	0.4265712	7.5572391	90.2188992
C	5.3522236	8.1395952	86.9269574
C	4.7586163	6.9136695	86.8924638
C	4.0141272	6.8072283	88.1716487
O	4.2217670	7.8714412	88.9557639
C	5.0506881	8.8052476	88.2320424

H	0.1665468	3.8477096	93.1884645
H	-0.5492526	5.2059307	92.2698243
H	0.7150203	4.1933299	91.5156530
C	-2.4281814	3.0951709	92.6114221
H	-0.7544155	2.1938395	91.6080689
H	-2.0932084	2.7912717	93.6249257
H	-3.1786846	2.3571831	92.2622504
H	-2.9447217	4.0733536	92.7049415
H	7.7120192	5.6490777	87.2425911
H	7.1021686	2.2851607	92.0997532
H	6.7342765	-0.0361383	84.5200223
C	7.9635821	5.1703158	88.2166950
H	3.9559087	2.7499154	92.6847699
H	8.3279417	7.1395244	89.0903361
H	4.8759051	1.6106025	83.9291204
C	7.0594518	3.9473318	88.3400074
C	6.3566148	1.4816411	91.9230286
C	7.7481989	6.2208183	89.3145370
H	8.0917188	5.8562730	90.3048341
C	6.4986028	3.5341678	89.5577426
C	6.9511454	0.5470673	85.4388038
H	9.6202305	4.0211506	87.3283455
C	6.7878965	3.1658948	87.2022106
C	9.4430750	4.7415801	88.1517314
H	10.1077506	5.6162602	87.9935557
H	7.2258465	3.4704198	86.2366435
C	4.4074660	3.1121993	91.7385639
H	5.9873883	1.1419797	92.9128509
H	6.8857446	0.6332368	91.4434643
C	5.6930581	2.3841159	89.6638342
C	5.1239473	2.1999645	84.8354438
C	5.9651047	2.0262103	87.2416862
H	7.3435732	-0.1526287	86.2042039
H	7.7655758	1.2627356	85.1993932
C	5.1901765	1.9805183	91.0485090
C	5.4161217	1.6208986	88.4957257
C	5.6911672	1.2824086	85.9324723
H	3.5912970	3.4886100	91.0922367
H	4.1958288	2.6937962	85.1820930
H	5.0648204	3.9687124	91.9965127
H	6.6803018	6.5002589	89.4174151
H	5.8442166	2.9872267	84.5299902
H	9.7456917	4.2471990	89.0983534
H	4.4962420	1.1259877	90.9253026
H	4.9149177	0.5187211	86.1347013
H	6.6940992	4.1180067	90.4690026
H	4.8388811	6.1424464	84.8713009
H	5.4316924	5.0358830	86.1605612
H	5.9687065	8.6009870	86.1432804
C	-5.0140909	6.3448218	70.6957641
C	-4.9277318	6.6836416	72.0499558
C	-5.0812535	8.0286804	72.4513936
C	-5.3197963	9.0268684	71.4851106
C	-5.4063543	8.6864217	70.1276503
C	-5.2536827	7.3458287	69.7345019
H	-4.8954930	5.2970796	70.3792415
H	-4.7419481	5.9288128	72.8295510
C	-4.9919701	8.3885452	73.8912321
H	-5.4367053	10.0748020	71.8079240
H	-5.5930784	9.4648058	69.3722432
H	-5.3218183	7.0763732	68.6689916
O	-4.7858043	7.5957260	74.7945545
H	-5.1347440	9.4933352	74.1016574



Energy (Hartree) = -11625.0703854

Zn	1.6043875	1.4769200	2.0211921
Br	3.8650111	1.7657327	2.0062855
C	1.8704952	6.0672279	1.4530647
C	0.8836998	5.1289087	1.3069274
C	1.0948031	4.1866887	2.4234353
O	2.0682758	4.5998379	3.2444441
C	2.6751776	5.7743274	2.6730493
O	0.5482323	3.0750880	2.6021135
C	-0.1826442	4.9731873	0.3109644
H	3.7373617	5.5137885	2.4649737
H	2.6624917	6.5866322	3.4327653
Zn	-0.6087656	3.3415058	-0.8004040
Br	-2.2623237	3.5831439	-2.4374102
C	-1.9895437	-1.5783220	0.3710503
C	-1.6958999	-2.6807547	-0.4354275
C	-2.0044119	-3.9930009	0.0863014
C	-1.6159036	-5.2012988	-0.5666295
C	-2.7029487	-4.0954377	1.3464089
C	-3.0477730	-5.3855273	1.8497038
C	-2.9821332	-2.9188232	2.1000400
H	-3.4820573	-3.0210712	3.0749769
C	-2.5877924	-1.6587519	1.6685314
C	1.0136232	-1.6410811	-2.9589460
C	0.5864707	-2.3049455	-4.1033978
H	1.2122749	-2.2702679	-5.0082559
C	-0.6629439	-2.9872227	-4.1558868
C	-1.1300231	-3.5784216	-5.3679788
C	-1.4893594	-3.0606574	-2.9741474
C	-2.7741133	-3.6718365	-3.0833381
C	-1.0015172	-2.4893616	-1.7423804
C	0.1856767	-1.7494526	-1.8005200
O	-1.6823737	-0.3012270	-0.1107889
O	0.6610442	-1.1229054	-0.6504799
P	-0.1214172	0.1576269	-0.0135529
O	0.3405158	0.1811692	1.4650209
O	0.0545597	1.4491243	-0.8095590
C	-2.6879727	-6.5382754	1.1690642
C	-1.9496401	-6.4412468	-0.0394724
H	-3.5924633	-5.4464334	2.8050179
H	-2.9556968	-7.5267076	1.5723700
H	-1.0360539	-5.1448937	-1.4975310
H	-1.6333614	-7.3566561	-0.5623707
C	-3.2057504	-4.2204859	-4.2827448
C	-2.3731026	-4.1886262	-5.4326633
H	-3.4309619	-3.6943520	-2.2024881
H	-4.2050933	-4.6776737	-4.3437585
H	-2.7234395	-4.6328472	-6.3767022
H	-0.4860474	-3.5238330	-6.2597447
C	-1.7769175	-0.2727885	3.6225633
C	-2.6582020	-0.4227558	2.5102052
C	-1.7401140	0.9666881	4.2829228
C	-3.5039147	0.6511715	2.1248583
C	-3.4163110	1.8741425	2.8159387
C	-2.5251348	2.0625178	3.8839471
H	-1.0485406	1.1021094	5.1303422

7.5 Interconversion of Complexes 13

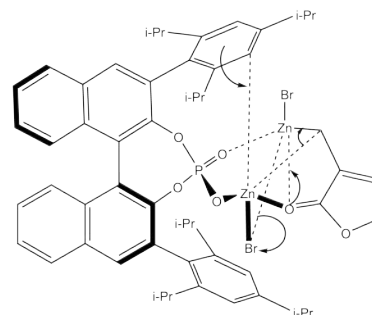
7.5.1 Pathway 13d-ma ↔ 13d-mi

TS1-dma-dmi; COSMO

C	-4.5462395	0.4926565	1.0205192
H	-4.0668706	2.7030928	2.4988916
C	-4.4528661	1.5821545	-0.0570552
H	-4.6757188	2.5918399	0.3465182
H	-5.1818933	1.3917855	-0.8708528
H	-3.4484269	1.6201584	-0.5187884
C	-5.9575399	0.4199024	1.6359620
H	-4.3625107	-0.4815546	0.5221292
H	-6.2153912	1.3656152	2.1572290
H	-6.0348775	-0.4022348	2.3763535
H	-6.7211629	0.2497502	0.8489378
C	-2.4140858	3.3827436	4.6373846
C	-2.6391457	4.6168731	3.7533460
H	-2.4233678	5.5470702	4.3174044
H	-3.6888794	4.6886228	3.4008815
H	-1.9855616	4.5944896	2.8583230
C	-3.3596302	3.3911136	5.8547018
H	-1.3707096	3.4338265	5.0216485
H	-3.2427165	4.3221654	6.4477855
H	-3.1637185	2.5288798	6.5232334
H	-4.4181512	3.3249957	5.5266210
C	-0.8950789	-1.4139040	4.1332803
C	0.5402460	-0.9955792	4.4955609
H	1.1284065	-1.8796927	4.8152863
H	0.5728612	-0.2657981	5.3304851
H	1.0630457	-0.5568704	3.6233184
C	-1.5645364	-2.0952540	5.3444850
H	-0.8142232	-2.1657182	3.3223036
H	-0.9746891	-2.9710800	5.6862415
H	-2.5887767	-2.4434912	5.1048883
H	-1.6500944	-1.3871488	6.1952248
H	5.6459529	2.5775509	-3.2373328
H	5.3657285	-3.1382458	-1.7337432
H	0.7615429	1.0453725	-6.7104096
C	5.8665679	1.6414427	-2.6776752
H	3.4518719	-3.1866843	0.8392402
H	7.1025254	2.7201147	-1.2236594
H	-0.0307378	2.6406150	-4.8661717
C	4.6096033	0.7837804	-2.7465672
C	4.3248959	-3.5181811	-1.8014120
C	6.2292452	2.0354081	-1.2361362
H	6.4969872	1.1480425	-0.6258318
C	4.4852266	-0.3964465	-1.9933158
C	1.6023791	0.7221774	-6.0626519
H	6.7980399	0.7040462	-4.4376167
C	3.5399590	1.1396149	-3.5808908
C	7.0462146	0.9478742	-3.3850849
H	7.9487727	1.5939951	-3.3826721
H	3.6209449	2.0658469	-4.1729121
C	3.5543706	-2.2431475	0.2643988
H	4.2776039	-4.4736446	-1.2386197
H	4.1176190	-3.7363663	-2.8686462
C	3.3405155	-1.2079465	-2.0543800
C	0.8321244	2.3213048	-4.2482671
C	2.3617309	0.3735961	-3.6721158
H	1.8504892	-0.3279928	-6.3194058
H	2.4861224	1.3420790	-6.3223849
C	3.3187656	-2.4980572	-1.2351708
C	2.2643476	-0.8212312	-2.9050497
C	1.2350045	0.8746433	-4.5747789
H	2.8225201	-1.5161358	0.6658974
H	0.5167447	2.4108147	-3.1921297
H	4.5701362	-1.8426280	0.4618583
H	5.3823875	2.5365457	-0.7260269
H	1.6594471	3.0384878	-4.4297850
H	7.3103442	-0.0024334	-2.8751736
H	2.3136421	-2.9540883	-1.3371231
H	0.3415374	0.2469136	-4.3844883
H	5.3120347	-0.7000159	-1.3321019
H	-1.1692719	5.0145114	0.8289302
H	-0.1712820	5.8080019	-0.4173237

H 2.0639790 6.9211102 0.7897179

TS1-dma-dmi



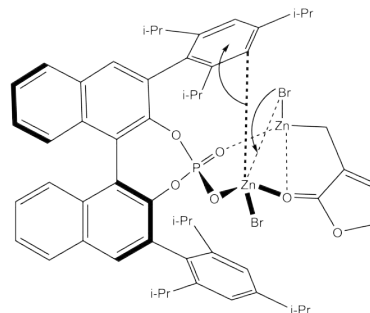
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number of imaginary frequencies: 3

Zn	1.6047122	1.4753400	2.0223212
Br	3.8658090	1.7609451	2.0080787
C	1.8743493	6.0658790	1.4507657
C	0.8866498	5.1284152	1.3054007
C	1.0974651	4.1862086	2.4218541
O	2.0717613	4.5985523	3.2422181
C	2.6794315	5.7725175	2.6703072
O	0.5498064	3.0751010	2.6009883
C	-0.1805419	4.9735147	0.3101211
H	3.7412934	5.5111562	2.4616992
H	2.6677913	6.5849463	3.4298728
Zn	-0.6080361	3.3416953	-0.8003745
Br	-2.2626217	3.5832503	-2.4366693
C	-1.9901926	-1.5785779	0.3710856
C	-1.6963739	-2.6809260	-0.4354346
C	-2.0047532	-3.9932462	0.0862165
C	-1.6160349	-5.2014874	-0.5667293
C	-2.7033325	-4.0958221	1.3463054
C	-3.0480228	-5.3859804	1.8495802
C	-2.9826744	-2.9192781	2.1000110
H	-3.4826002	-3.0216450	3.0749354
C	-2.5884464	-1.6591489	1.6685430
C	1.0134147	-1.6409695	-2.9585574
C	0.5864943	-2.3048997	-4.1030774
H	1.2124184	-2.2702178	-5.0078552
C	-0.6628756	-2.9872656	-4.1557389
C	-1.1297103	-3.5784996	-5.3679355
C	-1.4894810	-3.0607280	-2.9741276
C	-2.7742067	-3.6719692	-3.0835174
C	-1.0018432	-2.4894025	-1.7422863
C	0.1853192	-1.7494066	-1.8002097
O	-1.6830900	-0.3013626	-0.1106253
O	0.6604213	-1.1229550	-0.6500058
P	-0.1221384	0.1575403	-0.0130371
O	0.3396881	0.1809338	1.4655375
O	0.0542334	1.4489712	-0.8090661
C	-2.6880185	-6.5386801	1.1689082
C	-1.9496232	-6.4415179	-0.0396136
H	-3.5927525	-5.4469842	2.8048666
H	-2.9556218	-7.5271638	1.5721730
H	-1.0361279	-5.1450051	-1.4975938
H	-1.6331822	-7.3568721	-0.5625160
C	-3.2056356	-4.2206566	-4.2830087
C	-2.3727805	-4.1887691	-5.4328136
H	-3.4312131	-3.6945143	-2.2027793
H	-4.2049493	-4.6778937	-4.3441828

H	-2.7229436	-4.6330222	-6.3769045
H	-0.4855826	-3.5239031	-6.2595933
C	-1.7773719	-0.2732445	3.6224794
C	-2.6588257	-0.4231893	2.5102516
C	-1.7402922	0.9663166	4.2827055
C	-3.5045080	0.6507783	2.1249504
C	-3.4166608	1.8738260	2.8158727
C	-2.5252296	2.0622215	3.8836903
H	-1.0485919	1.1017326	5.1300215
C	-4.5470365	0.4922029	1.0208055
H	-4.0671944	2.7028203	2.4988749
C	-4.4537991	1.5816255	-0.0568423
H	-4.6765298	2.5913367	0.3467413
H	-5.1829871	1.3912229	-0.8705099
H	-3.4493930	1.6195514	-0.5186703
C	-5.9582576	0.4195664	1.6364472
H	-4.3634273	-0.4820476	0.5224463
H	-6.2159828	1.3653424	2.1576738
H	-6.0355136	-0.4025206	2.3769107
H	-6.7220023	0.2493699	0.8495421
C	-2.4137988	3.3825965	4.6367969
C	-2.6387111	4.6165219	3.7524342
H	-2.4226561	5.5468216	4.3162137
H	-3.6884757	4.6883788	3.4000612
H	-1.9851986	4.5937300	2.8573616
C	-3.3592131	3.3914703	5.8542152
H	-1.3703752	3.4335517	5.0209273
H	-3.2420225	4.3226585	6.4470273
H	-3.1633968	2.5293733	6.5229688
H	-4.4177938	3.3255095	5.5262604
C	-0.8956162	-1.4144516	4.1331255
C	0.5398251	-0.9963451	4.4951685
H	1.1278728	-1.8805513	4.8148581
H	0.5726894	-0.2665035	5.3300268
H	1.0626097	-0.5577917	3.6228361
C	-1.5650232	-2.0956609	5.3444426
H	-0.8149963	-2.1663164	3.3221740
H	-0.9752478	-2.9715577	5.6861421
H	-2.5893489	-2.4437687	5.1049804
H	-1.6503481	-1.3875050	6.1951717
H	5.6444553	2.5791311	-3.2365160
H	5.3659666	-3.1366891	-1.7327259
H	0.7616453	1.0448986	-6.7105785
C	5.8653042	1.6431992	-2.6766660
H	3.4517897	-3.1858613	0.8399242
H	7.1004243	2.7225958	-1.2224981
H	-0.0316116	2.6400922	-4.8667607
C	4.6087016	0.7850168	-2.7457623
C	4.3252785	-3.5170061	-1.8005714
C	6.2274393	2.0375131	-1.2350864
H	6.4953895	1.1503349	-0.6245926
C	4.4845845	-0.3952278	-1.9924532
C	1.6023984	0.7220318	-6.0625410
H	6.7976591	0.7059613	-4.4362329
C	3.5391069	1.1404003	-3.5803647
C	7.0454382	0.9500242	-3.3836521
H	7.9477063	1.5965489	-3.3810795
H	3.6199077	2.0665946	-4.1724805
C	3.5540204	-2.2422669	0.2651233
H	4.2782280	-4.4724838	-1.2377816
H	4.1182347	-3.7352737	-2.8678437
C	3.3401371	-1.2071345	-2.0536937
C	0.8311512	2.3210967	-4.2485320
C	2.3611553	0.3739540	-3.6717457
H	1.8508971	-0.3280960	-6.3191067
H	2.4860238	1.3421987	-6.3220635
C	3.3186950	-2.4972424	-1.2344749
C	2.2639649	-0.8208323	-2.9045722
C	1.2345301	0.8745183	-4.5747888
H	2.8218557	-1.5155251	0.6665450
H	0.5154586	2.4106179	-3.1924777

H	4.5696209	-1.8413791	0.4627020
H	5.3802375	2.5383697	-0.7252593
H	1.6583194	3.0384975	-4.4298795
H	7.3098445	-0.0000975	-2.8735212
H	2.3137409	-2.9536157	-1.3365745
H	0.3412108	0.2465204	-4.3846949
H	5.3113716	-0.6984729	-1.3310629
H	-1.1668493	5.0159033	0.8286288
H	-0.1687644	5.8081182	-0.4184126
H	2.0682771	6.9194491	0.7871404

TS2-dma-dmi; COSMO



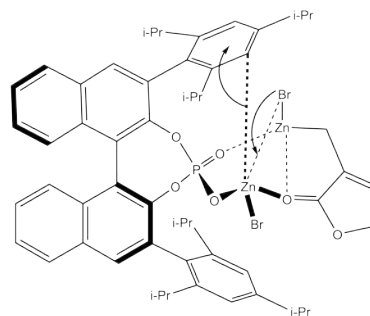
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Zn	2.4097082	0.5180607	2.1700913
Br	4.6925084	0.5401065	2.6122846
C	2.4396885	5.8581582	1.5950083
C	1.7280498	4.8032504	1.0969475
C	2.4611828	3.6017988	1.5506210
O	3.5630265	3.9092066	2.2332766
C	3.6313444	5.3520859	2.3401912
O	2.0684020	2.4297511	1.3769730
C	0.4515035	4.6273678	0.3859629
H	4.6060989	5.6844541	1.9210005
H	3.6260533	5.5986532	3.4247237
Zn	-0.3856420	3.0634447	1.3482592
Br	-0.3574677	2.5750515	3.6693466
C	-1.3106367	-2.3598995	0.7110270
C	-1.7567679	-2.8273421	-0.5288657
C	-1.6792188	-4.2501173	-0.7779742
C	-1.9529146	-4.8357366	-2.0509333
C	-1.2692313	-5.1264763	0.2957540
C	-1.2445235	-6.5368784	0.0773480
C	-0.7991979	-4.5702993	1.5213349
H	-0.3993174	-5.2461888	2.2933291
C	-0.7398387	-3.1974017	1.7204231
C	-1.6378217	0.1643313	-2.9389947
C	-2.7675714	-0.0696864	-3.7157431
H	-2.9823344	0.5947329	-4.5663165
C	-3.6942570	-1.1059608	-3.4065108
C	-4.9027641	-1.2599263	-4.1511620
C	-3.4350995	-1.9868025	-2.2927131
C	-4.4407542	-2.9339034	-1.9327528
C	-2.1929278	-1.8535707	-1.5700648
C	-1.3714554	-0.7595037	-1.8801358
O	-1.4194068	-1.0038476	1.0024286
O	-0.1963952	-0.5598787	-1.1604062
P	-0.3243747	0.0415050	0.3643373
O	1.0740647	-0.1644465	0.9594662
O	-0.9897899	1.4153039	0.3931285
C	-1.5634751	-7.0741553	-1.1607704
C	-1.8989860	-6.2108565	-2.2370740
H	-0.9435507	-7.1909558	0.9108127
H	-1.5344297	-8.1632489	-1.3171384
H	-2.2034621	-4.1845212	-2.8989035

H	-2.1126001	-6.6330476	-3.2309349
C	-5.6158847	-3.0436844	-2.6637791
C	-5.8443101	-2.2134312	-3.7939514
H	-4.2804882	-3.5762339	-1.0555761
H	-6.3791089	-3.7766273	-2.3606537
H	-6.7755878	-2.3161148	-4.3715681
H	-5.0811362	-0.5896429	-5.0067377
C	1.4845782	-2.6168920	2.7066921
C	0.0670438	-2.5414247	2.7947315
C	2.2516766	-1.8390712	3.6026533
C	-0.5498850	-1.7187200	3.7801583
C	0.2566494	-0.9522233	4.6381703
C	1.6653715	-0.9971092	4.5753779
H	3.3493018	-1.9227346	3.5799620
C	-2.0646434	-1.7322900	3.9665978
H	-0.2261198	-0.3178704	5.3965800
C	-2.6946811	-0.3331688	4.0167727
H	-2.3544963	0.2465653	4.8990976
H	-3.7993480	-0.4159657	4.0782834
H	-2.4356403	0.2573314	3.1177140
C	-2.4242080	-2.5609695	5.2162467
H	-2.4989507	-2.2604584	3.0926621
H	-2.0147166	-2.0923739	6.1357469
H	-2.0145554	-3.5896698	5.1518461
H	-3.5251933	-2.6343990	5.3344689
C	2.5459719	-0.3120506	5.6160229
C	2.2848046	1.1930146	5.7601802
H	2.9624410	1.6292007	6.5224485
H	1.2414526	1.4116307	6.0653426
H	2.4640563	1.7300966	4.8060077
C	2.4121391	-1.0382511	6.9689559
H	3.5946350	-0.4318823	5.2682529
H	3.1104322	-0.6060960	7.7151162
H	2.6372900	-2.1195368	6.8712311
H	1.3825669	-0.9429917	7.3733717
C	2.2241671	-3.4919531	1.6942087
C	3.1751575	-2.6897848	0.7881384
H	3.6774800	-3.3669500	0.0670884
H	3.9687848	-2.1689045	1.3633364
C	2.6167526	-1.9279460	0.2099360
C	2.9601859	-4.6399729	2.4113194
H	1.4693711	-3.9540067	1.0295689
H	3.4423172	-5.3144954	1.6740019
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H	3.7552104	-4.2548904	3.0836471
H	1.2274200	5.7376590	-3.3023410
H	2.2616174	0.4237559	-5.6658519
H	-4.6045138	3.6228289	-3.3908752
C	1.8314696	4.8524742	-3.6008484
H	2.8226074	-1.4985203	-3.1370054
H	3.6695004	5.7135716	-2.7687957
H	-3.9058988	3.9296981	-0.9593264
C	0.9323700	3.6324632	-3.4415646
C	1.5077793	-0.3183494	-5.3287821
C	3.0571895	4.7931607	-2.6714268
H	3.7113708	3.9309324	-2.9174640
C	1.4206857	2.3319361	-3.6567652
C	-3.5407134	3.4870695	-3.6764158
H	1.3686673	5.1281006	-5.7340458
C	-0.4177722	3.7702024	-3.0817547
C	2.2522397	5.0488083	-5.0690481
H	2.8588871	5.9704594	-5.1884184
H	-0.8138857	4.7841967	-2.9099244
C	2.4695383	-0.4592262	-2.9744683
H	1.9036576	-1.3293972	-5.5588512
H	0.5903769	-0.1626160	-5.9322542
C	0.6095556	1.1926851	-3.5168852
C	-2.8449178	3.8382390	-1.2694239
C	-1.2739532	2.6643926	-2.9127089
H	-3.5060782	2.8189718	-4.5604286
H	-3.1461105	4.4751169	-3.9939184

C	1.2166876	-0.1757220	-3.8226392
C	-0.7545403	1.3564076	-3.1395365
C	-2.7239671	2.9213077	-2.4983942
H	2.2549611	-0.3351089	-1.8952442
H	-2.2738418	3.4276454	-0.4150145
H	3.3076105	0.2184855	-3.2402622
H	2.7541415	4.6945347	-1.6098172
H	-2.4685744	4.8628113	-1.4686879
H	2.8653577	4.1946398	-5.4257987
H	0.4648125	-0.9488745	-3.5681258
H	-3.1700564	1.9478418	-2.2134309
H	2.4740300	2.1963069	-3.9498103
H	-0.1266880	5.5630926	0.2830987
H	0.6075924	4.1772609	-0.6187632
H	2.1995379	6.9257054	1.4997324

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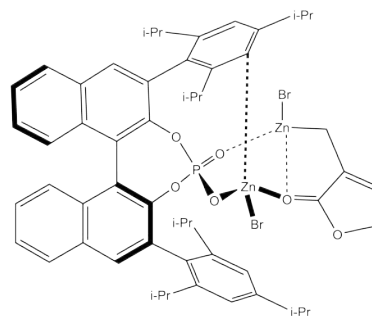


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C	1.7436706	4.7982904	1.0935818
C	2.4758710	3.5944147	1.5487277
O	3.5728840	3.9021245	2.2409867
C	3.6365044	5.3418051	2.3555263
O	2.0847599	2.4251712	1.3696641
C	0.4725785	4.6205312	0.3776017
H	4.6154056	5.6781977	1.9479824
H	3.6206121	5.5814663	3.4420161
Zn	-0.3652285	3.0595643	1.3488599
Br	-0.3556230	2.5826174	3.6646143
C	-1.3021367	-2.3589650	0.7074316
C	-1.7493446	-2.8279271	-0.5316215
C	-1.6767639	-4.2512971	-0.7780071
C	-1.9520802	-4.8382074	-2.0497552
C	-1.2710569	-5.1271570	0.2974056
C	-1.2520437	-6.5374743	0.0810035
C	-0.8009108	-4.5698988	1.5220949
H	-0.4044513	-5.2451084	2.2964902
C	-0.7363814	-3.1971789	1.7193309
C	-1.6331074	0.1629503	-2.9426046
C	-2.7643705	-0.0709817	-3.7167057
H	-2.9804339	0.5948435	-4.5658401
C	-3.6903387	-1.1070827	-3.4064675
C	-4.9003426	-1.2613054	-4.1477422
C	-3.4285095	-1.9876855	-2.2934656
C	-4.4334886	-2.9343294	-1.9313590
C	-2.1847545	-1.8549758	-1.5735683
C	-1.3632705	-0.7614080	-1.8850713
O	-1.4057383	-1.0032362	0.9964038
O	-0.1866013	-0.5622538	-1.1687723
P	-0.3096307	0.0396091	0.3571257
O	1.0890990	-0.1714028	0.9504349

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C	-1.9038350	-6.2134625	-2.2332149	C	-2.8486159	3.8228315	-1.2570021
H	-0.9540212	-7.1911450	0.9158460	C	-1.2764562	2.6630872	-2.9099754
H	-1.5476912	-8.1653205	-1.3097898	H	-3.5109552	2.8190479	-4.5525498
H	-2.1997315	-4.1868702	-2.8983948	H	-3.1564212	4.4728590	-3.9793825
H	-2.1188947	-6.6364463	-3.2263692	C	1.2191731	-0.1668910	-3.8349919
C	-5.6098969	-3.0440784	-2.6594788	C	-0.7536962	1.3576887	-3.1424870
C	-5.8409232	-2.2142907	-3.7887361	C	-2.7264140	2.9136015	-2.4912669
H	-4.2705236	-3.5761946	-1.0545188	H	2.2641734	-0.3300074	-1.9111328
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H	-6.7734930	-2.3167241	-4.3642084	H	3.3114431	0.2293463	-3.2572700
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C	-0.5514295	-1.7166934	3.7771555	H	-3.1685856	1.9373452	-2.2101284
C	0.2537584	-0.9514775	4.6373646	H	2.4690339	2.2092196	-3.9598500
C	1.6622622	-1.0011930	4.5816293	H	-0.1053543	5.5551822	0.2657640
C	3.3480639	-1.9304764	3.5940212	H	0.6315625	4.1602760	-0.6219690
C	-2.0672054	-1.7240031	3.9560662	H	2.2074730	6.9187778	1.5094553
H	-0.2307228	-0.3124843	5.3907515				
C	-2.6929035	-0.3227440	3.9997484				
H	-2.3562832	0.2591151	4.8818926				
H	-3.7980578	-0.4016997	4.0558214				
H	-2.4287682	0.2652212	3.1007921				
C	-2.4353012	-2.5492424	5.2054377				
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H	-2.0286757	-3.5793076	5.1454860				
H	-3.5369417	-2.6188799	5.3193965				
C	2.5404977	-0.3135784	5.6225104				
C	2.2818781	1.1925959	5.7590325				
H	2.9580674	1.6307634	6.5214300				
H	1.2382747	1.4165265	6.0592435				
H	2.4667850	1.7246839	4.8035104				
C	2.4008502	-1.0342294	6.9776998				
H	3.5899686	-0.4355551	5.2777965				
H	3.0970835	-0.6009257	7.7251167				
H	2.6237823	-2.1163340	6.8852469				
H	1.3702560	-0.9361684	7.3786480				
C	2.2271178	-3.5018018	1.7073267				
C	3.1841816	-2.7036733	0.8040631				
H	3.6875747	-3.3830008	0.0858127				
H	3.9769628	-2.1829377	1.3804430				
H	2.6299658	-1.9419565	0.2218644				
C	2.9569317	-4.6504864	2.4295120				
H	1.4738714	-3.9631817	1.0403241				
H	3.4410466	-5.3278737	1.6961504				
H	2.2574864	-5.2526246	3.0449648				
H	3.7498681	-4.2666739	3.1047919				
H	1.2126175	5.7455378	-3.3049422				
H	2.2553936	0.4400555	-5.6809781				
H	-4.6108760	3.6131520	-3.3780223				
C	1.8185121	4.8627248	-3.6072929				
H	2.8299496	-1.4881859	-3.1577185				
H	3.6580499	5.7319722	-2.7862336				
H	-3.9091481	3.9088937	-0.9441640				
C	0.9247687	3.6393193	-3.4433539				
C	1.5048904	-0.3046452	-5.3425019				
C	3.0498324	4.8092450	-2.6851158				
H	3.7064684	3.9499604	-2.9344730				
C	1.4162585	2.3410983	-3.6631818				
C	-3.5469232	3.4822749	-3.6651045				
H	1.3413831	5.1356995	-5.7373146				
C	-0.4241947	3.7716766	-3.0781608				
C	2.2292620	5.0609901	-5.0779320				
H	2.8315464	5.9848353	-5.2020829				
H	-0.8229603	4.7839684	-2.9022349				
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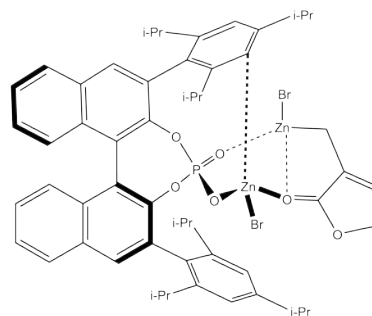


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C	2.9813582	3.6709655	1.6974712
C	3.1224735	2.4005343	2.4326679
O	4.1198214	2.4373042	3.3168205
C	4.7034122	3.7604038	3.2765871
O	2.3797895	1.4007768	2.3119795
C	1.9157713	3.8000527	0.6919589
H	5.7838559	3.6509078	3.0371046
H	4.6204951	4.1867489	4.3004174
Zn	0.3063488	2.9162637	1.5222852
Br	-0.7592818	3.1278677	3.6049037
C	-1.1813585	-2.3553448	0.3975802
C	-1.9074504	-2.6421526	-0.7631621
C	-2.0045909	-4.0269337	-1.1642443
C	-2.5663331	-4.4339944	-2.4116328
C	-1.4829649	-5.0505192	-0.2870929
C	-1.6225113	-6.4226879	-0.6550371
C	-0.7700181	-4.6802795	0.8914534
H	-0.3361606	-5.4734459	1.5198515
C	-0.5510917	-3.3480404	1.2147746
C	-2.1893387	0.7111451	-2.6318291
C	-3.4930394	0.6511825	-3.1097250
H	-3.8823368	1.4809279	-3.7194521
C	-4.3691196	-0.4207815	-2.7726960
C	-5.7324429	-0.4134322	-3.1964907
C	-3.8951217	-1.4986125	-1.9360390
C	-4.8407870	-2.4742886	-1.4976064
C	-2.5039806	-1.5215736	-1.5469884
C	-1.7148714	-0.4139918	-1.8866144

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O	-0.3748131	-0.3930089	-1.5121705	H	-1.0155639	5.1212650	-1.5636356
P	-0.0084898	-0.0392671	0.0490316	C	1.6818614	0.1059194	-3.9956104
O	1.4472941	-0.5119724	0.1910634	H	0.3600340	0.0155711	-6.4440132
O	-0.4142107	1.3641274	0.4650715	H	-0.8990163	1.2476286	-6.0926965
C	-2.2104807	-6.7835076	-1.8582151	C	-0.1073331	1.8585710	-3.5155388
C	-2.6670019	-5.7768789	-2.7499568	C	-2.7618182	3.7730734	0.1578838
H	-1.2329789	-7.1920406	0.0301677	C	-1.6564005	3.1115122	-2.0633338
H	-2.3052543	-7.8451776	-2.1324766	H	-4.1168747	3.8131207	-3.0818735
H	-2.9164411	-3.6671890	-3.1161338	H	-3.5236389	5.2152804	-2.1450886
H	-3.0999945	-6.0619825	-3.7209420	C	0.2760047	0.6294605	-4.3374249
C	-6.1656443	-2.4270166	-1.9104396	C	-1.3161335	1.9192715	-2.7686317
C	-6.6147807	-1.4002041	-2.7830121	C	-2.9616812	3.2718466	-1.2814040
H	-4.5136122	-3.2685810	-0.8128688	H	1.7762208	-0.1013653	-2.9117225
H	-6.8744352	-3.1891151	-1.5520419	H	-2.1857979	3.0429362	0.7578139
H	-7.6650471	-1.3781225	-3.1114962	H	2.4714597	0.8328969	-4.2787397
H	-6.0752142	0.4078636	-3.8453833	H	3.0888292	4.4507268	-1.9684507
C	1.8101747	-3.0255627	2.0265994	H	-2.2428923	4.7530500	0.2012792
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C	-0.0412129	-2.0541609	3.3318512	H	-3.4367666	2.2739582	-1.2040569
C	0.8935243	-1.3727680	4.1334218	H	1.6692257	2.9264848	-4.1275500
C	2.2775537	-1.4705805	3.9188960	H	1.7894838	4.8341283	0.3236112
H	3.8005448	-2.5154301	2.7598954	H	2.1022390	3.1262756	-0.1730386
C	-1.5223083	-1.9593567	3.6782173	H	4.1404827	5.5381218	1.9530292
H	0.5218811	-0.7385293	4.9490631				
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C	-1.8209207	-2.8677490	4.8888907				
H	-2.0933082	-2.3669610	2.8198079				
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H	-1.5255706	-3.9184823	4.6920616				
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C	3.3004619	-0.7740673	4.8099360				
C	2.7221828	0.3994168	5.6097925				
H	3.5407932	0.9674679	6.0939530				
H	2.0431593	0.0487491	6.4149935				
H	2.1552889	1.0977586	4.9633540				
C	3.9792862	-1.8019317	5.7384948				
H	4.0872920	-0.3700180	4.1323174				
H	4.7646762	-1.3117043	6.3489620				
H	4.4560775	-2.6236379	5.1673710				
H	3.2382495	-2.2534338	6.4307835				
C	2.3672726	-3.9696321	0.9645051				
C	3.4023736	-3.3235199	0.0317591				
H	3.7206324	-4.0535314	-0.7398319				
H	4.3155546	-2.9887477	0.5645069				
H	2.9707989	-2.4478163	-0.4937399				
C	2.9287242	-5.2349747	1.6436680				
H	1.5199797	-4.2850456	0.3264568				
H	3.2683929	-5.9644077	0.8803588				
H	2.1667399	-5.7303403	2.2794903				
H	3.7981908	-4.9921028	2.2898262				
H	1.0949534	6.0068516	-2.0066335				
H	0.8258762	1.7244190	-6.1658844				
H	-4.9098289	4.2557825	-1.5323557				
C	1.3352806	5.3916545	-2.9026921				
H	1.8891208	-0.8348422	-4.5463541				
H	3.4336024	5.9999005	-2.8081263				
H	-3.7406967	3.9019014	0.6636193				
C	0.4391219	4.1601678	-2.8374225				
C	0.1310628	0.9205844	-5.8436428				
C	2.8359311	5.0665328	-2.8544569				
H	3.1661763	4.5140501	-3.7586183				
C	0.7404528	2.9806896	-3.5390769				
C	-3.9327279	4.1870925	-2.0540515				
H	-0.0820305	6.5159269	-4.1585207				
C	-0.7648850	4.1994105	-2.1138865				
C	0.9903875	6.2350104	-4.1466352				
H	1.5931406	7.1666547	-4.1775006				
H	-1.0155639	5.1212650	-1.5636356				
C	1.6818614	0.1059194	-3.9956104				
H	0.3600340	0.0155711	-6.4440132				
H	-0.8990163	1.2476286	-6.0926965				
C	-0.1073331	1.8585710	-3.5155388				
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C	-1.6564005	3.1115122	-2.0633338				
H	-4.1168747	3.8131207	-3.0818735				
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C	0.2760047	0.6294605	-4.3374249				
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H	1.7762208	-0.1013653	-2.9117225				
H	-2.1857979	3.0429362	0.7578139				
H	2.4714597	0.8328969	-4.2787397				
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H	-0.4442513	-0.1782875	-4.0959859				
H	-3.4367666	2.2739582	-1.2040569				
H	1.6692257	2.9264848	-4.1275500				
H	1.7894838	4.8341283	0.3236112				
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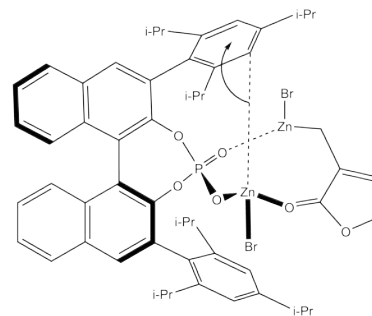
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C	2.9260640	3.7123636	1.7081324
C	3.1133924	2.4194431	2.3966936
O	4.1256293	2.4524594	3.2658851
C	4.6721753	3.7894854	3.2631603
O	2.3933054	1.4095566	2.2544335
C	1.8365361	3.8452833	0.7334022
H	5.7515669	3.7160148	3.0036444
H	4.5951180	4.1753300	4.3040725
Zn	0.2732329	2.8942616	1.5926463
Br	-0.7248580	3.0179916	3.7004748
C	-1.1758972	-2.3644959	0.3922604
C	-1.9052824	-2.6456843	-0.7678385
C	-2.0057349	-4.0284135	-1.1745024
C	-2.5729191	-4.4290004	-2.4212512
C	-1.4830949	-5.0568320	-0.3039080
C	-1.6268064	-6.4263778	-0.6781119
C	-0.7679319	-4.6925420	0.8749213
H	-0.3358709	-5.4888394	1.5008580
C	-0.5464466	-3.3624794	1.2047114
C	-2.1872111	0.7185099	-2.6160481
C	-3.4934961	0.6651826	-3.0867698
H	-3.8825254	1.5004803	-3.6890446
C	-4.3707001	-0.4064636	-2.7529118
C	-5.7356605	-0.3935577	-3.1695603
C	-3.8947955	-1.4916616	-1.9272254

C	-4.8403419	-2.4689705	-1.4929147
C	-2.5022610	-1.5200477	-1.5440337
C	-1.7119442	-0.4118378	-1.8792177
O	-1.0610440	-1.0528260	0.8216111
O	-0.3714049	-0.3947776	-1.5099125
P	0.0012555	-0.0492361	0.0523096
O	1.4540838	-0.5326492	0.1884596
O	-0.3953750	1.3539465	0.4743800
C	-2.2194343	-6.7809133	-1.8802734
C	-2.6776112	-5.7697386	-2.7650392
H	-1.2366019	-7.1995451	0.0024226
H	-2.3172736	-7.8411988	-2.1586011
H	-2.9247838	-3.6574985	-3.1195914
H	-3.1152445	-6.0495091	-3.7354028
C	-6.1664915	-2.4161492	-1.8994501
C	-6.6178339	-1.3816354	-2.7607100
H	-4.5105684	-3.2691565	-0.8165078
H	-6.8748221	-3.1800246	-1.5440894
H	-7.6695391	-1.3545657	-3.0840418
H	-6.0797710	0.4340771	-3.8095974
C	1.8120669	-3.0424236	2.0303308
C	0.4154111	-2.8726748	2.2406733
C	2.7157934	-2.3148266	2.8543352
C	-0.0477960	-2.0644221	3.3184646
C	0.8805010	-1.3658474	4.1118104
C	2.2659508	-1.4607803	3.9027783
H	3.7972656	-2.5145014	2.7642631
C	-1.5299905	-1.9865991	3.6655187
H	0.5025339	-0.7192018	4.9147456
C	-2.0312028	-0.5544973	3.8993128
H	-1.5943225	-0.0968281	4.8100663
H	-3.1322215	-0.5537001	4.0308042
H	-1.7850266	0.1096130	3.0498307
C	-1.8125548	-2.8961502	4.8792893
H	-2.0953223	-2.4064302	2.8090625
H	-1.2676435	-2.5405682	5.7787807
H	-1.4999710	-3.9426641	4.6867059
H	-2.8957220	-2.8975523	5.1186532
C	3.2829029	-0.7438179	4.7850479
C	2.6947977	0.4355159	5.5690287
H	3.5089954	1.0190144	6.0422972
H	2.0224481	0.0907756	6.3824095
H	2.1157804	1.1193128	4.9176976
C	3.9706226	-1.7524123	5.7277614
H	4.0672444	-0.3429632	4.1024763
H	4.7526342	-1.2481036	6.3310765
H	4.4541699	-2.5783149	5.1686564
H	3.2346141	-2.2010045	6.4273073
C	2.3781461	-3.9923448	0.9775256
C	3.3727261	-3.3318653	0.0106454
H	3.7040341	-4.0668724	-0.7508116
H	4.2826060	-2.9513003	0.5179683
H	2.8999477	-2.4845035	-0.5253096
C	2.9915249	-5.2261339	1.6687862
H	1.5286549	-4.3467849	0.3633261
H	3.3383786	-5.9609525	0.9138549
H	2.2581005	-5.7311916	2.3302360
H	3.8667021	-4.9466777	2.2919413
H	1.0967984	6.0242576	-2.0566335
H	0.8018981	1.7188483	-6.1764811
H	-4.8755977	4.2738988	-1.4760640
C	1.3627132	5.3769888	-2.9224464
H	1.8592767	-0.8508190	-4.5704707
H	3.4646764	5.9691535	-2.7809375
H	-3.6839819	3.9236316	0.7032035
C	0.4563298	4.1536498	-2.8460849
C	0.1040044	0.9197608	-5.8495202
C	2.8577757	5.0408755	-2.8076425
H	3.2132503	4.4462013	-3.6745471
C	0.7439728	2.9725302	-3.5505638
C	-3.9043875	4.2014918	-2.0080187

H	0.0020412	6.4669488	-4.2670668
C	-0.7388086	4.1988687	-2.1094846
C	1.0707438	6.1792056	-4.2059562
H	1.6824775	7.1045166	-4.2479265
H	-0.9785884	5.1219657	-1.5565053
C	1.6624988	0.0890496	-4.0146298
H	0.3214003	0.0146125	-6.4538524
H	-0.9250020	1.2557832	-6.0899870
C	-0.1088630	1.8552582	-3.5183249
C	-2.7117110	3.7777717	0.1899163
C	-1.6342407	3.1147497	-2.0468927
H	-4.1008978	3.8312416	-3.0347686
H	-3.4923634	5.2280574	-2.1023695
C	0.2587162	0.6246978	-4.3452372
C	-1.3085979	1.9221075	-2.7572571
C	-2.9290185	3.2801550	-1.2483044
H	1.7627060	-0.1244954	-2.9327537
H	-2.1484811	3.0356374	0.7873894
H	2.4564605	0.8104237	-4.2996303
H	3.0733080	4.4614537	-1.8880812
H	-2.1752535	4.7482438	0.2317414
H	1.3058516	5.5743526	-5.1068134
H	-0.4660259	-0.1777039	-4.0995127
H	-3.4080676	2.2843940	-1.1672765
H	1.6661962	2.9137077	-4.1491007
H	1.6774545	4.8841972	0.3929560
H	2.0059568	3.1903265	-0.1487340
H	4.0388523	5.5989269	2.0113222

7.5.2 Pathway 13j-ma ↔ 13d-ma

TS1-jma-dma; COSMO

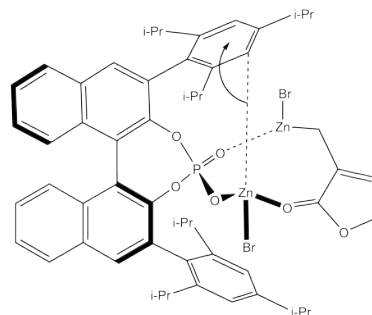


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H	2.3336499	6.5554247	2.0020080
Br	-1.0011853	5.4876658	-1.4580488
H	-2.1691980	4.3460697	2.0529449
Zn	-0.9966177	3.5989336	-0.0831854
C	0.2597026	5.9269259	2.3113006
C	1.6610231	6.1251671	2.7769844
C	-0.0518253	4.5920071	2.3441727
C	-1.2128730	3.8064839	1.9165772
C	1.1661551	3.9251795	2.8351874
O	2.1472511	4.7994589	3.0902893
O	1.3212675	2.7046836	3.0365882
H	1.7620518	6.7472079	3.6937338
H	-1.2446476	2.8229862	2.4205637
H	-0.3834226	6.7441374	1.9591287
C	-1.9521747	-1.4166818	0.4278606
C	-1.9881242	-2.2782664	-0.6730358
C	-2.2444573	-3.6811657	-0.4220635
C	-2.1480278	-4.6874992	-1.4309683
C	-2.5719066	-4.1028906	0.9205070

C	-2.8767837	-5.4747545	1.1713037	C	5.3561461	1.8604197	-3.4138215
C	-2.5000270	-3.1660613	1.9909763	H	2.9286827	-3.3401241	-0.5527142
H	-2.6766336	-3.5183207	3.0190838	H	6.8002704	2.5491221	-1.9120243
C	-2.1294697	-1.8444219	1.7806605	H	-0.6343997	3.7443373	-4.5336448
C	0.1625758	-0.8527475	-3.5046134	C	4.0211879	1.1317303	-3.4967320
C	-0.5600703	-1.2527353	-4.6230062	C	3.3627222	-3.2428819	-3.3259055
H	-0.1268275	-1.1084873	-5.6245520	C	5.8701240	1.9463401	-1.9652388
C	-1.8675077	-1.8097956	-4.5116816	H	6.1019488	0.9415465	-1.5548200
C	-2.6445672	-2.1104204	-5.6708896	C	3.8710738	-0.1685319	-2.9826079
C	-2.4256681	-2.0702277	-3.2056567	C	0.5962717	1.9251526	-6.2777042
C	-3.7580330	-2.5744672	-3.1241764	H	6.0460080	1.1923430	-5.3937604
C	-1.6310306	-1.7872833	-2.0352742	C	2.8972802	1.7375169	-4.0785369
C	-0.4285031	-1.0947230	-2.2264224	C	6.4034936	1.2213462	-4.3445811
O	-1.7501175	-0.0526049	0.2148719	H	7.3568156	1.7892029	-4.3196674
O	0.3141391	-0.6873496	-1.1230286	H	3.0010107	2.7544375	-4.4908026
P	-0.2482368	0.5008564	-0.1478765	C	3.0709982	-2.3217798	-0.9700783
O	0.6742840	0.4314916	1.0722008	H	3.2809963	-4.2799267	-2.9388133
O	-0.4391319	1.8409358	-0.8615851	H	2.9764214	-3.2315537	-4.3654755
C	-2.8193922	-6.4165321	0.1553684	C	2.6405734	-0.8444247	-3.0000205
C	-2.4298245	-6.0179620	-1.1505504	C	0.2801439	3.2585841	-4.1365423
H	-3.1387997	-5.7737283	2.1984458	C	1.6371000	1.1080151	-4.1233215
H	-3.0510828	-7.4722745	0.3629917	H	0.6723933	0.9139489	-6.7276177
H	-1.8365248	-4.4054555	-2.4449931	H	1.5062323	2.4881487	-6.5744532
H	-2.3431033	-6.7703887	-1.9492441	C	2.5835254	-2.2617184	-2.4294006
C	-4.4943471	-2.8376021	-4.2713795	C	1.5044713	-0.1944928	-3.5670482
C	-3.9309209	-2.6169105	-5.5568783	C	0.4621066	1.8602202	-4.7447256
H	-4.2042542	-2.7428398	-2.1334826	H	2.5133823	-1.6067700	-0.3358101
H	-5.5246253	-3.2149713	-4.1835021	H	0.1759847	3.2064503	-3.0366994
H	-4.5213754	-2.8357841	-6.4595954	H	4.1498201	-2.0762411	-0.8842744
H	-2.2052292	-1.9168368	-6.6621218	H	5.1186026	2.4067195	-1.2923183
C	-0.5236608	-1.1003140	3.5664890	H	1.1325507	3.9317319	-4.3647175
C	-1.7670551	-0.9119365	2.8928734	H	6.6257250	0.1778944	-4.0364198
C	-0.1203163	-0.1357653	4.5073552	H	1.5260173	-2.5948167	-2.4374308
C	-2.5877735	0.1990086	3.2103459	H	-0.4608495	1.2912439	-4.5142425
C	-2.1516986	1.1173821	4.1867166	H	4.7429602	-0.6716369	-2.5354698
C	-0.9129592	0.9827917	4.8342129				
H	0.8401527	-0.2698528	5.0344183				
C	-3.9519956	0.3865633	2.5507989				
H	-2.8016071	1.9694981	4.4345975				
C	-4.0990741	1.7488873	1.8534525				
H	-4.0459053	2.5905024	2.5745699				
H	-5.0784506	1.8154534	1.3369012				
H	-3.3023258	1.8939878	1.0977075				
C	-5.0816554	0.1470980	3.5704189				
H	-4.0506903	-0.3940626	1.7684258				
H	-5.0437175	0.8895255	4.3950611				
H	-5.0063556	-0.8621941	4.0236766				
H	-6.0755825	0.2337263	3.0845780				
C	-0.4224087	1.9551145	5.9020773				
C	-1.0688458	3.3441875	5.8344897				
H	-0.5800388	4.0320917	6.5535168				
H	-2.1459535	3.3081325	6.1011432				
H	-0.9893726	3.7881827	4.8226518				
C	-0.5955686	1.3399947	7.3057482				
H	0.6687228	2.0837663	5.7229823				
H	-0.1779019	2.0088482	8.0865430				
H	-0.0869560	0.3583916	7.3869408				
H	-1.6710717	1.1801678	7.5304953				
C	0.3547141	-2.3329778	3.3426942				
C	1.8192739	-2.0021104	3.0218525				
H	2.4298104	-2.9261445	2.9609205				
H	2.2968239	-1.3614556	3.7932032				
H	1.9053801	-1.5010124	2.0379969				
C	0.2509861	-3.2765876	4.5577452				
H	-0.0438966	-2.8802605	2.4661064				
H	0.8197410	-4.2123038	4.3789104				
H	-0.8027355	-3.5492657	4.7702759				
H	0.6610672	-2.7987030	5.4721788				
H	5.1786597	2.8985699	-3.7718733				
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TS1-jma-dma

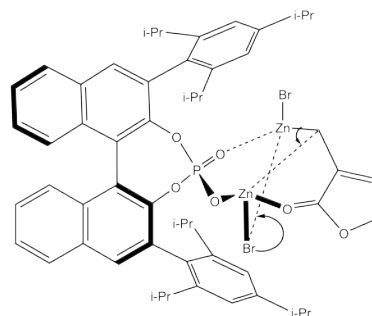


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Br	4.3444612	0.7280639	2.1306760
H	2.3539190	6.5233575	1.9437301
Br	-0.9316180	5.4958995	-1.4380348
H	-2.1584330	4.3364403	2.0431315
Zn	-0.9736553	3.6011205	-0.0911919
C	0.2781750	5.9107152	2.2762516
C	1.6849584	6.1055630	2.7292988
C	-0.0393744	4.5773899	2.3276282
C	-1.2034145	3.7942751	1.9107152
C	1.1804139	3.9095549	2.8157283
O	2.1678192	4.7831826	3.0540252
O	1.3329064	2.6906670	3.0227349
H	1.7977575	6.7376390	3.6384206
H	-1.2356825	2.8100877	2.4129683
H	-0.3629912	6.7243073	1.9128903
C	-1.9518060	-1.4167968	0.4283414

C	-1.9907338	-2.2786427	-0.6724710	H	0.6594850	-2.7988982	5.4783607
C	-2.2489427	-3.6810831	-0.4206538	H	5.1565453	2.9195666	-3.7406455
C	-2.1560036	-4.6871065	-1.4298595	H	4.4528646	-2.9645117	-3.3614514
C	-2.5752352	-4.1027286	0.9219682	H	-0.2747955	2.4341902	-6.7344623
C	-2.8820630	-5.4737641	1.1721557	C	5.3386632	1.8809140	-3.3859639
C	-2.5012163	-3.1657192	1.9916627	H	2.9279157	-3.3471762	-0.5591945
H	-2.6774122	-3.5167376	3.0202872	H	6.7707655	2.5723094	-1.8732850
C	-2.1292641	-1.8446916	1.7811871	H	-0.6548309	3.7352500	-4.5399134
C	0.1605465	-0.8565833	-3.5052531	C	4.0085623	1.1448157	-3.4792065
C	-0.5629978	-1.2565981	-4.6227936	C	3.3761696	-3.2324894	-3.3286650
H	-0.1299398	-1.1107402	-5.6241496	C	5.8445129	1.9643924	-1.9344946
C	-1.8706423	-1.8127805	-4.5114103	H	6.0800491	0.9600294	-1.5255439
C	-2.6482313	-2.1134789	-5.6696670	C	3.8634034	-0.1577872	-2.9704647
C	-2.4293040	-2.0718111	-3.2055123	C	0.5995529	1.9256106	-6.2779704
C	-3.7618433	-2.5746324	-3.1240894	H	6.0418816	1.2247536	-5.3650514
C	-1.6343392	-1.7894351	-2.0354493	C	2.8846467	1.7455795	-4.0649688
C	-0.4309245	-1.0990095	-2.2273256	C	6.3943682	1.2525059	-4.3143620
O	-1.7464575	-0.0532431	0.2161889	H	7.3443648	1.8255582	-4.2829325
O	0.3131256	-0.6939213	-1.1243909	H	2.9841797	2.7646283	-4.4725963
P	-0.2431388	0.4941397	-0.1473801	C	3.0654151	-2.3256155	-0.9702751
O	0.6827431	0.4176018	1.0712582	H	3.2993675	-4.2720588	-2.9474390
O	-0.4239180	1.8372638	-0.8575995	H	2.9964046	-3.2181458	-4.3703818
C	-2.8280498	-6.4149965	0.1563065	C	2.6372737	-0.8404511	-2.9962262
C	-2.4399039	-6.0166450	-1.1494681	C	0.2584762	3.2528350	-4.1364650
H	-3.1430443	-5.7725704	2.1995971	C	1.6284049	1.1098370	-4.1186306
H	-3.0614031	-7.4703019	0.3639877	H	0.6857789	0.9159878	-6.7296899
H	-1.8456075	-4.4044879	-2.4439483	H	1.5085945	2.4938449	-6.5668439
H	-2.3558697	-6.7687385	-1.9486661	C	2.5857099	-2.2606378	-2.4320466
C	-4.4980774	-2.8378769	-4.2708241	C	1.5005048	-0.1945848	-3.5660129
C	-3.9345902	-2.6185979	-5.5558689	C	0.4535948	1.8571318	-4.7462312
H	-4.2075483	-2.7419863	-2.1330962	H	2.5001876	-1.6179565	-0.3347989
H	-5.5286285	-3.2142534	-4.1826522	H	0.1460671	3.983130	-3.0379627
H	-4.5249981	-2.8372485	-6.4585942	H	4.1417990	-2.0733591	-0.8757199
H	-2.2087086	-1.9202901	-6.6608495	H	5.0870905	2.4172799	-1.2635186
C	-0.5237744	-1.1033744	3.5688746	H	1.1086443	3.9318524	-4.3543204
C	-1.7658154	-0.9129493	2.8935377	H	6.6214769	0.2092158	-4.0097669
C	-0.1204328	-0.1389163	4.5093820	H	1.5302810	-2.6004491	-2.4481144
C	-2.5843257	0.2000598	3.2085772	H	-0.4679920	1.2825367	-4.5244625
C	-2.1475758	1.1184686	4.1842081	H	4.7357368	-0.6573776	-2.5203801
C	-0.9105534	0.9815619	4.8339559				
H	0.8395498	-0.2740017	5.0371591				
C	-3.9481481	0.3881973	2.5482905				
H	-2.7956716	1.9725639	4.4298725				
C	-4.0952979	1.7499012	1.8501774				
H	-4.0436067	2.5924686	2.5703043				
H	-5.0737850	1.8161871	1.3321637				
H	-3.2982379	1.8939790	1.0948254				
C	-5.0778995	0.1478163	3.5674019				
H	-4.0461742	-0.3923523	1.7658442				
H	-5.0403681	0.8889209	4.3931105				
H	-5.0022871	-0.8615311	4.0199684				
H	-6.0720217	0.2346390	3.0821378				
C	-0.4190686	1.9536349	5.9016498				
C	-1.0590195	3.3454369	5.8295691				
H	-0.5709851	4.0323974	6.5500164				
H	-2.1371136	3.3144690	6.0924790				
H	-0.9741704	3.7880437	4.8176128				
C	-0.5993434	1.3418122	7.3057589				
H	0.6731942	2.0778253	5.7253877				
H	-0.1816155	2.0094427	8.0875163				
H	-0.0962213	0.3578482	7.3901366				
H	-1.6760269	1.1864430	7.5269689				
C	0.3532870	-2.3374997	3.3474389				
C	1.8182961	-2.0101829	3.0239806				
H	2.4281744	-2.9347572	2.9667989				
H	2.2990240	-1.3668757	3.7912004				
H	1.9054614	-1.5150835	2.0373911				
C	0.2487682	-3.2778314	4.5648861				
H	-0.0470044	-2.8864091	2.4726082				
H	0.8156784	-4.2151178	4.3887945				
H	-0.8051267	-3.5479543	4.7791733				

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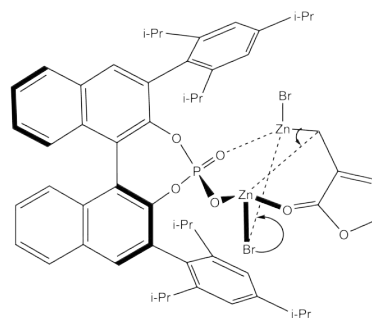


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Zn	2.5064520	0.7019142	1.8979441
Br	4.7580047	0.5250211	1.5324489
H	1.9890337	5.8961170	4.3248992
Br	0.5308838	5.2546141	-1.1932064
H	-1.5292078	3.3391308	1.9044381
Zn	0.0635795	3.3016610	-0.0246528
C	0.2118773	4.9102446	3.4898780
C	1.2667186	5.0742908	4.5265517
C	0.3136073	3.6721577	2.9136805
C	-0.4788401	2.9826837	1.8935555
C	1.4775519	3.0400671	3.5661253
O	2.0031352	3.8338802	4.5098134
O	1.9848066	1.9165410	3.3737941
H	0.8652171	5.2222418	5.5538277
H	-0.4835049	1.8917750	2.0794068

H	-0.5385673	5.6793141	3.2630630	H	1.1392141	-3.9879248	4.7808743
C	-1.4303454	-1.8415350	0.1772387	H	-0.6050716	-3.5741501	4.8834485
C	-1.3011696	-2.7563706	-0.8761852	H	0.6021478	-2.5655432	5.7325994
C	-1.3855740	-4.1632904	-0.5582345	H	3.4954779	4.5045491	-2.9314719
C	-1.1020898	-5.1918217	-1.5074141	H	5.1558186	-1.1277509	-4.1856698
C	-1.7302685	-4.5582979	0.7875431	H	-1.1161656	2.4534359	-6.6021347
C	-1.8573509	-5.9458875	1.0988542	C	4.0220088	3.5749454	-2.6242394
C	-1.8752924	-3.5657295	1.7985624	H	4.2345632	-2.7397752	-1.5513615
H	-2.1024553	-3.8852919	2.8274805	H	4.6687410	4.4530813	-0.7152591
C	-1.6742610	-2.2154280	1.5359027	H	-2.0957487	3.1067270	-4.3470530
C	0.4543247	-0.8725828	-3.7347106	C	3.1766636	2.4052893	-3.1100638
C	-0.2216597	-1.3576042	-4.8473421	C	4.2665093	-1.7925872	-4.1934882
H	0.0775921	-1.0191090	-5.8513469	C	4.0958394	3.5770803	-1.0847881
C	-1.3423745	-2.2314461	-4.7217284	H	4.5837626	2.6596597	-0.6951580
C	-2.0801356	-2.6461608	-5.8713621	C	3.6024530	1.0761991	-2.9252051
C	-1.7802983	-2.6605654	-3.4130502	C	-0.1332979	2.2701256	-6.1197317
C	-2.9815437	-3.4253209	-3.3198206	H	5.3711982	3.6071921	-4.3606914
C	-1.0087828	-2.2700270	-2.2563017	C	1.9198952	2.6176181	-3.6974766
C	0.0488663	-1.3790061	-2.4589893	C	5.4255154	3.5929586	-3.2531744
O	-1.3385553	-0.4754519	-0.0911674	H	5.9927944	4.4882169	-2.9243627
O	0.7917048	-0.9613643	-1.3551720	H	1.5851711	3.6540218	-3.8585891
P	0.1509197	0.1616352	-0.3565359	C	3.9611450	-1.6712450	-1.6723867
O	0.9924055	0.0711804	0.9270781	H	4.6237431	-2.8396998	-4.1028536
O	-0.0540994	1.5340088	-0.9937298	H	3.7727935	-1.6796267	-5.1801043
C	-1.6137420	-6.9176101	0.1401900	C	2.7755704	-0.0162016	-3.2280586
C	-1.2141364	-6.5331816	-1.1675732	C	-1.1040618	2.9542612	-3.8727062
H	-2.1354594	-6.2296831	2.1261018	C	1.0471127	1.5589391	-4.0169453
H	-1.7089791	-7.9841442	0.3948164	H	0.3878671	1.4730139	-6.6890093
H	-0.7808110	-4.9130595	-2.5200424	H	0.4709904	3.1964504	-6.2180712
H	-0.9845637	-7.3047804	-1.9182280	C	3.3051465	-1.4370078	-3.0420168
C	-3.6864743	-3.7958238	-4.4573997	C	1.4668153	0.2273798	-3.7358078
C	-3.2251262	-3.4192485	-5.7467457	C	-0.3114849	1.8829151	-4.6384816
H	-3.3545331	-3.7160094	-2.3278668	H	3.2773290	-1.3932579	-0.8476035
H	-4.6132215	-4.3812121	-4.3570656	H	-1.2619178	2.6467615	-2.8213496
H	-3.7865923	-3.7256827	-6.6424631	H	4.8904320	-1.0788785	-1.5466527
H	-1.7293308	-2.3222320	-6.8638559	H	3.0773531	3.6378854	-0.6477016
C	-0.5326042	-1.1864146	3.5429570	H	-0.5873505	3.9350123	-3.8545487
C	-1.6248889	-1.1872930	2.6238478	H	6.0155867	2.7007975	-2.9558221
C	-0.4766679	-0.1799219	4.5226329	H	2.4418755	-2.1304519	-3.1190558
C	-2.6289878	-0.1878103	2.7247278	H	-0.9239897	0.9598188	-4.6132841
C	-2.5376247	0.7785598	3.7455071	H	4.5995115	0.8845884	-2.4987427
C	-1.4673507	0.8104890	4.6525460				
H	0.3753097	-0.1647949	5.2225680				
C	-3.8282176	-0.1438321	1.7799629				
H	-3.3290029	1.5388021	3.8162175				
C	-3.9213762	1.1941065	1.0240693				
H	-4.0967335	2.0444004	1.7161599				
H	-4.7650805	1.1753005	0.3039187				
H	-2.9922148	1.3942257	0.4559016				
C	-5.1342009	-0.4616706	2.5321250				
H	-3.6909994	-0.9408084	1.0214838				
H	-5.3518750	0.3026079	3.3074625				
H	-5.0767230	-1.4466201	3.0385849				
H	-5.9950658	-0.4842481	1.8323017				
C	-1.3556894	1.8395155	5.7747172				
C	-2.2360993	3.0801384	5.5829524				
H	-2.0203345	3.8314864	6.3695545				
H	-3.3148346	2.8301893	5.6599942				
H	-2.0651711	3.5568153	4.5974517				
C	-1.6369347	1.1792179	7.1400864				
H	-0.2934311	2.1777235	5.7867408				
H	-1.4896299	1.9014898	7.9696149				
H	-0.9717662	0.3110239	7.3192489				
H	-2.6843839	0.8141577	7.1845723				
C	0.5551314	-2.2642234	3.5497326				
C	1.9860286	-1.7063179	3.4320513				
H	2.7456427	-2.4789379	3.6662563				
H	2.1739640	-0.8545112	4.1192776				
H	2.1920103	-1.4140354	2.3794480				
C	0.4154165	-3.1473745	4.8059189				
H	0.3985968	-2.9174019	2.6693398				

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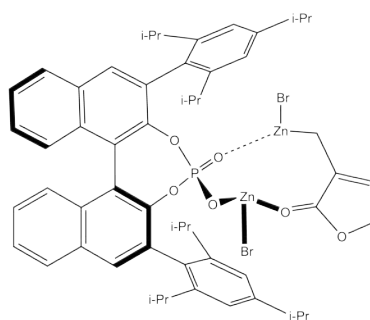


Energy (Hartree) = -11625.07555976
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Zn	2.5135883	0.7101123	1.8939107
Br	4.7592957	0.5385328	1.5234910
H	1.9604695	5.9059413	4.3106575
Br	0.5508904	5.2487198	-1.1832227
H	-1.5426412	3.3209902	1.8927939
Zn	0.0720167	3.3012432	-0.0264581
C	0.1872426	4.9087009	3.4760065
C	1.2415727	5.0806656	4.5135600
C	0.2954359	3.6689964	2.9044936
C	-0.4896146	2.9725194	1.8866871
C	1.4646135	3.0443245	3.5599676

O	1.9841241	3.8462997	4.5027657	H	2.1726987	-0.8625210	4.1304328
O	1.9796103	1.9268351	3.3695396	H	2.1941376	-1.4197303	2.3920801
H	0.8383113	5.2296242	5.5406129	C	0.4069491	-3.1537132	4.8116297
H	-0.4850523	1.8814903	2.0710048	H	0.3952921	-2.9203193	2.6753887
H	-0.5660200	5.6730765	3.2433550	H	1.1287165	-3.9960497	4.7880126
C	-1.4274340	-1.8402301	0.1806429	H	-0.6145744	-3.5781073	4.8865239
C	-1.2990291	-2.7551818	-0.8729667	H	0.5919013	-2.5741414	5.7400099
C	-1.3844792	-4.1619796	-0.5554954	H	3.5101422	4.5046078	-2.9486629
C	-1.1025115	-5.1896707	-1.5056358	H	5.1532980	-1.1289533	-4.1930520
C	-1.7292887	-4.5578437	0.7897631	H	-1.1177046	2.4588572	-6.5923094
C	-1.8568108	-5.9453031	1.0993630	C	4.0368769	3.5748617	-2.6422653
C	-1.8746065	-3.5654826	1.8004766	H	4.2388794	-2.7395694	-1.5539337
H	-2.1029080	-3.8846100	2.8293079	H	4.7053440	4.4605135	-0.7451275
C	-1.6728366	-2.2152550	1.5387795	H	-2.0929800	3.1152687	-4.3357454
C	0.4552051	-0.8688212	-3.7300264	C	3.1838772	2.4058237	-3.1158729
C	-0.2228841	-1.3517233	-4.8421365	C	4.2636434	-1.7930453	-4.1972717
H	0.0758553	-1.0106466	-5.8453805	C	4.1259400	3.5844095	-1.1038167
C	-1.3435025	-2.2254245	-4.7174671	H	4.6151910	2.6680092	-0.7135167
C	-2.0825391	-2.6383772	-5.8663250	C	3.6076253	1.0764283	-2.9304053
C	-1.7799922	-2.6573124	-3.4094149	C	-0.1347380	2.2736274	-6.1108723
C	-2.9801986	-3.4232163	-3.3167233	H	5.3685735	3.5944024	-4.3924945
C	-1.0074649	-2.2684788	-2.2530037	C	1.9240487	2.6195967	-3.6955471
C	0.0505219	-1.3779652	-2.4553359	C	5.4338097	3.5853326	-3.2856783
O	-1.3339690	-0.4747821	-0.0866837	H	6.0077429	4.4798118	-2.9666109
O	0.7952459	-0.9625319	-1.3519465	H	1.5903464	3.6564199	-3.8556156
P	0.1569763	0.1601233	-0.3528269	C	3.9661624	-1.6709346	-1.6749076
O	0.9975771	0.0697256	0.9317091	H	4.6205787	-2.8403750	-4.1080803
O	-0.0450053	1.5321885	-0.9913986	C	3.7669306	-1.6791944	-5.1820676
C	-1.6141267	-6.9160426	0.1402671	H	2.7778842	-0.0149509	-3.2277909
C	-1.2152482	-6.5307668	-1.1668831	C	-1.1004957	2.9620214	-3.8635660
H	-2.1347784	-6.2298738	2.1264375	C	1.0484815	1.5623381	-4.0105817
H	-1.7097622	-7.9826639	0.3941599	H	0.3848427	1.4758580	-6.6805422
H	-0.7822425	-4.9091654	-2.5179943	H	0.4714753	3.1982387	-6.2108880
H	-0.9867675	-7.3017613	-1.9183912	C	3.3065810	-1.4362409	-3.0427897
C	-3.6857499	-3.7919428	-4.4539999	C	1.4681084	0.2304679	-3.7312382
C	-3.2264004	-3.4123165	-5.7424919	C	-0.3112107	1.8880259	-4.6290487
H	-3.3513280	-3.7161120	-2.3248115	H	3.2855718	-1.3923123	-0.8478580
H	-4.6117173	-4.3784975	-4.3538228	H	-1.2577346	2.6562153	-2.8118640
H	-3.7884863	-3.7170883	-6.6383220	H	4.8964502	-1.0800304	-1.5509744
H	-1.7331166	-2.3118836	-6.8584306	H	3.1122061	3.6516518	-0.6573201
C	-0.5342113	-1.1894659	3.5491799	H	-0.5832559	3.9423592	-3.8471397
C	-1.6242800	-1.1883230	2.6277372	H	6.0240836	2.6927344	-2.9904803
C	-0.4797855	-0.1844341	4.5300705	H	2.4424882	-2.1291111	-3.1171986
C	-2.6276954	-0.1883525	2.7277267	H	-0.9256392	0.9661530	-4.6016292
C	-2.5376314	0.7765325	3.7497357	H	4.6063948	0.8838925	-2.5085342
C	-1.4697342	0.8063361	4.6591925				
H	0.3709059	-0.1707747	5.2317158				
C	-3.8254445	-0.1435019	1.7811865				
H	-3.3288828	1.5369312	3.8197170				
C	-3.9173950	1.1939388	1.0245864				
H	-4.0945823	2.0449037	1.7155138				
H	-4.7595325	1.1750546	0.3028840				
H	-2.9878847	1.3930840	0.4569965				
C	-5.1321335	-0.4621137	2.5315990				
H	-3.6867603	-0.9402573	1.0228610				
H	-5.3514792	0.3013247	3.3071734				
H	-5.0748744	-1.4468856	3.0379749				
H	-5.9923458	-0.4847996	1.8311121				
C	-1.3604819	1.8323503	5.7845003				
C	-2.2393988	3.0741538	5.5935074				
H	-2.0266247	3.8235848	6.3828729				
H	-3.3184031	2.8248703	5.6670833				
H	-2.0655336	3.5531851	4.6097209				
C	-1.6468624	1.1688696	7.1471784				
H	-0.2979280	2.1701904	5.8003403				
H	-1.5019741	1.8879061	7.9799635				
H	-0.9839243	0.2991367	7.3259246				
H	-2.6943988	0.8042153	7.1868624				
C	0.5518700	-2.2689334	3.5571481				
C	1.9842498	-1.7138913	3.4429257				
H	2.7416792	-2.4882449	3.6788088				

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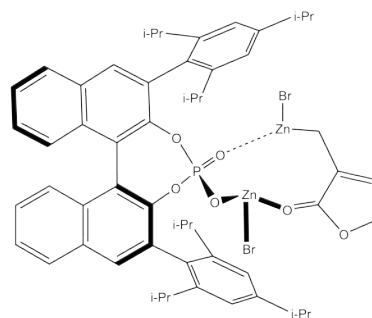


Energy (Hartree) = -11625.08859186

Zn	2.1376165	1.0205745	1.9289833
Br	4.2556638	0.2865830	2.4011377
H	3.3883861	6.3138750	0.7849092
Br	0.5937641	4.4308213	-3.1295383
H	-1.2538192	4.4691595	0.4354587
Zn	0.0686734	3.1200143	-1.2573126
C	1.2426048	5.8809981	0.7612969
C	2.5293157	6.1267730	1.4674864
C	0.7993683	4.6135667	1.0353028

C	-0.3559412	3.8360901	0.5755628	C	1.1031078	-1.6457285	3.6418449
C	1.8175870	4.0348725	1.9314920	H	1.5833596	-2.6087699	3.9101158
O	2.8034738	4.9049153	2.1862668	H	1.5525729	-0.8709104	4.2984300
O	1.8349037	2.9046385	2.4618432	H	1.3843679	-1.4284410	2.5928153
H	2.4985500	6.9579946	2.2058972	C	-0.8232582	-2.2380946	5.1899437
H	-0.5896453	3.0035342	1.2661124	H	-0.7653816	-2.4937234	3.0589539
H	0.7585544	6.6203920	0.1094755	H	-0.3602547	-3.2242349	5.4006327
C	-1.9884347	-1.5136714	0.2957431	H	-1.9231811	-2.3478217	5.2808103
C	-1.8975610	-2.6655645	-0.4962281	H	-0.4929034	-1.5325062	5.9808748
C	-2.3604664	-3.9088535	0.0817906	H	4.6950805	2.9386527	-2.7856338
C	-2.1755606	-5.1773306	-0.5472812	H	5.3220628	-2.8408433	-2.1848208
C	-3.0035557	-3.8841055	1.3758654	H	0.7006954	1.4940549	-6.8712498
C	-3.5123443	-5.0980220	1.9287344	C	4.5455039	2.2552369	-1.9205001
C	-3.0364467	-2.6730391	2.1261879	H	3.5026007	-3.6689278	0.3398894
H	-3.4503976	-2.6911190	3.1464262	H	4.2470843	3.9049494	-0.4841763
C	-2.4724803	-1.4999298	1.6412692	H	-1.2022067	0.8787659	-5.3177646
C	0.7895871	-1.9472635	-3.1614283	C	3.7566182	1.0535982	-2.4312406
C	0.2856842	-2.6361887	-4.2569073	C	4.3613206	-3.3823149	-2.3135730
H	0.8704636	-2.6845477	-5.1877704	C	3.7004706	3.0243024	-0.8820527
C	-1.0132761	-3.2265908	-4.2350511	H	3.4676643	2.3652460	-0.0167966
C	-1.5632647	-3.8273083	-5.4075175	C	3.8821602	-0.2197894	-1.8501433
C	-1.8158999	-3.1678566	-3.0348338	C	1.3857865	1.4846280	-5.9990583
C	-3.1596012	-3.6433282	-3.0948729	H	6.5243334	1.3042665	-2.0506836
C	-1.2386473	-2.6078884	-1.8349221	C	2.8173926	1.2177278	-3.4671852
C	0.0114043	-1.9928321	-1.9563377	C	5.9228791	1.9060027	-1.3399300
O	-1.5934142	-0.2844404	-0.2326265	H	6.4893978	2.8299835	-1.1053862
O	0.5769519	-1.3957281	-0.8282466	H	2.7442033	2.2000424	-3.9566418
P	0.0010349	0.0619786	-0.3674148	C	3.4623695	-2.6343928	-0.0586092
O	0.6270860	0.3318687	1.0105026	H	4.4948629	-4.4115341	-1.9197554
O	0.1245409	1.1438943	-1.4367708	H	4.1579320	-3.4514250	-3.4015132
C	-3.3574199	-6.3056419	1.2651886	C	3.0142301	-1.2723035	-2.1910272
C	-2.6627281	-6.3437703	0.0273266	C	-0.4966443	0.8104552	-4.4639095
H	-4.0128709	-5.0578829	2.9090207	C	1.9260787	0.1983025	-3.8490154
H	-3.7489283	-7.2352199	1.7056318	H	2.4086618	1.2666345	-6.3680052
H	-1.6300583	-5.2311820	-1.4985992	H	1.3814676	2.5084744	-5.5717339
H	-2.5017835	-7.3070619	-0.4803650	C	3.2195590	-2.6549089	-1.5748316
C	-3.6722333	-4.1991529	-4.2596227	C	1.9789719	-1.0388518	-3.1372882
C	-2.8635698	-4.3104608	-5.4217858	C	0.9110265	0.4420588	-4.9737771
H	-3.7965050	-3.5576346	-2.2031803	H	2.6528811	-2.0940157	0.4684054
H	-4.7147431	-4.5515810	-4.2823707	H	-0.8943004	0.0664106	-3.7482650
H	-3.2761692	-4.7621305	-6.3367810	H	4.4199025	-2.1426274	0.2078263
H	-0.9376523	-3.8794242	-6.3124606	H	2.7507217	3.3861122	-1.3270854
C	-1.1383895	-0.4184090	3.4735624	H	-0.4768002	1.7919100	-3.9515262
C	-2.1796526	-0.3104739	2.5026580	H	5.8313819	1.3320573	-0.3943045
C	-0.7537389	0.7363865	4.1767020	H	2.2952218	-3.2426633	-1.7559410
C	-2.8144247	0.9394021	2.2838261	H	0.8147688	-0.5175496	-5.5221580
C	-2.4092071	2.0583423	3.0388291	H	4.6517028	-0.3954331	-1.0848233
C	-1.3707902	1.9864808	3.9815112				
H	0.0588906	0.6625498	4.9193441				
C	-3.9491989	1.0943839	1.2739818				
H	-2.9168749	3.0187146	2.8665506				
C	-3.6733785	2.1975172	0.2369321				
H	-3.6167540	3.2008747	0.7078499				
H	-4.4855247	2.2316970	-0.5177995				
H	-2.7204006	2.0143112	-0.2971488				
C	-5.2911485	1.3243914	1.9949819				
H	-4.0370279	0.1365705	0.7212678				
H	-5.2808006	2.2734563	2.5711589				
H	-5.5110676	0.5022207	2.7058436				
H	-6.1254139	1.3818040	1.2655072				
C	-0.9165309	3.1780351	4.8194922				
C	-1.3087257	4.5437937	4.2429521				
H	-0.8475130	5.3587980	4.8364999				
H	-2.4073998	4.7005105	4.2731182				
H	-0.9813314	4.6566696	3.1906394				
C	-1.4188028	3.0346192	6.2706296				
H	0.1956860	3.1301928	4.8430354				
H	-1.0336626	3.8581638	6.9069421				
H	-1.0979904	2.0742071	6.7216344				
H	-2.5282162	3.0665644	6.3025836				
C	-0.4242914	-1.7346122	3.7893186				

int-jma-dma



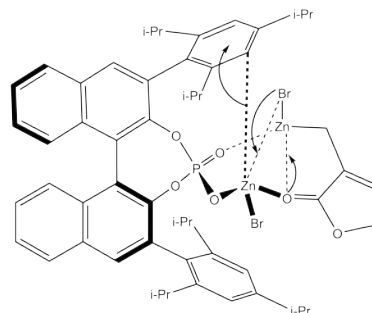
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Zn	2.1713419	1.0177143	1.9010998
Br	4.2754183	0.2854229	2.3985624
H	3.3685408	6.2798463	0.6628387
Br	0.6372508	4.4533960	-3.1060969
H	-1.2881591	4.4656301	0.4022921
Zn	0.0654564	3.1181632	-1.2774225
C	1.2178413	5.8768462	0.6948956
C	2.5240415	6.1151569	1.3699169

C	0.7691948	4.6163696	0.9924064	C	-0.4274059	-1.7428736	3.8014641
C	-0.3896630	3.8368341	0.5540755	C	1.1007887	-1.6533111	3.6634230
C	1.8026562	4.0359855	1.8728482	H	1.5787109	-2.6197778	3.9230369
O	2.8012518	4.9025233	2.0986988	H	1.5487736	-0.8868103	4.3303998
O	1.8220597	2.9094917	2.4046980	H	1.3894647	-1.4230205	2.6195386
H	2.5237110	6.9575472	2.0971082	C	-0.8344874	-2.2510466	5.1979700
H	-0.6181338	3.0077464	1.2500900	H	-0.7640794	-2.4996500	3.0664711
H	0.7314031	6.6065120	0.0342910	H	-0.3721331	-3.2372476	5.4096924
C	-1.9872347	-1.5157344	0.3057605	H	-1.9347173	-2.3614097	5.2828459
C	-1.8979159	-2.6644191	-0.4912743	H	-0.5104903	-1.5474765	5.9932205
C	-2.3628599	-3.9094649	0.0811627	H	4.7225873	2.9287998	-2.7875117
C	-2.1799739	-5.1749553	-0.5540031	H	5.3201198	-2.8365150	-2.1758402
C	-3.0061748	-3.8903121	1.3749991	H	0.7104496	1.5174048	-6.8542963
C	-3.5164927	-5.1061196	1.9210203	C	4.5704846	2.2511610	-1.9182004
C	-3.0381513	-2.6825627	2.1300767	H	3.4995305	-3.6711675	0.3451824
H	-3.4524691	-2.7034456	3.1501255	H	4.2973911	3.9089460	-0.4870524
C	-2.4731250	-1.5079721	1.6508137	H	-1.1963272	0.9050851	-5.3015471
C	0.7898120	-1.9349803	-3.1525525	C	3.7679154	1.0553555	-2.4210957
C	0.2847457	-2.6187689	-4.2505956	C	4.3591999	-3.3768030	-2.3066346
H	0.8706544	-2.6624095	-5.1809835	C	3.7384376	3.0333085	-0.8794459
C	-1.0139751	-3.2090233	-4.2323068	H	3.5069787	2.3808286	-0.0089272
C	-1.5644428	-3.8043588	-5.4067215	C	3.8873675	-0.2179711	-1.8391937
C	-1.8164704	-3.1559350	-3.0319903	C	1.3943772	1.5041476	-5.9813425
C	-3.1598538	-3.6311434	-3.0943600	H	6.5373959	1.2766644	-2.0518838
C	-1.2388640	-2.6020984	-1.8296301	C	2.8264647	1.2252415	-3.4536405
C	0.0116743	-1.9876096	-1.9477754	C	5.9466945	1.8899941	-1.3422315
O	-1.5901355	-0.2846313	-0.2144097	H	6.5259275	2.8083595	-1.1166867
O	0.5769736	-1.3979346	-0.8161053	H	2.7571086	2.2080424	-3.9424953
P	0.0047533	0.0602455	-0.3527715	C	3.4584110	-2.6355141	-0.0501510
O	0.6336137	0.3286966	1.0247997	H	4.4922376	-4.4074184	-1.9164051
O	0.1278208	1.1412862	-1.4222335	H	4.1572719	-3.4414598	-3.3949256
C	-3.3637571	-6.3102398	1.2517728	C	3.0146314	-1.2663365	-2.1796395
C	-2.6693493	-6.3430241	0.0142709	C	-0.4905093	0.8339348	-4.4483498
H	-4.0169721	-5.0700017	2.9014842	C	1.9304459	0.2102397	-3.8351286
H	-3.7569120	-7.2412395	1.6875867	H	2.4170449	1.2843294	-6.3493648
H	-1.6346330	-5.2236459	-1.5055779	H	1.3908452	2.5271642	-5.5523917
H	-2.5099900	-7.3037832	-0.4985652	C	3.2174590	-2.6508297	-1.5666885
C	-3.6722177	-4.1820051	-4.2610681	C	1.9800691	-1.0281412	-3.1253228
C	-2.8640356	-4.2877812	-5.4233444	C	0.9156573	0.4608799	-4.9586578
H	-3.7956930	-3.5494690	-2.2016516	H	2.6475850	-2.0990371	0.4785630
H	-4.7145914	-4.5345599	-4.2851043	H	-0.8915798	0.0921573	-3.7324081
H	-3.2763556	-4.7352118	-6.3404685	H	4.4144446	-2.1437066	0.2209969
H	-0.9390255	-3.8519680	-6.3120437	H	2.7897933	3.4029631	-1.3204504
C	-1.1421844	-0.4269377	3.4861006	H	-0.4671373	1.8169696	-3.9390604
C	-2.1831568	-0.3202750	2.5152543	H	5.8535821	1.3243717	-0.3918591
C	-0.7595537	0.7285064	4.1884713	H	2.2928176	-3.2372605	-1.7509259
C	-2.8206268	0.9280918	2.2969201	H	0.8152193	-0.4971654	-5.5092148
C	-2.4152320	2.0480729	3.0494840	H	4.6577816	-0.3977947	-1.0757799
C	-1.3757070	1.9780437	3.9907335				
H	0.0540538	0.6559162	4.9301579				
C	-3.9591321	1.0787287	1.2905567				
H	-2.9239102	3.0078084	2.8768065				
C	-3.6917495	2.1813346	0.2510995				
H	-3.6357342	3.1855654	0.7203780				
H	-4.5079068	2.2132726	-0.4993178				
H	-2.7415756	1.9995576	-0.2879913				
C	-5.2990506	1.3030457	2.0167734				
H	-4.0446821	0.1201399	0.7388046				
H	-5.2906878	2.2516887	2.5935107				
H	-5.5123441	0.4805702	2.7289966				
H	-6.1371433	1.3571948	1.2914989				
C	-0.9190134	3.1719257	4.8241938				
C	-1.3061584	4.5361365	4.2406565				
H	-0.8433474	5.3531538	4.8302335				
H	-2.4041882	4.6971971	4.2704649				
H	-0.9786643	4.6426957	3.1877330				
C	-1.4230619	3.0367605	6.2752546				
H	0.1932624	3.1219429	4.8479416				
H	-1.0364967	3.8611149	6.9096331				
H	-1.1073745	2.0767999	6.7304396				
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7.5.3 Pathway 13j-ma ↔ 13d-mi

TS-jma-dmi; COSMO

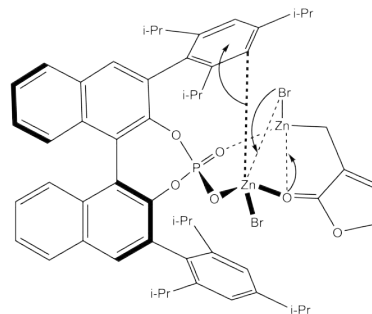


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Zn	1.2105627	-0.6217820	2.9544295
Br	2.7564704	-0.2481003	4.6812551
C	0.5996615	4.1189861	1.4192477

C	-0.2652434	3.3346812	2.1305729	H	-0.6455426	-4.1002947	6.0371598
C	0.5103726	2.1409864	2.5024404	H	-2.3323900	-3.6041665	5.6824167
O	1.7780557	2.2200346	2.0831205	C	2.4643735	-3.8219430	1.6911504
C	1.9280335	3.4467363	1.3283125	C	3.5008156	-2.7143455	1.9316929
O	0.0644525	1.1199504	3.0698343	H	4.5029746	-3.0575836	1.6032261
C	-1.7054720	3.3553700	2.3967768	H	3.5857657	-2.4285554	2.9997080
H	2.2027583	3.1651923	0.2867228	H	3.2512647	-1.8057907	1.3465431
H	2.7749286	4.0186422	1.7652083	C	2.8456984	-5.1230606	2.4253736
Zn	-2.3721203	1.5982671	1.6548039	H	2.4827713	-4.0395383	0.6062444
Br	-4.2809425	0.3449924	2.1045836	H	3.8571130	-5.4590346	2.1176513
C	-0.0748611	-2.6055837	-1.1323614	H	2.1281223	-5.9398094	2.2055617
C	0.3231570	-2.4750099	-2.4624598	H	2.8600048	-4.9757027	3.5256481
C	1.0917947	-3.5519230	-3.0451027	H	1.0319776	7.0448522	-1.1058160
C	1.6881540	-3.4702258	-4.3390757	H	4.6466106	3.1760016	-3.7659224
C	1.2981340	-4.7578046	-2.2758943	H	-3.5654599	3.7290879	-3.7678548
C	2.0141716	-5.8450969	-2.8609418	C	1.9106971	6.5622518	-1.5893823
C	0.8488199	-4.8235251	-0.9236608	H	4.6473051	0.6471783	-1.8598256
H	1.0520391	-5.7355391	-0.3413798	H	3.2934056	7.6834714	-0.3188076
C	0.2210033	-3.7453848	-0.3150352	H	-3.5610966	3.2348585	-1.2248941
C	0.2205244	1.2507290	-3.3932500	C	1.4887015	5.1415890	-1.9483847
C	-0.2865436	1.1875656	-4.6864834	C	4.0786398	2.2673401	-4.0557296
H	-0.3470488	2.1100400	-5.2839973	C	3.0831513	6.6313313	-0.5988972
C	-0.7640266	-0.0290383	-5.2494939	H	4.0161599	6.2177854	-1.0346857
C	-1.3763261	-0.0578340	-6.5387488	C	2.4279661	4.1321878	-2.2260818
C	-0.6462393	-1.2527319	-4.4946560	C	-2.4829459	3.9690529	-3.7272262
C	-1.2099089	-2.4425042	-5.0476117	H	1.3631083	7.3554964	-3.5685476
C	0.0005877	-1.2237708	-3.2045109	C	0.1265545	4.8157642	-2.0664324
C	0.3305605	0.0284952	-2.6619609	C	2.2250387	7.3591083	-2.8715813
O	-0.8214477	-1.5801235	-0.5608887	H	2.4747946	8.4140530	-2.6341837
O	0.8797889	0.1200194	-1.3888027	H	-0.6228638	5.5873800	-1.8246448
P	-0.0119797	-0.2391722	-0.0482549	C	3.8981423	1.4388782	-1.6515705
O	1.0614731	-0.5927616	0.9926941	H	4.8178166	1.4737837	-4.2899971
O	-1.0705511	0.8111534	0.2643743	H	3.5199159	2.5016580	-4.9845627
C	2.5479306	-5.7447742	-4.1372380	C	2.0438182	2.8451852	-2.6507217
C	2.3976677	-4.5387244	-4.8715737	C	-2.5118913	3.5952804	-1.2180126
H	2.1513858	-6.7628631	-2.2677219	C	-0.3117934	3.5431037	-2.4790732
H	3.1031445	-6.5888909	-4.5737592	H	-2.0313538	3.6729828	-4.6951662
H	1.5885881	-2.5418903	-4.9177500	H	-2.3836005	5.0710317	-3.6344003
H	2.8511732	-4.4464869	-5.8702442	C	3.1290507	1.8082930	-2.9345295
C	-1.8177134	-2.4341285	-6.2955652	C	0.6597612	2.5584626	-2.8095337
C	-1.8895312	-1.2369914	-7.0574724	C	-1.8104020	3.2523478	-2.5424515
H	-1.1719219	-3.3740487	-4.4658876	H	3.2100870	1.0576518	-0.8713560
H	-2.2537175	-3.3627112	-6.6945371	H	-1.9847885	3.1191697	-0.3693218
H	-2.3667280	-1.2450132	-8.0492470	H	4.4454010	2.3135887	-1.2406985
H	-1.4476576	0.8826544	-7.1074720	H	2.8694162	6.0716248	0.3339643
C	1.0329198	-3.4339843	2.0505629	H	-2.5378059	4.6879450	-1.0249163
C	-0.0480422	-3.5936388	1.1463639	H	3.0909250	6.9144053	-3.4058187
C	0.7509434	-2.9233445	3.3491430	H	2.6303133	0.8857895	-3.2940752
C	-1.3897009	-3.3844263	1.5836569	H	-1.9285738	2.1600940	-2.6945536
C	-1.6226908	-2.8420488	2.8575345	H	3.5021337	4.3539419	-2.1261299
C	-0.5690088	-2.5807414	3.7560902	H	-1.9251982	3.2473582	3.4802563
H	1.5516858	-2.9116109	4.1076739	H	-2.2160491	4.2518579	1.9999173
C	-2.5495035	-3.8459485	0.7080957	H	0.3749881	5.0725972	0.9254290
H	-2.6572909	-2.6326165	3.1666805				
C	-3.6989899	-2.8422348	0.5830214				
H	-4.2183336	-2.6747625	1.5478587				
H	-4.4536704	-3.2187673	-0.1373105				
H	-3.3388457	-1.8575707	0.2313710				
C	-3.0430826	-5.2114937	1.2326193				
H	-2.1442231	-4.0208185	-0.3097941				
H	-3.4585079	-5.1149328	2.2576432				
H	-2.2216085	-5.9556803	1.2692474				
H	-3.8436951	-5.6112358	0.5768097				
C	-0.8325785	-2.0818167	5.1720955				
C	-1.7847786	-0.8755561	5.2170627				
H	-1.9219899	-0.5383420	6.2642335				
H	-2.7876994	-1.1164729	4.8091975				
H	-1.3899700	-0.0208519	4.6333282				
C	-1.3478419	-3.2423892	6.0459454				
H	0.1476956	-1.7562267	5.5860302				
H	-1.4736516	-2.9102546	7.0967068				

TS-jma-dmi



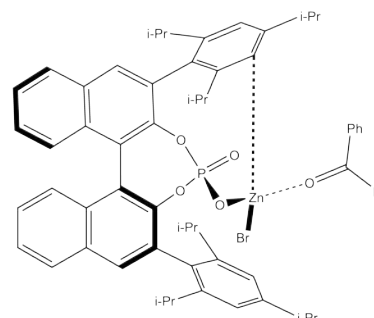
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Zn 1.2291078 -0.6152222 2.9635535

Br	2.7632441	-0.2876250	4.6944183	H	0.1483390	-1.7588738	5.5802896
C	0.5976653	4.1193795	1.4089801	H	-1.4783642	-2.9047510	7.0948404
C	-0.2612585	3.3372504	2.1298049	H	-0.6554000	-4.0997957	6.0376251
C	0.5201773	2.1462122	2.5031884	H	-2.3394073	-3.5976193	5.6821571
O	1.7859236	2.2272116	2.0752848	C	2.4590133	-3.8415844	1.6950268
C	1.9270132	3.4479123	1.3127419	C	3.4991646	-2.7374520	1.9352252
O	0.0804737	1.1277262	3.0755681	H	4.5003374	-3.0835057	1.6064396
C	-1.6981085	3.3520084	2.4052805	H	3.5855627	-2.4483980	3.0021918
H	2.1957131	3.1613649	0.2709749	H	3.2525194	-1.8289056	1.3490880
H	2.7764600	4.0245566	1.7396349	C	2.8351057	-5.1437029	2.4299269
Zn	-2.3709959	1.5893823	1.6728066	H	2.4770639	-4.0604374	0.6102350
Br	-4.2618120	0.3323566	2.1370503	H	3.8457304	-5.4845334	2.1247007
C	-0.0673918	-2.6062691	-1.1279623	H	2.1145745	-5.9581619	2.2111135
C	0.3320424	-2.4747010	-2.4576380	H	2.8489316	-4.9962574	3.5300904
C	1.0961061	-3.5535350	-3.0425745	H	1.0245189	7.0506876	-1.1080547
C	1.6941491	-3.4708993	-4.3354518	H	4.6469315	3.1854610	-3.7674324
C	1.2950573	-4.7629841	-2.2774646	H	-3.5706113	3.7046293	-3.7531285
C	2.0055378	-5.8513683	-2.8660493	C	1.9015251	6.5728218	-1.6000358
C	0.8428918	-4.8303150	-0.9264939	H	4.6539454	0.6603849	-1.8522374
H	1.0393984	-5.7451339	-0.3461848	H	3.2884390	7.7051258	-0.3423681
C	0.2207914	-3.7510601	-0.3144923	H	-3.5535282	3.2238992	-1.2052742
C	0.2269320	1.2514414	-3.3852922	C	1.4846316	5.1489841	-1.9525916
C	-0.2790849	1.1882926	-4.6786603	C	4.0799225	2.2748178	-4.0527324
H	-0.3394046	2.1118961	-5.2744611	C	3.0825769	6.6517647	-0.6208198
C	-0.7545626	-0.0278605	-5.2432186	H	4.0148037	6.2458930	-1.0652198
C	-1.3658991	-0.0572784	-6.5323637	C	2.4264786	4.1416104	-2.2271964
C	-0.6355427	-1.2512505	-4.4886471	C	-2.4891459	3.9495839	-3.7180215
C	-1.1979247	-2.4409676	-5.0424755	H	1.3286902	7.3586493	-3.5744491
C	0.0108822	-1.2225187	-3.1982553	C	0.1237041	4.8182241	-2.0677322
C	0.3391648	0.0294391	-2.6535755	C	2.1971748	7.3702418	-2.8861309
O	-0.8101060	-1.5816937	-0.5542432	H	2.4423538	8.4274141	-2.6541731
O	0.8872170	0.1215527	-1.3810848	H	-0.6283234	5.5880799	-1.8280291
P	-0.0058577	-0.2387518	-0.0385534	C	3.9039978	1.4516469	-1.6458468
O	1.0698842	-0.5883590	1.0013627	H	4.8207752	1.4827641	-4.2864207
O	-1.0671878	0.8083221	0.2717844	H	3.5193995	2.5058455	-4.9810738
C	2.5407102	-5.7501165	-4.1411282	C	2.0459688	2.8520839	-2.6469578
C	2.3977548	-4.5412048	-4.8710346	C	-2.5073879	3.5929116	-1.2061122
H	2.1372967	-6.7718701	-2.2758011	C	-0.3113915	3.5429476	-2.4745211
H	3.0915253	-6.5959171	-4.5798151	H	-2.0404711	3.6487193	-4.6856384
H	1.5989981	-2.5398223	-4.9103290	H	-2.3947488	5.0526992	-3.6346278
H	2.8522787	-4.4479505	-5.8690895	C	3.1332975	1.8169721	-2.9287799
C	-1.8045978	-2.4328285	-6.2904648	C	0.6629601	2.5608599	-2.8035358
C	-1.8772447	-1.2361847	-7.0519505	C	-1.8088702	3.2448775	-2.5306794
H	-1.1591286	-3.3719947	-4.4602857	H	3.2179687	1.0708300	-0.8638176
H	-2.2394768	-3.3617753	-6.6896288	H	-1.9740025	3.1273370	-0.3556478
H	-2.3538980	-1.2441712	-8.0439100	H	4.4514984	2.3274135	-1.2374142
H	-1.4384170	0.8835479	-7.1003704	H	2.8824158	6.0898465	0.3137190
C	1.0282005	-3.4485969	2.0529247	H	-2.5428878	4.6869626	-1.0219778
C	-0.0516355	-3.6022553	1.1464004	H	3.0597206	6.9300635	-3.4290347
C	0.7459591	-2.9366953	3.3498908	H	2.6356166	0.8927561	-3.2851621
C	-1.3932667	-3.3842048	1.5794343	H	-1.9217123	2.1509624	-2.6743233
C	-1.6254791	-2.8391289	2.8521142	H	3.5001640	4.3664955	-2.1292431
C	-0.5718747	-2.5856083	3.7533106	H	-1.9110168	3.2369658	3.4891374
H	1.5469312	-2.9206923	4.1079007	H	-2.2161907	4.2477206	2.0167350
C	-2.5532136	-3.8372378	0.6991698	H	0.3682783	5.0686048	0.9093873
H	-2.6589811	-2.6173566	3.1563588				
C	-3.6972325	-2.8279376	0.5703424				
H	-4.2205686	-2.6572429	1.5322449				
H	-4.4512410	-3.2000459	-0.1529237				
H	-3.3329384	-1.8443100	0.2205592				
C	-3.0554007	-5.2012024	1.2194261				
H	-2.1444943	-4.0131446	-0.3173362				
H	-3.4739986	-5.1045058	2.2430419				
H	-2.2382496	-5.9499729	1.2586452				
H	-3.8560934	-5.5965073	0.5610441				
C	-0.8336847	-2.0818740	5.1681262				
C	-1.7801192	-0.8712501	5.2110744				
H	-1.9126017	-0.5292943	6.2573188				
H	-2.7857680	-1.1049121	4.8059487				
H	-1.3819165	-0.0200866	4.6249134				
C	-1.3534870	-3.2384494	6.0444599				

7.6 Complexes 12

12d-ma

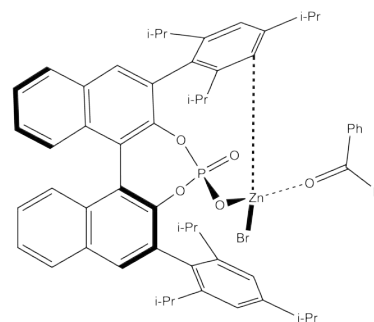


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C	2.7940644	6.5625353	86.2572704
C	2.3492315	7.6085678	87.1046571
C	2.9194878	8.9015457	87.0131994
C	3.9099463	9.1576662	86.0596108
C	4.3441756	8.1202714	85.2129586
H	4.1600921	6.0164555	84.6721309
H	2.3883181	5.5478011	86.4083558
C	1.3467693	7.3412251	88.1272182
H	2.5791973	9.6965379	87.6960160
H	4.3558169	10.1602157	85.9787640
H	5.1338499	8.3189390	84.4715230
O	0.6925256	6.2827261	88.1788627
C	0.0676347	0.9859379	89.0037883
C	0.8449383	-0.1404326	89.3053501
C	0.2898330	-1.1172273	90.2143564
C	1.0479583	-2.2075963	90.7381606
C	-1.0822777	-0.9787865	90.6461779
C	-1.6516848	-1.9731257	91.4968489
C	-1.8197519	0.1875959	90.2891286
H	-2.8426273	0.3090024	90.6790798
C	-1.2444102	1.2041297	89.5391220
C	4.4225017	0.8013545	88.2548234
C	4.8818265	-0.4005724	87.7319056
H	5.9132335	-0.4626860	87.3519724
C	4.0299148	-1.5337929	87.5929234
C	4.4913617	-2.7260724	86.9587812
C	2.6571128	-1.4528225	88.0332409
C	1.7924176	-2.5482603	87.7316952
C	2.2096892	-0.2617774	88.7183559
C	3.0922212	0.8276116	88.7861267
O	0.5414358	1.9330642	88.1269019
O	2.6970820	1.9878854	89.4235869
P	1.6931787	3.0420570	88.6192464
O	1.1297500	3.8699099	89.8075996
O	2.2479239	3.6802029	87.3834230
C	-0.8964362	-3.0431770	91.9513992
C	0.4708084	-3.1456982	91.5828618
H	-2.7033440	-1.8598928	91.8045341
H	-1.3466072	-3.7987473	92.6130840
H	2.1093368	-2.2960831	90.4696947
H	1.0822232	-3.9730094	91.9744648
C	2.2670542	-3.6858967	87.0932226
C	3.6329204	-3.7882300	86.7197833
H	0.7300555	-2.4809282	88.0029168
H	1.5750459	-4.5121949	86.8693689
H	4.0013662	-4.6988184	86.2232148
H	5.5451761	-2.7757549	86.6420291
C	-1.8689042	3.4148356	90.5524762
C	-1.8150971	2.5791712	89.4002167
C	-2.1713989	4.7913141	90.3793931
C	-2.1222229	3.1196179	88.1190373
C	-2.4344361	4.4867743	87.9971943
C	-2.4635602	5.3508443	89.1042847
H	-2.2839633	5.4296518	91.2711103
C	-2.1627186	2.2445127	86.8712150
H	-2.6587347	4.8881505	86.9992684
C	-1.3524917	2.8316664	85.7030950
H	-1.8124405	3.7607467	85.3057768
H	-1.3123377	2.1057045	84.8657258
H	-0.3137902	3.0587600	86.0119685
C	-3.6267345	1.9727219	86.4719228
H	-1.7091585	1.2684464	87.1345068
H	-4.1515150	2.9131220	86.2014246
H	-4.1912969	1.4982932	87.2999498
H	-3.6713030	1.2966076	85.5934638
C	-2.8672914	6.8172352	89.0071204

C	-2.6459000	7.4313613	87.6196978
H	-2.8197365	8.5253834	87.6535230
H	-3.3472274	7.0146528	86.8668895
H	-1.6140061	7.2558425	87.2569326
C	-4.3290877	6.9906302	89.4667051
H	-2.2220326	7.3653648	89.7315247
H	-4.6144576	8.0624328	89.4654110
H	-4.4851723	6.5979535	90.4912753
H	-5.0213087	6.4500052	88.7877664
C	-1.6184415	2.9028879	91.9693321
C	-0.5103040	3.6693365	92.7102293
H	-0.3534839	3.2285259	93.7156795
H	-0.7508103	4.7428037	92.8559529
H	0.4485072	3.6009479	92.1583683
C	-2.9374160	2.8947483	92.7662358
H	-1.2761913	1.8542805	91.8871136
H	-2.7790752	2.4551589	93.7721761
H	-3.7222725	2.3030574	92.2521047
H	-3.3323982	3.9225938	92.9082965
H	7.0404689	6.2991210	86.8046728
H	7.5432568	2.5579775	91.4013434
H	5.8262163	0.9342194	83.9017544
C	7.0042200	6.0426336	87.8871141
H	4.6040165	2.5004088	92.6932956
H	6.4854448	8.1069583	88.4360073
C	3.7089969	2.3941564	83.8262950
C	6.4145375	4.6415584	87.9868576
C	6.8732408	1.6830763	91.2653938
C	6.0944166	7.0773191	88.5746927
H	6.0253233	6.8880601	89.6662599
C	6.2335376	4.0122596	89.2311266
C	6.1510198	1.4558473	84.8262445
H	9.1020766	5.3832319	87.9119618
C	6.0011115	3.9503052	86.8384186
C	8.4419688	6.1072498	88.4306556
H	8.8714611	7.1223895	88.3004543
H	6.1420502	4.4320253	85.8573037
C	4.7599527	3.0271479	91.7291338
H	6.7759737	1.1767125	92.2483876
H	7.3748024	0.9839647	90.5657837
C	5.6308341	2.7485974	89.3484130
C	4.1036583	2.9539964	84.6992584
C	5.3865030	2.6856545	86.8965079
H	6.7262568	0.7354447	85.4422802
H	6.8496017	2.2669460	84.5304828
C	5.4943981	2.1152476	90.7312256
C	5.1936741	2.0807541	88.1712894
C	4.9410906	2.0230704	85.5923596
H	3.7689153	3.3268041	91.3364502
H	3.2507895	3.3656928	85.2720773
H	5.3397711	3.9479017	91.9492332
H	5.0663949	7.0409369	88.1631336
H	4.7086000	3.7935389	84.2949168
H	8.4724023	5.8701819	89.5146714
H	4.8875171	1.1937297	90.6198465
H	4.2840321	1.1713661	85.8574044
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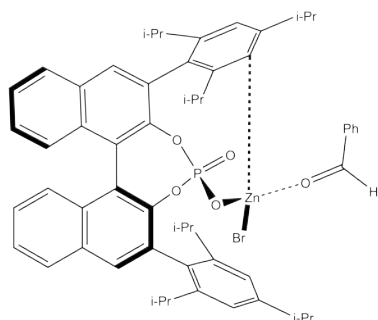
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C	0.9042078	6.0829757	83.5603897
C	0.5399812	5.9445493	84.9028071
C	1.5248254	6.0579174	85.9107893
C	2.8715075	6.3011995	85.5628765
C	3.2302878	6.4474488	84.2178251
C	2.2474745	6.3376839	83.2185506
H	0.1442382	5.9910855	82.7697700
H	-0.5000280	5.7381358	85.1967414
C	1.1774168	5.9053780	87.3212378
H	3.6345151	6.3511561	86.3552033
H	4.2791720	6.6349674	83.9432795
H	2.5301395	6.4453373	82.1598891
O	0.0009397	5.7618929	87.7208048
C	-0.1795714	0.8797773	89.1255184
C	0.5982174	-0.2330641	89.4706855
C	0.0434484	-1.1756809	90.4141992
C	0.8014041	-2.2478341	90.9750723
C	-1.3272491	-1.0170268	90.8434421
C	-1.8958773	-1.9748262	91.7363225
C	-2.0673341	0.1309427	90.4350308
H	-3.0911961	0.2649904	90.8169579
C	-1.4953185	1.1147037	89.6396070
C	4.1664869	0.6862979	88.3747258
C	4.6217502	-0.5242977	87.8676403
H	5.6470785	-0.5919995	87.4729881
C	3.7721109	-1.6635385	87.7668896
C	4.2301930	-2.8682296	87.1528296
C	2.4050906	-1.5783876	88.2248919
C	1.5404309	-2.6841699	87.9622997
C	1.9627769	-0.3730956	88.8874152
C	2.8456212	0.7161465	88.9263876
O	0.3080163	1.8025622	88.2237668
O	2.4512966	1.8899669	89.5488441
P	1.4465183	2.9166340	88.7219464
O	0.8643523	3.7992860	89.8568391
O	2.0221507	3.5475397	87.4825144
C	-1.1404550	-3.0279653	92.2300075
C	0.2251641	-3.1503470	91.8588912
H	-2.9461118	-1.8474694	92.0431212
H	-1.5892829	-3.7552557	92.9235896
H	1.8613954	-2.3509776	90.7053675
H	0.8352013	-3.9643079	92.2796577
C	2.0110171	-3.8343231	87.3426724
C	3.3722474	-3.9390707	86.9508220
H	0.4818287	-2.6162691	88.2481093
H	1.3200394	-4.6690048	87.1485280
H	3.7370826	-4.8593478	86.4695982
H	5.2795099	-2.9213353	86.8220734
C	-2.1445860	3.3791544	90.5121385
C	-2.0952414	2.4673287	89.4175296
C	-2.5161523	4.7261739	90.2562586
C	-2.4617733	2.9061501	88.1140172
C	-2.8652739	4.2409247	87.9160736
C	-2.8956345	5.1767124	88.9615644
H	-2.6207962	5.4230296	91.1040232
C	-2.4472172	1.9637877	86.9155048
H	-3.1449289	4.5634741	86.9034409
C	-1.6252987	2.5251351	85.7411153
H	-2.1022358	3.4246233	85.2982360
H	-1.5450604	1.7674170	84.9350931
H	-0.6011808	2.7965290	86.0632961
C	-3.8875682	1.6175610	86.4909271
H	-1.9652424	1.0193764	87.2381082
H	-4.4378305	2.5218742	86.1557945
H	-4.4581068	1.1658147	87.3275959
H	-3.8812729	0.8950721	85.6490684
C	-3.3706476	6.6120673	88.7829072
C	-3.1129007	7.1824907	87.3824986
H	-3.3696968	8.2603210	87.3579880

H	-3.7349930	6.6818645	86.6110898
H	-2.0486927	7.0714553	87.0957941
C	-4.8597394	6.7177523	89.1705188
H	-2.7878612	7.2230258	89.5088911
H	-5.2027046	7.7710378	89.1134067
H	-5.0403031	6.3540630	90.2021489
H	-5.4884254	6.1139477	88.4828696
C	-1.8455374	2.9688316	91.9522192
C	-0.8651018	3.9040047	92.6787860
H	-0.6933121	3.5366682	93.7108304
H	-1.2389796	4.9453563	92.7597259
H	0.1142962	3.9268004	92.1615523
C	-3.1700944	2.8313002	92.7304387
H	-1.3699590	1.9696781	91.9212344
H	-2.9782742	2.4588158	93.7573820
H	-3.8680746	2.1271950	92.2336686
H	-3.6866906	3.8103880	92.8158830
H	6.8319586	6.1328569	86.8026040
H	7.3626932	2.4620069	91.4457344
H	5.3987724	0.7336372	84.0073590
C	6.8292256	5.8809958	87.8866254
H	4.4489456	2.4357234	92.7806711
H	6.4218317	7.9646624	88.4563642
H	3.3516348	2.2837263	83.9374079
C	6.1962016	4.5011166	88.0165858
C	6.6884379	1.5875345	91.3287297
C	5.9937295	6.9526036	88.6112862
H	5.9606602	6.7653305	89.7047716
C	6.0402857	3.8856976	89.2716596
C	5.7644026	1.2581865	84.9148640
H	8.8997723	5.1428469	87.8257522
C	5.7277081	3.8132139	86.8863000
C	8.2903995	5.8924625	88.3697593
H	8.7513845	6.8902672	88.2162678
H	5.8430921	4.2858005	85.8972353
C	4.5875497	2.9463756	91.8051605
H	6.6027080	1.0930731	92.3188139
H	7.1777131	0.8779501	90.6306811
C	5.4175157	2.6341834	89.4166893
C	3.7877380	2.8446680	84.7901165
C	5.0932534	2.5593975	86.9732353
H	6.3209069	0.5251565	85.5331472
H	6.4889665	2.0343416	84.5890088
C	5.3034352	2.0174975	90.8090040
C	4.9367891	1.9643991	88.2580496
C	4.5938930	1.8934107	85.6902447
H	3.5897988	3.2402954	91.4246749
H	2.9675998	3.3163576	85.3633052
H	5.1723949	3.8701029	91.9977749
H	4.9453112	6.9641667	88.2482615
H	4.4198535	3.6485367	84.3586715
H	8.3565370	5.6573919	89.4527535
H	4.6917835	1.0965867	90.7192250
H	3.9051131	1.0770891	85.9862449
H	6.4077114	4.4016215	90.1734390
H	2.0155713	6.0040986	88.0505143

Zn	-0.3206902	5.3646652	89.7492136
Br	-0.1160477	7.3475738	90.9488143
C	0.9626698	6.1412166	83.5909044
C	0.5816538	5.9904114	84.9272307
C	1.5579993	6.0638653	85.9460451
C	2.9132088	6.2780290	85.6153139
C	3.2887616	6.4369995	84.2764381
C	2.3143958	6.3685009	83.2660503
H	0.2086927	6.0799104	82.7916185
H	-0.4653773	5.8045122	85.2096144
C	1.1910037	5.8999859	87.3521599
H	3.6697565	6.2904979	86.4152175
H	4.3452636	6.6007867	84.0161294
H	2.6103126	6.4857571	82.2120446
O	0.0081269	5.7760327	87.7363061
C	-0.1883119	0.8715506	89.1220060
C	0.5930023	-0.2376802	89.4709378
C	0.0392015	-1.1809063	90.4143715
C	0.7999546	-2.2485978	90.9792760
C	-1.3334638	-1.0281977	90.8388501
C	-1.9001152	-1.9878884	91.7302017
C	-2.0760935	0.1166452	90.4275102
H	-3.1011156	0.2487555	90.8074167
C	-1.5059076	1.1025170	89.6335254
C	4.1588373	0.6937638	88.3777076
C	4.6207577	-0.5175081	87.8789474
H	5.6470848	-0.5805365	87.4861046
C	3.7775254	-1.6613771	87.7824436
C	4.2422295	-2.8670786	87.1766220
C	2.4089977	-1.5797639	88.2357872
C	1.5503184	-2.6904526	87.9758867
C	1.9596114	-0.3735144	88.8917538
C	2.8373037	0.7200051	88.9275096
O	0.2966987	1.7950330	88.2202602
O	2.4386015	1.8946716	89.5446457
P	1.4279298	2.9145743	88.7193725
O	0.8412534	3.7948955	89.8531600
O	1.9996235	3.5519248	87.4800984
C	-1.1421265	-3.0368412	92.2272369
C	0.2248334	-3.1528703	91.8612723
H	-2.9519510	-1.8649365	92.0333280
H	-1.5902171	-3.7655687	92.9196936
H	1.8610947	-2.3461796	90.7126076
H	0.8373352	-3.9634517	92.2847965
C	2.0280297	-3.8416365	87.3647151
C	3.3903596	-3.9426402	86.9780149
H	0.4907091	-2.6249253	88.2580180
H	1.3412151	-4.6802366	87.1730379
H	3.7610004	-4.8638066	86.5031248
H	5.2926881	-2.9168681	86.8490741
C	-2.1677625	3.3602710	90.5135492
C	-2.1079569	2.4544547	89.4144516
C	-2.5397574	4.7068779	90.2622514
C	-2.4638333	2.9003552	88.1104482
C	-2.8647459	4.2361376	87.9171558
C	-2.9057992	5.1658206	88.9677908
H	-2.6424882	5.4016517	91.1117774
C	-2.4422420	1.9639911	86.9069351
H	-3.1341444	4.5647798	86.9037118
C	-1.6182192	2.5317636	85.7373501
H	-2.0957467	3.4317648	85.2957788
H	-1.5330950	1.7780075	84.9282643
H	-0.5953171	2.8030926	86.0627993
C	-3.8801693	1.6149562	86.4769925
H	-1.9581055	1.0197805	87.2266622
H	-4.4335906	2.5188665	86.1460743
H	-4.4513509	1.1571128	87.3097267
H	-3.8708273	0.8972740	85.6310589
C	-3.3768325	6.6032511	88.7936036
C	-3.1142998	7.1785014	87.3962263
H	-3.3661812	8.2575144	87.3752418

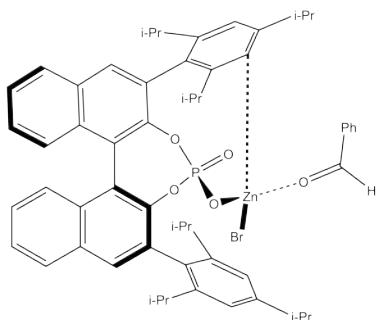
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Energy (Hartree) = -7274.231097117

H	-3.7371626	6.6847654	86.6207215	Zn	0.1144447	5.4220625	90.0457877
H	-2.0496927	7.0654311	87.1122099	Br	0.3756433	7.2705382	91.4913783
C	-4.8658842	6.7135784	89.1789009	C	0.0027338	0.9233097	89.2046662
H	-2.7912424	7.2093862	89.5216106	C	0.7544260	-0.2140884	89.5293557
H	-5.2055547	7.7681699	89.1264730	C	0.1863607	-1.1483795	90.4744297
H	-5.0502308	6.3459464	90.2083781	C	0.9223274	-2.2431737	91.0207858
H	-5.4968845	6.1152689	88.4885694	C	-1.1753342	-0.9589987	90.9203548
C	-1.8732726	2.9464633	91.9539998	C	-1.7597698	-1.9110310	91.8091474
C	-0.8710814	3.8639601	92.6739822	C	-1.8871342	0.2158157	90.5381293
H	-0.7075293	3.5013783	93.7090893	H	-2.9007096	0.3755224	90.9380515
H	-1.2172022	4.9155828	92.7458318	C	-1.2955166	1.1932484	89.7495539
H	0.1083027	3.8589950	92.1566550	C	4.3377728	0.6050533	88.3964841
C	-3.1970135	2.8343759	92.7369950	C	4.7586534	-0.6220940	87.8999399
H	-1.4172895	1.9383102	91.9237599	H	5.7806604	-0.7217672	87.5028938
H	-3.0096553	2.4600437	93.7640966	C	3.8763300	-1.7372635	87.8086185
H	-3.9097295	2.1425840	92.2435750	C	4.2980030	-2.9581139	87.2004945
H	-3.6967773	3.8219931	92.8237996	C	2.5132741	-1.6096326	88.2688550
H	6.8015608	6.1367307	86.7591165	C	1.6165204	-2.6910316	88.0121503
H	7.3457473	2.5024835	91.4321647	C	2.1070932	-0.3888181	88.9270950
H	5.3923845	0.7167819	84.0042733	C	3.0185098	0.6785791	88.9508904
C	6.8259690	5.8820273	87.8425900	O	0.4911572	1.8309881	88.2937789
H	4.4317859	2.4877272	92.7701068	O	2.6628192	1.8646964	89.5638272
H	6.4718398	7.9711839	88.4277318	P	1.6760796	2.9244085	88.7425828
H	3.3273521	2.2464819	83.9352423	O	1.1508811	3.7977550	89.9152319
C	6.1799376	4.5094170	87.9863715	O	2.2327665	3.5106920	87.4825036
C	6.6708317	1.6275648	91.3235622	C	-1.0267912	-2.9874978	92.2862230
C	6.0315463	6.9661703	88.5935106	C	0.3322173	-3.1901026	91.9023058
H	6.0278394	6.7790111	89.6872802	H	-2.8034041	-1.7596905	92.1275247
C	6.0200205	3.9076317	89.2472015	H	-1.4874685	-3.7099552	92.9771129
C	5.7560570	1.2499617	84.9073858	H	1.9771890	-2.3698683	90.7414807
H	8.8807724	5.1100562	87.7167013	H	0.9263753	-3.9707940	92.3110104
C	5.7145282	3.8095636	86.8625152	C	2.0519430	-3.8576381	87.3974233
C	8.3011346	5.8673431	88.2816208	C	3.4089998	-4.0046531	87.0049211
H	8.7751934	6.8578456	88.1206862	O	0.5605725	-2.5905303	88.2982907
H	5.8342770	4.2700604	85.8681843	H	1.3360858	-4.6721523	87.2076131
C	4.5693608	2.9897901	91.7901766	H	3.7461385	-4.9376362	86.5279248
H	6.5867631	1.1417310	92.3179684	H	5.3448376	-3.0433662	86.8684572
H	7.1596365	0.9126345	90.6309856	C	-1.8445544	3.4508377	90.7012114
C	5.3993003	2.6568690	89.4039863	C	-1.8318052	2.5784466	89.5752017
C	3.7631241	2.8161396	84.7820651	C	-2.1139774	4.8295520	90.4896828
C	5.0804468	2.5566102	86.9608690	C	-2.1471169	3.0865524	88.2827609
H	6.3221881	0.5261316	85.5275993	C	-2.4292497	4.4566376	88.1227293
H	6.4729137	2.0301621	84.5746485	C	-2.4171447	5.3555573	89.2020361
C	5.2852969	2.0530266	90.8018259	H	-2.2028243	5.4959601	91.3635220
C	4.9228911	1.9744940	88.2511493	C	-2.2278032	2.1754685	87.0631588
C	4.5827708	1.8781726	85.6837542	H	-2.6633304	4.8318817	87.1169788
C	3.5707415	3.2797958	91.4096043	C	-1.4171188	2.7065519	85.8685082
H	2.9410823	3.2831031	85.3564192	H	-1.8587012	3.6351182	85.4498930
H	5.1527089	3.9159254	91.9752848	H	-1.4064537	1.9549384	85.0529871
H	4.9726383	6.9972559	88.2640671	H	-0.3696276	2.9169838	86.1596732
H	4.3852809	3.6230949	84.3418523	C	-3.7035151	1.9323548	86.6887243
H	8.3945557	5.6233393	89.3604894	H	-1.7978508	1.1953279	87.3500794
H	4.6737427	1.1313679	90.7202567	H	-4.2048132	2.8785048	86.3946926
H	3.9027367	1.0572202	85.9864613	H	-4.2706055	1.4989079	87.5373945
H	6.3852566	4.4324736	90.1446222	H	-3.7757924	1.2308858	85.8322397
H	2.0224765	5.9794472	88.0916022	C	-2.7893426	6.8271079	89.0650693
				C	-2.5921924	7.3892110	87.6522107
				H	-2.7421776	8.4872190	87.6542217
				H	-3.3225221	6.9619789	86.9337549
				H	-1.5744496	7.1797134	87.2681117
				C	-4.2346030	7.0490550	89.5560920
				H	-2.1142709	7.3845751	89.7543341
				H	-4.4950044	8.1266597	89.5236702
				H	-4.3721084	6.6957910	90.5976339
				H	-4.9551379	6.5014229	88.9131958
				C	-1.5915701	2.9740528	92.1294222
				C	-0.4763914	3.7504655	92.8484418
				H	-0.3174606	3.3294676	93.8620035
				H	-0.7125783	4.8274604	92.9726957
				H	0.4792727	3.6664599	92.2929438
				C	-2.9087614	2.9974327	92.9295319

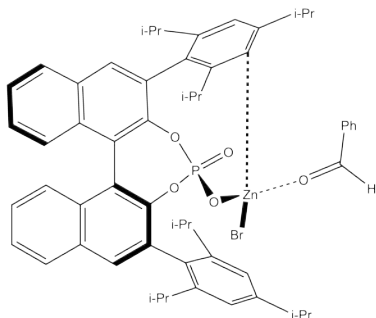
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H	-1.2574223	1.9210922	92.0733361	Zn	0.0989982	5.4261790	90.0568008
H	-2.7502023	2.5837724	93.9463945	Br	0.3007913	7.2906501	91.4761170
H	-3.6989298	2.3977146	92.4332318	C	-0.0060158	0.9237497	89.2055843
H	-3.2942754	4.0323968	93.0431522	C	0.7516645	-0.2091923	89.5313378
H	7.0248149	6.0061286	86.7232760	C	0.1900132	-1.1443426	90.4791691
H	7.5570843	2.4027636	91.4259470	C	0.9327641	-2.2339402	91.0260561
H	5.6556033	0.5739114	84.0164823	C	-1.1719924	-0.9624522	90.9265283
C	6.9882651	5.7921682	87.8147043	C	-1.7491822	-1.9167675	91.8168461
H	4.6463435	2.4340562	92.7760842	C	-1.8901565	0.2075330	90.5428647
H	6.4783530	7.8779686	88.2835053	H	-2.9042985	0.3631051	90.9433184
H	3.5677091	2.0741822	83.9341836	C	-1.3050824	1.1870456	89.7522016
C	6.3893726	4.4000158	87.9698431	C	4.3289452	0.6209325	88.3895772
C	6.8712294	1.5346770	91.3302174	C	4.7530884	-0.6064120	87.8968897
C	6.0823839	6.8563845	88.4619783	H	5.7754443	-0.7023035	87.4998696
H	6.0131158	6.7082561	89.5600757	C	3.8753163	-1.7249162	87.8097783
C	6.2269719	3.8108676	89.2365918	C	4.2998091	-2.9461661	87.2056652
C	6.0092789	1.1176736	84.9174413	C	2.5129006	-1.6004400	88.2717229
H	9.0839833	5.1258664	87.8664475	C	1.6199495	-2.6858531	88.0203723
C	5.9415224	3.6803866	86.8517180	C	2.1034962	-0.3791392	88.9267685
C	8.4262265	5.8726573	88.3555535	C	3.0101733	0.6922653	88.9448841
H	8.8588763	6.8800510	88.1827026	O	0.4749975	1.8325804	88.2927899
H	6.0657614	4.1314521	85.8539822	O	2.6519691	1.8797437	89.5535933
C	4.7905151	2.9279606	91.7927354	P	1.6563771	2.9313668	88.7357347
H	6.7849056	1.0606902	92.3303106	O	1.1281027	3.8033647	89.9086779
H	7.3474965	0.8055001	90.6434476	O	2.2039348	3.5233533	87.4740393
C	5.6070768	2.5609180	89.4048691	C	-1.0098962	-2.9880670	92.2941275
C	3.9903188	2.6536761	84.7810829	C	0.3489440	-3.1320417	91.9087723
C	5.3095134	2.4275189	86.9615153	H	-2.7933259	-1.7710662	92.1362484
H	6.5814943	0.4048975	85.5453453	H	-1.4657028	-3.7123089	92.9862888
H	6.7170408	1.9052735	84.5821570	H	1.9876617	-2.3540618	90.7445269
C	5.4890342	1.9728196	90.8092932	H	0.9485268	-3.9597403	92.3174760
C	5.1338714	1.8646567	88.2582989	C	2.0586915	-3.8529314	87.4099867
C	4.8257843	1.7337326	85.6875894	C	3.4149716	-3.9964927	87.0157694
H	3.7966425	3.2316655	91.4099169	H	0.5643588	-2.5873581	88.3080725
H	3.1585983	3.1017741	85.3577917	H	1.3454109	-4.6706661	87.2247183
H	5.3906538	3.8447679	91.9709865	H	3.7548908	-4.9299259	86.5417843
H	5.0546602	6.8087721	88.0506622	H	5.3463060	-3.0284183	86.8719004
H	4.6036297	3.4678710	84.3397799	C	-1.8694695	3.4426594	90.7006705
H	8.4560906	5.6817113	89.4488148	C	-1.8489889	2.5686657	89.5760307
H	4.8652465	1.0584227	90.7388687	C	-2.1440407	4.8192181	90.4860763
H	4.1575706	0.9041884	85.9921943	C	-2.1621078	3.0735350	88.2818307
H	6.5817496	4.3499022	90.1298223	C	-2.4461804	4.4425480	88.1189364
C	3.7481531	6.5667761	85.2428557	C	-2.4409416	5.3429590	89.1969174
C	2.7679396	6.3487942	86.2153906	H	-2.2314459	5.4886040	91.3576678
C	2.3453332	7.4347849	87.0239480	C	-2.2388160	2.1593106	87.0640554
C	2.9175536	8.7203390	86.8608951	H	-2.6751962	4.8157639	87.1112392
C	3.8889691	8.9275116	85.8758134	C	-1.4330728	2.6904705	85.8664557
C	4.3012503	7.8504653	85.0682298	H	-1.8792928	3.6154513	85.4446454
H	4.0979235	5.7265665	84.6253598	H	-1.4196841	1.9367201	85.0531245
H	2.3616027	5.3442758	86.4211137	H	-0.3857514	2.9057140	86.1538970
C	1.3669944	7.2211729	88.0801005	C	-3.7138070	1.9064695	86.6937240
H	2.5937278	9.5477484	87.5122714	H	-1.8024246	1.1827108	87.3530324
H	4.3360927	9.9234312	85.7391868	H	-4.2222347	2.8487217	86.3994747
H	5.0750816	8.0111129	84.3013889	H	-4.2765482	1.4715760	87.5444024
O	0.7169362	6.1643356	88.2032134	H	-3.7851368	1.2032413	85.8386392
H	1.2263158	8.0434873	88.8286581	C	-2.8118150	6.8144542	89.0558264
				C	-2.5986064	7.3755841	87.6449030
				H	-2.7458518	8.4740428	87.6437526
				H	-3.3219364	6.9507251	86.9178912
				H	-1.5772640	7.1628999	87.2723407
				C	-4.2614665	7.0387091	89.5315408
				H	-2.1422943	7.3712856	89.7510645
				H	-4.5212126	8.1164592	89.4977759
				H	-4.4103989	6.6850567	90.5712834
				H	-4.9771347	6.4922883	88.8822279
				C	-1.6130293	2.9713010	92.1304416
				C	-0.4830254	3.7394855	92.8356185
				H	-0.3236840	3.3274888	93.8528212
				H	-0.7017133	4.8213949	92.9499688
				H	0.4684724	3.6354207	92.2766716
				C	-2.9234317	3.0135024	92.9402896

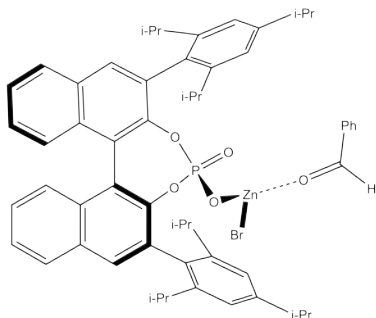
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Energy (Hartree) = -7274.225769422

H	-1.2912138	1.9143393	92.0780857	Zn	1.3878586	5.3428809	90.1327029
H	-2.7628735	2.6030016	93.9581036	Br	3.1233975	6.2254475	91.3454450
H	-3.7246087	2.4209822	92.4529796	C	2.4795674	6.3896147	85.9709432
H	-3.2974577	4.0526973	93.0532473	C	1.6505392	6.4351524	87.0931953
H	7.0305263	6.0110214	86.7070350	C	1.1305144	7.6749832	87.5423339
H	7.5502495	2.4116572	91.4139367	C	1.4293383	8.8635668	86.8294732
H	5.6404961	0.5836465	84.0063766	C	2.2735388	8.8139781	85.7150958
C	7.0116838	5.7906022	87.7978571	C	2.8003544	7.5795767	85.2897249
H	4.6381460	2.4587235	92.7654805	H	2.8670628	5.4157042	85.6379985
H	6.5481991	7.8824083	88.2889606	H	1.3682749	5.4875405	87.5736054
C	3.5527856	2.0863148	83.9284934	C	0.2955226	7.7697645	88.7319896
C	6.3948612	4.4066444	87.9556546	H	1.0104709	9.8236071	87.1705418
C	6.8596394	1.5472796	91.3201697	H	2.5221786	9.7370960	85.1707765
C	6.1385860	6.8665594	88.4694334	H	3.4608280	7.5439025	84.4095973
H	6.0885753	6.7144405	89.5678242	O	0.1588858	6.8951673	89.6111131
C	6.2269577	3.8220155	89.2233501	C	-0.1542088	0.8095250	89.0362238
C	5.9962883	1.1277002	84.9062221	C	0.6584770	-0.2729237	89.3950799
H	9.0951697	5.0867446	87.8017066	C	0.2161154	-1.1211716	90.4780791
C	5.9426050	3.6878260	86.8392219	C	1.0221945	-2.1611163	91.0331042
C	8.4616139	5.8414822	88.3095890	C	-1.0853080	-0.8885890	91.0622582
H	8.9096355	6.8422559	88.1373567	C	-1.5498105	-1.7508129	92.1009559
H	6.0726937	4.1345552	85.8402110	C	-1.8522642	0.2408744	90.6523543
C	4.7844201	2.9502771	91.7814276	H	-2.8134351	0.4392497	91.1524064
H	6.7722591	1.0752661	92.3210272	C	-1.3844760	1.1333986	89.6956380
H	7.3321855	0.8154238	90.6340062	C	4.2130314	0.5683841	88.2158671
C	5.6002189	2.5762688	89.3943334	C	4.6603544	-0.6635062	87.7569149
C	3.9784535	2.6651059	84.7741121	H	5.7002204	-0.7688752	87.4111506
C	5.3028633	2.4393823	86.9513178	C	3.7930472	-1.7937002	87.6830011
H	6.5697773	0.4152817	85.5330934	C	4.2403865	-3.0293947	87.1256868
H	6.7049575	1.9136079	84.5692842	C	2.4305514	-1.6863273	88.1520817
C	5.4792790	1.9911301	90.7996390	C	1.5663115	-2.8094273	87.9806863
C	5.1244420	1.8803298	88.2489672	C	1.9860399	-0.4441545	88.7361260
C	4.8155245	1.7452037	85.6789592	C	2.8636978	0.6471853	88.6872743
H	3.7915341	3.2573407	91.3992878	O	0.2261170	1.6139297	87.9762448
H	3.1474956	3.1136555	85.3514508	O	2.4409592	1.8791307	89.1595398
H	5.3871284	3.8654635	91.9590048	P	1.4091692	2.7519782	88.1898982
H	5.1015978	6.8391005	88.0803564	O	0.8497289	3.8191574	89.1728601
H	4.5919011	3.4779083	84.3298832	O	1.9272209	3.1810812	86.8521260
H	8.5098857	5.6391610	89.4000179	C	-0.7556569	-2.7792402	92.5859577
H	4.8513882	1.0795434	90.7305960	C	0.5488708	-2.9698680	92.0578881
H	4.1467080	0.9168126	85.9852443	H	-2.5501201	-1.5688480	92.5249738
H	6.5850864	4.3602628	90.1156719	H	-1.1244573	-3.4327881	93.3912305
C	3.7659626	6.5665461	85.2661434	H	2.0379382	-2.3167128	90.6453963
C	2.7805367	6.3506509	86.2340712	H	1.1945269	-3.7618626	92.4674086
C	2.3766624	7.4306412	87.0590239	C	2.0284369	-3.9914270	87.4173875
C	2.9724238	8.7074653	86.9171062	C	3.3806238	-4.1107714	86.9987506
C	3.9473755	8.9135517	85.9358294	H	0.5155385	-2.7257064	88.2925933
C	4.3411318	7.8423337	85.1118264	H	1.3391956	-4.8402103	87.2895209
H	4.1005401	5.7281828	84.6379674	H	3.7389066	-5.0549358	86.5607688
H	2.3563063	5.3502042	86.4239857	H	5.2846027	-3.1021557	86.7826462
C	1.3913690	7.2157466	88.1102109	C	-1.9445731	3.4771034	90.4308391
H	2.6640383	9.5294628	87.5828844	C	-2.0115844	2.4650647	89.4288645
H	4.4127158	9.9032315	85.8157297	C	-2.3704967	4.7782316	90.1055654
H	5.1189325	8.0015095	84.3486246	C	-2.5377136	2.7774029	88.1451237
O	0.7151132	6.1743362	88.2068965	C	-2.9565892	4.0923961	87.8769557
H	1.2688511	8.0213069	88.8814659	C	-2.8602122	5.1168135	88.8337250
				H	-2.2998240	5.5733431	90.8662951
				C	-2.6942098	1.7150422	87.0597326
				H	-3.3594712	4.3235988	86.8788076
				C	-2.0510683	2.1313743	85.7255326
				H	-2.5780258	2.9942422	85.2668228
				H	-2.0977048	1.2952903	84.9976194
				H	-0.9879062	2.4079666	85.8652718
				C	-4.1791553	1.3440320	86.8815750
				H	-2.1718338	0.8007679	87.4069377
				H	-4.7720765	2.2172857	86.5364149
				H	-4.6235002	0.9920834	87.8348714
				H	-4.2962606	0.5371144	86.1285281
				C	-3.3017686	6.5436475	88.5330703
				C	-2.8291913	7.0400191	87.1565895
				H	-3.0455426	8.1211278	87.0325878

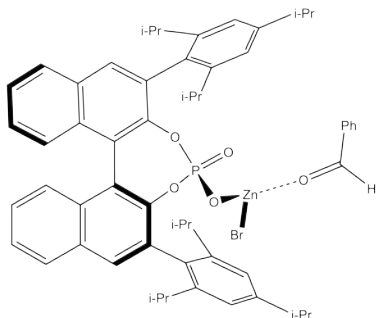
12j-mi; COSMO



Energy (Hartree)= -7274.220915627

H	-3.3451488	6.5079323	86.3306008	Zn	1.4513559	5.3297808	90.1351440
H	-1.7403476	6.8841001	87.0143425	Br	3.1238301	6.2523783	91.3887003
C	-4.8289349	6.6871735	88.6793303	C	2.4490116	6.3206815	85.8995455
H	-2.8299360	7.1892826	89.3069655	C	1.6524400	6.3903753	87.0442353
H	-5.1506952	7.7362329	88.5111395	C	1.1507497	7.6391386	87.4864179
H	-5.1663879	6.3798773	89.6896257	C	1.4360159	8.8138620	86.7462262
H	-5.3546618	6.0466410	87.9403164	C	2.2470250	8.7413657	85.6093392
C	-1.4106178	3.2296481	91.8442940	C	2.7547851	7.4968961	85.1897970
C	-0.1755518	4.0866002	92.1825155	H	2.8219893	5.3377704	85.5766230
H	0.1154342	3.9871220	93.2477506	H	1.3843295	5.4525786	87.5507263
H	-0.3602368	5.1712086	92.0112311	C	0.3447354	7.7524811	88.6957176
H	0.6993409	3.7338504	91.5952461	H	1.0318336	9.7819528	87.0830599
C	-2.5235162	3.4249621	92.8911327	H	2.4850554	9.6540432	85.0429542
H	-1.0813636	2.1748449	91.9090623	H	3.3899228	7.4428035	84.2920246
H	-2.1572103	3.1745837	93.9081443	O	0.2176945	6.8901783	89.5844049
H	-3.3948037	2.7757696	92.6695907	C	-0.1485535	0.8089799	89.0312560
H	-2.8861756	4.4738648	92.9112842	C	0.6567411	-0.2803186	89.3874206
H	7.5104265	5.8928009	87.4976975	C	0.2005938	-1.1362487	90.4587635
H	7.0968900	2.1662208	91.6927751	C	0.9975815	-2.1836657	91.0122677
H	6.1215633	0.8261519	84.0668205	C	-1.1055598	-0.9051172	91.0323816
C	6.7731313	5.8259758	88.3300858	C	-1.5828432	-1.7760155	92.0572275
H	4.0858233	1.8947422	92.7149354	C	-1.8630471	0.2319098	90.6271333
H	6.0083414	7.8590623	87.9717338	H	-2.8274409	0.4313479	91.1206038
H	4.1129285	2.3595435	83.7281074	C	-1.3822798	1.1322351	89.6846980
C	6.2356417	4.3978538	88.3247385	C	4.2205821	0.5644197	88.2375556
C	6.4877058	1.2743621	91.4354771	C	4.6706085	-0.6657278	87.7771287
C	5.6313513	6.8156382	88.0163299	H	5.7118480	-0.7675826	87.4343909
H	4.8461648	6.7633209	88.7999011	C	3.8046594	-1.7960723	87.6943548
C	5.9611394	3.6866542	89.5040790	C	4.2555862	-3.0294385	87.1360757
C	6.3306914	1.3219089	85.0378032	C	2.4385445	-1.6905504	88.1527668
H	8.2934063	5.5044421	89.8906123	C	1.5756524	-2.8121842	87.9684823
C	5.9381160	3.7723820	87.0999296	C	1.9900996	-0.4513950	88.7400144
C	7.4916508	6.2233129	89.6257596	C	2.8695542	0.6385598	88.7046102
H	7.9516019	7.2268605	89.5205600	O	0.2397538	1.6220978	87.9816042
H	6.1702273	4.3092901	86.1654264	O	2.4444425	1.8673513	89.1830591
C	4.2819325	2.4887952	91.7982652	P	1.4283378	2.7496353	88.2071288
H	6.3292272	0.6936858	92.3681472	O	0.8671756	3.8168026	89.1943028
H	7.0833938	0.6506411	90.7381486	O	1.9601098	3.1905948	86.8795583
C	5.3665615	2.4118894	89.4849492	C	-0.7975626	-2.8115190	92.5399149
C	4.3473699	2.8718622	84.6841871	C	0.5111675	-3.0007307	92.0235876
C	5.3294763	2.5069955	87.0229201	H	-2.5867928	-1.5946559	92.4727973
H	6.8071234	0.5776042	85.7079909	H	-1.1768587	-3.4717436	93.3347203
H	7.0744736	2.1263660	84.8557130	H	2.0165277	-2.3380325	90.6329344
C	5.1401602	1.6823212	90.8090303	H	1.1503555	-3.7985718	92.4317202
C	5.0238516	1.8259376	88.2358874	C	2.0422423	-3.9917573	87.4048818
C	5.0394049	1.8972732	85.6516314	C	3.3973538	-4.1099062	86.9977467
H	3.3093843	2.7593713	91.3442579	H	0.5225438	-2.7284012	88.2718980
H	3.4009557	3.2322086	85.1304021	H	1.3536992	-4.8395562	87.2675977
H	4.7787487	3.4306793	92.1086083	H	3.7593746	-5.0522740	86.5591137
H	5.1479523	6.5836300	87.0468709	H	5.3024488	-3.1006350	86.8009623
H	4.9891337	3.7437806	84.4375277	C	-1.9284134	3.4706991	90.4450695
H	6.7846318	6.2765043	90.4798811	C	-1.9976183	2.4718164	89.4302254
H	4.5925096	0.7432208	90.5884433	C	-2.3424676	4.7785201	90.1336765
H	4.3363436	1.0538762	85.8066549	C	-2.5127628	2.8042220	88.1475566
H	6.1992315	4.1393923	90.4773469	C	-2.9200424	4.1256008	87.8936080
H	-0.2710576	8.7243475	88.8682839	C	-2.8231917	5.1365055	88.8638859
				H	-2.2698106	5.5634312	90.9049524
				C	-2.6710892	1.7564911	87.0484491
				H	-3.3145901	4.3712958	86.8957595
				C	-2.0175224	2.1828726	85.7227327
				H	-2.5333169	3.0565057	85.2716111
				H	-2.0697183	1.3566965	84.9841535
				H	-0.9517983	2.4451726	85.8690277
				C	-4.1579119	1.3989550	86.8597119
				H	-2.1571087	0.8345994	87.3877819
				H	-4.7433062	2.2802210	86.5223900
				H	-4.6094239	1.0400312	87.8068015
				H	-4.2783572	0.6018541	86.0969114
				C	-3.2599224	6.5693296	88.5844982
				C	-2.8261716	7.0735627	87.1985328
				H	-3.0363558	8.1576501	87.0896900

12j-mi



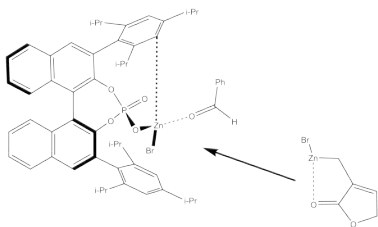
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H	-3.3740158	6.5552962	86.3845129
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C	-4.7805103	6.7246557	88.7791531
H	-2.7587789	7.2050704	89.3485884
H	-5.1003605	7.7770712	88.6289976
H	-5.0889464	6.4110071	89.7964672
H	-5.3336157	6.0928505	88.0529986
C	-1.4045529	3.2005186	91.8581658
C	-0.1661777	4.0440100	92.2157265
H	0.1226898	3.9183122	93.2788770
H	-0.3421211	5.1328461	92.0663994
H	0.7069534	3.7048296	91.6192919
C	-2.5235174	3.3870998	92.8999997
H	-1.0829186	2.1425161	91.9091736
H	-2.1670154	3.1199836	93.9162726
H	-3.3978972	2.7477777	92.6630285
H	-2.8809419	4.4374645	92.9333212
H	7.4518892	5.9229522	87.4928760
H	7.0821454	2.2096070	91.7038232
H	6.1801367	0.8219832	84.0963350
C	6.7136294	5.8525030	88.3242408
H	4.0741553	1.9198980	92.7347015
H	5.9230577	7.8724079	87.9448064
H	4.1357950	2.3020368	83.7357011
C	6.1965373	4.4169056	88.3279386
C	6.4788986	1.3118704	91.4537424
C	5.5595697	6.8247949	88.0015306
H	4.7777498	6.7733734	88.7884764
C	5.9230331	3.7129138	89.5116045
C	6.3704286	1.3303654	85.0646124
H	8.2335753	5.5618874	89.8902560
C	5.9190693	3.7753257	87.1073615
C	7.4239725	6.2689499	89.6183384
H	7.8721250	7.2771418	89.5070440
H	6.1527930	4.3058379	86.1695095
C	4.2647291	2.5108159	91.8149896
H	6.3275872	0.7355261	92.3902277
H	7.0777874	0.6894596	90.7583556
C	5.3481913	2.4294521	89.4996276
C	4.3467276	2.8242927	84.6917642
C	5.3296732	2.5007529	87.0368357
H	6.8634615	0.6046853	85.7431124
H	7.0945832	2.1519293	84.8805555
C	5.1270387	1.7062864	90.8280388
C	5.0229282	1.8272254	88.2536131
C	5.0614566	1.8753234	85.6681107
H	3.2886714	2.7705499	91.3622415
H	3.3856742	3.1554024	85.1294186
H	4.7528676	3.4583079	92.1214802
H	5.0772853	6.5759014	87.0356469
H	4.9634836	3.7146665	84.4462265
H	6.7140562	6.3208086	90.4699376
H	4.5864057	0.7618221	90.6128923
H	4.3800847	1.0147946	85.8242734
H	6.1470780	4.1780330	90.4822584
H	-0.2097148	8.7161880	88.8319848

7.7 Agglomeration to Complexes 12

7.7.1 Pathway 12d-ma → 14d-ma

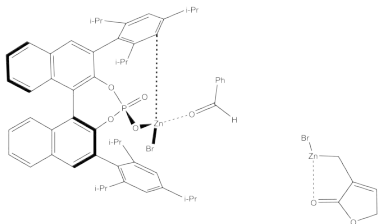
TS-7-d-ma; woelfling data



Energy (Hartree) = -11969.928995

C	1.914707	2.314193	1.800735	H	-0.476303	6.664803	0.465374
C	3.316279	2.309259	1.794368	H	-1.614282	6.345047	-0.875658
C	3.995976	3.584576	1.785391	H	1.415254	-6.036851	-2.024880
C	5.404857	3.713947	1.594158	H	5.446552	-2.156344	-3.867294
C	3.221141	4.793014	1.941464	H	4.006580	-4.922433	3.421408
C	3.889397	6.053224	1.981497	C	1.717072	-5.202135	-2.695836
C	1.799990	4.716752	1.987848	H	4.059636	0.715550	-3.665014
H	1.221258	5.649720	2.072780	H	-0.184567	-5.290767	-3.807508
C	1.126242	3.509316	1.853451	H	1.642518	-3.853347	3.526622
C	4.365180	-1.224489	0.692713	C	2.482285	-4.203317	-1.837188
C	5.462576	-1.454308	1.513090	C	5.720003	-1.448127	-3.057033
H	6.013500	-2.403281	1.421741	C	0.425524	-4.561533	-3.234149
C	5.843198	-0.533911	2.531797	H	0.654439	-3.708141	-3.907957
C	6.906767	-0.834828	3.434730	C	3.119693	-3.084129	-2.401528
C	5.098005	0.691577	2.701272	C	4.003603	-4.790312	2.319430
C	5.411390	1.516748	3.823579	H	3.483744	-6.282342	-3.429264
C	4.049635	1.011478	1.760325	C	2.517740	-4.341574	-0.442542
C	3.700643	0.037761	0.813215	C	2.568190	-5.800245	-3.826786
O	1.229388	1.113115	1.796188	H	1.993402	-6.563556	-4.391370
O	2.694273	0.298555	-0.093994	H	2.013639	-5.209178	0.013721
P	1.100641	0.256763	0.383459	C	3.531108	-0.156718	-3.228478
O	0.478011	1.226970	-0.680033	H	6.268604	-0.601398	-3.519429
O	0.497634	-1.085671	0.641811	H	6.414718	-1.976848	-2.373295
C	5.264778	6.138190	1.830880	C	3.766263	-2.116480	-1.613482
C	6.022784	4.956893	1.616459	C	1.651226	-3.808740	2.417562
H	3.282764	6.963126	2.114356	C	3.143529	-3.399657	0.394863
H	5.766167	7.117712	1.856567	H	5.050547	-4.625607	1.991508
H	6.004469	2.810677	1.417635	H	3.663434	-5.744973	1.865343
H	7.110240	5.026112	1.460586	C	4.470917	-0.951180	-2.304427
C	6.438299	1.184717	4.696436	C	3.779380	-2.273303	-0.199716
C	7.207540	0.008646	4.493265	C	3.090472	-3.621014	1.905984
H	4.818477	2.424383	4.000453	H	2.655364	0.225251	-2.667958
H	6.652010	1.836741	5.557204	H	1.012455	-2.966267	2.086098
H	8.024826	-0.241110	5.186945	H	3.162478	-0.773430	-4.074819
H	7.472398	-1.767971	3.284408	H	-0.195148	-4.173818	-2.403000
C	-0.925783	3.949512	0.453720	H	1.200711	-4.754332	2.048569
C	-0.353510	3.425880	1.652614	H	2.886034	-5.022813	-4.552379
C	-2.299557	3.755044	0.223582	H	4.821851	-0.254412	-1.516473
C	-1.180748	2.760404	2.595825	H	3.482208	-2.707379	2.394405
C	-2.555790	2.620369	2.326885	H	3.110802	-2.954375	-3.495877
C	-3.139166	3.099120	1.143993	C	-11.354491	-1.698120	-2.619440
H	-2.743053	4.147882	-0.707281	C	-10.103244	-1.177470	-2.672486
C	-0.638109	2.236955	3.923892	C	-9.894932	-0.663842	-4.067049
H	-3.183534	2.114826	3.075071	O	-11.052059	-0.877434	-4.783695
C	-0.949946	0.745844	4.140176	C	-12.017316	-1.520384	-3.951962
H	-2.040017	0.567006	4.253304	O	-8.909888	-0.142038	-4.540219
H	-0.460158	0.379436	5.065897	C	-9.013937	-1.071643	-1.672720
H	-0.583448	0.135757	3.292124	H	-9.399818	-0.918751	-0.644340
C	-1.148883	3.099840	5.093769	H	-11.844661	-2.177497	-1.759786
H	0.464870	2.343380	3.903166	H	-12.317807	-2.484918	-4.423073
H	-2.253962	3.041978	5.186001	H	-12.932129	-0.886249	-3.895375
H	-0.880276	4.166801	4.955103	Zn	-7.993509	-2.739657	-1.642005
H	-0.713047	2.757118	6.055245	H	-8.331368	-0.238892	-1.938689
C	-4.634884	2.994134	0.855179	Br	-7.097361	-4.808636	-1.483660
C	-5.365534	1.939637	1.696127	Zn	-0.664150	0.888263	-2.108221
H	-6.418437	1.838790	1.362395	Br	-1.053858	1.404487	-4.311058
H	-5.392918	2.223787	2.769107	C	-3.454487	-4.705286	-1.200501
H	-4.882430	0.944207	1.624150	C	-2.885255	-3.434010	-1.280846
C	-5.308353	4.373196	1.011002	C	-2.620921	-2.873791	-2.555431
H	-4.731008	2.698249	-0.214879	C	-2.920108	-3.595792	-3.734667
H	-6.384656	4.325994	0.743863	C	-3.492171	-4.867989	-3.644458
H	-4.828444	5.136162	0.366415	C	-3.758750	-5.417789	-2.378916
H	-5.229513	4.726676	2.060420	H	-3.676252	-5.151964	-0.220352
C	-0.122684	4.752825	-0.572556	H	-2.613680	-2.857059	-0.383475
C	-0.190102	4.177828	-1.994278	C	-1.999910	-1.569797	-2.688891
H	0.314348	4.849222	-2.718877	H	-2.689546	-3.149056	-4.714970
H	-1.228827	4.034334	-2.356843	H	-3.730936	-5.434198	-4.556671
H	0.340134	3.207751	-2.041797	H	-4.217543	-6.415318	-2.306936
C	-0.558514	6.230685	-0.551772	O	-1.734512	-0.826643	-1.722379
H	0.942504	4.718564	-0.273512	H	-1.752011	-1.227529	-3.727184
H	0.071478	6.834798	-1.237086				

agg-7-d-ma



Energy (Hartree)=-11969.96497

C	2.952877	2.568828	2.244162
C	4.353657	2.568828	2.244162
C	5.026472	3.847942	2.244162
C	6.436497	3.983063	2.062582
C	4.247343	5.054653	2.401759
C	4.913040	6.315787	2.460953
C	2.823206	4.978905	2.409154
H	2.242302	5.913060	2.465398
C	2.164856	3.766275	2.258777
C	5.356295	-0.975926	1.139926
C	6.464717	-1.211688	1.942927
H	7.004781	-2.165789	1.846944
C	6.872995	-0.290161	2.949400
C	7.950637	-0.597118	3.832454
C	6.140849	0.941493	3.129007
C	6.476561	1.762683	4.247387
C	5.082736	1.269111	2.201346
C	4.710406	0.298046	1.258462
O	2.265569	1.378571	2.267449
O	3.695956	0.570413	0.361046
P	2.118840	0.458489	0.877867
O	1.396471	1.295259	-0.214949
O	1.648258	-0.900450	1.295692
C	6.290034	6.403365	2.324023
C	7.052007	5.226595	2.101966
H	4.305416	7.223983	2.595836
H	6.789815	7.384042	2.364758
H	7.038167	3.082990	1.880545
H	8.139704	5.298884	1.954288
C	7.517487	1.424164	5.102283
C	8.277028	0.244791	4.884008
H	5.891861	2.672435	4.437749
H	7.749475	2.074107	5.959639
H	9.106646	-0.008625	5.562134
H	8.507350	-1.534352	3.672595
C	0.258583	4.071270	0.653053
C	0.712997	3.628698	1.928408
C	-1.052175	3.717832	0.238948
C	-0.167421	2.901456	2.779203
C	-1.465532	2.588822	2.334160
C	-1.938811	2.977538	1.070147
H	-1.436830	4.115013	-0.715531
C	0.245020	2.483748	4.186398
H	-2.127120	2.018939	3.001207
C	-0.027956	0.997070	4.472334
H	-1.115175	0.776841	4.513455
H	0.397959	0.715397	5.456452
H	0.431735	0.351099	3.700422
C	-0.434134	3.400406	5.223193
H	1.338916	2.645216	4.273850
H	-1.539175	3.298893	5.188087
H	-0.187238	4.466469	5.044741
H	-0.104029	3.137539	6.249580
C	-3.361606	2.712121	0.594586
C	-4.030607	1.513494	1.276723
H	-4.999206	1.287037	0.788063
H	-4.246852	1.714025	2.346526
H	-3.395503	0.607358	1.222280
C	-4.213578	3.988598	0.749647

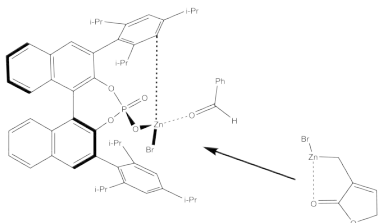
H	-3.288546	2.490484	-0.495129
H	-5.232994	3.829018	0.345195
H	-3.764169	4.847765	0.213726
H	-4.308450	4.269445	1.819552
C	1.113851	4.910536	-0.294131
C	1.271934	4.288148	-1.690955
H	1.928871	4.925454	-2.317489
H	0.306314	4.184062	-2.229105
H	1.739924	3.285549	-1.621840
C	0.559910	6.346701	-0.368891
H	2.129150	4.971053	0.141279
H	1.217402	6.983282	-0.995832
H	0.489902	6.811029	0.636280
H	-0.455014	6.367661	-0.818834
H	2.076880	-5.616250	-1.485259
H	6.350590	-1.958986	-3.416771
H	5.092245	-4.640786	3.866381
C	2.495189	-4.856215	-2.181611
H	5.044616	0.965607	-3.190001
H	0.666173	-4.855307	-3.400423
H	2.728056	-3.647836	4.075313
C	3.316132	-3.891321	-1.336195
C	6.653078	-1.255710	-2.612464
C	1.307103	-4.137292	-2.846573
H	1.655185	-3.370778	-3.569099
C	3.989455	-2.801723	-1.916359
C	5.051466	-4.502423	2.765897
H	4.194818	-6.138646	-2.733347
C	3.395848	-4.041596	0.057183
C	3.358275	-5.596427	-3.218443
H	2.752199	-6.332122	-3.786633
H	2.875817	-4.894529	0.522615
C	4.500386	0.096604	-2.765741
H	7.217236	-0.425327	-3.085655
H	7.343207	-1.799371	-1.936189
C	4.695357	-1.863566	-1.145638
C	2.684600	-3.603705	2.967204
C	4.083989	-3.129778	0.877670
H	6.082335	-4.305692	2.407409
H	4.723681	-5.463090	2.314675
C	5.426169	-0.721465	-1.849135
C	4.737006	-2.022069	0.267034
C	4.089123	-3.359949	2.390443
H	3.625098	0.478569	-2.204947
H	2.003402	-2.782775	2.671042
H	4.129050	-0.506849	-3.620715
H	0.677295	-3.625261	-2.092267
H	2.258158	-4.570591	2.623539
H	3.798351	-4.889568	-3.952471
H	5.806505	-0.034005	-1.067772
H	4.466500	-2.434305	2.868496
H	3.953104	-2.666949	-3.009325
C	-21.155475	-3.913619	-7.253424
C	-19.946960	-3.323465	-7.425118
C	-19.849094	-3.005177	-8.876018
O	-20.985779	-3.345310	-9.518802
C	-21.877598	-3.954139	-8.567916
O	-18.864254	-2.534760	-9.448538
C	-18.783977	-2.982205	-6.561835
H	-18.596043	-3.743825	-5.780918
H	-21.585224	-4.305734	-6.319623
H	-22.103641	-4.984651	-8.920594
H	-22.834242	-3.387075	-8.558432
Zn	-17.269808	-2.620141	-7.816612
H	-18.972890	-2.020330	-6.030745
Br	-15.171178	-2.227274	-8.600166
Zn	-0.435661	1.638563	-0.699798
Br	-1.501415	1.800588	-2.789473
C	-0.468591	-4.330410	0.727781
C	-0.608276	-2.952636	0.537959
C	-1.513700	-2.479615	-0.445750

C	-2.256649	-3.389115	-1.236969
C	-2.117515	-4.765057	-1.029054
C	-1.224409	-5.232226	-0.045539
H	0.248536	-4.704579	1.472790
H	0.014855	-2.221679	1.081336
C	-1.634463	-1.050363	-0.696636
H	-2.937525	-3.005306	-2.013629
H	-2.692968	-5.478775	-1.636450
H	-1.105395	-6.316182	0.108230
O	-1.135602	-0.183945	0.045135
H	-2.178352	-0.729095	-1.624683

H	-3.399432	-6.577989	3.477488
H	-4.842369	-7.879428	1.902606
H	-4.669244	-4.634073	-0.965911
H	-5.427063	-6.906622	-0.344564
C	-7.417148	-2.254338	-0.477586
C	-7.748529	-1.745869	-1.761255
H	-5.847657	-2.787581	0.901559
H	-8.217937	-2.528936	0.226099
H	-8.803998	-1.642448	-2.055995
H	-6.983288	-0.933763	-3.616474
C	0.665459	-2.978228	3.285209
C	-0.603281	-2.329830	3.377330
C	1.755957	-2.427132	3.985480
C	-0.729153	-1.126919	4.123017
C	0.391083	-0.631391	4.822912
C	1.640880	-1.274914	4.787192
H	2.734716	-2.928277	3.930864
C	-2.055707	-0.378283	4.227009
H	0.265789	0.274965	5.436932
C	-1.937298	1.070018	3.719130
H	-1.248028	1.673325	4.347943
H	-2.926407	1.571857	3.744792
H	-1.575036	1.096856	2.672410
C	-2.619069	-0.440612	5.658731
H	-2.782822	-0.895800	3.570443
H	-1.952445	0.071634	6.384060
H	-2.739737	-1.489705	5.996855
H	-3.611643	0.052698	5.710642
C	2.815760	-0.858347	5.666915
C	3.053904	0.654998	5.754414
H	3.903251	0.876079	6.431776
H	2.169655	1.193350	6.157351
H	3.310985	1.078658	4.763271
C	2.643366	-1.469145	7.072556
H	3.724999	-1.304788	5.208897
H	3.520596	-1.244404	7.714242
H	2.525502	-2.569820	7.020774
H	1.739957	-1.059947	7.572004
C	0.879681	-4.273386	2.497887
C	2.074019	-4.211846	1.531003
H	2.179425	-5.178181	0.996964
H	3.035341	-4.011044	2.046182
H	1.920254	-3.429487	0.762670
C	1.018422	-5.470424	3.459330
H	-0.023204	-4.442252	1.879001
H	1.112916	-6.418896	2.891421
H	0.142938	-5.562165	4.132738
H	1.920354	-5.367304	4.098484
H	1.245327	-2.940158	-5.098055
H	-0.172734	-2.776975	-6.117940
H	-4.720969	3.232978	-3.710309
C	1.414982	1.861886	-5.313914
H	0.505135	-4.186300	-3.308360
H	3.586350	2.104429	-5.118875
H	-3.430181	3.549464	-1.497687
C	0.255895	1.103013	-4.680468
C	-0.977650	-3.102703	-5.426154
C	2.772000	1.477832	-4.699620
H	3.029735	0.419048	-4.910773
C	0.242425	-0.301675	-4.615500
C	-3.860154	2.659805	-4.113876
H	0.454116	2.014073	-7.284859
C	-0.845232	1.790524	-4.151244
C	1.417686	1.688358	-6.843847
H	2.230157	2.281875	-7.312909
H	-0.846069	2.892117	-4.192966
C	0.541885	-3.079663	-3.383466
H	-0.985094	-4.212706	-5.413541
H	-1.942196	-2.756370	-5.849692
C	-0.812265	-1.013205	-4.019780
C	-2.570180	3.004948	-1.940699

7.7.2 Pathway 12d-mi → 14d-mi

TS-7-d-mi; woelfling data



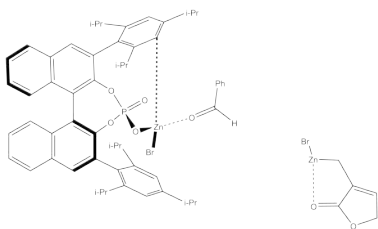
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Br	4.292899	-0.938841	1.830538
C	0.470826	5.385330	1.773616
C	0.770056	4.038681	1.545764
C	1.252753	3.250323	2.618443
C	1.421305	3.812646	3.905616
C	1.126859	5.161693	4.122182
C	0.651942	5.944481	3.055073
H	0.091505	6.012210	0.952930
H	0.625642	3.567326	0.561079
C	1.591366	1.845854	2.447380
H	1.796089	3.178233	4.723930
H	1.266157	5.604326	5.119696
H	0.416349	7.006386	3.225716
O	1.603505	1.257423	1.352347
C	-2.265208	-2.301141	1.463586
C	-3.186910	-2.910536	0.600331
C	-3.624156	-4.251631	0.913589
C	-4.407763	-5.042735	0.019444
C	-3.228004	-4.843888	2.169512
C	-3.699974	-6.147432	2.509065
C	-2.311338	-4.153147	3.012195
H	-1.977339	-4.638357	3.942229
C	-1.765161	-2.928783	2.647525
C	-2.996539	-0.997501	-2.726146
C	-4.331657	-0.985128	-3.112638
H	-4.608110	-0.532620	-4.077729
C	-5.365168	-1.474984	-2.262335
C	-6.739397	-1.358965	-2.630031
C	-5.025633	-2.045818	-0.980161
C	-6.090132	-2.401566	-0.098213
C	-3.633675	-2.198094	-0.629210
C	-2.677523	-1.637075	-1.486231
O	-1.830535	-1.016985	1.214072
O	-1.337745	-1.731753	-1.158975
P	-0.731610	-0.713160	-0.002292
O	0.601559	-1.468146	0.341023
O	-0.739861	0.754061	-0.284469
C	-4.493153	-6.871191	1.632279
C	-4.830430	-6.317733	0.368860

C	-1.932128	1.131381	-3.547276
H	-4.250991	1.915512	-4.838083
H	-3.221353	3.367361	-4.683402
C	-0.756786	-2.540476	-4.009375
C	-1.912573	-0.290781	-3.475681
C	-3.067445	1.983367	-2.979487
H	0.691396	-2.671095	-2.365381
H	-2.012764	2.489036	-1.134466
H	1.431496	-2.822783	-3.995990
H	2.768353	1.609894	-3.599053
H	-1.899546	3.763568	-2.396790
H	1.571272	0.624632	-7.122356
H	-1.596748	-2.906234	-3.385355
H	-3.765038	1.308224	-2.446333
H	1.090295	-0.866845	-5.034309
H	1.858266	1.289583	3.377168
C	9.495689	7.861025	-3.180683
C	8.401120	7.121922	-3.487837
C	8.651658	5.742527	-2.977295
O	9.923224	5.666802	-2.481913
C	10.517788	6.971234	-2.537471
O	7.852847	4.820868	-2.939525
C	7.103950	7.403822	-4.133329
H	7.011431	6.803641	-5.066096
H	9.652966	8.932430	-3.367371
H	11.467366	6.920654	-3.117745
H	10.783808	7.276054	-1.499376
Zn	5.675985	6.661097	-2.996079
H	6.960267	8.472040	-4.381564
Br	3.792193	6.280983	-1.790036

C	-5.932983	-2.531294	-3.019733
C	-7.231880	-2.485875	-3.608408
C	-5.750431	-3.222148	-1.764260
C	-6.906151	-3.757215	-1.119613
C	-4.423911	-3.306517	-1.198949
C	-3.395759	-2.586687	-1.825038
O	-3.068530	-2.123227	0.965396
O	-2.111278	-2.640260	-1.308381
P	-1.757068	-1.714449	0.019088
O	-0.474018	-2.391776	0.566727
O	-1.802781	-0.222926	-0.184177
C	-5.246746	-8.175936	0.657817
C	-5.413920	-7.576241	-0.618308
H	-4.507462	-7.910773	2.675344
H	-5.550091	-9.222175	0.818278
H	-5.174087	-5.807952	-1.827122
H	-5.831633	-8.165574	-1.448133
C	-8.160889	-3.677210	-1.709629
C	-8.326550	-3.053959	-2.974187
H	-6.798626	-4.232468	-0.135850
H	-9.034586	-4.094573	-1.186633
H	-9.323717	-3.004146	-3.437512
H	-7.351050	-1.966863	-4.573341
C	-0.768941	-3.922683	3.259209
C	-2.103043	-3.420753	3.207743
C	0.216258	-3.158021	3.938141
C	-2.426808	-2.203230	3.870209
C	-1.423111	-1.500739	4.564487
C	-0.092151	-1.945180	4.611157
H	1.237916	-3.562512	4.030438
C	-3.842943	-1.639037	3.867187
H	-1.688848	-0.561399	5.068255
C	-3.889673	-0.174334	3.395026
H	-3.392222	0.506729	4.117277
H	-4.941965	0.163045	3.299810
H	-3.400474	-0.056520	2.408600
C	-4.488811	-1.812969	5.255394
H	-4.439764	-2.238258	3.151284
H	-3.937918	-1.241617	6.032410
H	-4.499842	-2.877587	5.565468
H	-5.536199	-1.446612	5.247226
C	1.001250	-1.227873	5.390261
C	0.794331	0.288868	5.499819
H	1.680838	0.761426	5.967756
H	-0.081226	0.542320	6.133804
H	0.644456	0.743495	4.501527
C	1.163213	-1.877016	6.779513
H	1.944757	-1.397447	4.823126
H	2.004159	-1.412086	7.332650
H	1.364055	-2.964043	6.701141
H	0.241304	-1.747418	7.384771
C	-0.353142	-5.254426	2.638267
C	0.888779	-5.161093	1.736036
H	1.127548	-6.162272	1.323508
H	1.791956	-4.803495	2.272678
H	0.704146	-4.480269	0.882731
C	-0.161433	-6.302611	3.753228
H	-1.187471	-5.598032	1.997396
H	0.065949	-7.296253	3.316730
H	-1.067375	-6.403416	4.384095
H	0.681370	-6.027654	4.422391
H	0.451423	2.850011	-4.151109
H	-0.188526	-2.679701	-6.238799
H	-5.712583	2.193143	-3.424727
C	0.795254	1.824262	-4.416180
H	0.232840	-4.551617	-3.669733
H	2.846033	2.248549	-3.748575
H	-4.627061	2.460233	-1.110195
C	-0.358001	0.878950	-4.101134
C	-1.048526	-3.181779	-5.749443
C	2.036402	1.513546	-3.560333

agg-7-d-mi



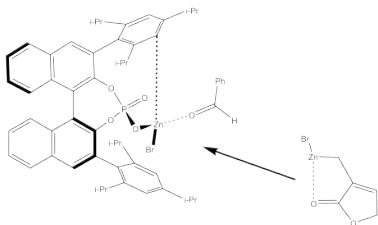
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Br	3.034805	-1.845365	2.026283
C	-1.693363	4.020215	2.026283
C	-1.166623	2.729891	2.128481
C	-0.492063	2.159700	1.025648
C	-0.361013	2.885771	-0.177267
C	-0.882923	4.181185	-0.272483
C	-1.547641	4.746971	0.829045
H	-2.223830	4.468749	2.879539
H	-1.270578	2.136563	3.049168
C	0.060932	0.807980	1.099453
H	0.128475	2.413586	-1.043652
H	-0.784211	4.747413	-1.210172
H	-1.965414	5.762745	0.752391
O	0.049068	0.124618	2.145961
C	-3.432680	-3.447540	1.085088
C	-4.129847	-4.075235	0.044032
C	-4.495976	-5.461152	0.218886
C	-5.047718	-6.254898	-0.832063
C	-4.267284	-6.093802	1.497107
C	-4.675863	-7.447600	1.690082
C	-3.568916	-5.387577	2.519604
H	-3.351272	-5.903277	3.467423
C	-3.087891	-4.101858	2.312114
C	-3.585089	-1.800836	-3.007167
C	-4.834610	-1.847717	-3.613687
H	-5.000583	-1.286819	-4.545849

H	2.440358	0.505830	-3.786050	C	-1.854908	1.911343	2.426595
C	-0.233965	-0.508655	-4.291047	C	-3.115609	2.254699	2.900548
C	-4.760597	1.785064	-3.823693	H	-3.345509	2.108601	3.967029
H	0.253413	2.082428	-6.531502	C	-4.138846	2.739163	2.037400
C	-1.573810	1.365917	-3.600530	C	-5.461047	2.978208	2.518318
C	1.138817	1.824929	-5.916349	C	-3.846248	2.953394	0.640671
H	1.942091	2.557670	-6.141081	C	-4.917884	3.339381	-0.220280
H	-1.684441	2.452124	-3.446619	C	-2.504144	2.726325	0.162938
C	0.167323	-3.453192	-3.527152	C	-1.574520	2.154731	1.045121
H	-0.957484	-4.270733	-5.942221	O	-1.300539	0.802056	-1.486503
H	-1.972165	-2.819916	-6.245957	O	-0.302412	1.847515	0.595467
C	-1.273828	-1.400630	-3.977466	P	-0.123710	0.484985	-0.350387
C	-3.666079	2.135284	-1.561098	O	1.262734	0.781395	-1.015850
C	-2.647038	0.518894	-3.263560	O	-0.413411	-0.826347	0.303846
H	-5.007478	1.060158	-4.626014	C	-2.611590	6.920115	-3.027063
H	-4.203918	2.621654	-4.295843	C	-2.928206	6.725659	-1.656809
C	-1.077644	-2.892854	-4.236250	H	-1.806252	6.015144	-4.821553
C	-2.492442	-0.883607	-3.457736	H	-2.764762	7.905282	-3.493568
C	-3.928041	1.136488	-2.701100	H	-2.994518	5.353760	0.004026
H	0.130570	-3.249397	-2.440135	H	-3.312047	7.567038	-1.059727
H	-3.044496	1.668990	-0.774054	C	-6.198225	3.543292	0.275046
H	1.103331	-3.013876	-3.931669	C	-6.473074	3.376466	1.658436
H	1.799337	1.535226	-2.476516	H	-4.721306	3.460827	-1.294569
H	-3.150457	3.051225	-1.917337	H	-7.008729	3.828869	-0.412933
H	1.495096	0.827353	-6.245516	H	-7.491301	3.545463	2.040903
H	-1.959503	-3.423518	-3.822927	H	-5.666143	2.818317	3.588691
H	-4.531872	0.314765	-2.267752	C	1.295395	1.446384	-4.010911
H	0.707861	-0.916616	-4.691950	C	-0.113156	1.256344	-3.948988
H	0.583095	0.437225	0.186067	C	2.101430	0.360091	-4.414645
C	19.287639	15.613770	0.330938	C	-0.686291	0.016091	-4.338909
C	18.360995	14.775376	-0.199116	C	0.158881	-1.034223	-4.736524
C	18.979143	13.421603	-0.186358	C	1.557417	-0.893699	-4.768703
O	20.201907	13.458198	0.384875	H	3.190464	0.497875	-4.497592
C	20.496188	14.823480	0.731769	C	-2.199110	-0.176317	-4.382873
O	18.488668	12.396641	-0.662558	H	-0.292232	-1.991766	-5.040853
C	16.993262	14.905807	-0.769502	C	-2.664993	-1.405093	-3.589295
H	16.861562	15.843670	-1.344282	H	-2.288950	-2.352982	-4.029478
H	19.204301	16.699976	0.473845	H	-3.772568	-1.467411	-3.581072
H	21.423264	15.122043	0.192585	H	-2.321463	-1.353299	-2.539065
H	20.712414	14.876756	1.822846	C	-2.689087	-0.211239	-5.843596
Zn	16.663758	13.207232	-1.771774	H	-2.660455	0.714336	-3.909226
H	16.239487	14.924948	0.049321	H	-2.268252	-1.081989	-6.389313
Br	15.704241	11.672922	-3.149588	H	-2.389270	0.704534	-6.392758

7.7.3 Pathway 12j-ma → 14j-ma

TS-7-j-ma-woelfling data



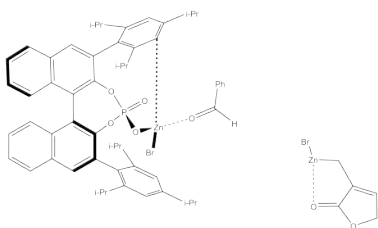
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C	-1.447338	2.076358	-1.996519
C	-2.084842	3.055562	-1.226976
C	-2.254020	4.370714	-1.800302
C	-2.752564	5.484860	-1.059399
C	-1.875550	4.588550	-3.177204
C	-2.086865	5.870908	-3.766068
C	-1.241134	3.541849	-3.906897
H	-0.916876	3.736422	-4.940854
C	-0.966686	2.312222	-3.325249

C	-1.854908	1.911343	2.426595
C	-3.115609	2.254699	2.900548
H	-3.345509	2.108601	3.967029
C	-4.138846	2.739163	2.037400
C	-5.461047	2.978208	2.518318
C	-3.846248	2.953394	0.640671
C	-4.917884	3.339381	-0.220280
C	-2.504144	2.726325	0.162938
C	-1.574520	2.154731	1.045121
O	-1.300539	0.802056	-1.486503
O	-0.302412	1.847515	0.595467
P	-0.123710	0.484985	-0.350387
O	1.262734	0.781395	-1.015850
O	-0.413411	-0.826347	0.303846
C	-2.611590	6.920115	-3.027063
C	-2.928206	6.725659	-1.656809
H	-1.806252	6.015144	-4.821553
H	-2.764762	7.905282	-3.493568
H	-2.994518	5.353760	0.004026
H	-3.312047	7.567038	-1.059727
C	-6.198225	3.543292	0.275046
C	-6.473074	3.376466	1.658436
H	-4.721306	3.460827	-1.294569
H	-7.008729	3.828869	-0.412933
H	-7.491301	3.545463	2.040903
H	-5.666143	2.818317	3.588691
C	1.295395	1.446384	-4.010911
C	-0.113156	1.256344	-3.948988
C	2.101430	0.360091	-4.414645
C	-0.686291	0.016091	-4.338909
C	0.158881	-1.034223	-4.736524
C	1.557417	-0.893699	-4.768703
H	3.190464	0.497875	-4.497592
C	-2.199110	-0.176317	-4.382873
H	-0.292232	-1.991766	-5.040853
C	-2.664993	-1.405093	-3.589295
H	-2.288950	-2.352982	-4.029478
H	-3.772568	-1.467411	-3.581072
H	-2.321463	-1.353299	-2.539065
C	-2.689087	-0.211239	-5.843596
H	-2.660455	0.714336	-3.909226
H	-2.268252	-1.081989	-6.389313
H	-2.389270	0.704534	-6.392758
H	-3.795335	-0.290217	-5.884445
C	2.459556	-2.017338	-5.261531
C	2.213876	-3.345444	-4.527483
H	2.912199	-4.126119	-4.892538
H	1.183397	-3.725358	-4.688090
H	2.366247	-3.249848	-3.433232
C	2.324182	-2.177221	-6.789115
H	3.504249	-1.706372	-5.043970
H	3.031182	-2.941653	-7.173051
H	2.531778	-1.222690	-7.314026
H	1.297629	-2.494546	-7.069576
C	1.949606	2.795314	-3.710981
C	3.197217	2.712637	-2.818008
H	3.614822	3.726849	-2.652932
H	4.005368	2.094113	-3.258958
H	2.938867	2.302019	-1.821844
C	2.272604	3.519596	-5.033567
H	1.207067	3.410086	-3.164689
H	2.683784	4.531642	-4.838068
H	1.371606	3.631578	-5.669513
H	3.025206	2.953847	-5.621906
H	1.806086	-1.582916	6.135490
H	1.414109	4.212237	5.069214
H	-4.144051	-1.561161	4.257377
C	2.116117	-0.524324	5.988226
H	2.070301	4.535490	1.960430
H	4.239442	-1.070019	6.081599
H	-2.733344	-2.825389	2.546605

C	1.104363	0.101872	5.036610	Br	4.853945	1.180845	-1.805576
C	0.604271	4.423266	4.339459	C	-1.590190	3.244492	-1.805576
C	3.538763	-0.539746	5.403807	C	-2.227373	4.280141	-1.108947
H	3.930536	0.489007	5.262711	C	-2.445083	5.525867	-1.808608
C	1.293597	1.392281	4.513231	C	-2.915533	6.707541	-1.159249
C	-3.247369	-0.986349	4.569428	C	-2.147476	5.603504	-3.220791
H	1.063580	0.135643	7.802332	C	-2.417322	6.814162	-3.926857
C	-0.063014	-0.585200	4.669521	C	-1.513114	4.503837	-3.869007
C	2.081438	0.166053	7.364436	H	-1.235986	4.601854	-4.930047
H	2.780258	-0.321543	8.075941	C	-1.163827	3.357112	-3.169469
H	-0.225653	-1.598007	5.071962	C	-1.950425	3.307125	2.600790
C	1.930413	3.510516	2.362111	C	-3.184304	3.718971	3.086861
H	0.746884	5.460707	3.971909	H	-3.412154	3.588310	4.155651
H	-0.358665	4.381838	4.887875	C	-4.199435	4.227787	2.225922
C	0.354826	2.000074	3.661719	C	-5.495435	4.549088	2.729329
C	-1.838191	-2.276508	2.901467	C	-3.938577	4.351130	0.811412
C	-1.025660	-0.035735	3.801682	C	-5.028371	4.708709	-0.039951
H	-3.584959	0.010940	4.915992	C	-2.610522	4.071597	0.315345
H	-2.799270	-1.505928	5.442873	C	-1.672585	3.541406	1.214886
C	0.623288	3.421200	3.170116	O	-1.378936	2.032371	-1.191301
C	-0.823612	1.284194	3.310688	O	-0.393981	3.252133	0.776859
C	-2.237764	-0.881981	3.411594	P	-0.139669	1.851587	-0.083093
H	1.912435	2.805885	1.507868	O	1.214031	2.176664	-0.773673
H	-1.148678	-2.182264	2.040843	O	-0.384551	0.567060	0.647262
H	2.816094	3.277805	2.990227	C	-2.915280	7.928910	-3.271073
H	3.563629	-1.047197	4.418995	C	-3.145008	7.877144	-1.870940
H	-1.367620	-2.892194	3.697892	H	-2.198772	6.850588	-5.005705
H	2.375421	1.233191	7.279383	H	-3.111025	8.858055	-3.827258
H	-0.202518	3.706916	2.488276	H	-3.089599	6.686372	-0.074984
H	-2.740242	-0.372268	2.565064	H	-3.503857	8.773138	-1.341355
H	2.201730	1.954414	4.784036	C	-6.283972	4.994074	0.478440
C	1.869750	-3.586063	3.816072	C	-6.518595	4.934285	1.876933
C	2.017369	-2.870127	2.624417	H	-4.866819	4.748041	-1.126334
C	3.287686	-2.823217	1.998852	H	-7.105480	5.262242	-0.204456
C	4.400916	-3.465547	2.590201	H	-7.515908	5.172458	2.278508
C	4.243060	-4.176029	3.785890	H	-5.672117	4.462145	3.812662
C	2.975547	-4.241271	4.392064	C	1.149008	2.658979	-3.856196
H	0.886885	-3.629229	4.307501	C	-0.220947	2.312086	-3.675155
H	1.176285	-2.328615	2.162785	C	2.086703	1.619159	-4.090104
C	3.456080	-2.129910	0.722547	C	-0.628058	0.952678	-3.792139
H	5.385688	-3.408747	2.099342	C	0.334685	-0.043191	-4.042626
H	5.103890	-4.682745	4.247597	C	1.699048	0.254003	-4.191907
H	2.848964	-4.803910	5.330375	H	3.136526	1.884039	-4.301186
O	2.509182	-1.619593	0.106496	C	-2.094956	0.546287	-3.693564
H	4.492985	-2.070681	0.296848	H	0.002664	-1.087951	-4.119191
C	0.490073	-8.250819	0.278139	C	-2.327439	-0.620096	-2.717712
C	0.101267	-7.247403	-0.546970	H	-1.886297	-1.566998	-3.092604
C	1.316873	-6.430551	-0.853027	H	-3.413833	-0.796990	-2.588890
O	2.404016	-7.018686	-0.247349	H	-1.892516	-0.400941	-1.723422
C	1.970056	-8.161162	0.495996	C	-2.645441	0.234294	-5.099318
O	1.391189	-5.404630	-1.499674	H	-2.656941	1.419720	-3.308409
C	-1.205450	-6.889811	-1.133477	H	-2.119339	-0.632213	-5.553974
H	-1.997945	-7.610584	-0.848065	H	-2.525120	1.097803	-5.783197
H	-0.141949	-9.037881	0.713866	H	-3.724742	-0.016019	-5.047172
H	2.255718	-8.022424	1.564143	C	2.748466	-0.797162	-4.531201
H	2.506989	-9.066816	0.128905	C	2.361139	-2.220206	-4.110439
Zn	-1.863120	-5.076111	-0.753207	H	3.218505	-2.907599	-4.250511
H	-1.124655	-6.884625	-2.243540	H	1.523488	-2.617436	-4.720704
Br	-3.214303	-3.299085	-0.430548	H	2.055000	-2.260762	-3.045729
				C	3.089588	-0.734168	-6.033351
				H	3.666922	-0.511777	-3.968032
				H	3.900691	-1.448125	-6.280441
				H	3.422914	0.278179	-6.335141
				H	2.202258	-0.995865	-6.648587
				C	1.658831	4.097294	-3.815282
				C	2.790727	4.317658	-2.797739
				H	3.091243	5.384879	-2.791920
				H	3.698600	3.721561	-3.026009
				H	2.452705	4.056408	-1.775399
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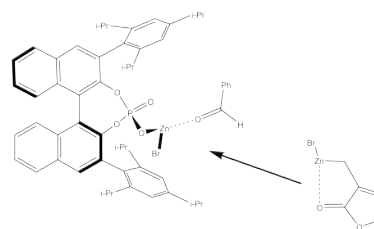
agg-7-j-ma



Energy (Hartree)= -11969.965166

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H	1.236224	4.433428	-5.954384
H	2.928943	3.960408	-5.611543
H	1.539983	-0.973818	5.546243
H	1.570566	4.970807	5.350648
H	-4.511940	0.049766	4.541833
C	2.022090	0.013161	5.366027
H	2.172780	5.653449	2.271944
H	3.936385	-0.931499	4.844762
H	-3.547304	-1.175809	2.496093
C	0.967061	0.906664	4.725981
C	0.768751	5.341812	4.677892
C	3.205067	-0.220761	4.408960
H	3.742462	0.727961	4.197221
C	1.253144	2.236220	4.370789
C	-3.507086	0.466270	4.764220
H	1.645194	0.694000	7.422454
C	-0.315705	0.415234	4.439713
C	2.495137	0.557173	6.725220
H	3.222926	-0.134890	7.198502
H	-0.552792	-0.624696	4.717268
C	1.981003	4.600377	2.563328
H	0.990830	6.403558	4.441467
H	-0.184957	5.306481	5.242150
C	0.314517	3.054630	3.719592
C	-2.541350	-0.814722	2.794833
C	-1.293420	1.187671	3.784316
H	-3.644868	1.460751	5.236437
H	-3.026291	-0.192173	5.518758
C	0.688492	4.498755	3.390456
C	-0.968965	2.524371	3.413810
C	-2.652877	0.555330	3.486333
H	1.908777	3.995421	1.639726
H	-1.908616	-0.735256	1.890170
H	2.865665	4.254360	3.137919
H	2.859135	-0.632448	3.440296
H	-2.111855	-1.584834	3.471261
H	2.996667	1.540401	6.611506
H	-0.129389	4.924789	2.775132
H	-3.182240	1.219841	2.775720
H	2.249190	2.651131	4.596156
C	0.831114	-2.832023	2.531226
C	1.159231	-2.059245	1.413620
C	2.478561	-2.118887	0.897831
C	3.455721	-2.936666	1.513254
C	3.111767	-3.715345	2.622838
C	1.798524	-3.660987	3.128627
H	-0.184210	-2.773050	2.950943
H	0.443672	-1.351110	0.960589
C	2.857457	-1.281777	-0.232961
H	4.482809	-2.952270	1.114577
H	3.863561	-4.356402	3.106076
H	1.531900	-4.263668	4.011084
O	2.031729	-0.651530	-0.920784
H	3.950383	-1.182507	-0.463178
C	1.545201	-17.884743	0.731767
C	1.247261	-16.966935	-0.222617
C	2.543098	-16.343909	-0.609504
O	3.569288	-16.918635	0.054211
C	3.027776	-17.905145	0.952278
O	2.689006	-15.403549	-1.390817
C	0.014896	-16.468490	-0.887530
H	-0.850243	-16.422059	-0.197272
H	0.847742	-18.538650	1.273638
H	3.329258	-17.627912	1.987539
H	3.491403	-18.890589	0.722636
Zn	0.532910	-14.747618	-1.762013
H	-0.275462	-17.153050	-1.715858
Br	0.382450	-12.747724	-2.837591



Energy (Hartree) = -11969.945713

C	1.165102	1.998690	2.307794
C	2.560844	2.002006	2.417187
C	3.219511	3.269754	2.634218
C	4.637968	3.425952	2.590009
C	2.415607	4.446640	2.867713
C	3.060408	5.692362	3.130306
C	0.997018	4.361729	2.766755
H	0.398817	5.275327	2.908969
C	0.357354	3.175092	2.431012
C	3.930642	-1.144432	0.693485
C	4.986884	-1.475670	1.533640
H	5.668438	-2.291886	1.247424
C	5.192466	-0.813178	2.779097
C	6.213242	-1.236000	3.682108
C	4.338713	0.290235	3.151018
C	4.512190	0.874278	4.441291
C	3.331265	0.740706	2.221619
C	3.109857	-0.032389	1.074393
O	0.505809	0.801422	2.107261
O	2.105348	0.332555	0.196794
P	0.516795	0.091306	0.609477
O	-0.212125	1.083076	-0.355090
O	0.031009	-1.317427	0.731008
C	4.442702	5.798452	3.120939
C	5.233753	4.656764	2.827271
H	2.432456	6.576668	3.322903
H	4.926467	6.766989	3.319145
H	5.264332	2.555510	2.353659
H	6.329789	4.747004	2.780488
C	5.500666	0.423891	5.305548
C	6.370672	-0.629904	4.919537
H	3.839494	1.686131	4.752045
H	5.606416	0.884554	6.299680
H	7.156889	-0.973876	5.608779
H	6.865787	-2.070764	3.381061
C	-1.592177	3.700831	0.912924
C	-1.102280	3.098442	2.109541
C	-2.948895	3.536627	0.582095
C	-1.987632	2.364773	2.943075
C	-3.337715	2.236792	2.566993
C	-3.842256	2.807360	1.387991
H	-3.332000	3.995272	-0.345069
C	-1.531320	1.750355	4.264536
H	-4.012700	1.669808	3.225029
C	-1.802886	0.237649	4.333534
H	-2.889331	0.012256	4.291849
H	-1.415349	-0.182185	5.284630
H	-1.302523	-0.288650	3.497833
C	-2.161776	2.498260	5.455152
H	-0.434171	1.891061	4.339899
H	-3.267427	2.395874	5.458604
H	-1.926751	3.581449	5.420061
H	-1.784361	2.095455	6.417925
C	-5.314613	2.718492	0.998298
C	-6.041128	1.492096	1.566278
H	-7.064842	1.418182	1.146346
H	-6.149602	1.558434	2.668951
H	-5.504267	0.550462	1.335393
C	-6.048962	4.018767	1.385675

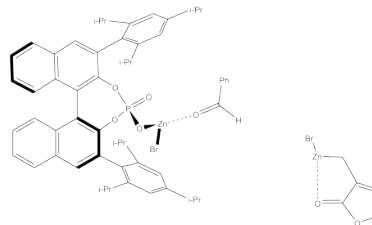
7.7.4 Pathway 12j-mi → 14j-mi

TS-7-j-mi; woelfling data

H	-5.343703	2.642771	-0.113976
H	-7.107875	3.996944	1.053414
H	-5.563981	4.908735	0.937210
H	-6.038609	4.153948	2.487498
C	-0.711475	4.556997	-0.001125
C	-0.707017	4.106405	-1.472655
H	-0.170916	4.834782	-2.113663
H	-1.724190	3.977330	-1.895513
H	-0.135350	3.157694	-1.568457
C	-1.109676	6.041912	0.114042
H	0.333173	4.468673	0.355604
H	-0.428977	6.682440	-0.484150
H	-1.067402	6.386418	1.167021
H	-2.144757	6.213677	-0.248410
H	1.766851	-4.810127	-3.915360
H	5.491201	-0.331577	-3.703607
H	3.800103	-5.941548	1.573077
C	1.881259	-3.724202	-4.130881
H	3.880131	2.224205	-2.630918
H	-0.026545	-3.594202	-5.223865
H	1.673912	-4.676816	2.345317
C	2.536713	-3.099876	-2.905094
C	5.629826	0.041440	-2.667139
C	0.470159	-3.137713	-4.341132
H	0.512564	-2.040616	-4.506154
C	3.085218	-1.805473	-2.947061
C	3.708435	-5.420634	0.597512
H	3.759327	-4.004730	-5.239313
C	2.574722	-3.787917	-1.682524
C	2.742254	-3.592127	-5.398186
H	2.279619	-4.133071	-6.249272
H	2.165804	-4.810715	-1.642381
C	3.382098	1.232443	-2.626954
H	6.154957	1.017770	-2.725454
H	6.291842	-0.675467	-2.140231
C	3.613356	-1.184242	-1.804707
C	1.648497	-4.140083	1.373425
C	3.090746	-3.213836	-0.504214
H	4.720501	-5.347701	0.148764
H	3.097164	-6.071704	-0.061910
C	4.276338	0.186265	-1.943849
C	3.579626	-1.878081	-0.560579
C	3.067177	-4.033851	0.786199
H	2.416564	1.332973	-2.096054
H	1.199265	-3.139634	1.524442
H	3.156790	0.970823	-3.680860
H	-0.170664	-3.311326	-3.451519
H	0.971834	-4.697639	0.691729
H	2.854280	-2.532472	-5.708019
H	4.499746	0.561248	-0.924422
H	3.680930	-3.496589	1.535044
C	3.094178	-1.253376	-3.899386
C	-6.168756	-5.434073	-5.992406
C	-5.067598	-5.018330	-5.320225
C	-4.965769	-3.541272	-5.514635
O	-5.949464	-3.141015	-6.385705
C	-6.764767	-4.269852	-6.723143
O	-4.190196	-2.770406	-4.980570
C	-4.054697	-5.736986	-4.524177
H	-4.344232	-6.788410	-4.329615
H	-6.567150	-6.457137	-6.045475
H	-6.754191	-4.421463	-7.827698
H	-7.817219	-4.046463	-6.434808
Zn	-3.471892	-4.910377	-2.842820
H	-3.090957	-5.748542	-5.083834
Br	-2.512311	-4.855376	-0.789330
Zn	-0.839439	1.166606	-2.128579
Br	-0.129946	0.958560	-4.287883
C	-3.225491	-1.650510	0.758598
C	-3.069660	-0.577717	-0.118978
C	-4.051851	-0.316838	-1.105212

C	-5.205566	-1.137348	-1.190794
C	-5.357435	-2.209840	-0.307900
C	-4.369628	-2.463581	0.664547
H	-2.428134	-1.859964	1.485957
H	-2.194885	0.079583	-0.031319
C	-3.901128	0.795194	-2.028307
H	-5.964347	-0.932383	-1.962782
H	-6.240664	-2.862779	-0.375463
H	-4.485772	-3.319316	1.346050
O	-2.870358	1.472268	-2.209799
H	-4.807866	1.072637	-2.624833

agg-7-j-mi



Energy (Hartree) = -11969.950117

C	1.966380	2.711877	3.038038
C	3.367194	2.711877	3.038038
C	4.042711	3.989968	3.038038
C	5.456537	4.124074	2.888315
C	3.256735	5.197585	3.155635
C	3.919886	6.460330	3.205501
C	1.834347	5.118259	3.136982
H	1.250526	6.051826	3.160009
C	1.172047	3.903831	3.013559
C	4.469705	-0.671383	1.598402
C	5.567669	-0.975123	2.392205
H	6.158761	-1.878319	2.176400
C	5.926762	-0.168751	3.512271
C	7.002982	-0.540704	4.371596
C	5.175820	1.030170	3.806078
C	5.503721	1.760379	4.987135
C	4.102679	1.419418	2.922557
C	3.752749	0.531026	1.896878
O	1.291586	1.505397	3.079729
O	2.674469	0.831398	1.081390
P	1.155407	0.586766	1.711553
O	0.253968	1.376586	0.716086
O	0.781434	-0.813754	2.081832
C	5.299689	6.549951	3.101071
C	6.068651	5.370292	2.920658
H	3.307220	7.370046	3.309812
H	5.796744	7.531292	3.135182
H	6.066247	3.223519	2.736777
H	7.160368	5.441962	2.799842
C	6.546099	1.361270	5.812163
C	7.314033	0.209614	5.496648
H	4.909806	2.648692	5.244888
H	6.774659	1.938967	6.720588
H	8.143064	-0.095022	6.153172
H	7.575662	-1.449335	4.130881
C	-0.767303	4.194563	1.432107
C	-0.288905	3.784435	2.711186
C	-2.101384	3.910504	1.087860
C	-1.169123	3.135778	3.618610
C	-2.495574	2.883621	3.225190
C	-2.979201	3.241099	1.956045
H	-2.473499	4.203085	0.092773
C	-0.724867	2.736616	5.024511

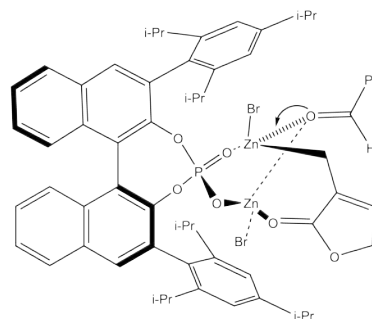
H	-3.166938	2.378235	3.936456
C	-1.017827	1.261162	5.343188
H	-2.108208	1.057579	5.389184
H	-0.593421	0.988777	6.331509
H	-0.571051	0.591682	4.582599
C	-1.350697	3.679335	6.070247
H	0.373267	2.874836	5.079502
H	-2.458079	3.599802	6.071072
H	-1.090438	4.737416	5.865765
H	-0.994060	3.427477	7.090613
C	-4.415035	2.961979	1.531251
C	-4.909888	1.568802	1.950498
H	-5.901119	1.350202	1.502499
H	-5.028590	1.491915	3.051520
H	-4.203250	0.770157	1.644176
C	-5.361899	4.064167	2.045463
H	-4.426784	3.005125	0.418276
H	-6.401389	3.897005	1.695500
H	-5.036555	5.065402	1.699891
H	-5.373268	4.081825	3.155354
C	0.102611	4.914163	0.398470
C	0.251134	4.129291	-0.919040
H	0.785517	4.719714	-1.690527
H	-0.734841	3.858044	-1.359115
H	0.865257	3.219549	-0.749703
C	-0.421021	6.339557	0.140466
H	1.123332	5.011158	0.816036
H	0.250156	6.888432	-0.551808
H	-0.487371	6.915635	1.084971
H	-1.434313	6.326936	-0.311318
H	1.973327	-4.718734	-2.536816
H	5.717091	-0.546726	-3.020702
H	4.343665	-4.950570	3.251557
C	1.814305	-3.627503	-2.691811
H	4.473821	-2.242550	-2.088355
H	-0.306705	-3.894358	-3.216933
H	1.925556	-4.236426	3.626573
C	2.634199	-2.911284	-1.622143
C	6.004710	-0.091861	-2.049683
C	0.312857	-3.343278	-2.479592
H	0.103089	-2.259327	-2.593883
C	3.324732	-1.713925	-1.871198
C	4.304325	-4.525053	2.226617
H	3.313077	-3.453593	-4.295195
C	2.663034	-3.421472	-0.310979
C	2.228276	-3.292893	-4.129948
H	1.674216	-3.928092	-4.850101
H	2.146748	-4.373620	-0.107167
C	3.890469	1.315264	-1.909486
H	6.603482	0.816377	-2.267028
H	6.656802	-0.816742	-1.519907
C	3.989023	-1.009992	-0.850116
C	1.884112	-3.837568	2.592104
C	3.296756	-2.751732	0.749553
H	5.323905	-4.185596	1.955367
H	4.035689	-5.346592	1.528001
C	4.761418	0.258696	-1.209248
C	3.953367	-1.517083	0.477331
C	3.280720	-3.376264	2.145291
H	3.011655	1.573880	-1.288053
H	1.184914	-2.980306	2.575789
H	3.512821	0.963165	-2.890296
H	-0.016972	-3.640088	-1.463938
H	1.483363	-4.648607	1.947542
H	1.995858	-2.236955	-4.382290
H	5.129365	0.709148	-0.264927
H	3.597098	-2.593690	2.863046
H	3.338638	-1.299042	-2.888533
C	-12.399466	-8.347426	-12.583011
C	-11.468330	-7.928557	-11.688667
C	-11.054878	-6.568989	-12.134113

O	-11.762631	-6.184745	-13.217817
C	-12.636541	-7.265466	-13.592614
O	-10.163879	-5.882015	-11.632602
C	-10.803614	-8.492085	-10.483088
H	-11.455717	-8.356567	-9.590196
H	-12.927990	-9.310958	-12.598188
H	-12.384794	-7.563337	-14.635058
H	-13.684442	-6.892119	-13.596106
Zn	-9.200205	-7.342330	-10.164088
H	-10.613704	-9.580037	-10.573808
Br	-7.225312	-6.587707	-9.324407
Zn	-0.347077	1.261836	-1.056273
Br	0.217451	0.800853	-3.221982
C	-1.619521	-2.637496	0.701355
C	-1.841005	-1.322770	0.287674
C	-2.987912	-1.003627	-0.479857
C	-3.925435	-2.017415	-0.800357
C	-3.691008	-3.335427	-0.395768
C	-2.538115	-3.644289	0.350281
H	-0.722808	-2.857076	1.299208
H	-1.137935	-0.545957	0.617958
C	-3.232006	0.352149	-0.958164
H	-4.824766	-1.763603	-1.383952
H	-4.407676	-4.127762	-0.658738
H	-2.358986	-4.682546	0.670392
O	-2.409287	1.284748	-0.991308
H	-4.266191	0.565201	-1.333503

7.8 Interconversion of Complexes 14 - Mechanism 1

7.8.1 Pathway 14j-ma ↔ 14d-ma

jma-dma-TS1-mech1; COSMO

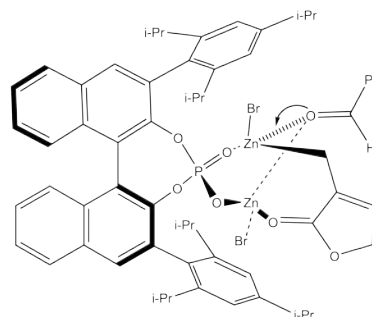


Energy (Hartree) = -11970.02355299

Zn	2.7431148	1.0438682	0.8458810
Br	4.9511147	0.7006529	0.2591669
H	1.9313901	6.1220841	1.1186878
Br	-2.3822538	4.3629694	-0.4271883
H	-1.6128396	3.1750805	3.0614624
Zn	-1.3065197	2.5499229	0.6268935
C	0.3691691	5.1680936	2.3151355
C	1.7701523	5.6367945	2.1086581
C	0.3558020	3.8041408	2.4516012
C	-0.7126649	2.8077668	2.5331769
C	1.7681005	3.3838790	2.3487881
O	2.5799443	4.4429374	2.1452611
O	2.2242733	2.2319514	2.4179671
H	2.1512427	6.3301746	2.8915237
H	-0.3606170	1.8561612	2.9707554
H	-0.5046579	5.8322796	2.2904203
C	0.5884218	6.0847711	-2.3572570
C	0.9842849	4.8985589	-1.7358497

C	2.3617614	4.6108030	-1.5848613	H	1.2199445	2.1069481	8.3391561
C	3.3368013	5.5188106	-2.0634201	H	1.5752755	0.4353155	7.7853381
C	2.9335387	6.7054388	-2.6853008	H	-0.1182397	0.9411415	8.0637445
C	1.5613960	6.9850524	-2.8332022	C	2.1991454	-2.3875771	3.7113408
H	-0.4855391	6.3008106	-2.4623100	C	3.3910230	-1.7018054	3.0310272
H	0.2274758	4.1930189	-1.3622113	H	4.2042601	-2.4301409	2.8350573
C	2.7908344	3.3777431	-0.9385917	H	3.8273121	-0.8845220	3.6406498
H	4.4059336	5.2806509	-1.9455135	H	3.0945279	-1.2799574	2.0526453
H	3.6849565	7.4157833	-3.0611187	C	2.6458339	-3.1690873	4.9632009
H	1.2472575	7.9179795	-3.3268330	H	1.8035320	-3.1254295	2.9861737
O	1.9968750	2.5684102	-0.4234146	H	3.4172553	-3.9231505	4.7027414
C	-0.9590500	-2.4737456	1.3925351	H	1.7951643	-3.6967481	5.4409450
C	-1.1420575	-3.4453884	0.4023820	H	3.0812021	-2.4890847	5.7252094
C	-0.8665520	-4.8215817	0.7492439	H	0.9974027	3.3300664	-6.0462079
C	-0.8325346	-5.8736524	-0.2150966	H	2.9735656	-2.1893638	-5.4441789
C	-0.5787318	-5.1528521	2.1243367	H	-4.5035285	0.6593225	-4.9750425
C	-0.3452802	-6.5144796	2.4823311	C	1.7417639	2.5282531	-5.8440266
C	-0.4770852	-4.1129479	3.0910204	H	3.5131302	-2.5684012	-2.3188512
H	-0.2357145	-4.3766022	4.1323165	H	3.3315232	3.9993482	-5.4739663
C	-0.6016039	-2.7731119	2.7447884	H	-3.8877288	2.2154042	-2.9905882
C	-1.1488219	-1.7536362	-3.0574168	C	0.9984738	1.4124233	-5.1204056
C	-2.1500919	-2.4781681	-3.6954979	C	2.2836840	-2.7940377	-4.8190410
H	-2.3482039	-2.2904827	-4.7612353	C	2.8485203	3.1386137	-4.9660138
C	-2.9640761	-3.4183863	-3.0031880	H	3.6425011	2.3961632	-4.7400776
C	-4.0540496	-4.0715620	-3.6532473	C	1.6658633	0.2620402	-4.6680098
C	-2.7072725	-3.6928918	-1.6104144	C	-3.4258889	0.5132245	-5.1950440
C	-3.6022641	-4.5624844	-0.9175694	H	1.4848834	1.6569844	-7.8458283
C	-1.5778280	-3.0606256	-0.9710784	C	-0.3783446	1.5016037	-4.8773364
C	-0.8890492	-2.0741793	-1.6884115	C	2.2936517	2.0545605	-7.2005674
O	-1.1827886	-1.1359829	1.0764936	H	2.7911215	2.8861312	-7.7418264
O	0.1677667	-1.4078598	-1.0801493	H	-0.9152449	2.4020642	-5.2158544
P	-0.1139317	-0.3292398	0.1191534	C	2.9901925	-1.6500022	-2.6563848
O	1.2493722	-0.1920882	0.8047467	H	2.8238076	-3.7157816	-4.5184107
O	-0.8661660	0.9087697	-0.3803815	H	1.4265141	-3.0899061	-5.4572584
C	-0.3526522	-7.5158935	1.5240693	C	1.0049541	-0.7781322	-3.9920166
C	-0.5810569	-7.1854848	0.1622063	C	-2.8397628	2.1230980	-3.3357247
H	-0.1383981	-6.7503597	3.5381309	C	-1.0924024	0.4983266	-4.1949399
H	-0.1630678	-8.5609934	1.8125491	H	-3.2980239	-0.5039878	-5.6160553
H	-0.9975777	-5.6343371	-1.2742864	H	-3.1412636	1.2365770	-5.9879763
H	-0.5525832	-7.9751224	-0.6040361	C	1.8121844	-2.0087106	-3.5805586
C	-4.6660076	-5.1655749	-1.5737251	C	-0.3955608	-0.6642159	-3.7565578
C	-4.8872275	-4.9335656	-2.9572477	C	-2.5782984	0.7298469	-3.9272846
H	-3.4479134	-4.7444370	0.1549543	H	2.6453473	-1.1079391	-1.7544878
H	-5.3470976	-5.8245213	-1.0138650	H	-2.1964738	2.3087496	-2.4548449
H	-5.7293061	-5.4241012	-3.4686921	H	3.7404651	-1.0161353	-3.1737382
H	-4.2309999	-3.8604394	-4.7196141	H	2.4395722	3.4975359	-4.0005007
C	1.0633353	-1.4297701	4.0748899	H	-2.6590740	2.9316765	-4.0746413
C	-0.2909331	-1.6616249	3.6954912	H	3.0425923	1.2459531	-7.0675904
C	1.3518647	-0.3037087	4.8648688	H	1.1425469	-2.6838963	-3.0118122
C	-1.3196697	-0.8054994	4.1694191	H	-2.9040160	-0.0090619	-3.1671131
C	-0.9763876	0.2899517	4.9851088	H	2.7434332	0.1667040	-4.8652376
C	0.3566637	0.5759271	5.3248712	H	3.8902376	3.1607440	-0.8998290
H	2.4000428	-0.1003682	5.1405340				
C	-2.7921413	-1.0846569	3.8701827				
H	-1.7808682	0.9434562	5.3553436				
C	-3.4955775	0.0863370	3.1661399				
H	-3.5110044	1.0024744	3.7914031				
H	-4.5465609	-0.1686174	2.9222475				
H	-2.9859336	0.3331866	2.2142055				
C	-3.5353042	-1.4965326	5.1554260				
H	-2.8339088	-1.9535301	3.1815053				
H	-3.5453694	-0.6712422	5.8977378				
H	-3.0518949	-2.3715817	5.6351520				
H	-4.5896811	-1.7623027	4.9338780				
C	0.7510967	1.7471851	6.2187572				
C	-0.1721380	2.9676030	6.1041189				
H	0.2316245	3.8148176	6.6950956				
H	-1.1873644	2.7541515	6.4991922				
H	-0.2868529	3.3007949	5.0540889				
C	0.8677122	1.2825952	7.6844288				
H	1.7652671	2.0628137	5.8854052				

jma-dma-TS1-mech1

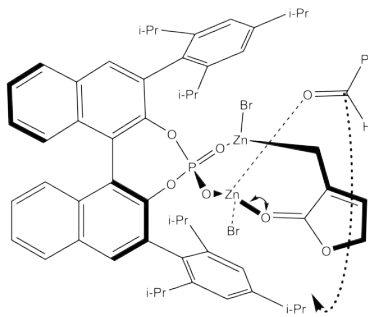


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number of imaginary frequencies: 2

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Br	4.1562258	1.7501215	1.3481566

H	-0.6650778	5.4823545	2.6606033	C	-3.7135800	-2.0095644	2.0761034
Br	-3.7586459	3.0081042	-0.1847429	H	-4.1180248	-1.4001166	2.9106532
H	-3.1855421	1.1861757	3.0795231	H	-4.5776117	-2.4147233	1.5106726
Zn	-2.3024244	1.3783856	0.7014908	H	-3.1508211	-1.3348936	1.4006576
C	-1.9409005	3.8096789	3.2579611	C	-3.5948070	-4.1433418	3.4606200
C	-0.7759218	4.7186457	3.4643890	H	-2.4651843	-3.7115730	1.6922275
C	-1.4963366	2.5239763	3.0899181	H	-3.9892899	-3.6525670	4.3749888
C	-2.1450494	1.2680556	2.7125662	H	-2.9494102	-4.9845156	3.7849669
C	-0.0262090	2.5980153	3.2029751	H	-4.4586847	-4.5650377	2.9061632
O	0.3867599	3.8646349	3.4156350	C	-0.8219308	-0.4242409	6.4091862
O	0.7854428	1.6638705	3.1101451	C	-2.1010434	0.4233549	6.4236232
H	-0.7657008	5.2515885	4.4414618	H	-2.1013374	1.1075387	7.2963530
H	-1.5496536	0.3869099	3.0142582	H	-3.0107382	-0.2073469	6.5086292
H	-2.9795212	4.1586768	3.1894141	H	-2.1981264	1.0341937	5.5045545
C	-1.3601446	6.0562823	-0.9951327	C	-0.7225378	-1.2923636	7.6797578
C	-0.6839808	4.9181886	-0.5504758	H	0.0437540	0.2758939	6.4138662
C	0.6756798	5.0142816	-0.1696380	H	-0.7715798	-0.6682538	8.5963946
C	1.3505766	6.2568382	-0.2404259	H	0.2244439	-1.8680145	7.7039968
C	0.6675168	7.3928499	-0.6880028	H	-1.5579966	-2.0225844	7.7170898
C	-0.6848998	7.2903460	-1.0663687	C	2.3060984	-2.8669542	3.2958251
H	-2.4185613	5.9710833	-1.2842946	C	3.2118131	-1.6487375	3.0595851
H	-1.2080097	3.9521579	-0.4957289	H	4.2594758	-1.9645984	2.8795362
C	1.3990456	3.8360989	0.2887329	H	3.2232461	-0.9472977	3.9187819
H	2.4108603	6.3169492	0.0525510	H	2.8873492	-1.0922897	2.1608844
H	1.1854697	8.3616137	-0.7484778	C	2.8878212	-3.7936539	4.3815278
H	-1.2186827	8.1853267	-1.4225126	C	2.2942634	-3.4391360	2.3474593
O	0.8649418	2.1797192	0.4306299	H	3.9070699	-4.1337418	4.1043558
C	-0.2895989	-3.2977321	0.3887669	H	2.2545824	-4.6916077	4.5328907
C	0.0217410	-3.9708299	-0.7978108	H	2.9602622	-3.2727211	5.3592435
C	0.7231898	-5.2308075	-0.6927478	H	0.4367379	4.6152877	-5.0463566
C	1.2634836	-5.9159173	-1.8227105	H	4.1849908	0.0966810	-5.1312666
C	0.9190097	-5.8158254	0.6121298	H	-3.7887519	0.1675110	-5.8438624
C	1.5706636	-7.0809200	0.7212548	C	1.3837366	4.0712039	-4.8342336
C	0.5122029	-5.0979686	1.7721685	H	4.3713168	-0.9696607	-2.1266334
H	0.6905558	-5.5434954	2.7630472	H	2.2590404	5.8344574	-3.8592999
C	-0.0311230	-3.8211069	1.6936675	H	-4.1043528	1.1156587	-3.4454570
C	-0.1086370	-1.4949896	-3.7414659	C	1.0008007	2.6313813	-4.5139807
C	-0.6676828	-2.2962934	-4.7307357	C	3.6824590	-0.8477818	-4.8349726
H	-0.7621858	-1.8976225	-5.7518814	C	2.0547994	4.7661307	-3.6378880
C	-1.1748137	-3.5967610	-4.4526067	C	3.0230652	4.2872258	-3.3806971
C	-1.8437685	-4.3583838	-5.4574075	H	1.9736334	1.6750265	-4.1738348
C	-1.0442697	-4.1427878	-3.1233771	C	-2.7178752	0.4576429	-5.8163544
C	-1.6555225	-5.4031995	-2.8495492	H	1.7552245	3.6907780	-6.9682330
C	-0.3291969	-3.3851750	-2.1230924	C	-0.3361719	2.2106744	-4.5702497
C	0.0453780	-2.0744394	-2.4443083	C	2.2607704	4.1526808	-6.0965683
O	-0.9417677	-2.0699204	0.3212689	H	2.4951953	5.2073135	-6.3511902
O	0.6775678	-1.2902636	-1.4887636	H	-1.1121997	2.9532092	-4.8171596
P	-0.1255960	-0.7351818	-0.1745980	C	3.5996340	-0.2107959	-2.3699953
O	0.9894497	-0.3638679	0.8065268	H	4.4737967	-1.5969676	-4.6248047
O	-1.2049977	0.2930949	-0.5383848	H	3.0952231	-1.2018857	-5.7065314
C	2.0527104	-7.7350058	-0.4017049	C	1.6487445	0.3326549	-3.9127519
C	1.9120385	-7.1347540	-1.6807245	C	-3.0620551	1.4869436	-3.5237110
H	1.7010235	-7.5181319	1.7237105	C	-0.7214958	0.8809198	-4.3128938
H	2.5605893	-8.7063956	-0.3026269	H	-2.1497864	-0.2743799	-6.4246942
H	1.1727907	-5.4613145	-2.8184022	H	-2.6229403	1.4449336	-6.3155542
H	2.3262563	-7.6361479	-2.5687213	C	2.7830112	-0.6430048	-3.6010540
C	-2.3181863	-6.1092303	-3.8438319	C	0.2860949	-0.0741980	-3.9965149
C	-2.4004293	-5.5936604	-5.1645355	C	-2.2076804	0.5264999	-4.3644638
H	-1.6060065	-5.8113014	-1.8305535	H	2.9556332	-0.0909840	-1.4780936
H	-2.7885872	-7.0749430	-3.6036360	H	-2.6652593	1.5861546	-2.4963243
H	-2.9209522	-6.1667643	-5.9468333	H	4.1271008	0.7510028	-2.5378133
H	-1.9253475	-3.9326919	-6.4699412	H	1.4085946	4.7222117	-2.7403822
C	0.8632798	-2.4900943	3.6375370	H	-3.1120841	2.5043753	-3.9643089
C	-0.2602949	-2.9765992	2.9068182	H	3.2244021	3.6217040	-5.9492163
C	0.6324558	-1.6480225	4.7388067	H	2.3332573	-1.6289415	-3.3685031
C	-1.5759836	-2.6304903	3.3156491	H	-2.3257453	-0.4812719	-3.9179399
C	-1.7478715	-1.8103015	4.4469078	H	3.0310431	1.9805144	-4.1204368
C	-0.6580428	-1.2932986	5.1665355	H	2.4882173	3.9511539	0.5291309
H	1.4974636	-1.2470386	5.2926105				
C	-2.8119752	-3.1489431	2.5825343				
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7.8.2 Pathway 14j-ma ↔ 14j-mi jma-jmi-TS1-mech1; COSMO



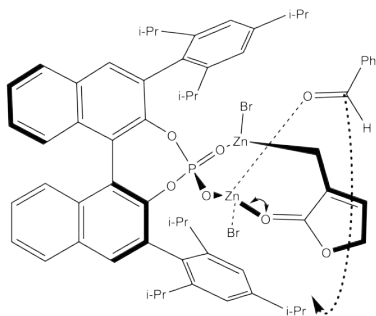
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Zn	-1.9353640	1.7909425	1.3906132
Br	-3.0602313	2.7479010	-0.4437508
C	-1.7869728	-1.1117111	-2.0559217
C	-1.6362576	-0.3510432	-3.2219694
C	-1.8763790	-1.0120592	-4.4860207
C	-1.5894554	-0.4039559	-5.7460556
C	-2.3927722	-2.3605887	-4.4881514
C	-2.6759553	-3.0005728	-5.7324879
C	-2.5534463	-3.0555430	-3.2554756
H	-2.9196077	-4.0932974	-3.2741668
C	-2.2013835	-2.4802511	-2.0415958
C	0.6053659	2.6575462	-2.3952282
C	0.0095155	3.6628518	-3.1454698
H	0.4667959	4.6628784	-3.1759149
C	-1.2190969	3.4520902	-3.8370515
C	-1.8736189	4.5264133	-4.5107778
C	-1.8418108	2.1500785	-3.8198226
C	-3.1276610	2.0065828	-4.4191799
C	-1.1635191	1.0617286	-3.1600305
C	-0.0097675	1.3684336	-2.4361284
O	-1.5715260	-0.5255813	-0.8084153
O	0.6253412	0.3537587	-1.7252226
P	-0.0628419	-0.1399696	-0.3199497
O	0.7427943	-1.4098501	0.0280025
O	-0.1868587	0.9567689	0.7351795
C	-2.4227123	-2.3633581	-6.9377420
C	-1.8559711	-1.0611049	-6.9397097
H	-3.0835194	-4.0237106	-5.7143945
H	-2.6398891	-2.8706177	-7.8901749
H	-1.1415994	0.5985412	-5.7680899
H	-1.6196165	-0.5685972	-7.8953766
C	-3.7486415	3.0776753	-5.0467755
C	-3.1114909	4.3456262	-5.1096441
H	-3.6366524	1.0343724	-4.3634716
H	-4.7467688	2.9446857	-5.4914354
H	-3.6100341	5.1862948	-5.6160226
H	-1.3836230	5.5127806	-4.5259126
C	-1.1250928	-4.1841364	-0.5257731
C	-2.1672003	-3.2419820	-0.7539927
C	-1.0587446	-4.8188341	0.7291927
C	-3.1172910	-2.9660804	0.2656724
C	-3.0060513	-3.6305732	1.4977440
C	-1.9750462	-4.5495678	1.7584913
H	-0.2498770	-5.5419978	0.9234729
C	-4.2563411	-1.9745675	0.0446644
H	-3.7352744	-3.4017296	2.2905021
C	-4.3508775	-0.9384860	1.1751044
H	-4.7335132	-1.3842074	2.1173017
H	-5.0272118	-0.1061436	0.8936809
H	-3.3502912	-0.5203978	1.3960611
C	-5.5914761	-2.7101653	-0.1717819
H	-4.0399780	-1.4145086	-0.8873221
H	-5.8651540	-3.3090016	0.7225395

H	-5.5332133	-3.4036280	-1.0355662
H	-6.4136777	-1.9894593	-0.3633225
C	-1.8333225	-5.2112355	3.1232600
C	-1.5839863	-4.1704268	4.2301348
H	-1.3961658	-4.6687893	5.2043793
H	-2.4628601	-3.5045068	4.3571149
H	-0.7244354	-3.5148125	3.9901454
C	-3.0410917	-6.1062824	3.4541221
H	-0.9358682	-5.8670463	3.0697513
H	-2.8995401	-6.6200006	4.4278752
H	-3.1966363	-6.8802298	2.6752646
H	-3.9742871	-5.5086991	3.5248640
C	-0.0960686	-4.5372825	-1.6010665
C	1.3489789	-4.5949763	-1.0815057
H	2.0570386	-4.7666045	-1.9175053
H	1.5052566	-5.4102618	-0.3455347
H	1.6372316	-3.6411816	-0.6005837
C	-0.4680258	-5.8650238	-2.2907862
H	-0.1289846	-3.7381069	-2.3695425
H	0.2467205	-6.1033291	-3.1058364
H	-1.4858801	-5.8282999	-2.7272904
H	-0.4490215	-6.7038002	-1.5634367
H	4.6424154	3.3752941	2.3287353
H	5.2174955	2.1137164	-3.4644486
H	-0.3601406	6.4542897	-0.2429949
C	5.0206916	2.8178101	1.4430835
H	3.6814145	-0.6744341	-3.7924665
H	6.0407738	1.3666227	2.7381518
H	-1.0414872	4.7187410	1.5985400
C	3.9159942	2.8562104	0.3949338
C	4.2203152	2.0644627	-3.9503560
C	5.3206847	1.3773865	1.8939669
H	5.7557893	0.7708937	1.0733832
C	4.0199855	2.1237449	-0.8013908
C	0.5801241	5.8913141	-0.4181407
H	6.0872231	4.5776936	0.6649029
C	2.7513682	3.6140758	0.5983549
C	6.2955718	3.5272750	0.9521673
H	7.0765680	3.5325858	1.7408348
H	2.6693859	4.2075788	1.5223145
C	3.6120232	-0.1348107	-2.8255162
H	4.3424178	1.5406659	-4.9211769
H	3.8958261	3.1043818	-4.1581755
C	2.9890427	2.1037280	-1.7564695
C	-0.0054377	4.3413382	1.4800937
C	1.6775650	3.6122927	-0.3132246
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jma-jmi-TS1-mech1



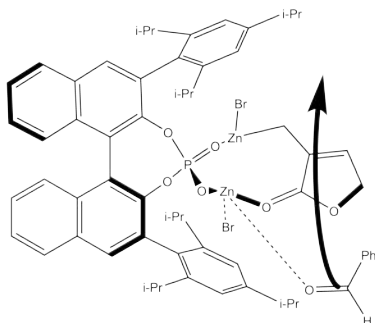
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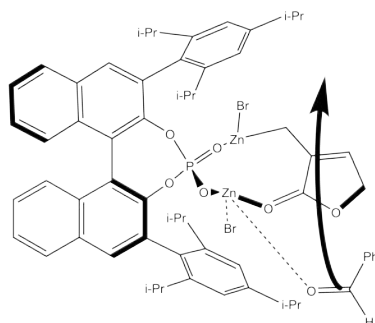
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H	-3.7875620	-4.9925337	-4.2803754
H	-3.1851243	-4.7821083	-6.6989638
H	-1.2495270	-0.9862670	-5.9046380
H	-1.8658743	-2.7873386	-7.4855463
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C	-2.9433488	2.8611724	-6.7878563
H	-3.7329496	0.1002474	-4.9061344
H	-4.6546128	1.5014261	-6.7278738
H	-3.3573817	3.4724368	-7.6041703
H	-1.1669531	4.0777585	-6.5602250
C	-1.7377508	-3.6176870	0.5573023
C	-2.6437599	-2.6221561	0.0916958
C	-1.5811874	-3.7837101	1.9457155
C	-3.3783152	-1.8349028	1.0222842
C	-3.1586765	-2.0261032	2.3963671
C	-2.2494066	-2.9822550	2.8829235
H	-0.8785786	-4.5497216	2.3123022
C	-4.4318147	-0.8265913	0.5689627
H	-3.7125827	-1.3975039	3.1109686
C	-4.2502705	0.5619915	1.2028448
H	-4.3965681	0.5433985	2.3025034
H	-4.9918242	1.2762480	0.7901624
H	-3.2426133	0.9763080	1.0099294
C	-5.8438097	-1.3877541	0.8289570
H	-4.3310390	-0.7061547	-0.5290961
H	-6.0202200	-1.5376786	1.9149089
H	-5.9886388	-2.3666944	0.3281264
H	-6.6205241	-0.6893757	0.4538604
C	-1.9860924	-3.1393295	4.3752148
C	-1.6134558	-1.8023024	5.0386039
H	-1.2864930	-1.9594551	6.0874589
H	-2.4769688	-1.1055883	5.0611860
H	-0.7967131	-1.2894555	4.4938934
C	-3.1702277	-3.8163298	5.0892462
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C	-0.8944989	-4.4827106	-0.3814375
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H	1.1910087	-4.8639459	-0.9170806
H	0.9254922	-4.7235170	0.8437658
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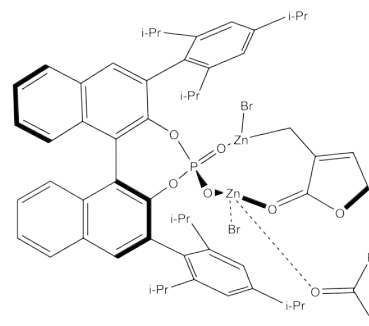
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H	-0.7369339	-6.5744371	-1.0275474
H	-2.3968554	-6.0839511	-0.5487684
H	-1.1566036	-6.3807256	0.7037344
H	4.3283417	5.0411100	0.6671858
H	5.1768496	1.2557267	-3.8024730
H	-0.4341456	6.6842091	-2.8117817
C	4.7931742	4.2540534	0.0310422
H	3.6632380	-1.4136174	-2.8675780
H	6.2121567	3.7135562	1.6053622
H	-1.3690236	5.7273129	-0.7067270
C	3.6769325	3.6714099	-0.8279334
C	4.2094434	0.9585153	-4.2588299
C	5.4479771	3.2254472	0.9659214
H	5.9615974	2.4233773	0.3969600
C	3.8421884	2.4741738	-1.5436524
C	0.4897679	6.0929324	-2.6439512
H	5.3827238	5.7138411	-1.5106317
C	2.4637320	4.3603418	-0.9868562
C	5.8449100	4.9436783	-0.8605986
H	6.6299878	5.4324949	-0.2467726
H	2.3223018	5.3050700	-0.4354009
C	3.5415305	-0.4859833	-2.2711405
H	4.3906712	0.0495318	-4.8693392
H	3.8961198	1.7748347	-4.9409554
C	2.8448663	1.9626914	-2.3923265
C	-0.5447937	4.9924131	-0.6027013
C	1.4295643	3.8987976	-1.8229043
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H	1.1810994	6.7131360	-2.0360535
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C	1.6223114	2.6782664	-2.5360863
C	0.1673576	4.7573650	-1.9458572
H	2.7734130	-0.6718301	-1.4968369
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H	4.5009722	-0.2984207	-1.7470545
H	4.7047882	2.7321174	1.6217246
H	0.1366333	5.3861808	0.1809416
H	6.3428283	4.2035652	-1.5215944
H	2.2164796	0.3943219	-3.7152968
H	-0.5545961	4.2169783	-2.5878099
H	4.7842001	1.9141975	-1.4420373
C	2.2417093	-1.7788024	6.7518508
C	2.0081423	-1.9519510	5.3862604
C	1.9113929	-3.2562708	4.8489532
C	2.0640367	-4.3820852	5.6923911
C	2.3015446	-4.2035153	7.0596457
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H	2.2989913	-0.7621758	7.1679886
H	1.8802065	-1.0924357	4.7180168
C	1.6227122	-3.4691386	3.4315658
H	1.9869595	-5.3953950	5.2659851
H	2.4173998	-5.0758452	7.7199257
H	2.5687179	-2.7626277	8.6649201
O	1.4051389	-2.5954997	2.5864137
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C	1.6460670	3.4276341	4.7729783
C	1.6083514	2.6744637	3.6304041
C	1.0629287	1.3667743	4.0514237
O	0.8312091	1.3305905	5.3742627
C	1.1174184	2.6359118	5.9193573
O	0.7899524	0.3684967	3.3593172
C	1.8137757	2.9788697	2.2152321
H	1.8272642	2.5068553	6.7664405
H	0.1618058	3.0377241	6.3261655
H	2.3761771	2.1868226	1.6803995
H	2.2965084	3.9580945	2.0468948
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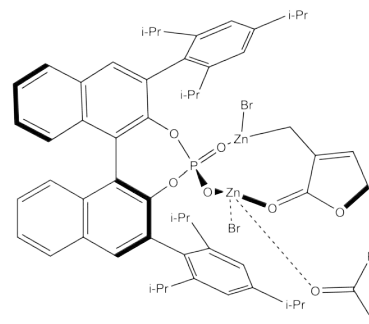
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Br	0.1126555	-1.9718211	4.1285971
Zn	-3.0360270	-0.6753512	0.7551751
Br	-4.2158548	0.8367198	-0.5739145
C	0.1961458	1.1859418	-2.0938532
C	-0.0514191	2.5632718	-2.1278187
C	0.6048186	3.3429111	-3.1505597
C	0.5605832	4.7700247	-3.1829715
C	1.3671028	2.6629220	-4.1705936
C	1.9913559	3.4260306	-5.2031123
C	1.5121267	1.2478152	-4.1117417
H	2.0889871	0.7386897	-4.8990090
C	0.9788603	0.4983924	-3.0696360
C	-1.3785797	3.6577677	1.3052013
C	-2.3968106	4.5285940	0.9363849
H	-2.9411717	5.0808976	1.7168299
C	-2.7893815	4.6980452	-0.4224699
C	-3.9063636	5.5155449	-0.7696325
C	-2.0706643	4.0091950	-1.4666811
C	-2.5447473	4.1257843	-2.8068580
C	-0.9332506	3.1985339	-1.1090399
C	-0.6726195	3.0053038	0.2488789
O	-0.3919207	0.4015870	-1.1124145
O	0.3618128	2.1362254	0.6143511
P	0.0034858	0.5455234	0.4788387
O	1.2903689	-0.2182290	0.8482642
O	-1.2406766	0.1126761	1.2533052
C	1.9035758	4.8098625	-5.2201072
C	1.1939150	5.4845465	-4.1906656
H	2.5593532	2.8909181	-5.9804756
H	2.3947026	5.3870583	-6.0183692
H	0.0233835	5.3072902	-2.3893674
H	1.1494795	6.5844238	-4.1877108
C	-3.6472391	4.9131709	-3.1091762
C	-4.3273189	5.6269121	-2.0863747
H	-2.0351027	3.5679708	-3.6048242
H	-4.0017122	4.9781565	-4.1493216
H	-5.1969594	6.2527163	-2.3388493
H	-4.4415456	6.0426981	0.0358539
C	2.5027356	-1.4535462	-2.5844325
C	1.2202376	-0.9765193	-2.9730164
C	2.7449506	-2.8387120	-2.6236192
C	0.1914537	-1.8956992	-3.3095309
C	0.4875484	-3.2718634	-3.3343724
C	1.7650959	-3.7657659	-3.0219559
H	3.7453055	-3.2134486	-2.3483633
C	-1.2212401	-1.4304958	-3.6569181
H	-0.3089522	-3.9763737	-3.6172440
C	-2.2514062	-1.9699347	-2.6502806
H	-2.3387440	-3.0749207	-2.7092489
H	-3.2547820	-1.5356430	-2.8323270
H	-1.9586036	-1.6986162	-1.6168509
C	-1.6035501	-1.7858581	-5.1044820
H	-1.2442904	-0.3250615	-3.5779365
H	-1.6226032	-2.8846594	-5.2629262

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H	-0.8807739	-1.3546826	-5.8266307
H	-2.6119477	-1.3941383	-5.3511676
C	2.1408049	-5.2355792	-3.1820651
C	0.9872512	-6.2147009	-2.9285713
H	1.3539099	-7.2614256	-2.9568067
H	0.2009175	-6.1267839	-3.7074710
H	0.5170177	-6.0321972	-1.9439896
C	2.7677189	-5.4680430	-4.5720167
H	2.9330301	-5.4434919	-2.4269027
H	3.1080979	-6.5184801	-4.6869026
H	3.6373604	-4.8014746	-4.7401758
H	2.0258427	-5.2585617	-5.3711142
C	3.6195378	-0.5060640	-2.1467841
C	4.2553349	-0.9238973	-0.8102221
H	4.9936499	-0.1625718	-0.4840077
H	4.7990281	-1.8889156	-0.8945747
H	3.4875407	-1.0235179	-0.0205479
C	4.6868576	-0.3572452	-3.2473081
H	3.1611815	0.4916691	-1.9870378
H	5.4760070	0.3586388	-2.9367377
H	4.2489394	0.0091178	-4.1973922
H	5.1770156	-1.3311817	-3.4586501
H	-0.7088791	1.8738983	7.2848287
H	1.7995227	6.0561561	3.9791707
H	-5.3573830	2.6364062	3.0600272
C	0.1787853	2.3361209	6.7990433
H	3.2449587	4.5176154	1.5712055
H	1.5488921	0.8958160	7.7382462
H	-4.3551530	0.2324955	2.9172806
C	-0.2533553	2.7514193	5.3988076
C	1.3667600	6.0663417	2.9567703
C	1.2788396	1.2593417	6.7246079
H	2.1990038	1.6678125	6.2556320
C	0.5930659	3.4980922	4.5610478
C	-4.4012812	3.0105763	3.4817813
H	-0.1835360	4.2961514	7.7305006
C	-1.4904294	2.3392458	4.8789072
C	0.6149360	3.5293492	7.6653824
H	0.8600847	3.1982943	8.6958254
H	-2.1560999	1.7434339	5.5232829
C	2.5837435	3.9416566	2.2515873
H	2.0367172	6.6746729	2.3139802
H	0.3850158	6.5793012	3.0133554
C	0.2430326	3.8180471	3.2376013
C	-3.5020521	0.6516505	3.4950286
C	-1.8902862	2.6274680	3.5606565
H	-4.2637161	4.0534036	3.1346551
H	-4.4992925	3.0369851	4.5878154
C	1.2191714	4.6393838	2.3966806
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C	-3.2324624	2.1024203	3.0570873
H	2.4620815	2.9222550	1.8362211
H	-2.6067769	0.0147033	3.3515904
H	3.1048816	3.8578456	3.2282714
H	0.9516363	0.3917221	6.1160236
H	-3.7880742	0.5789989	4.5652016
H	1.5211158	4.0210655	7.2535201
H	0.7913966	4.7379806	1.3781875
H	-3.1939511	2.1039040	1.9482685
H	1.5701419	3.8328749	4.9449049
C	0.0221473	-6.3905882	2.3447725
C	0.8358743	-5.2626381	2.2149023
C	1.8865339	-5.2600633	1.2642474
C	2.1348449	-6.4152766	0.4868722
C	1.3098978	-7.5391243	0.6138653
C	0.2497313	-7.5229535	1.5369183
H	-0.7952620	-6.3922036	3.0814077
H	0.6650265	-4.3820646	2.8552311
C	2.7199398	-4.0802079	1.0329810
H	2.9660724	-6.4145303	-0.2356588
H	1.4903837	-8.4289695	-0.0072153

H	-0.3990204	-8.4067292	1.6399111
O	2.5078756	-2.9329593	1.4526551
H	3.6350811	-4.2434242	0.4073976
C	-3.2129012	-4.6146823	0.0867415
C	-2.5787483	-3.5691738	0.7007321
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O	-0.9909785	-4.6866570	-0.5884802
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O	-0.2134545	-2.9003532	0.5010097
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H	-2.1041595	-6.4276345	-0.4549859
H	-2.4913517	-5.3607690	-1.8478393
H	-2.3460322	-2.3694851	2.4419294
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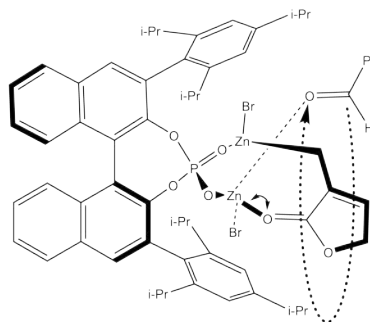


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Zn	-3.0322978	-0.6687463	0.7546041
Br	-4.2044485	0.8287145	-0.5774991
C	0.2035683	1.1854876	-2.0967594
C	-0.0452754	2.5623517	-2.1301517
C	0.6116434	3.3425284	-3.1519917
C	0.5653038	4.7692444	-3.1843070
C	1.3759788	2.6637936	-4.1710968
C	2.0001866	3.4281645	-5.2019863
C	1.5217838	1.2490662	-4.1125299
H	2.0996514	0.7393519	-4.8986793
C	0.9875433	0.4987901	-3.0718161
C	-1.3792478	3.6510398	1.3022078
C	-2.3963114	4.5222196	0.9316504
H	-2.9416837	5.0723858	1.7127869
C	-2.7864421	4.6940539	-0.4272196
C	-3.9022324	5.5117185	-0.7757729
C	-2.0658543	4.0068046	-1.4709565
C	-2.5369981	4.1257270	-2.8116968
C	-0.9292210	3.1955711	-1.1120689
C	-0.6718529	3.0001369	0.2461267
O	-0.3841602	0.3996377	-1.1160575
O	0.3634177	2.1320926	0.6136465
P	0.0186041	0.5408673	0.4730534
O	1.3077764	-0.2210298	0.8396616
O	-1.2150996	0.0805518	1.2524523
C	1.9103499	4.8112688	-5.2190801
C	1.1984167	5.4843661	-4.1910288
H	2.5703395	2.8940047	-5.9784027
H	2.4017888	5.3891063	-6.0166067
H	0.0252808	5.3043923	-2.3913672
H	1.1517716	6.5840787	-4.1881513
C	-3.6379724	4.9141357	-3.1147379
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H	-2.0259003	3.5683052	-3.6088057

H	-3.9904186	4.9803127	-4.1553873	H	-2.6218028	0.0101544	3.3412124
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C	2.5087431	-1.4576126	-2.5944353	H	-3.8028400	0.5739169	4.5521363
C	1.2261913	-0.9765388	-2.9770179	H	1.4944682	4.0114637	7.2594037
C	2.7463920	-2.8434445	-2.6369626	H	0.7942354	4.7242366	1.3788697
C	0.1929543	-1.8922102	-3.3094352	H	-3.2038881	2.1055326	1.9406234
C	0.4848449	-3.2688645	-3.3371406	H	1.5650307	3.8115818	4.9446596
C	1.7621693	-3.7668750	-3.0315015	C	0.0676824	-6.3788133	2.3913155
H	3.7479324	-3.2206434	-2.3688300	C	0.8673913	-5.2422322	2.2471882
C	-1.2201508	-1.4229899	-3.6492626	C	1.8971929	-5.2284969	1.2750186
H	-0.3151507	-3.9701098	-3.6184973	C	2.1389337	-6.3785773	0.4897391
C	-2.2478117	-1.9657579	-2.6421253	C	1.3289292	-7.5113036	0.6322226
H	-2.3438434	-3.0696673	-2.7127497	C	0.2894071	-7.5077263	1.5781665
H	-3.2487575	-1.5207910	-2.8101589	H	-0.7343076	-6.3870629	3.1447139
H	-1.9459806	-1.7077123	-1.6079944	H	0.6994181	-4.3624234	2.8903027
C	-1.6071579	-1.7686358	-5.0976840	C	2.7132897	-4.0354306	1.0313453
H	-1.2419716	-0.3182402	-3.5635144	H	2.9515959	-6.3563405	-0.2536617
H	-1.6268554	-2.8662478	-5.2642488	H	1.5045594	-8.3974628	0.0044030
H	-0.8864802	-1.3334340	-5.8191922	H	-0.3470290	-8.3990005	1.6941499
H	-2.6160841	-1.3751405	-5.3387426	O	2.4956679	-2.8964936	1.4607612
C	2.1317448	-5.2374856	-3.1982994	H	3.6165111	-4.1864795	0.3830567
C	0.9798301	-6.2132719	-2.9239479	C	-3.2282538	-4.6003065	0.0924489
H	1.3418486	-7.2616543	-2.9555290	C	-2.5849571	-3.5632966	0.7126053
H	0.1832652	-6.1257831	-3.6923552	C	-1.1769456	-3.6471646	0.2529544
H	0.5227775	-6.0258011	-1.9339649	O	-1.0059363	-4.6952122	-0.5792128
C	2.7339247	-5.4722338	-4.5984401	C	-2.2682395	-5.3586346	-0.7591682
H	2.9364545	-5.4475433	-2.4563976	O	-0.2109172	-2.9211816	0.5154464
H	3.0692583	-6.5234540	-4.7208604	C	-3.0448957	-2.4993919	1.6066062
H	3.6014930	-4.8073477	-4.7816502	H	-2.1366408	-6.4233174	-0.4607181
H	1.9793849	-5.2591096	-5.3842738	H	-2.5082043	-5.3404252	-1.8468961
C	3.6302673	-0.5146522	-2.1592928	H	-2.3321395	-2.3609051	2.4484184
C	4.2635852	-0.9311430	-0.8211245	H	-4.0550635	-2.7117682	2.0065193
H	5.0078574	-0.1743360	-0.4986471	H	-4.2922880	-4.8567418	0.1823418
H	4.8020415	-1.8996990	-0.9018812				
H	3.4971959	-1.0198831	-0.0287293				
C	4.6978140	-0.3741950	-3.2604685				
H	3.1768982	0.4857171	-2.0025499				
H	5.4902261	0.3389562	-2.9525055				
H	4.2617136	-0.0087023	-4.2115688				
H	5.1840053	-1.3504260	-3.4700343				
H	-0.7181611	1.8467571	7.2750849				
H	1.7840144	6.0466325	3.9843624				
H	-5.3636000	2.6427123	3.0513962				
C	0.1685150	2.3165192	6.7944689				
H	3.2467623	4.5096334	1.5802835				
H	1.5462777	0.8853391	7.7362220				
H	-4.3693810	0.2358870	2.9023389				
C	-0.2612709	2.7341778	5.3943590				
C	1.3580606	6.0547977	2.9592040				
C	1.2763481	1.2479553	6.7222602				
H	2.1950775	1.6630346	6.2566602				
C	0.5874714	3.4803693	4.5591546				
C	-4.4070493	3.0109792	3.4768304				
H	-0.2136543	4.2716240	7.7283712				
C	-1.4988104	2.3272509	4.8726523				
C	0.5906966	3.5110582	7.6658676				
H	0.8343855	3.1803687	8.6967494				
H	-2.1666648	1.7320347	5.5151837				
C	2.5850166	3.9335037	2.2598934				
H	2.0301086	6.6653779	2.3207693				
H	0.3745721	6.5645387	3.0104723				
C	0.2399211	3.8046035	3.2366412				
C	-3.5154999	0.6499176	3.4825742				
C	-1.8970273	2.6198659	3.5552168				
H	-4.2652233	4.0547716	3.1348094				
H	-4.5058369	3.0341389	4.5827626				
C	1.2179770	4.6271368	2.3992253				
C	-1.0153403	3.3698437	2.7268720				
C	-3.2407700	2.1010735	3.0496137				
H	2.4693754	2.9123845	1.8474688				

7.8.3 Pathway 14j-ma ↔ 14d-mi TS1; COSMO

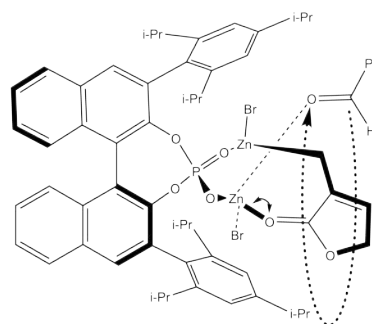


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Br	3.3546501	-2.5446226	1.8370236
Zn	-3.3800182	0.7616259	-0.0830441
Br	-3.3758428	3.0482898	-0.5474694
C	0.3818214	1.5928429	-2.5633910
C	0.7932018	2.8642682	-2.1512788
C	1.7619455	3.5525260	-2.9759738
C	2.3820554	4.7788448	-2.5876119
C	2.1567732	2.9634311	-4.2348468
C	3.0767583	3.6600265	-5.0754276
C	1.6844750	1.6661156	-4.5870360
H	2.0397813	1.2052679	-5.5218628
C	0.8530194	0.9394243	-3.7443666
C	0.1574017	3.1738288	1.6221514
C	-0.2726084	4.4896163	1.7258873

H	-0.4525845	4.9249237	2.7204156	C	2.2567001	-1.5737862	5.7417916
C	-0.5212141	5.2870789	0.5711204	H	3.2363879	-1.0527573	5.7519014
C	-1.0682413	6.5995862	0.6888288	C	1.9284740	0.9930407	4.1873560
C	-0.2483845	4.7541044	-0.7418400	C	-2.7013692	3.1309508	4.0312833
C	-0.5990248	5.5411208	-1.8782600	H	0.4426994	0.8127933	7.5641502
C	0.3160204	3.4319009	-0.8580192	C	-0.4463521	0.7419362	4.4962083
C	0.4220846	2.6732367	0.3115541	C	1.3015107	0.1488124	7.3392906
O	-0.5689714	0.9032943	-1.8155624	H	1.4225678	-0.5604168	8.1847523
O	0.8653194	1.3516803	0.2323158	H	-1.2912958	0.2681902	5.0219624
P	-0.1887660	0.2442709	-0.3713430	C	3.8174338	1.4533662	1.7896231
O	0.6750340	-1.0182117	-0.5605253	H	4.5910897	3.8963307	2.8849489
O	-1.4927980	0.1004866	0.4033400	H	3.1086942	4.2165345	3.8471806
C	3.6275445	4.8709147	-4.6837829	C	1.7196587	1.9194414	3.1499115
C	3.2892027	5.4217631	-3.4193163	C	-3.0965305	0.8084624	3.1194217
H	3.3557029	3.2031337	-6.0380814	C	-0.7114084	1.6704057	3.4715974
H	4.3398638	5.3944736	-5.3395702	H	-2.0664908	4.0381788	4.0064627
H	2.1402850	5.2155032	-1.6094094	H	-2.7483273	2.7843458	5.0855403
H	3.7533616	6.3643764	-3.0910425	C	2.9335954	2.5269989	2.4486910
C	-1.1505840	6.8061116	-1.7303647	C	0.3879134	2.2638390	2.7899007
C	-1.3742651	7.3493188	-0.4371182	C	-2.1528347	2.0220726	3.1137637
H	-0.4468620	5.1239560	-2.8834255	H	3.2279544	0.8293491	1.0904777
H	-1.4261197	7.3881153	-2.6231314	H	-2.6671291	-0.0430526	2.5563277
H	-1.8076884	8.3556239	-0.3316211	H	4.2721202	0.7747438	2.5406053
H	-1.2640379	6.9980969	1.6967748	H	2.1676983	-2.0683322	4.7534506
C	1.5877039	-1.4645007	-3.7329651	H	-3.3250280	0.4546834	4.1468914
C	0.5484171	-0.5120520	-3.9345832	H	2.2120327	0.7824543	7.2920760
C	1.2612399	-2.8334937	-3.7779290	H	2.5609667	3.1880811	1.6401668
C	-0.7815132	-0.9503046	-4.1842566	H	-2.1456193	2.4225811	2.0783299
C	-1.0498377	-2.3282251	-4.2196630	H	2.9626311	0.7295973	4.4570988
C	-0.0461228	-3.2895873	-4.0060713	C	-0.1541871	-4.2384055	4.6037697
H	2.0557962	-3.5803136	-3.6121874	C	0.0787181	-4.0542401	3.2379253
C	-1.9163120	0.0413757	-4.4288128	C	-0.4405860	-4.9820043	2.3040536
H	-2.0840984	-2.6615611	-4.3963210	C	-1.1906739	-6.0926215	2.7598763
C	-3.1367808	-0.2320497	-3.5344465	C	-1.4214448	-6.2729200	4.1281244
H	-3.6820934	-1.1485479	-3.8416740	C	-0.9042093	-5.3444365	5.0489857
H	-3.8502800	0.6161929	-3.5735942	H	0.2525794	-3.5191393	5.3287101
H	-2.8275767	-0.3886155	-2.4831024	H	0.6728498	-3.1931620	2.8970983
C	-2.3007172	0.0749056	-5.9198326	C	-0.2748822	-4.8292969	0.8610110
H	-1.5423060	1.0523220	-4.1697180	H	-1.5999328	-6.8047375	2.0260603
H	-2.6742132	-0.9148437	-6.2574266	H	-2.0065988	-7.1349851	4.4810812
H	-1.4300616	0.3399503	-6.5538583	H	-1.0859499	-5.4814068	6.1259694
H	-3.1014885	0.8210128	-6.1045003	O	0.3539218	-3.9380834	0.2646006
C	-0.3630519	-4.7792041	-4.0001335	H	-0.7603583	-5.6130285	0.2310563
C	-1.4197011	-5.1255689	-2.9367214	C	-4.3732606	-2.3234845	1.9832897
H	-1.5402271	-6.2253836	-2.8435388	C	-4.1983120	-1.8506276	0.7178383
H	-2.4100086	-4.6976460	-3.1946265	C	-3.1596817	-2.7087566	0.0751043
H	-1.1461135	-4.6974941	-1.9532150	O	-2.7723319	-3.6854026	0.9811586
C	-0.7788600	-5.2776178	-5.3959216	C	-3.4698130	-3.4909250	2.2194858
H	0.5785583	-5.3039597	-3.7234682	O	-2.6769067	-2.6487221	-1.0371042
H	-0.9630905	-6.3722905	-5.3888899	C	-4.7539447	-0.6983258	0.0018668
H	0.0042071	-5.0641383	-6.1514999	H	-2.7196280	-3.3115083	3.0249976
H	-1.7141623	-4.7824512	-5.7319269	H	-4.0092447	-4.4303784	2.4781335
C	3.0406669	-1.0684739	-3.4610681	H	-5.6717290	-0.3000020	0.4764800
C	3.5913880	-1.6651303	-2.1545442	H	-4.9603527	-0.9467271	-1.0600050
H	4.6464481	-1.3631149	-1.9934953	H	-5.0537878	-1.9257745	2.7487163
H	3.5616023	-2.7747481	-2.1470828				
H	3.0134910	-1.2878985	-1.2876139				
C	3.9375398	-1.4270416	-4.6611000				
H	3.0778195	0.0321103	-3.3420140				
H	4.9806811	-1.0881698	-4.4913852				
H	3.5690301	-0.9527262	-5.5934593				
H	3.9613371	-2.5235765	-4.8337759				
H	0.1627968	-1.2002892	6.1056227				
H	4.1605136	2.8244758	4.2539080				
H	-3.7247232	3.4244563	3.7178268				
C	1.0967816	-0.6008416	6.0083306				
H	4.6445749	1.9260403	1.2203712				
H	2.3013999	-2.3567133	6.5268906				
H	-4.0692033	1.0815995	2.6563391				
C	0.8617294	0.3836586	4.8686257				
C	3.7412797	3.4158069	3.4127643				

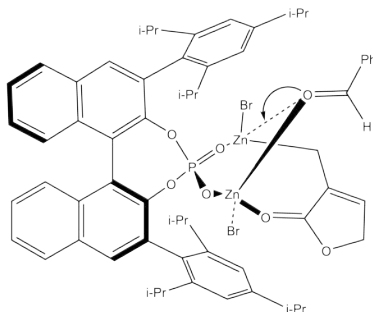
TS1



Energy (Hartree) = -11970.00155227
number of imaginary frequencies: 1

Zn	1.5210956	-2.3099902	0.5082119	H	3.0156853	-1.2935600	-1.2853314
Br	3.3542723	-2.5567698	1.8472798	C	3.9347697	-1.4363458	-4.6596786
Zn	-3.3785653	0.7633894	-0.0890877	H	3.0787255	0.0248418	-3.3402335
Br	-3.3782372	3.0451587	-0.5391413	H	4.9788174	-1.0993328	-4.4919888
C	0.3829957	1.5925924	-2.5594364	H	3.5655892	-0.9626112	-5.5918505
C	0.7933202	2.8654875	-2.1506961	H	3.9564835	-2.5327159	-4.8329247
C	1.7611506	3.5522244	-2.9776402	H	0.1421465	-1.1914280	6.1034513
C	2.3796178	4.7802242	-2.5930725	H	4.1563067	2.8200003	4.2604060
C	2.1561454	2.9602757	-4.2348797	H	-3.7240442	3.4515219	3.7138601
C	3.0746982	3.6558514	-5.0769762	C	1.0785992	-0.5948757	6.0075515
C	1.6846566	1.6619558	-4.5831578	H	4.6401702	1.9226221	1.2251243
H	2.0395671	1.1981939	-5.5167024	H	2.2784223	-2.3553608	6.5267865
C	0.8540685	0.9364297	-3.7389750	H	-4.0782522	1.1122870	2.6526899
C	0.1572407	3.1840433	1.6218944	C	0.8482060	0.3909123	4.8678216
C	-0.2708659	4.5004294	1.7223355	C	3.7400348	3.4133327	3.4193005
H	-0.4503195	4.9373073	2.7162071	C	2.2350248	-1.5721807	5.7414649
C	-0.5191158	5.2955862	0.5662537	H	3.2165719	-1.0550836	5.7524659
C	-1.0644348	6.6085372	0.6805085	C	1.9176880	0.9971197	4.1887556
C	-0.2478934	4.7591267	-0.7454935	C	-2.7030025	3.1529681	4.0292744
C	-0.5987001	5.5433472	-1.8834138	H	0.4292794	0.8213823	7.5623494
C	0.3158709	3.4364479	-0.8588959	C	-0.4577711	0.7543299	4.4944051
C	0.4216969	2.6809095	0.3124903	C	1.2850193	0.1534260	7.3388482
O	-0.5671911	0.9041887	-1.8102438	H	1.4032036	-0.5551371	8.1854034
O	0.8654065	1.3591528	0.2371729	H	-1.3052539	0.2840706	5.0193894
P	-0.1876832	0.2506017	-0.3643257	C	3.8107958	1.4528057	1.7932071
O	0.6810654	-1.0099309	-0.5514288	H	4.5923650	3.8914591	2.8935485
O	-1.4909867	0.1030869	0.4098994	H	3.1099605	4.2154030	3.8543653
C	3.6238729	4.8680757	-4.6892464	C	1.7134393	1.9252504	3.1522543
C	3.2852287	5.4217189	-3.4267824	C	-3.1077602	0.8333647	3.1165798
H	3.3539098	3.1964864	-6.0383545	C	-0.7187392	1.6843871	3.4704814
H	4.3352279	5.3905857	-5.3468312	H	-2.0642033	4.0571932	4.0050435
H	2.1365561	5.2189908	-1.6162431	H	-2.7519637	2.8073754	5.0837507
H	3.7478425	6.3659944	-3.1013371	C	2.9304117	2.5288484	2.4530839
C	-1.1482782	6.8089660	-1.7380069	C	0.3835352	2.2742402	2.7906422
C	-1.3701433	7.3555418	-0.4465767	C	-2.1583463	2.0423457	3.1118739
H	-0.4486076	5.1224403	-2.8871519	H	3.2199539	0.8324999	1.0921095
H	-1.4245457	7.3885093	-2.6319975	H	-2.6823569	-0.0198699	2.5528867
H	-1.8028788	8.3622537	-0.3431696	H	4.2628938	0.7706839	2.5425274
H	-1.2601768	7.0092207	1.6875114	H	2.1472994	-2.0653073	4.7523243
C	1.5856244	-1.4691550	-3.7295135	H	-3.3390842	0.4801433	4.1438746
C	0.5478642	-0.5148306	-3.9286427	H	2.1972348	0.7842142	7.2915921
C	1.2571231	-2.8373009	-3.7769068	H	2.5607316	3.1925540	1.6453607
C	-0.7826744	-0.9507336	-4.1780941	H	-2.1508938	2.4428646	2.0763978
C	-1.0527906	-2.3279863	-4.2154111	H	2.9507397	0.7297857	4.4588286
C	-0.0507363	-3.2911028	-4.0047774	C	-0.1079725	-4.2961082	4.6043009
H	2.0510756	-3.5857256	-3.6150480	C	0.1106666	-4.0908794	3.2387255
C	-1.9162928	0.0425725	-4.4207621	C	-0.4338452	-4.9933927	2.2956608
H	-2.0878574	-2.6591147	-4.3911721	C	-1.1940612	-6.1004685	2.7413736
C	-3.1363331	-0.2306277	-3.5260891	C	-1.4105060	-6.3024138	4.1086240
H	-3.6833282	-1.1463095	-3.8329447	C	-0.8682632	-5.3982982	5.0391830
H	-3.8483348	0.6187347	-3.5625260	H	0.3203112	-3.5948345	5.3345497
H	-2.8255299	-0.3882014	-2.4754650	H	0.7154873	-3.2342922	2.9058196
C	-2.3007611	0.0786880	-5.9115639	C	-0.2804369	-4.8164696	0.8517879
H	-1.5415526	1.0528187	-4.1603674	H	-1.6240879	-6.7920527	1.9996262
H	-2.6751566	-0.9099325	-6.2511338	H	-2.0036817	-7.1623638	4.4534487
H	-1.4299398	0.3433497	-6.5451818	H	-1.0384205	-5.5524973	6.1158487
H	-3.1005818	0.8258980	-6.0951762	O	0.3513012	-3.9230700	0.2660672
C	-0.3698903	-4.7803070	-4.0036415	H	-0.7817974	-5.5834713	0.2122535
C	-1.4268582	-5.1295895	-2.9414080	C	-4.3642658	-2.3213370	1.9860559
H	-1.5491455	-6.2296479	-2.8521720	C	-4.1820238	-1.8547029	0.7189614
H	-2.4171137	-4.7001230	-3.1964009	C	-3.1301636	-2.7086939	0.0911011
H	-1.1533051	-4.7041255	-1.9566891	O	-2.7437454	-3.6782128	1.0104703
C	-0.7861808	-5.2733883	-5.4009969	C	-3.4534923	-3.4798518	2.2395459
H	0.5712904	-5.3073358	-3.7290184	O	-2.6336986	-2.6536455	-1.0135701
H	-0.9722113	-6.3677553	-5.3987787	C	-4.7395228	-0.7120039	-0.0071478
H	-0.0031944	-5.0573549	-6.1555343	H	-2.7111378	-3.2896655	3.0506089
H	-1.7203119	-4.7754923	-5.7355481	H	-3.9878944	-4.4224412	2.5002608
C	3.0396136	-1.0757567	-3.4591242	H	-5.6655806	-0.3193949	0.4554451
C	3.5910811	-1.6727094	-2.1530564	H	-4.9320949	-0.9670544	-1.0697516
H	4.6471016	-1.3739914	-1.9926806	H	-5.0556115	-1.9231406	2.7412903
H	3.5597267	-2.7824474	-2.1451700				

TS2; COSMO



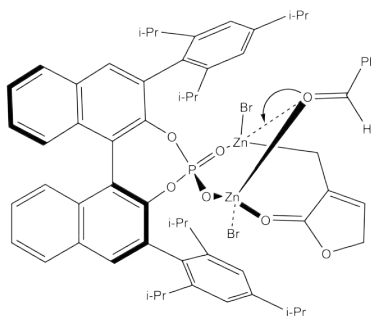
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Zn	2.9761004	0.6106141	-0.1860845
Br	5.2003952	0.0236394	-0.5314403
Zn	-1.2754313	2.4075106	0.3320669
Br	-3.5630486	2.0539859	0.0845950
C	-1.4954756	-1.8953348	0.2986293
C	-2.3385194	-2.3638457	-0.7203191
C	-2.7887166	-3.7339640	-0.6462193
C	-3.4954698	-4.3728973	-1.7104791
C	-2.4905055	-4.5110467	0.5325810
C	-2.9609962	-5.8557544	0.6237737
C	-1.7108701	-3.9317456	1.5727788
H	-1.5107932	-4.5217849	2.4803793
C	-1.1714924	-2.6551135	1.4625729
C	-1.9921753	0.0131346	-3.7234081
C	-3.3137161	0.1209458	-4.1389477
H	-3.5545023	0.7217907	-5.0280469
C	-4.3852335	-0.4691679	-3.4063683
C	-5.7420689	-0.2572053	-3.7951020
C	-4.1072350	-1.2437683	-2.2205079
C	-5.2074597	-1.7075926	-1.4406710
C	-2.7319432	-1.4814896	-1.8561048
C	-1.7448731	-0.8293223	-2.5935755
O	-0.9853753	-0.6056351	0.2534225
O	-0.4153663	-1.0090123	-2.2088151
P	0.0607735	-0.1123576	-0.9294376
O	1.5001721	-0.5704483	-0.6462817
O	-0.2191916	1.3800485	-1.0818995
C	-3.6695710	-6.4354816	-0.4176712
C	-3.9232464	-5.6888272	-1.5995878
H	-2.7348012	-6.4298363	1.5361557
H	-4.0212842	-7.4754528	-0.3383274
H	-3.6912054	-3.8130591	-2.6352454
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C	-6.5164619	-1.4655790	-1.8348769
C	-6.7896001	-0.7494096	-3.0306592
H	-5.0090380	-2.2526081	-0.5074466
H	-7.3487948	-1.8259073	-1.2110705
H	-7.8313627	-0.5700500	-3.3376325
H	-5.9414242	0.3266654	-4.7075700
C	1.0262946	-2.5541462	2.7140757
C	-0.3158656	-2.1069832	2.5648123
C	1.7288349	-2.2022377	3.8806012
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H	2.7613336	-2.5667388	4.0084396
C	-2.2738061	-0.6315955	3.3459592
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H	-2.0771316	1.1623174	4.6234183
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H	-2.5861828	-0.7979441	2.2956518
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H	-4.3171386	-0.9387107	4.0860288
C	1.9085736	-1.2201747	6.2158346
C	1.2463647	-0.2282870	7.1788978
H	1.9024480	-0.0457381	8.0538404
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H	1.0505278	0.7497766	6.6987409
C	2.1474587	-2.5690087	6.9254205
H	2.9064130	-0.8081211	5.9429436
H	2.7550677	-2.4297393	7.8436312
H	2.6764584	-3.2926463	6.2740231
H	1.1810104	-3.0287588	7.2211758
C	1.7014252	-3.4200220	1.6507585
C	3.1070768	-2.9155385	1.2891193
H	3.5161948	-3.4805946	0.4276071
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H	3.0890014	-1.8497143	0.9972465
C	1.7441666	-4.9004164	2.0739348
H	1.0850095	-3.3472802	0.7303938
H	2.2172665	-5.5215697	1.2854025
H	0.7289043	-5.3028312	2.2608210
H	2.3334477	-5.0272837	3.0066449
H	2.6678045	4.0278204	-4.8275655
H	0.9641495	-1.1939291	-7.2262092
H	-3.7328185	4.0898805	-4.2634374
C	2.8533865	2.9657088	-5.1023700
H	1.3268340	-3.2327596	-4.7382765
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H	-2.4467144	4.5038710	-2.0272220
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H	4.1803107	1.3662772	-4.3720731
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H	2.5391332	3.3477412	-7.2471622
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C	3.3135985	2.9329755	-6.5703320
H	4.2436331	3.5231054	-6.7063595
H	0.4672713	3.9668554	-4.2278082
C	1.4530251	-2.1399571	-4.5933023
H	0.0188240	-2.6861092	-6.9118708
H	-0.8179065	-1.1040337	-7.0691749
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C	-0.7916407	2.2049445	-4.0938492
H	-3.1932394	2.7822251	-5.3664243
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C	0.2399282	-1.3811602	-5.1585487
C	-0.8448063	0.7925799	-4.2873908
C	-1.9731025	2.9962434	-3.5345410
H	1.5732614	-1.9445901	-3.5099127
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H	2.3951244	-1.8496441	-5.1035424
H	3.6244807	2.4904138	-3.0964777
H	-1.1081481	4.9872620	-3.1106340
H	3.5279750	1.8949439	-6.9007881
H	-0.6670237	-1.8055160	-4.6815167
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H	2.3099006	0.3053485	-5.5522345
C	2.6841779	2.7758299	5.7240411
C	2.6071008	2.2014515	4.4536077
C	3.6153350	1.3010841	4.0297435
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C	4.7561544	1.5531983	6.1687146
C	3.7558400	2.4510043	6.5808313
H	1.9068387	3.4785293	6.0594686
H	1.7804886	2.4382957	3.7676151
C	3.5968564	0.7316165	2.6882680
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H	5.5882149	1.3044610	6.8438709

H	3.8084420	2.9040283	7.5827935
O	2.7093475	0.9797747	1.8518107
H	4.4553918	0.0731164	2.3988475
C	0.7655866	5.4668967	-0.1747492
C	0.9336818	4.1709309	0.2312370
C	1.9719762	3.6112785	-0.6768553
O	2.3441367	4.5271585	-1.5938719
C	1.6289197	5.7508171	-1.3536610
O	2.5211128	2.5051997	-0.6825688
C	0.2346870	3.3782035	1.2550205
H	1.0537403	6.0008463	-2.2736060
H	2.3757149	6.5599629	-1.1941103
H	-0.1582422	4.0091338	2.0749632
H	0.8841352	2.5768657	1.6612980
H	0.0735978	6.2030294	0.2565550

TS2



Energy (Hartree) = -11970.02557841
number of imaginary frequencies: 1

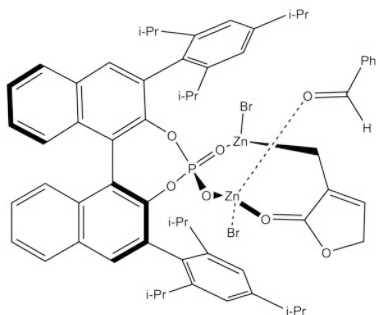
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Zn	-1.2857301	2.3846944	0.3316792
Br	-3.5657887	2.0448686	0.0870665
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C	-2.3293311	-2.3594804	-0.7207291
C	-2.7819152	-3.7284734	-0.6408186
C	-3.4889789	-4.3701595	-1.7027877
C	-2.4872944	-4.5010669	0.5415077
C	-2.9610782	-5.8437139	0.6374515
C	-1.7090660	-3.9179733	1.5801670
H	-1.5120667	-4.5022161	2.4922410
C	-1.1667232	-2.6433139	1.4647206
C	-1.9882554	0.0105253	-3.7299177
C	-3.3101288	0.1132251	-4.1450672
H	-3.5514471	0.7119592	-5.0353912
C	-4.3802505	-0.4769111	-3.4111148
C	-5.7373680	-0.2694540	-3.7994874
C	-4.1001766	-1.2463591	-2.2226256
C	-5.1989391	-1.7085830	-1.4402583
C	-2.7240706	-1.4808503	-1.8587703
C	-1.7386278	-0.8292880	-2.5987488
O	-0.9704797	-0.6010894	0.2475207
O	-0.4082382	-1.0073613	-2.2161145
P	0.0720685	-0.1094278	-0.9402210
O	1.5115676	-0.5688339	-0.6600151
O	-0.2095594	1.3831453	-1.0896292
C	-3.6697238	-6.4260137	-0.4017178
C	-3.9202238	-5.6839580	-1.5864614
H	-2.7369874	-6.4144150	1.5524546
H	-4.0239543	-7.4647351	-0.3181567
H	-3.6822532	-3.8127714	-2.6293917
H	-4.4564370	-6.1558820	-2.4239247
C	-6.5080536	-1.4708643	-1.8350688
C	-6.7831638	-0.7606028	-3.0331143

H	-4.9984189	-2.2482049	-0.5045351
H	-7.3391203	-1.8293427	-1.2087037
H	-7.8252930	-0.5838109	-3.3400195
H	-5.9380495	0.3114512	-4.7134862
C	1.0253059	-2.5352947	2.7254845
C	-0.3163900	-2.0903351	2.5684186
C	1.7210304	-2.1786908	3.8946447
C	-0.8842307	-1.2040067	3.5187145
C	-0.1538001	-0.8968355	4.6841138
C	1.1332251	-1.4072732	4.9171933
H	2.7531265	-2.5423793	4.0288892
C	-2.2815299	-0.6171623	3.3340346
H	-0.6261721	-0.2518748	5.4384468
C	-2.3065546	0.9011450	3.5732435
H	-2.1187932	1.1634258	4.6355631
H	-3.2882829	1.3248328	3.2827043
H	-1.5358641	1.4104315	2.9573233
C	-3.3132052	-1.3498068	4.2105498
H	-2.5800681	-0.7715287	2.2779479
H	-3.0726223	-1.2396973	5.2890373
H	-3.3344682	-2.4341215	3.9791297
H	-4.3319981	-0.9430282	4.0441898
C	1.8843557	-1.1948712	6.2303541
C	1.2150493	-0.2023588	7.1879343
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H	0.2491352	-0.5965346	7.5676847
H	1.0190363	0.7743494	6.7050610
C	2.1170876	-2.5425871	6.9437564
H	2.8844517	-0.7829175	5.9650129
H	2.7180508	-2.4040301	7.8664780
H	2.6487334	-3.2681513	6.2969603
H	1.1482031	-3.0013218	7.2320108
C	1.7050371	-3.4058423	1.6689354
C	3.1121383	-2.9047187	1.3096570
H	3.5253889	-3.4742351	0.4533859
H	3.8268923	-3.0164250	2.1518606
H	3.0974147	-1.8412640	1.0096082
C	1.7444450	-4.8841192	2.0993818
H	1.0923080	-3.3373294	0.7458674
H	2.2204559	-5.5094737	1.3161505
H	0.7281494	-5.2849372	2.2828713
H	2.3287325	-5.0078725	3.0355732
H	2.6572547	4.0425069	-4.8269534
H	0.9674797	-1.1767014	-7.2351217
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H	1.3393357	-3.2251156	-4.7541562
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C	1.5366754	2.2326599	-4.8971892
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C	3.9403163	2.4491834	-4.1551591
H	4.1815739	1.3874571	-4.3708353
C	1.4415500	0.8523572	-5.1435591
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H	2.5303105	3.3616723	-7.2465492
C	0.3944143	2.8880820	-4.4121501
C	3.3069288	2.9511039	-6.5699529
H	4.2346159	3.5446453	-6.7066921
H	0.4546561	3.9732660	-4.2340803
C	1.4632302	-2.1326332	-4.6058142
H	0.0275216	-2.6729236	-6.9252487
H	-0.8134416	-1.0922468	-7.0743714
C	0.2795208	0.1196920	-4.8507155
C	-1.5805708	4.1222099	-2.5840121
C	-0.7967489	2.2063970	-4.1000771
H	-3.1962899	2.7741010	-5.3784983
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H	1.5855996	-1.9424723	-3.5219145
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H	-1.1322126	4.9880599	-3.1165537
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C	2.7457523	2.7253249	5.7324178
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C	3.8229901	2.3873162	6.5758209
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H	1.8216111	2.4099435	3.7801296
C	3.6148213	0.7050100	2.6657377
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H	5.6515170	1.2291861	6.8095874
H	3.8875757	2.8301955	7.5816317
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H	4.4673737	0.0463532	2.3567075
C	0.7406359	5.4459940	-0.1693072
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C	1.5963785	5.7283592	-1.3556897
O	2.5148732	2.4957590	-0.6669391
C	0.2265045	3.3551856	1.2634842
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O	0.0031249	1.3279101	1.0731472
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C	1.8676689	2.0965048	7.1912432
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H	3.2308765	3.2838979	5.9992188
H	2.3588098	2.3413483	8.1454016
H	-0.7439065	0.2249297	5.9783769
H	0.3871163	0.7765653	8.1128158
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H	-1.7517568	2.7231905	4.8662201
H	-3.7980043	3.3452579	6.1154536
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C	0.4560165	4.4730210	0.5874303
H	1.5796932	4.4625281	-1.9110741
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H	-0.0159451	5.7097843	-1.1801191
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H	1.5686419	5.3294569	2.2864096
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C	3.6618153	3.1867279	-3.1559676
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C	4.1712921	4.5953197	-3.5088102
H	4.5140476	2.4831534	-3.2918740
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H	5.1708939	-0.8299127	1.6032397
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H	3.6878656	-0.7470372	0.5947685
C	5.5836967	1.8869354	1.9170590
H	3.6856711	0.9837172	2.3681552
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H	-1.5335374	-6.1008221	2.7734646
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C	-2.8427614	-5.4289491	-1.9348450
H	1.1226129	-4.3158525	3.0113975
H	-1.5451928	-6.1109504	-3.5702834
H	-4.9006101	0.5222032	-1.3521069
C	-2.8202459	-4.4348890	-0.7808931
C	-1.5219405	-5.1711526	3.3804758
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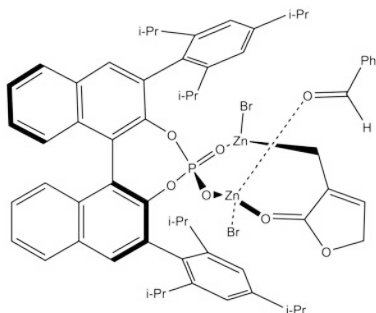
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Br	-3.2805423	2.5677880	0.6477291
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C	0.5624083	1.4608058	4.7388620
C	0.1139464	0.9114425	5.9780747
C	1.7298149	2.3118725	4.7544433
C	2.3488851	2.6240856	6.0022468
C	2.2707328	2.7938177	3.5267064
H	3.1656851	3.4346915	3.5547601
C	1.7301093	2.4268672	2.3016620
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C	-3.7399279	-1.1473559	3.2165325
H	-4.6554772	-1.7554298	3.1703703
C	-3.7235828	-0.0026434	4.0635460
C	-4.8809780	0.3727098	4.8099520

C	-5.9511369	-1.3684319	0.4774710
H	-4.2455623	-6.8233057	-0.9698086
C	-3.6343554	-3.2920419	-0.8019484
C	-3.2590594	-6.8375008	-1.4759325
H	-3.3231090	-7.5321455	-2.3391722
H	-4.3058052	-3.1437668	-1.6634792
C	0.4669503	-4.1941116	2.1244085
H	-0.8811053	-5.3555792	4.2677747
H	-2.5569094	-4.9888281	3.7353352
C	-1.9150226	-3.6835404	1.3813572
C	-4.4517804	-0.4919839	-1.3466385
C	-3.6099661	-2.3235085	0.2194371
H	-6.0278623	-1.7462560	1.5156742
H	-6.4037500	-2.1337902	-0.1881884
C	-0.9923625	-3.9774539	2.5627114
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H	-3.4094735	-0.4266829	-1.7199268
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H	-1.9024830	-2.0329329	-5.4915675
H	-2.2645107	2.4749377	-3.5430511
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H	-3.4621473	0.0417378	-4.5786992

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C	-0.0804127	1.1711467	3.4761070
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C	1.7262928	2.3175108	4.7548332
C	2.3407318	2.6321626	6.0037265
C	2.2680448	2.7998943	3.5280709
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C	1.7312732	2.4309959	2.3021216
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C	-3.7333868	-1.1525733	3.2135111
H	-4.6478001	-1.7621314	3.1658083
C	-3.7186879	-0.0091032	4.0617368
C	-4.8753483	0.3637024	4.8096232
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H	-1.4040235	5.3960069	-0.0884976
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C	0.9297665	5.6592687	1.4496354
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C	4.3059342	1.1803650	1.4653204
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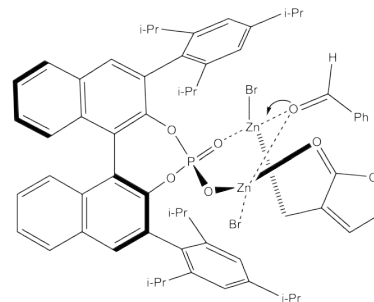
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Br	-3.2638657	2.5768151	0.6403064

H	5.3565849	2.8739042	2.4096717
H	6.2535145	2.1183219	1.0607031
H	-3.5969480	-5.0222945	-2.6918932
H	-1.5311976	-6.1022374	2.7293082
H	-6.5773218	-0.4590253	0.4280495
C	-2.8388165	-5.3995579	-1.9680551
H	1.1298530	-4.3284033	2.9866047
H	-1.5394068	-6.1073485	-3.5912034
H	-4.9256127	0.5409710	-1.3217351
C	-2.8117993	-4.4102563	-0.8100414
C	-1.5177505	-5.1771689	3.3430804
C	-1.4831997	-5.4556050	-2.6941918
H	-0.6883370	-5.8598434	-2.0345531
C	-1.9553627	-4.5888707	0.2893771
C	-5.9578106	-1.3778141	0.4869977
H	-4.2832323	-6.7634644	-1.0214648
C	-3.6336949	-3.2731681	-0.8163089
C	-3.2915361	-6.7990886	-1.5156919
H	-3.3589349	-7.4932223	-2.3790845
H	-4.3139144	-3.1234591	-1.6709186
C	0.4770684	-4.1959118	2.0992888
H	-0.8797260	-5.3707129	4.2303707
H	-2.5530474	-4.9948261	3.6963632
C	-1.9042966	-3.6748665	1.3563611
C	-4.4700686	-0.4699473	-1.3303183
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C	-0.9824548	-3.9789541	2.5356967
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H	0.8549148	-3.3326795	1.5189442
H	-3.4286670	-0.3904779	-1.7032240
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H	-1.1388318	-4.4497167	-3.0073616
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H	-0.9988969	-3.1027260	3.2145554
H	-4.1085842	-0.3000744	0.7654083
H	-1.2958370	-5.4703884	0.3181714
C	2.1853513	-1.7844588	-6.3315048
C	2.6300526	-1.6080770	-5.0185754
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C	4.3148130	-0.0203566	-5.8240824
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C	2.7876087	-1.0724684	-7.3859192
H	1.3630668	-2.4871096	-6.5335173
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C	4.1713501	-0.4347478	-3.3996599
H	5.1484609	0.6685186	-5.6121075
H	4.3286634	0.3548782	-7.9628185
H	2.4275373	-1.2121803	-8.4170266
O	3.6229160	-0.7361337	-2.3324601
H	5.1374138	0.1325286	-3.3397728
C	-2.4650593	-0.2998677	-4.2185658
C	-1.5047685	0.4448041	-3.5858246
C	-0.3779725	-0.4885287	-3.3682804
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H	-2.6020520	-2.4354198	-3.7742450
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H	-2.2188775	2.4759900	-3.5391167
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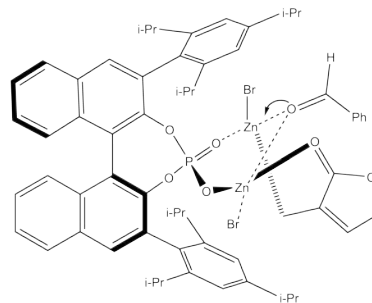
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C	4.5886004	3.6232890	1.2052199
C	2.3662227	4.6150270	1.5525195
C	2.9913302	5.8927750	1.6762875
C	0.9492796	4.4950248	1.5220182
H	0.3375252	5.4067071	1.6010068
C	0.3176017	3.2769048	1.2971176
C	3.8957255	-1.1555799	-0.1268629
C	5.0486990	-1.3179306	0.6345757
H	5.7415534	-2.1398208	0.3961324
C	5.3287337	-0.4914230	1.7612052
C	6.4497222	-0.7515098	2.6064104
C	4.4373817	0.5957456	2.0877020
C	4.6709010	1.3220225	3.2936875
C	3.3408764	0.8933099	1.1959122
C	3.0740628	-0.0189468	0.1678945
O	0.4796560	0.8814350	1.2478350
O	1.9940492	0.2117129	-0.6767480
P	0.4741909	-0.0417998	-0.1151007
O	-0.4285248	0.5646567	-1.2040574
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C	4.3667221	6.0272459	1.5660211
C	5.1655674	4.8821805	1.3050534
H	2.3521331	6.7753844	1.8364624
H	4.8371840	7.0183585	1.6546756
H	5.2249294	2.7547513	0.9904444
H	6.2528741	4.9924266	1.1732735
C	5.7551261	1.0269117	4.1093198
C	6.6650646	-0.0052717	3.7556902
H	3.9714758	2.1199184	3.5800152
H	5.9072362	1.5949337	5.0397864
H	7.5275071	-0.2229876	4.4040053
H	7.1301278	-1.5748774	2.3376042
C	-1.5291062	3.7860412	-0.3100854
C	-1.1411103	3.2524172	0.9542682
C	-2.8994171	3.9408373	-0.5812606
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C	-3.4890864	2.9626185	1.5371849
C	-3.8971547	3.5701775	0.3352607
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H	-4.2505845	2.6422472	2.2672540
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H	-3.3333956	0.6382362	3.2560318
H	-1.9095812	0.2559276	4.2678760
H	-1.8006328	0.0893592	2.4978489
C	-2.2558651	3.0183311	4.3887975
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H	-1.8814043	4.0605102	4.3265454
H	-1.9159919	2.5871868	5.3531085
C	-5.3547500	3.9127837	0.0466577
C	-6.3214031	2.7333791	0.2227345
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H	-6.3229411	2.3634180	1.2698508

7.8.4 Pathway 14j-mi ↔ 14d-mi

TS1; COSMO

H	-6.0534392	1.8979499	-0.4557332	O	-4.0539159	-2.6663050	-2.3097567
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H	-6.8275519	5.4311295	0.6493028	C	-1.1981950	-4.3525998	-0.6812084
H	-5.1215320	5.9885749	0.7380855	H	-5.2937788	-4.2943355	-2.6605673
H	-5.7625880	4.8713127	1.9811973	H	-5.5602239	-3.4289242	-1.1085056
C	-0.5124972	4.2091847	-1.3737002	Zn	-0.7964231	-3.0901656	0.8409423
C	-0.7868776	3.5601528	-2.7417630	Br	-1.2273099	-3.1212355	3.1598662
H	0.0160953	3.8302868	-3.4585156	H	-0.3880095	-4.1167825	-1.4005762
H	-1.7512403	3.8916553	-3.1782054	H	-1.1088555	-5.3968201	-0.3260283
H	-0.8156752	2.4581586	-2.6569030	H	-3.5045248	-2.9330150	1.5287569
C	-0.4400993	5.7425585	-1.5023675	H	-3.9815278	-5.5987609	-0.6252707
H	0.4845686	3.8523137	-1.0455462	H	-4.5759784	0.4661845	0.1260764
H	0.3233750	6.0379832	-2.2516437	H	-3.2089005	4.3712071	-1.5465431
H	-0.1768517	6.2249810	-0.5399213				
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H	4.7349735	-1.2625949	-4.7898127				
H	4.3611985	-5.6479097	1.6825244				
C	1.3472422	-4.8224520	-3.9007369				
H	3.0191133	1.3780120	-4.0854001				
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H	2.2249073	-4.5327025	2.5123818				
C	2.1091794	-3.9007166	-2.9572089				
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C	4.1040455	-5.3269977	0.6520589				
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C	2.4056387	-4.3002310	-1.6446452				
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H	1.7438774	-6.1813109	-5.5826197				
H	2.0870459	-5.3036103	-1.3169296				
C	2.6356576	0.3751784	-3.8054784				
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H	5.7636673	-1.1562884	-3.3274241				
C	3.2051357	-1.7477371	-2.4943827				
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C	3.7113260	-0.4122632	-3.0376581				
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H	1.7264995	0.5141125	-3.1891130				
H	1.5724972	-3.1220507	1.6438315				
H	2.3435100	-0.1361970	-4.7465749				
H	-0.4691271	-3.5792864	-3.8669109				
H	1.2987977	-4.7973263	1.0087320				
H	2.7676487	-4.7087585	-5.5703076				
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H	2.3790763	-2.3138562	-4.4087576				
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C	-5.3205587	-3.3559566	2.6408276				
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C	-6.5941316	-2.8832816	3.0134758				
H	-4.9551409	-4.3248928	3.0121992				
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H	-8.0524370	-1.2719694	2.8547989				
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TS1

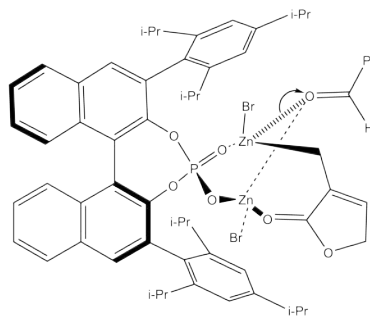


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C	2.3607733	4.6150283	1.5505186
C	2.9852259	5.8925028	1.6746833
C	0.9443376	4.4926350	1.5250626
H	0.3302514	5.4023660	1.6082469
C	0.3130844	3.2747644	1.2989922
C	3.8908178	-1.1565451	-0.1308797
C	5.0450019	-1.3165617	0.6287813
H	5.7354633	-2.1407102	0.3909148
C	5.3282601	-0.4869078	1.7517371
C	6.4512133	-0.7429293	2.5947787
C	4.4369839	0.6003973	2.0769411
C	4.6731172	1.3299642	3.2801517
C	3.3385308	0.8953932	1.1868004
C	3.0699546	-0.0188071	0.1610226
O	0.4770386	0.8803847	1.2414591
O	1.9902049	0.2100041	-0.6839565
P	0.4689535	-0.0392569	-0.1230741
O	-0.4310765	0.5763905	-1.2101393
O	0.2320097	-1.4699751	0.3234924
C	4.3595345	6.0288185	1.5603680
C	5.1582868	4.8855101	1.2947123
H	2.3454645	6.7740299	1.8384326
H	4.8290232	7.0202939	1.6494283
H	5.2182545	2.7586541	0.9753418
H	6.2450376	4.9969014	1.1598497
C	5.7596594	1.0386675	4.0932478
C	6.6693485	0.0067446	3.7405882
H	3.9733272	2.1278222	3.5650705
H	5.9135461	1.6098503	5.0213989
H	7.5338491	-0.2082358	4.3869724
H	7.1314058	-1.5666942	2.3266481
C	-1.5384153	3.7918462	-0.2993528

C	-1.1465506	3.2513714	0.9608156	H	4.0160648	0.1988369	-2.1845876
C	-2.9092946	3.9480839	-0.5648828	H	3.9386121	-3.2538138	1.2328087
C	-2.1299058	2.7891467	1.8736283	H	2.3875776	-2.3428630	-4.4091832
C	-3.4919944	2.9610547	1.5508656	Zn	-2.2246057	0.0581679	-1.7160483
C	-3.9037469	3.5744355	0.3534264	Br	-3.9759153	1.1817332	-2.7307329
C	-1.7472521	2.1571931	3.2095628	C	-5.3468931	-3.3542045	2.6224320
H	-4.2506536	2.6387768	2.2832052	C	-4.5294421	-2.5897305	1.7865887
C	-2.2223893	0.6972246	3.3041352	C	-4.9641762	-1.3148293	1.3516155
H	-3.3300702	0.6226727	3.2571036	C	-6.2287380	-0.8216911	1.7572298
H	-1.9019425	0.2342312	4.2592654	C	-7.0462054	-1.5960156	2.5871018
H	-1.7988242	0.0785423	2.4905552	C	-6.6037506	-2.8602946	3.0197998
C	-2.2472828	2.9981415	4.3979099	H	-4.9917298	-4.3323274	2.9794185
H	-0.6395603	2.1431137	3.2645166	C	-4.1354047	-0.4978662	0.4740623
H	-3.3562681	3.0417880	4.4298131	H	-6.5568816	0.1706491	1.4134570
H	-1.8729699	4.0404176	4.3396973	H	-8.0288871	-1.2162803	2.9041192
H	-1.9040895	2.5616962	5.3585354	H	-7.2448923	-3.4653567	3.6796997
C	-5.3613423	3.9215550	0.0701782	O	-3.0180753	-0.8546959	0.0493532
C	-6.3309567	2.7446995	0.2455971	C	-3.7168525	-4.6534664	-1.1910095
H	-7.3698445	3.0534873	0.0086758	C	-2.4928552	-4.0466724	-1.2831746
H	-6.3323250	2.3752229	1.2931366	C	-2.7378853	-2.7827006	-2.0123972
H	-6.0651236	1.9098370	-0.4343953	O	-4.0360933	-2.6518171	-2.3405019
C	-5.7924481	5.1289389	0.9254140	C	-4.7524664	-3.8002605	-1.8460108
H	-5.4108371	4.2273115	-0.9974343	O	-1.9056762	-1.9020351	-2.2837278
H	-6.8279575	5.4444873	0.6795646	C	-1.1728333	-4.3348278	-0.7259970
H	-5.1195382	5.9947938	0.7641402	H	-5.2699984	-4.2777104	-2.7078611
H	-5.7602636	4.8793584	2.0069875	H	-5.5350162	-3.4304389	-1.1447061
C	-0.5261099	4.2207398	-1.3647878	Zn	-0.8099954	-3.0896031	0.8266114
C	-0.8043970	3.5780506	-2.7349382	Br	-1.2935406	-3.1599886	3.1221962
H	-0.0048227	3.8530032	-3.4534472	H	-0.3601473	-4.0682187	-1.4309558
H	-1.7709940	3.9077317	-3.1673856	H	-1.0686554	-5.3829284	-0.3872163
H	-0.8297996	2.4756898	-2.6566092	H	-3.5368773	-2.9549829	1.4921950
C	-0.4566653	5.7547403	-1.4864445	H	-3.9457166	-5.6024110	-0.6878670
H	0.4727167	3.8642714	-1.0417871	H	-4.5469434	0.4896092	0.1537443
H	0.3036534	6.0551742	-2.2367439	H	-3.2219411	4.3808660	-1.5279431
H	-0.1908683	6.2336361	-0.5230843				
H	-1.4332405	6.1726703	-1.8092413				
H	0.9294849	-5.6595677	-3.2605922				
H	4.7393838	-1.2865930	-4.7887729				
H	4.3490732	-5.6282851	1.7165591				
C	1.3666671	-4.8540108	-3.8919868				
H	3.0125326	1.3539143	-4.1036521				
H	-0.4097861	-4.8734783	-5.1770789				
H	2.2014350	-4.5147330	2.5256429				
C	2.1177343	-3.9220379	-2.9497134				
C	4.9674914	-0.6567005	-3.9033554				
C	0.2049777	-4.1447828	-4.6097294				
H	0.5748150	-3.3925395	-5.3371423				
C	2.5613922	-2.6557172	-3.3680463				
C	4.0969772	-5.3149561	0.6825415				
H	3.1333630	-6.0729213	-4.3779781				
C	2.4078965	-4.3113090	-1.6328970				
C	2.3256662	-5.5187764	-4.8970611				
H	1.7848538	-6.2303418	-5.5553199				
H	2.0901461	-5.3132801	-1.3000396				
C	2.6316525	0.3515220	-3.8191449				
H	5.3750469	0.3083463	-4.2700118				
H	5.7624220	-1.1692604	-3.3245027				
C	3.2038891	-1.7626726	-2.4955512				
C	2.0133696	-4.1109734	1.5101405				
C	3.0608872	-3.4643568	-0.7166298				
H	5.0427230	-5.2167231	0.1115226				
H	3.5146069	-6.1398758	0.2217779				
C	3.7076038	-0.4288523	-3.0448142				
C	3.4199860	-2.1515220	-1.1418680				
C	3.3118724	-3.9916453	0.6981400				
H	1.7202055	0.4917705	-3.2066783				
H	1.5502483	-3.1133684	1.6444314				
H	2.3425270	-0.1647269	-4.7584578				
H	-0.4515226	-3.6120582	-3.8930462				
H	1.2862447	-4.7936763	1.0191588				
H	2.8064548	-4.7565377	-5.5455964				

7.8.5 Pathway 14d-ma ↔ 14j-mi TS1; COSMO

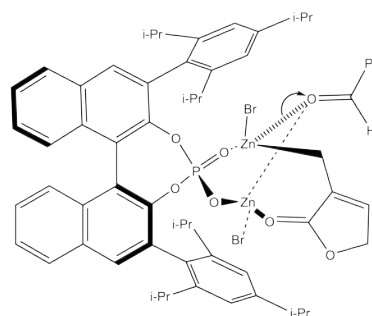


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C	1.9765381	1.9830327	1.7391123
C	2.7339626	3.1487756	2.1277478
C	4.1521843	3.1210652	2.2887070
C	2.0460229	4.3985217	2.3431717
C	2.7925837	5.5461092	2.7457127
C	0.6338447	4.4577638	2.1633218
H	0.1040780	5.3908332	2.4095351
C	-0.0868608	3.3728657	1.6809430
C	3.0981622	-1.5037918	0.5594323
C	3.7889451	-1.9503192	1.6801083
H	4.2834380	-2.9329469	1.6485412
C	3.8335076	-1.1997312	2.8885549
C	4.4623532	-1.7258824	4.0567793
C	3.1951144	0.0922901	2.9512402
C	3.1565618	0.7644957	4.2091104

C	2.5829797	0.6223788	1.7564183	C	4.0631851	-5.6833118	-4.3662684
C	2.5156867	-0.2035937	0.6348399	H	4.0056907	-6.4075311	-5.2056678
O	-0.1267655	1.1139367	0.9149038	H	1.5169168	-5.2990262	-1.6950476
O	1.8681358	0.2782361	-0.5047890	C	3.9168447	0.2094457	-3.0812308
P	0.2338114	0.2941339	-0.4848117	H	6.5605666	-0.1618795	-2.2645556
O	-0.1333060	1.0888589	-1.7526953	H	6.3372266	-1.7342141	-1.4261814
O	-0.4149576	-1.0674271	-0.2356318	C	3.6103692	-2.0011412	-1.8724530
C	4.1688872	5.4811995	2.9066534	C	-0.0942086	-4.2572896	0.3429915
C	4.8524300	4.2595267	2.6640002	C	2.1648986	-3.5422326	-0.6028208
H	2.2525613	6.4908114	2.9164292	H	3.0952498	-4.8855965	1.6620949
H	4.7339182	6.3754126	3.2111723	H	2.0573006	-6.0311236	0.7614241
H	4.6923420	2.1829288	2.0976302	C	4.4609128	-0.7383966	-1.9969848
H	5.9472234	4.2154508	2.7698664	C	2.9507445	-2.3558466	-0.6625959
C	3.7584106	0.2160547	5.3332521	C	1.3806569	-3.9398662	0.6466025
C	4.4330022	-1.0316215	5.2566626	H	2.8606161	0.4744890	-2.8794051
H	2.6246033	1.7220404	4.2900916	H	-0.5593036	-3.4240781	-0.2192778
H	3.7038328	0.7498010	6.2944569	H	3.9732691	-0.2509606	-4.0900207
H	4.9127918	-1.4530227	6.1532659	H	1.2383792	-3.7951269	-5.2522995
H	4.9548182	-2.7088569	3.9899716	H	-0.2137129	-5.1940893	-0.2424042
C	-2.2024512	3.8407472	0.3570979	H	4.8504532	-4.9407220	-4.6145186
C	-1.5801361	3.3961790	1.5540247	H	4.4087862	-0.1969936	-1.0309629
C	-3.6069096	3.8584623	0.2963280	H	1.3705148	-3.0694720	1.3326502
C	-2.3652364	2.9414663	2.6471854	H	4.0230682	-2.5791456	-3.9149227
C	-3.7691506	2.9904282	2.5389776	Zn	-1.7346239	0.6075398	-2.7816803
C	-4.4105866	3.4530743	1.3784669	Br	-2.5465398	1.4190016	-4.8099872
C	-1.7166265	2.4475104	3.9409113	Zn	-1.6302279	-1.1196813	1.4136951
H	-4.3734761	2.6487602	3.3910265	Br	-0.2017460	-1.5991093	3.2482777
C	-2.4390836	1.2472653	4.5699965	H	-4.1018783	4.1950241	-0.6280118
H	-3.4550563	1.5093984	4.9326526	C	-0.9881311	-5.6339492	-3.5721631
H	-1.8638835	0.8698338	5.4390005	C	-1.1394336	-4.2647073	-3.3421011
H	-2.5230683	0.4097270	3.8506107	C	-1.4792142	-3.4091989	-4.4183070
C	-1.5803407	3.6034053	4.9510994	C	-1.6548937	-3.9349689	-5.7202850
H	-0.6919455	2.1016591	3.6906843	C	-1.4966651	-5.3078564	-5.9434449
H	-2.5791349	3.9981362	5.2336652	C	-1.1656215	-6.1544279	-4.8696818
H	-0.9925050	4.4436704	4.5305790	H	-0.7238177	-6.3055424	-2.7414091
H	-1.0732745	3.2600894	5.8767241	C	-1.6447247	-1.9769523	-4.2015103
C	-5.9275933	3.5762312	1.2701010	H	-1.9122935	-3.2575642	-6.5499898
C	-6.7029170	2.6342356	2.2007019	H	-1.6284288	-5.7231527	-6.9535955
H	-7.7876649	2.6647234	1.9715546	H	-1.0394557	-7.2339081	-5.0457503
H	-6.5879175	2.9281062	3.2646819	O	-1.5378697	-1.4449984	-3.0822504
H	-6.3556075	1.5855129	2.1062574	H	-0.9875788	-3.8290095	-2.3442680
C	-6.3622705	5.0393831	1.4904142	H	-1.8851924	-1.3422163	-5.0937360
H	-6.1886080	3.3129449	0.2189717	C	-5.8648083	-0.4434770	0.3642001
H	-7.4573507	5.1570222	1.3521200	C	-4.5060200	-0.5122532	0.4501996
H	-5.8496603	5.7239531	0.7853807	C	-4.0134608	0.2210117	-0.7373442
H	-6.1088434	5.3663940	2.5206433	O	-5.0292215	0.7062090	-1.4741707
C	-1.3656930	4.2991649	-0.8350931	C	-6.2685701	0.3282990	-0.8447247
C	-2.0514026	4.0505014	-2.1836528	O	-2.8353081	0.3898408	-1.0775449
H	-1.3290704	4.1444135	-3.0181066	C	-3.6335317	-1.1830831	1.4597664
H	-2.8718008	4.7732546	-2.3760247	H	-6.8647132	-0.2631741	-1.5736120
H	-2.4986686	3.0392220	-2.2381355	H	-6.8386017	1.2545560	-0.6128534
C	-0.9696260	5.7835244	-0.7092815	H	-3.8886619	-2.2672869	1.4783945
H	-0.4333465	3.6947144	-0.8243566	H	-3.9226748	-0.8160434	2.4690242
H	-0.3574667	6.0988983	-1.5795221	H	-6.5888491	-0.8902046	1.0602260
H	-0.3812731	5.9797606	0.2072370				
H	-1.8751825	6.4251872	-0.6770043				
H	1.9629906	-5.7806453	-3.8917228				
H	6.0878015	-1.6169033	-3.1960272				
H	1.4940249	-5.3447391	2.3226101				
C	2.7061434	-4.9910116	-4.1392187				
H	4.5082884	1.1480449	-3.1107627				
H	2.1057553	-5.0086288	-6.2481358				
H	-0.6535972	-4.3852655	1.2925862				
C	2.7650307	-4.0519835	-2.9405972				
C	5.9429652	-1.0835207	-2.2331568				
C	2.2188414	-4.2843781	-5.4150053				
H	2.9357411	-3.5050229	-5.7477468				
C	3.5008732	-2.8549675	-2.9846000				
C	2.0458216	-5.1135553	1.3879015				
H	4.3928730	-6.2301363	-3.4598259				
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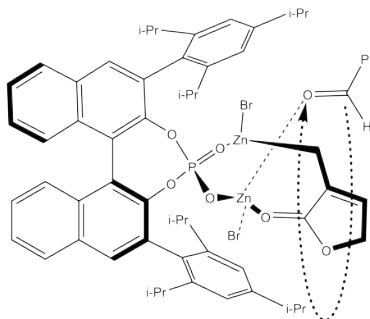
TS1



Energy (Hartree) = -11970.01716103
number of imaginary frequencies: 2

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C	1.9596952	1.9709390	1.7248571	H	1.9990113	-5.8102984	-3.8887804
C	2.7142729	3.1386342	2.1127826	H	6.0982382	-1.6264655	-3.1853681
C	4.1319520	3.1133953	2.2763868	H	1.4878781	-5.3540808	2.3200980
C	2.0244036	4.3874987	2.3254807	C	2.7423512	-5.0193853	-4.1329254
C	2.7686780	5.5360352	2.7277816	H	4.5093867	1.1344308	-3.1142552
C	0.6126519	4.4430016	2.1444592	H	2.1655986	-5.0518985	-6.2492208
H	0.0789979	5.3741696	2.3898352	H	-0.6543731	-4.3968095	1.2801694
C	-0.1057155	3.3561564	1.6632010	C	2.7853941	-4.0734824	-2.9390175
C	3.0918911	-1.5149738	0.5544225	C	5.9457315	-1.0915383	-2.2245669
C	3.7828114	-1.9566034	1.6766152	C	2.2668553	-4.3229541	-5.4185906
H	4.2796330	-2.9380634	1.6462837	H	2.9846509	-3.5434476	-5.7485921
C	3.8249321	-1.2034075	2.8830491	C	3.5144229	-2.8727218	-2.9836713
C	4.4553411	-1.7237098	4.0523866	C	2.0428446	-5.1272456	1.3865578
C	3.1821039	0.0863904	2.9421300	H	4.4249541	-6.2475856	-3.4261700
C	3.1414204	0.7616073	4.1980672	C	2.1215641	-4.3891207	-1.7425800
C	2.5688198	0.6116481	1.7456545	C	4.1038101	-5.7089014	-4.3401946
C	2.5046238	-0.2169317	0.6258172	H	4.0599077	-6.4386188	-5.1757192
O	-0.1402725	1.0979584	0.8959262	H	1.5395465	-5.3238007	-1.6941113
O	1.8600248	0.2600261	-0.5168457	C	3.9197299	0.1948364	-3.0850713
P	0.2265844	0.2806942	-0.5055763	H	6.5614410	-0.1686232	-2.2545637
O	-0.1309161	1.0834565	-1.7709583	H	6.3371655	-1.7399723	-1.4146672
O	-0.4306179	-1.0778352	-0.2613764	C	3.6149554	-2.0151974	-1.8738826
C	4.1441332	5.4734496	2.8916563	C	-0.0923453	-4.2706215	0.3321250
C	4.8294213	4.2528594	2.6519372	C	2.1703378	-3.5586813	-0.6064800
H	2.2268618	6.4801404	2.8960903	H	3.0913318	-4.8993340	1.6637335
H	4.7070908	6.3688492	3.1963374	H	2.0571161	-6.0467597	0.7630051
H	4.6725443	2.1751490	2.0879810	C	4.4616290	-0.7498364	-1.9972101
H	5.9239402	4.2101157	2.7604578	C	2.9514141	-2.3695955	-0.6663615
C	3.7459760	0.2185600	5.3227823	C	1.3817152	-3.9547971	0.6404436
C	4.4245466	-1.0263709	5.2497019	H	2.8628837	0.4600919	-2.8877950
H	2.6054006	-1.7169653	4.2764038	H	-0.5544004	-3.4361602	-0.2309024
H	3.6890516	0.7545645	6.2824875	H	3.9807152	-0.2664721	-4.0931978
H	4.9052654	-1.4440999	6.1474210	H	1.2838721	-3.8342145	-5.2704775
H	4.9495869	-2.7058845	3.9882593	H	-0.2115451	-5.2077915	-0.2533198
C	-2.2335222	3.8178202	0.3538670	H	4.8915723	-4.9652104	-4.5827456
C	-1.5999275	3.3787002	1.5468640	H	4.4029332	-0.2071954	-1.0323369
C	-3.6383481	3.8502466	0.3128825	H	1.3682353	-3.0841935	1.3262468
C	-2.3744264	2.9379441	2.6531251	H	4.0402674	-2.5970904	-3.9119565
C	-3.7790360	2.9995003	2.5633045	Zn	-1.7362049	0.6479545	-2.8058393
C	-4.4309023	3.4630643	1.4094357	Br	-2.5355123	1.4046522	-4.8490695
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C	-2.4211781	1.2421053	4.5763002	H	-4.1421327	4.1853455	-0.6072329
H	-3.4415222	1.4903953	4.9367456	C	-0.9518450	-5.6082203	-3.5925467
H	-1.8424538	0.8754790	5.4473407	C	-1.1045124	-4.2389066	-3.3623580
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C	-1.5844080	3.6077707	4.9516474	C	-1.6096039	-3.9098514	-5.7415704
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H	-1.0070211	4.4532319	4.5274364	H	-0.6894042	-6.2777050	-2.7595912
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C	-5.9471089	3.6125931	1.3250320	H	-1.8633770	-3.2318557	-6.5720650
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H	-6.3950934	1.6211841	2.1492357	H	-0.9559058	-3.8034275	-2.3637665
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H	-7.4479500	5.2202768	1.4463533	C	-4.5038490	-0.4687667	0.4563086
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TS2; COSMO



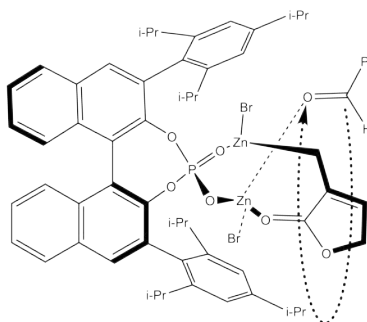
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C	-0.7856758	-4.4797203	-3.6473517
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H	3.6524409	-4.0039113	2.2421963
H	2.7266266	-5.5302888	2.1111420
C	3.3939721	-1.4036873	-2.2373372
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H	1.7503990	-0.2562402	-3.0970884
H	-0.7024212	-3.9410682	1.9491652
H	2.4948819	-1.4086655	-4.2577278
H	-1.4263271	-3.8054683	-3.0447130
H	0.1580303	-5.4916658	2.1198312
H	1.7042903	-5.6485089	-4.2805645
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H	1.4835367	-2.7083573	2.3539110
H	1.9141623	-3.3036533	-3.4862765
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Br	1.2422696	2.4856460	-2.0057551
Zn	-2.4352999	-2.5065378	1.6906572
Br	-3.4201831	-2.4646434	3.7996958
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C	-1.3239562	-1.0959513	-6.0240899
C	-0.3022991	-0.1207145	-5.9158192
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H	-2.1534058	-2.6957480	-7.2318511
C	-0.2008205	0.7091143	-4.7183215
H	1.4671940	0.7615764	-6.8327122
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H	-0.4398523	-2.4514050	-9.0417970

O	-1.0334731	0.6625679	-3.7961934
H	-2.0563380	-1.1847057	-5.2076784
H	0.6879341	1.3852766	-4.6258805
C	-4.6211545	-1.5664316	-0.9888936
C	-3.3549780	-2.0832526	-0.8960645
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O	-3.2123598	-0.0873294	-2.0895394
C	-4.5906006	-0.2631659	-1.7107883
O	-1.2534456	-1.1512455	-1.7743066
C	-2.8093260	-3.2278883	-0.1566695
H	-5.2105439	-0.2204898	-2.6331606
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H	-1.8453605	-3.5731426	-0.5781684
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TS2



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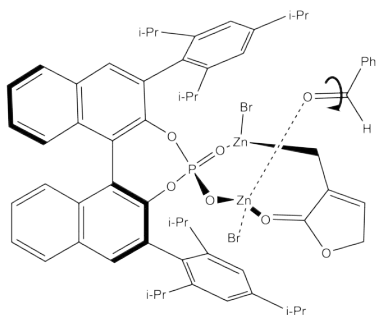
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C	4.5884557	4.6814307	0.5012889
H	1.9659714	6.7420151	1.3121856
H	4.3148168	6.8521291	0.4623209
H	4.5994717	2.5299673	0.6360448
H	5.6069514	4.7253967	0.0860410
C	5.8008684	1.3080586	3.9044799
C	6.5496892	0.1301800	3.6429450
H	4.0165989	2.4434853	3.4819550
H	6.1799223	2.0482664	4.6255627
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C	2.4837503	-2.4593513	-1.5927136
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C	1.5011046	-3.7508049	1.9233865
H	1.7008155	-0.2760929	-3.1252221
H	-0.6844818	-3.9010469	1.9906334
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H	-1.4647326	-3.8602509	-3.0100112

H	0.1380990	-5.4794285	2.1113164
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Br	-3.4638500	-2.4503773	3.7867859
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C	-0.2711099	-0.1241360	-5.9158783
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C	4.2677154	5.8638586	1.9540141
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H	2.2593612	6.6665453	2.0662468
H	4.7549298	6.8460944	2.0506043
H	5.0810549	2.5543068	1.5374526
H	6.1524317	4.7756891	1.7383301
C	5.1570999	0.9311471	4.8588144
C	6.0332096	-0.1746030	4.6930831
H	3.5360829	2.0893107	4.0340835
H	5.2239289	1.5506196	5.7662642
H	6.7860904	-0.3996662	5.4638447
H	6.5747906	-1.8576875	3.4426350
C	-1.8901009	3.6851893	0.1356125
C	-1.3113195	3.1234726	1.3125557
C	-3.2851413	3.6168380	-0.0266772
C	-2.1416533	2.4892608	2.2753634
C	-3.5330454	2.4474904	2.0595459
C	-4.1311344	3.0137360	0.9231934
C	-1.5865130	1.8916247	3.5665963
H	-4.1632843	1.9597771	2.8173971
C	-1.9272566	0.3984062	3.7039781
H	-3.0215383	0.2295155	3.7822975
H	-1.4630981	-0.0258211	4.6182393
H	-1.5597697	-0.1845922	2.8384646
C	-2.0560679	2.7001164	4.7911546
H	-0.4816933	1.9757922	3.5336823
H	-3.1594059	2.6556754	4.9070616
H	-1.7701123	3.7683286	4.7035361
H	-1.6049024	2.2980070	5.7219728
C	-5.6427377	3.0469790	0.7150451
C	-6.4125330	2.0114948	1.5428388
H	-7.4811941	1.9961127	1.2480430
H	-6.3750816	2.2491596	2.6264628
H	-6.0062906	0.9901690	1.4055570
C	-6.1871203	4.4668905	0.9728027
H	-5.8196346	2.8167657	-0.3606870
H	-7.2755435	4.5207609	0.7617150
H	-5.6763333	5.2210074	0.3410082
H	-6.0288620	4.7554747	2.0331061
C	-1.0506892	4.3793315	-0.9383164
C	-1.4275677	3.9597014	-2.3673027
H	-0.7035852	4.3714213	-3.0986990
H	-2.4343827	4.3238003	-2.6610971
H	-1.4212924	2.8616555	-2.4799303
C	-1.1344979	5.9124404	-0.7997799
H	0.0043474	4.0762595	-0.7806900
H	-0.4903377	6.4111931	-1.5533889
H	-0.8177019	6.2598496	0.2031861
H	-2.1763483	6.2629453	-0.9578032
H	1.2337560	-5.7999977	-3.1093850
H	5.4037267	-1.6077793	-3.9426946
H	3.3792418	-5.8091486	2.5407294
C	1.8911146	-5.0715675	-3.6346756
H	3.7398332	1.0832453	-3.5747027
H	0.5244781	-5.0618968	-5.3471265
H	1.2563315	-4.4037428	2.8219860
C	2.4439491	-4.1358767	-2.5665542
C	5.5168191	-0.9941829	-3.0243207
C	1.0323307	-4.3372640	-4.6782996
H	1.6479868	-3.6741086	-5.3206821
C	3.0099609	-2.8933094	-2.8975401
C	3.3855065	-5.5398661	1.4645555
H	3.6116198	-6.4426486	-3.5589148
C	2.4250993	-4.5040201	-1.2110224
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H	2.6214592	-6.5862716	-5.0516389

TS3; COSMO



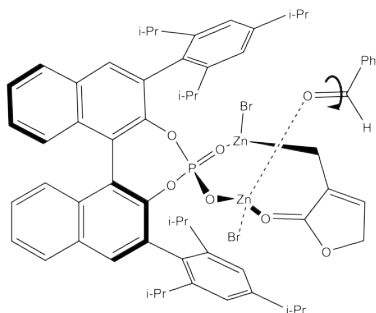
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C	4.4558596	3.4466795	1.6767307
C	2.2368566	4.4999400	1.8337070
C	2.8846384	5.7649502	1.9692773
C	0.8179462	4.4076886	1.7617578
H	0.2232401	5.3282741	1.8575552
C	0.1692697	3.2013686	1.5262120
C	3.7571194	-1.3926627	0.5220592
C	4.7721090	-1.5833522	1.4526968
H	5.4387295	-2.4544743	1.3546214
C	4.9433814	-0.7095809	2.5652851
C	5.9210317	-0.9803544	3.5698003
C	4.0890466	0.4461780	2.7051098
C	4.2115280	1.2348027	3.8885663
C	3.1366854	0.7443356	1.6604677
C	2.9621740	-0.2085468	0.6503140

H	1.9965457	-5.4827735	-0.9392576
C	3.2490918	0.1233204	-3.3132955
H	6.0256731	-0.0499660	-3.3094203
H	6.1812060	-1.5480002	-2.3299544
C	3.4960986	-2.0075427	-1.9214525
C	1.3428442	-4.0588759	1.7714750
C	2.9022509	-3.6597017	-0.1897580
H	4.4327276	-5.5897674	1.1030702
H	2.8073043	-6.3204259	0.9277436
C	4.1480230	-0.7027202	-2.3776153
C	3.4149035	-2.3787781	-0.5483226
C	2.7910538	-4.1362608	1.2606672
H	2.2800563	0.3621631	-2.8355610
H	0.9753568	-3.0126196	1.7447736
H	3.0363140	-0.4045094	-4.2656458
H	0.2617754	-3.7033874	-4.1958012
H	0.6726245	-4.7104382	1.1662766
H	3.7253108	-5.1885269	-4.8326941
H	4.3444271	-0.0858031	-1.4775344
H	3.3771772	-3.4433228	1.8934816
H	3.0669647	-2.5933093	-3.9551189
Zn	-0.8941984	0.3480273	-2.9874880
Br	-0.3006224	1.2017613	-5.0474001
Zn	-1.1090271	-3.1113033	0.3718743
Br	-2.3140803	-3.2081349	2.3928088
H	-3.7367880	4.0552517	-0.9319199
C	-5.1178576	-1.6863634	0.3874141
C	-4.2995028	-0.8517153	-0.3778252
C	-4.8775724	0.0087406	-1.3428948
C	-6.2801283	0.0400880	-1.5189117
C	-7.0957909	-0.8085566	-0.7592617
C	-6.5135560	-1.6704232	0.1882798
H	-4.6586884	-2.3471057	1.1401401
C	-4.0228776	0.8257008	-2.2045283
H	-6.7203241	0.7217727	-2.2641736
H	-8.1870959	-0.7962639	-0.8984924
H	-7.1552330	-2.3324735	0.7900202
O	-2.7986935	0.6833410	-2.2542191
H	-3.2071965	-0.8416543	-0.2366985
H	-4.5293229	1.5872361	-2.8545008
C	-3.5620078	-4.0704552	-2.4084657
C	-2.2758087	-3.6837780	-2.1422257
C	-2.1109360	-2.3854528	-2.8271173
O	-3.2318335	-2.0262356	-3.4772783
C	-4.2329857	-3.0461326	-3.2599857
O	-1.0954407	-1.6709955	-2.8245888
C	-1.2022664	-4.2237973	-1.3040395
H	-4.5610324	-3.4182135	-4.2554246
H	-5.1074505	-2.5588132	-2.7724547
H	-0.2088892	-4.0718834	-1.7692075
H	-1.3551201	-5.2876196	-1.0426637
H	-4.0654752	-4.9788123	-2.0515985

C	3.0223060	3.2978799	1.7218162
C	4.4417523	3.4441260	1.6785404
C	2.2210916	4.4926766	1.8338916
C	2.8665558	5.7576568	1.9752448
C	0.8029186	4.3976464	1.7585056
H	0.2051049	5.3160016	1.8559788
C	0.1567681	3.1913349	1.5174364
C	3.7552928	-1.3960286	0.5172681
C	4.7707343	-1.5826947	1.4478870
H	5.4393677	-2.4522245	1.3488514
C	4.9391282	-0.7088000	2.5603834
C	5.9170880	-0.9752925	3.5650385
C	4.0805653	0.4436195	2.6998515
C	4.1996796	1.2321025	3.8834158
C	3.1281976	0.7394398	1.6545352
C	2.9567458	-0.2143138	0.6446096
O	0.3001226	0.8036236	1.3243464
O	2.0362196	0.0173441	-0.3608845
P	0.4136333	-0.0069278	-0.0993635
O	-0.1475099	0.8190297	-1.2611295
O	-0.1325700	-1.3975163	0.1754177
C	4.2488993	5.8591863	1.9639859
C	5.0389121	4.6916242	1.7950706
H	2.2392624	6.6577210	2.0731927
H	4.7339719	6.8419590	2.0650827
H	5.0679937	2.5528525	1.5378752
H	6.1354922	4.7751849	1.7492804
C	5.1460734	0.9322098	4.8533599
C	6.0262140	-0.1695848	4.6879397
H	3.5206926	2.0838263	4.0277799
H	5.2101324	1.5519888	5.7607139
H	6.7798731	-0.3919112	5.4586441
H	6.5741242	-1.8501842	3.4379408
C	-1.9021862	3.6825182	0.1290403
C	-1.3236454	3.1135231	1.3024184
C	-3.2980639	3.6227571	-0.0291638
C	-2.1542634	2.4769071	2.2633646
C	-3.5462521	2.4440640	2.0511632
C	-4.1446671	3.0215645	0.9211102
C	-1.5998675	1.8683965	3.5497277
H	-4.1762243	1.9557848	2.8087377
C	-1.9466988	0.3758385	3.6783390
H	-3.0412534	0.2093185	3.7576417
H	-1.4832593	-0.0570820	4.5884950
H	-1.5816868	-0.2046539	2.8102180
C	-2.0637517	2.6719414	4.7795699
H	-0.4948647	1.9481067	3.5157046
H	-3.1669197	2.6321942	4.8978433
H	-1.7736739	3.7393252	4.6978721
H	-1.6132633	2.2622136	5.7072291
C	-5.6571887	3.0717683	0.7227820
C	-6.4331532	2.0447449	1.5553452
H	-7.5040112	2.0401141	1.2680282
H	-6.3871711	2.2835822	2.6382310
H	-6.0384793	1.0189927	1.4185062
C	-6.1839733	4.4972262	0.9855170
H	-5.8445985	2.8439439	-0.3520994
H	-7.2731992	4.5648958	0.7826303
H	-5.6683204	5.2466049	0.3523882
H	-6.0140892	4.7826396	2.0445964
C	-1.0619970	4.3760156	-0.9448346
C	-1.4422464	3.9612594	-2.3742787
H	-0.7179690	4.3694894	-3.1069061
H	-2.4473566	4.3313283	-2.6670766
H	-1.4404522	2.8637815	-2.4911407
C	-1.1399131	5.9090224	-0.8032185
H	-0.0078944	4.0685864	-0.7896033
H	-0.4953909	6.4068924	-1.5568921
H	-0.8204175	6.2538952	0.1995992
H	-2.1804604	6.2644355	-0.9582365
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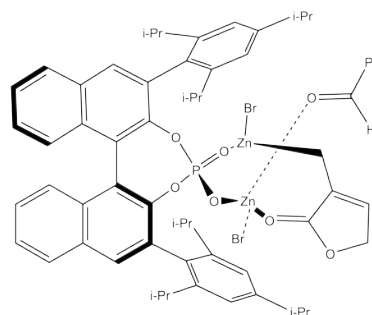
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number of imaginary frequencies: 1

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C	2.3593658	2.0167968	1.6243815

H	5.4037530	-1.6137804	-3.9454968
H	3.3859491	-5.8035275	2.5501184
C	1.9130276	-5.0937163	-3.6332955
H	3.7264571	1.0728410	-3.5859563
H	0.5543279	-5.0998974	-5.3524033
H	1.2529036	-4.4035400	2.8196829
C	2.4560773	-4.1509576	-2.5663236
C	5.5128417	-0.9971363	-3.0288321
C	1.0539755	-4.3696033	-4.6836004
H	1.6670377	-3.7046454	-5.3263724
C	3.0148950	-2.9060362	-2.8992390
C	3.3939078	-5.5373892	1.4731950
H	3.6421683	-6.4526930	-3.5438865
C	2.4365240	-4.5153185	-1.2100435
C	3.0548722	-5.8880302	-4.2956057
H	2.6604759	-6.6098125	-5.0409607
H	2.0123124	-5.4955483	-0.9365932
C	3.2408050	0.1112180	-3.3224775
H	6.0183493	-0.0520334	-3.3165313
H	6.1786270	-1.5468085	-2.3327842
C	3.4962619	-2.0157247	-1.9252254
C	1.3434699	-4.0643046	1.7677761
C	2.9075295	-3.6662241	-0.1903689
H	4.4419065	-5.5847723	1.1140372
H	2.8217228	-6.3235174	0.9381006
C	4.1423312	-0.7091205	-2.3844291
C	3.4159968	-2.3845914	-0.5516052
C	2.7934144	-4.1376272	1.2615937
H	2.2711226	0.3493866	-2.8460366
H	0.9712896	-3.0198405	1.7356260
H	3.0293408	-0.4173695	-4.2745764
H	0.2764292	-3.7392161	-4.2080845
H	0.6771015	-4.7211055	1.1641820
H	3.7536798	-5.2041364	-4.8213991
H	4.3357072	-0.0894441	-1.4856015
H	3.3744141	-3.4392654	1.8932684
H	3.0706806	-2.6073148	-3.9571710
Zn	-0.8631042	0.3653847	-3.0201903
Br	-0.3066107	1.2220649	-5.0748325
Zn	-1.1090680	-3.1226511	0.3696734
Br	-2.3295425	-3.2361329	2.3667074
H	-3.7493662	4.0707736	-0.9300470
C	-5.0951223	-1.6694135	0.4065380
C	-4.2769741	-0.8357889	-0.3609405
C	-4.8552443	0.0315368	-1.3187729
C	-6.2580743	0.0704555	-1.4866761
C	-7.0741068	-0.7775242	-0.7269893
C	-6.4911172	-1.6455327	0.2144084
H	-4.6310620	-2.3341925	1.1535789
C	-3.9980938	0.8479328	-2.1819585
H	-6.6989302	0.7588317	-2.2256798
H	-8.1661976	-0.7584753	-0.8598484
H	-7.1332304	-2.3058187	0.8177700
O	-2.7798479	0.6875494	-2.2528269
H	-3.1839781	-0.8330027	-0.2248862
H	-4.5037266	1.6275440	-2.8135276
C	-3.5454773	-4.0611308	-2.3966525
C	-2.2550571	-3.6764455	-2.1471399
C	-2.0987447	-2.3733288	-2.8296124
O	-3.2325741	-2.0111736	-3.4603693
C	-4.2291493	-3.0299629	-3.2313358
O	-1.0852593	-1.6605702	-2.8407131
C	-1.1724219	-4.2158506	-1.3251282
H	-4.5750256	-3.3949962	-4.2241414
H	-5.0943474	-2.5436927	-2.7253824
H	-0.1815041	-4.0377752	-1.7852540
H	-1.3088883	-5.2849191	-1.0771876
H	-4.0424611	-4.9705342	-2.0339594



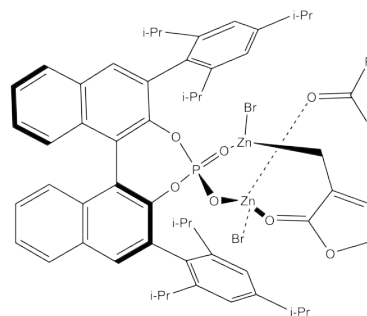
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C	4.4825288	3.1672239	0.6791246
C	2.5138648	4.4701137	1.3920161
C	3.2768124	5.6607782	1.1970241
C	1.1457889	4.5301862	1.7882348
H	0.6995873	5.5159025	1.9841840
C	0.3575846	3.3898501	1.8949606
C	2.9741142	-1.6832245	0.4147001
C	4.1261906	-1.9621405	1.1412668
H	4.6039602	-2.9473970	1.0279082
C	4.6960986	-1.0208398	2.0436056
C	5.8313094	-1.3575691	2.8410973
C	4.0989101	0.2859819	2.1758910
C	4.6346914	1.1725674	3.1593759
C	2.9682008	0.6282850	1.3447548
C	2.4128211	-0.3768028	0.5415337
O	0.2500775	0.9857459	1.8510420
O	1.2841849	-0.0954324	-0.2288510
P	-0.1648493	0.1269750	0.5230584
O	-1.0246508	0.9629867	-0.4340584
O	-0.7631202	-1.1745562	1.0557040
C	4.5904228	5.6031081	0.7552056
C	5.1908628	4.3449244	0.4816239
H	2.7934377	6.6314927	1.3899010
H	5.1640273	6.5299015	0.6016775
H	4.9547195	2.1995679	0.4578283
H	6.2243288	4.3028567	0.1049502
C	5.7277425	0.8084239	3.9337439
C	6.3446167	-0.4602261	3.7650889
H	4.1636731	2.1530172	3.3122550
H	6.1151384	1.5083083	4.6898883
H	7.2159380	-0.7337948	4.3794463
H	6.2819429	-2.3549653	2.7176355
C	-2.0229007	3.9566411	1.2334061
C	-1.1121647	3.4001834	2.1792214
C	-3.4051074	3.8229586	1.4705168
C	-1.6101071	2.7610603	3.3519496
C	-2.9989731	2.6635547	3.5390699
C	-3.9165806	3.1710590	2.6042238
C	-0.6895118	2.2216489	4.4461875
H	-3.3750694	2.1607642	4.4433043
C	-0.9919836	0.7576310	4.8091164
H	-1.9891284	0.6458827	5.2828377
H	-0.2394382	0.3770849	5.5304302
H	-0.9760088	0.1082865	3.9131707
C	-0.7437206	3.1357947	5.6858991
H	0.3522378	2.2604394	4.0693106
H	-1.7621888	3.1509042	6.1278161
H	-0.4731708	4.1805119	5.4293505
H	-0.0412899	2.7798292	6.4681989
C	-5.4182313	3.0395406	2.8221864
C	-5.8398147	1.5907654	3.1220637
H	-6.9456459	1.4956236	3.1356442

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H	-5.4677965	1.2561591	4.1119263	O	-1.2407458	-0.7192540	-3.2908951
H	-5.4303649	0.8775015	2.3786051	H	-2.7033043	-2.7227374	-3.9670832
C	-5.9080071	4.0030525	3.9195481	H	0.0293006	-0.1998181	-4.8017425
H	-5.9057386	3.3515681	1.8700038	C	-5.7270603	-0.0459658	-0.3458304
H	-7.0089401	3.9375740	4.0456711	C	-4.5052442	-0.2685755	-0.9224747
H	-5.6483484	5.0538294	3.6794004	C	-4.1878991	0.9829043	-1.6523478
H	-5.4406704	3.7551803	4.8956489	O	-5.1652627	1.8939297	-1.4944393
C	-1.5540644	4.7114747	-0.0106598	C	-6.2023218	1.3254126	-0.6735762
C	-2.3825945	4.4060730	-1.2664542	O	-3.2197341	1.2611927	-2.3794719
H	-1.9009578	4.8464122	-2.1621167	C	-3.6061689	-1.4341710	-0.8801425
H	-3.4117736	4.8165540	-1.2048254	H	-7.1528302	1.3542314	-1.2510192
H	-2.4742928	3.3191562	-1.4386125	H	-6.3297916	1.9793991	0.2172850
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H	-0.5136942	4.3905340	-0.2253577	H	-4.1748037	-2.3823535	-0.9653344
H	-1.1434564	6.7791799	-0.6288134	H	-6.2903296	-0.7484903	0.2833922
H	-0.9353653	6.5053643	1.1327494				
H	-2.5765289	6.5981127	0.4369940				
H	0.7545766	-6.7941043	-2.4134581				
H	4.5789432	-2.6874827	-4.0804790				
H	1.6994292	-4.6161551	3.4108825				
C	1.1513574	-6.0044304	-3.0889987				
H	3.2490029	0.1701939	-3.8145943				
H	-0.3323728	-6.4452010	-4.6532781				
H	-0.7281257	-3.9749718	2.6339999				
C	1.5706427	-4.8391915	-2.2004704				
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C	0.0127571	-5.5899571	-4.0352439				
H	0.3426451	-4.7870069	-4.7267558				
C	2.3135603	-3.7569706	-2.7048773				
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C	2.3324115	-6.6096959	-3.8660761				
H	2.0093433	-7.5053727	-4.4359602				
H	0.5879234	-5.6322504	-0.4491222				
C	2.6800061	-0.6937205	-3.4139537				
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H	5.4582710	-2.6558630	-2.5203025				
C	2.7412461	-2.6989863	-1.8813244				
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C	2.3954525	-2.7180383	-0.5033228				
C	1.1178864	-3.7704826	1.4726080				
H	1.8034630	-0.2898536	-2.8710793				
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H	-0.4520931	-5.3272657	1.4941824				
H	2.7513811	-5.8876079	-4.5979123				
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H	2.5891043	-3.7426526	-3.7717025				
Zn	-1.2002215	1.1399910	-2.3594462				
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Br	-3.6825459	-1.8248867	3.0478399				
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C	-0.6867300	-3.3552819	-7.2743320				
C	-1.7672009	-4.1885955	-6.9319847				
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C	-0.7195792	-0.9291305	-4.4021736				
H	0.4917477	-1.6168005	-6.6966281				
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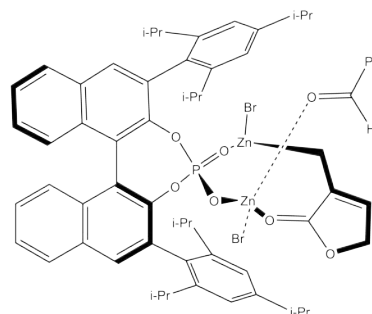


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C	2.5041179	4.4675248	1.3922716
C	3.2675093	5.6577729	1.2002796
C	1.1359196	4.5261233	1.7869567
H	0.6874885	5.5107097	1.9835668
C	0.3477335	3.3858916	1.8919757
C	2.9611725	-1.6843325	0.4059590
C	4.1117378	-1.9657359	1.1336882
H	4.5863275	-2.9523957	1.0188108
C	4.6829559	-1.0267590	2.0370560
C	5.8168714	-1.3651479	2.8347597
C	4.0879067	0.2807462	2.1697790
C	4.6248391	1.1657869	3.1536328
C	2.9582275	0.6257334	1.3385750
C	2.4018379	-0.3771771	0.5332333
O	0.2403924	0.9826496	1.8457881
O	1.2741894	-0.0931627	-0.2372230
P	-0.1747061	0.1238475	0.5183703
O	-1.0396426	0.9574699	-0.4365224
O	-0.7648839	-1.1814324	1.0490014
C	4.5816545	5.6011395	0.7617831
C	5.1825610	4.3439230	0.4880493
H	2.7831777	6.6280465	1.3927841
H	5.1552205	6.5282909	0.6107292
H	4.9458724	2.1985341	0.4602215
H	6.2169002	4.3023337	0.1139051
C	5.7170328	0.7996894	3.9274204
C	6.3315242	-0.4694325	3.7587207
H	4.1548703	2.1467319	3.3057090
H	6.1054160	1.4988346	4.6836517
H	7.2021020	-0.7449254	4.3731772
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C	-2.0326801	3.9524936	1.2331993

C	-1.1213169	3.3978242	2.1788641	H	3.8881089	-0.9073766	-1.6561124
C	-3.4141314	3.8321684	1.4797727	H	1.1374139	-2.7227075	1.8160570
C	-1.6166869	2.7665940	3.3564791	H	2.6033579	-3.7466298	-3.7800896
C	-3.0049930	2.6800118	3.5513934	Zn	-1.2079626	1.1525065	-2.3600986
C	-3.9237663	3.1926093	2.6211252	Br	0.1203551	2.4938724	-3.7051360
C	-0.6942501	2.2234366	4.4471316	Zn	-2.7389991	-1.5278211	0.9496607
H	-3.3790389	2.1823192	4.4590516	Br	-3.7388023	-1.7672568	3.0354079
C	-1.0019380	0.7609824	4.8117030	H	-4.1256250	4.2396633	0.7437684
H	-1.9980129	0.6517068	5.2878936	C	-2.4585032	-3.9649954	-5.7844998
H	-0.2491989	0.3769886	5.5307174	C	-2.1206630	-2.9180661	-4.9237235
H	-0.9910127	0.1099037	3.9171430	C	-1.0454669	-2.0586498	-5.2545610
C	-0.7386915	3.1390161	5.6860091	C	-0.3111671	-2.2649456	-6.4454988
H	0.3460946	2.2574210	4.0658064	C	-0.6424945	-3.3280838	-7.2938802
H	-1.7549283	3.1601450	6.1324486	C	-1.7180188	-4.1721452	-6.9646703
H	-0.4647222	4.1822021	5.4275441	H	-3.2967053	-4.6334717	-5.5376930
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H	-6.9726709	1.5742514	3.2263757	H	-1.9838115	-5.0031789	-7.6360279
H	-5.5006849	1.3538637	4.2117118	O	-1.2383725	-0.7318477	-3.2910062
H	-5.4635045	0.9052189	2.4974616	H	-2.6778783	-2.7344230	-3.9924715
C	-5.8935329	4.0952521	3.9189058	H	0.0308811	-0.1783127	-4.7872690
H	-5.9156392	3.3715211	1.8947335	C	-5.6968139	-0.0846847	-0.2835523
H	-6.9939829	4.0497839	4.0576593	C	-4.4951520	-0.3163626	-0.8983991
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C	-2.3975806	4.3655383	-1.2715261	C	-3.2331190	1.2068403	-2.3789883
H	-1.9121568	4.7786897	-2.1778205	O	-3.5985375	-1.4820122	-0.8753136
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H	-2.5039357	3.2762930	-1.4192132	H	-6.2507787	1.9445491	0.3074655
C	-1.5503893	6.2121160	0.2128079	H	-2.8353155	-1.4357972	-1.6737772
H	-0.5259781	4.3611961	-0.2359129	H	-4.1660991	-2.4314797	-0.9489000
H	-1.1526675	6.7445284	-0.6759161	H	-6.2366018	-0.7799765	0.3735565
H	-0.9349100	6.4977937	1.0883802				
H	-2.5791865	6.5846224	0.4017985				
H	0.7615045	-6.7975735	-2.4301680				
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H	-0.7660155	-3.9639354	2.5956648				
C	1.5745142	-4.8416478	-2.2147874				
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C	0.0419744	-5.6024838	-4.0680735				
H	0.3802252	-4.8014924	-4.7578685				
C	2.3188626	-3.7590834	-2.7155507				
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H	3.1703679	-6.9173058	-3.1654089				
C	1.1916309	-4.8058460	-0.8640308				
C	2.3597297	-6.6197752	-3.8603501				
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H	0.5808347	-5.6333924	-0.4692004				
C	2.6857189	-0.6903407	-3.4180356				
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H	5.4578827	-2.6601678	-2.5222563				
C	2.7399233	-2.6999855	-1.8904783				
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H	1.8102158	-0.2831383	-2.8761411				
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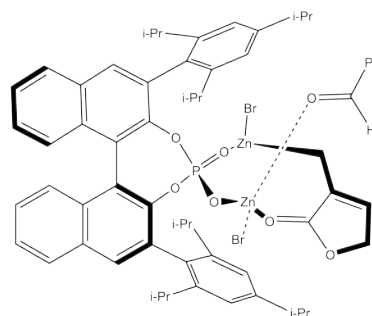


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C	2.4094969	4.5289650	1.6313194
C	3.0962208	5.7805753	1.6359776
C	0.9860090	4.4730452	1.6544172
H	0.4204202	5.4151582	1.7158199
C	0.2968703	3.2705098	1.5527655
C	3.6190940	-1.5344591	0.7411287
C	4.6409194	-1.7182985	1.6659293
H	5.2202543	-2.6543043	1.6491239
C	4.9224369	-0.7556846	2.6772487
C	5.9106535	-1.0078660	3.6763957
C	4.1661442	0.4737262	2.7256191
C	4.3911490	1.3586899	3.8232965
C	3.1967800	0.7395119	1.6881024
C	2.9288125	-0.2833441	0.7705784
O	0.3705034	0.8750163	1.5035906

O	1.9816736	-0.0720939	-0.2184363	C	3.0350018	-0.4784519	-3.2118444
P	0.3788955	-0.0531687	0.1524374	H	5.8178722	-0.6156545	-3.2881339
O	-0.2635172	0.6672085	-1.0408533	H	6.0240348	-2.0107962	-2.1757293
O	-0.1303196	-1.4193496	0.5994792	C	3.3462014	-2.4366502	-1.6182339
C	4.4785909	5.8377039	1.5392149	C	0.9223614	-4.3830680	2.1106599
C	5.2277690	4.6366915	1.4203660	C	2.6219569	-3.8082432	0.2969684
H	2.5007826	6.7049801	1.7004854	H	4.4001612	-4.8744765	2.1529874
H	4.9944750	6.8100144	1.5363799	H	3.1460704	-6.1129932	1.8508914
H	5.1838367	2.4831560	1.3315120	C	3.9831720	-1.1901750	-2.2314216
H	6.3220364	4.6832604	1.3103041	C	3.1976827	-2.6087313	-0.2121480
C	5.3451260	1.0741204	4.7910200	C	2.3895698	-4.0476350	1.7901219
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H	3.7890658	2.2740022	3.9056598	H	0.2584226	-3.5681322	1.7637308
H	5.4923919	1.7704830	5.6307419	H	2.7703842	-1.1192464	-4.0779208
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C	-1.1925653	3.1844802	1.4323715	H	4.2039672	-0.4787333	-1.4105978
C	-3.2286442	3.4924675	0.1331978	H	2.6208184	-3.1042944	2.3229723
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C	-3.3503962	2.4380861	2.2897971	Zn	-0.7115428	0.0822727	-2.8546455
C	-4.0082498	2.8820297	1.1326133	Br	-0.2612010	1.1553205	-4.8572397
C	-1.3336772	2.0959210	3.7700969	Zn	-1.7604900	-2.5423135	0.3363749
H	-3.9299062	1.9532906	3.0884366	Br	-3.6341188	-1.5541869	1.3408854
C	-1.6278948	0.6135184	4.0581513	H	-3.7314620	3.8446085	-0.7829219
H	-2.7094813	0.4340987	4.2288182	C	-6.8231802	-0.0832101	-1.2146350
H	-1.0873264	0.2840137	4.9698668	C	-5.4760936	-0.1097143	-1.5828381
H	-1.3145975	-0.0274556	3.2122918	C	-4.9848712	0.8512042	-2.5008504
C	-1.7704767	2.9984250	4.9402287	C	-5.8480936	1.8387829	-3.0329414
H	-0.2335854	2.2019986	3.6796856	C	-7.1958552	1.8604381	-2.6549606
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H	-1.2760118	2.6865068	5.8838487	C	-3.5816663	0.8479552	-2.8918487
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C	-6.1692081	1.6658935	1.7932242	H	-7.8719958	2.6276221	-3.0605137
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C	-6.2059795	4.1178832	1.1546839	H	-3.2461632	1.6389778	-3.6100875
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H	-7.2926988	4.0513023	0.9372978	C	-2.0106074	-3.8620749	-2.1423229
H	-5.7727249	4.9032457	0.5028811	C	-1.5146410	-2.7163575	-2.9316120
H	-6.0868962	4.4523440	2.2068541	O	-2.2021504	-2.5664628	-4.0732140
C	-1.0736566	4.3411142	-0.8815903	C	-3.2396076	-3.5716181	-4.1140761
C	-1.4252722	3.7813413	-2.2669989	O	-0.6058514	-1.9310996	-2.6062991
H	-0.7737888	4.2211109	-3.0486899	H	-1.4333848	-4.1527049	-0.8266722
H	-2.4756576	3.9987150	-2.5542927	C	-3.1142771	-4.1580097	-5.0508282
H	-1.2747709	2.6870373	-2.2962699	H	-4.2154576	-3.0398785	-4.1763296
C	-1.2860972	5.8667731	-0.8413817	H	-0.3250310	-4.1810359	-0.8757223
H	0.0061571	4.1450605	-0.7250445	H	-1.8292024	-5.0834516	-0.3795849
H	-0.6933400	6.3700434	-1.6333650	H	-3.7066643	-5.2089840	-2.5876230
H	-0.9901977	6.2988411	0.1357089				
H	-2.3552725	6.1194374	-1.0036001				
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H	5.1960706	-2.2312420	-3.7487770				
H	3.1989806	-5.2636242	3.4287343				
C	2.0060389	-5.7993933	-2.9534835				
H	3.4997046	0.4456438	-3.6120170				
H	0.6565296	-6.2003109	-4.6362842				
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C	2.3946792	-4.6755167	-2.0002381				
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H	4.0066213	-6.7151554	-2.9451237				
C	2.2471234	-4.8182945	-0.6113215				
C	3.2430095	-6.3708305	-3.6714760				
H	2.9656856	-7.2310350	-4.3156635				
H	1.8155396	-5.7550574	-0.2217107				

int2



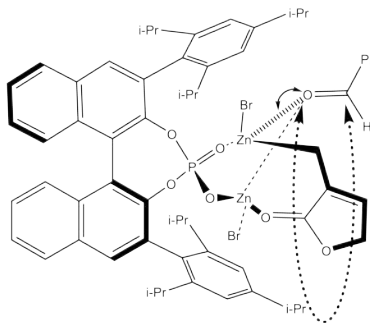
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C	3.1686358	3.3031384	1.5683820
C	4.5869356	3.3991241	1.4400193

C	2.4067277	4.5275743	1.6363974	C	2.0091752	-5.8039520	-2.9539336
C	3.0954248	5.7775169	1.6430794	H	3.4811121	0.4477910	-3.6120611
C	0.9834122	4.4732296	1.6584660	H	0.6574064	-6.2132137	-4.6336586
H	0.4179585	5.4153743	1.7199572	H	0.7678394	-4.4864288	3.2024256
C	0.2924149	3.2721482	1.5555995	C	2.3917182	-4.6782409	-2.0003548
C	3.6106585	-1.5363460	0.7414916	C	5.3142051	-1.5290236	-2.9029028
C	4.6337936	-1.7202389	1.6644680	C	0.9206423	-5.3762096	-3.9540235
H	5.2124275	-2.6566794	1.6450972	H	1.2582165	-4.5271651	-4.5840386
C	4.9163822	-0.7587358	2.6760480	C	2.9285915	-3.4705882	-2.4779490
C	5.9055460	-1.0103803	3.6736794	C	3.3186129	-5.1448004	2.3334671
C	4.1597937	0.4702161	2.7257271	H	4.0195751	-6.6965744	-2.9592041
C	4.3861290	1.3545811	3.8232742	C	2.2443397	-4.8213067	-0.6118460
C	3.1890653	0.7370046	1.6897236	C	3.2473039	-6.3614672	-3.6803235
C	2.9191099	-0.2860678	0.7728498	H	2.9762937	-7.2244401	-4.3234435
O	0.3629442	0.8776117	1.5048267	H	1.8159412	-5.7595242	-0.2221448
O	1.9711578	-0.0775885	-0.2151308	C	3.0175239	-0.4743609	-3.2068715
P	0.3684339	-0.0466563	0.1523385	H	5.8010192	-0.6116168	-3.2936088
O	-0.2675170	0.6774163	-1.0420149	H	6.0101772	-2.0101424	-2.1860899
O	-0.1543301	-1.4095248	0.5950167	C	3.3361769	-2.4365622	-1.6183882
C	4.4774314	5.8332113	1.5482607	C	0.9112138	-4.3684279	2.1088497
C	5.2247664	4.6318536	1.4289609	C	2.6165235	-3.8106342	0.2964520
H	2.5009275	6.7025159	1.7074248	H	4.3840527	-4.8979328	2.1504184
H	4.9943526	6.8049097	1.5471732	H	3.1187349	-6.1234177	1.8488753
H	5.1774928	2.4784174	1.3373526	C	3.9696793	-1.1884530	-2.2320505
H	6.3191958	4.6768655	1.3204694	C	3.1893798	-2.6099472	-0.2124053
C	5.3414878	1.0701867	4.7890021	C	2.3824502	-4.0498873	1.7894050
C	6.1224023	-0.1129141	4.7075824	H	2.0842128	-0.1733664	-2.6943622
H	3.7835714	2.2694287	3.9056920	H	0.2578039	-3.5432871	1.7663151
H	5.4896182	1.7665449	5.6284904	H	2.7420840	-1.1138001	-4.0704238
H	6.8835853	-0.3233830	5.4742333	H	-0.0023748	-5.0615473	-3.4291989
H	6.4828754	-1.9465359	3.6142931	H	0.5689301	-5.3064531	1.6245011
C	-1.8407895	3.6612670	0.2540357	H	3.7101398	-5.5905164	-4.3312119
C	-1.1968575	3.1867029	1.4340227	H	4.1934996	-0.4787676	-1.4105419
C	-3.2317296	3.4981144	0.1349318	H	2.6237878	-3.1099139	2.3236051
C	-1.9646274	2.5713807	2.4597484	H	3.0510312	-3.3303149	-3.5638969
C	-3.3542911	2.4347179	2.2864280	Zn	-0.6647086	0.1045555	-2.8703150
C	-4.0115200	2.8840170	1.1314442	Br	-0.3121436	1.1881277	-4.8746677
C	-1.3401724	2.0892471	3.7679886	Zn	-1.7930029	-2.5189736	0.3397980
H	-3.9335487	1.9455231	3.0823906	Br	-3.6823281	-1.6085082	1.3690628
C	-1.6377543	0.6071045	4.0534675	H	-3.7341201	3.8538593	-0.7801137
H	-2.7193584	0.4274634	4.2227887	C	-6.7830901	-0.0998736	-1.1903175
H	-1.0986656	0.2745945	4.9647346	C	-5.4360874	-0.1233842	-1.5597074
H	-1.3241863	-0.0342850	3.2082394	C	-4.9540181	0.8209584	-2.4985188
C	-1.7763518	2.9916355	4.9383395	C	-5.8256945	1.7896117	-3.0494206
H	-0.2398044	2.1935813	3.6790429	C	-7.1734002	1.8076444	-2.6716648
H	-2.8738596	2.9409693	5.0978345	C	-7.6501113	0.8604790	-1.7465511
H	-1.5141854	4.0525990	4.7493838	H	-7.1549865	-0.8206751	-0.4470665
H	-1.2844865	2.6775585	5.8825031	C	-3.5491076	0.8165060	-2.8915908
C	-5.5191796	2.7615645	0.9361053	H	-5.4343962	2.5263357	-3.7693303
C	-6.1737007	1.6703968	1.7913463	H	-7.8562423	2.5605655	-3.0925665
H	-7.2379157	1.5434956	1.5055839	H	-8.7091890	0.8793193	-1.4458283
H	-6.1562142	1.9311979	2.8702952	O	-2.7282550	-0.0099582	-2.4610522
H	-5.6622825	0.6945914	1.6688153	H	-4.7354142	-0.8381294	-1.0990656
C	-6.2065184	4.1235183	1.1575048	H	-3.2118583	1.5975627	-3.6214293
H	-5.6723223	2.4859108	-0.1314508	C	-3.0402227	-4.3234029	-2.8726878
H	-7.2938683	4.0609383	0.9418805	C	-1.9876001	-3.8312700	-2.1489886
H	-5.7715797	4.9098677	0.5082867	C	-1.4712022	-2.6944144	-2.9424274
H	-6.0846114	4.4554013	2.2098945	O	-2.1544203	-2.5423468	-4.0886673
C	-1.0767389	4.3482364	-0.8776381	C	-3.2034355	-3.5310528	-4.1281520
C	-1.4291950	3.7911933	-2.2637791	O	-0.5559064	-1.9192180	-2.6201404
H	-0.7759217	4.2268504	-3.0459799	C	-1.42411293	-4.1213434	-0.8305460
H	-2.4785850	4.0132982	-2.5520180	H	-3.0831121	-4.1221386	-5.0633831
H	-1.2828088	2.6965602	-2.2946015	H	-4.1717962	-2.9850187	-4.1958379
C	-1.2873747	5.8738848	-0.8347535	H	-0.3152341	-4.1332570	-0.8626606
H	0.0028817	4.1502303	-0.7222300	H	-1.8165399	-5.0562492	-0.3894029
H	-0.6950210	6.3783763	-1.6261732	H	-3.6983364	-5.1571346	-2.5943534
H	-0.9911617	6.3043142	0.1428299				
H	-2.3562999	6.1285971	-0.9947896				
H	1.5874457	-6.6242943	-2.3317852				
H	5.1781635	-2.2253418	-3.7566229				
H	3.1800358	-5.2756693	3.4267018				

7.8.6 Pathway 14d-ma ↔ 14d-mi

TS1; COSMO



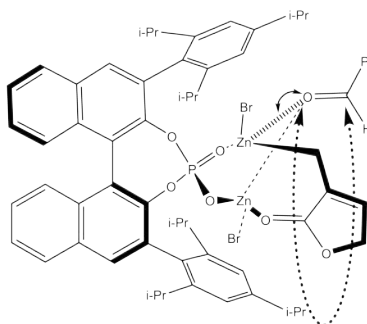
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C	4.5835439	3.3119398	2.1648917
C	2.3823101	4.4123119	2.0997623
C	3.0362438	5.6574940	2.3440651
C	0.9820770	4.3554511	1.8497714
H	0.4012120	5.2906612	1.8568854
C	0.3419978	3.1625921	1.5352645
C	3.8601001	-1.4016865	0.5392608
C	4.7568899	-1.7375497	1.5467345
H	5.3757117	-2.6403568	1.4356243
C	4.8632799	-0.9794392	2.7471871
C	5.7102909	-1.4039339	3.8142563
C	4.0709462	0.2143702	2.9106301
C	4.1161539	0.8912904	4.1652107
C	3.2325128	0.6473148	1.8212947
C	3.1154844	-0.1939387	0.7107076
O	0.4305141	0.7725020	1.3916615
O	2.2276629	0.1597889	-0.3101702
P	0.6481200	-0.1337814	0.0266103
O	-0.1521166	0.4596626	-1.1414497
O	0.3899267	-1.5789038	0.4462403
C	4.4131468	5.7240810	2.4927054
C	5.1912058	4.5405872	2.3843462
H	2.4222190	6.5705977	2.3943307
H	4.9055012	6.6915209	2.6749432
H	5.2010420	2.4081922	2.0741914
H	6.2872933	4.5970222	2.4689465
C	4.9348656	0.4409485	5.1914063
C	5.7519173	-0.7071838	5.0124578
H	3.4765641	1.7713551	4.3195750
H	4.9430967	0.9729797	6.1550438
H	6.4011481	-1.0522802	5.8316394
H	6.3161311	-2.3129724	3.6734926
C	-1.3839523	3.6435010	-0.2281387
C	-1.0787670	3.1346739	1.0657613
C	-2.7283197	3.6572537	-0.6435809
C	-2.1111819	2.6062255	1.8851638
C	-3.4403114	2.6448153	1.4206939
C	-3.7761401	3.1853147	0.1657456
C	-1.8118478	2.0447731	3.2736964
H	-4.2393408	2.2614323	2.0747927
C	-2.2533356	0.5801658	3.4105170
H	-3.3583580	0.4755914	3.3913715
H	-1.8862789	0.1374671	4.3582682
H	-1.8347988	-0.0247844	2.5821099
C	-2.4178248	2.9273080	4.3793411
H	-0.7123254	2.0598318	3.4122487
H	-3.5258700	2.9581857	4.3122416
H	-2.0486562	3.9702173	4.3049568
H	-2.1514485	2.5386898	5.3840680
C	-5.2192009	3.3716492	-0.2932948
C	-6.1474729	2.1911199	0.0231777
H	-7.1560880	2.3659581	-0.4044799

H	-6.2803280	2.0581241	1.1180038
H	-5.7488082	1.2443794	-0.3879861
C	-5.7811425	4.6884727	0.2797840
H	-5.1866444	3.4800081	-1.4005079
H	-6.8086862	4.8823314	-0.0931231
H	-5.1433171	5.5518522	0.0032685
H	-5.8216516	4.6457327	1.3887128
C	-0.3121274	4.1974406	-1.1679613
C	-0.3520308	3.5479932	-2.5608436
H	0.4744388	3.9385556	-3.1900255
H	-1.2997110	3.7605540	-3.0980511
H	-0.2372995	2.4503059	-2.4936006
C	-0.4081698	5.7319302	-1.2653210
H	0.6759459	3.9527885	-0.7287894
H	0.4008959	6.1359191	-1.9085075
H	-0.3258458	6.2132677	-0.2697443
H	-1.3779589	6.0441618	-1.7070332
H	2.1304168	-5.5647548	-3.8196900
H	6.0890639	-1.1300918	-3.6478721
H	3.3674959	-5.4671134	2.4030404
C	2.6621816	-4.6585389	-4.1858784
H	4.2626588	1.4824842	-3.2235902
H	1.3724153	-4.5364618	-5.9591137
H	0.8857302	-4.9267732	1.8935162
C	3.0268834	-3.8354745	-2.9570918
C	6.0513147	-0.6077873	-2.6686734
C	1.6994726	-3.8956031	-5.1140783
H	2.1845001	-2.9964198	-5.5478031
C	3.6238951	-2.5691260	-3.0806086
C	3.6476272	-5.1236777	1.3856295
H	4.5895813	-5.7140744	-4.2845806
C	2.7574033	-4.3076229	-1.6629762
C	3.9155961	-5.1314875	-4.9444811
H	3.6409421	-5.7702461	-5.8097046
H	2.2841612	-5.2968632	-1.5543550
C	3.7962862	0.4781731	-3.1511494
H	6.5577148	0.3725153	-2.7895556
H	6.6366242	-1.2109203	-1.9450286
C	3.9268078	-1.7717818	-1.9640790
C	1.2144058	-4.7198730	0.8529516
C	3.0250887	-3.5460025	-0.5090378
H	4.6682577	-4.6965449	1.4409478
H	3.6977920	-6.0141571	0.7235815
C	4.5985424	-0.4186904	-2.1919728
C	3.6204926	-2.2605730	-0.6621294
C	2.6238865	-4.1021777	0.8565612
H	2.7543474	0.6053868	-2.7979710
H	0.4889335	-4.0360838	0.3701712
H	3.7625631	0.0568156	-4.1776201
H	0.7969252	-3.5497930	-4.5701087
H	1.1733660	-5.6829940	0.3025445
H	4.4943190	-4.2682926	-5.3355582
H	4.6495004	0.1060998	-1.2169935
H	2.5941316	-3.2527245	1.5691869
H	3.8527577	-2.1790380	-4.0851066
Zn	-1.7856151	-0.2519946	-1.9946459
Br	-1.7091601	0.3189046	-4.2507308
Zn	-0.3832404	-2.2933558	2.1760192
Br	1.0813469	-1.9373209	3.9451470
H	-2.9741025	4.0644490	-1.6383358
C	-7.5459538	-3.2721205	-1.9404150
C	-6.2645094	-2.7170895	-1.9852577
C	-5.8857367	-1.9096675	-3.0851390
C	-6.8014941	-1.6670418	-4.1332099
C	-8.0844744	-2.2283583	-4.0850738
C	-8.4549189	-3.0280690	-2.9899100
H	-7.8461114	-3.9021374	-1.0893304
C	-4.5506616	-1.3029310	-3.1379990
H	-6.4971749	-1.0358147	-4.9834678
H	-8.7997305	-2.0434474	-4.9004105
H	-9.4634147	-3.4681427	-2.9517099

O	-3.6949337	-1.4888788	-2.2634118
H	-5.5318263	-2.8939126	-1.1830686
H	-4.3103594	-0.6419295	-4.0120662
C	-4.4997197	-2.2027831	2.2459938
C	-3.2974249	-2.3052417	1.6021386
C	-3.2960583	-1.2089579	0.6054743
O	-4.4601744	-0.5366462	0.6193943
C	-5.2867756	-1.0717271	1.6725879
O	-2.3677107	-0.8952312	-0.1463948
C	-2.1442325	-3.1989240	1.7512962
H	-6.2605363	-1.3739966	1.2265123
H	-5.4901606	-0.2442664	2.3894621
H	-1.8904387	-3.6460443	0.7655565
H	-2.3451322	-4.0094466	2.4776402
H	-4.8637787	-2.8381616	3.0645993

TS1



Energy (Hartree) = -11969.9988476
number of imaginary frequencies: 4

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C	2.4927525	1.9409891	1.8368841
C	3.1689262	3.2003832	2.0420006
C	4.5878691	3.3090052	2.1613573
C	2.3894991	4.4145172	2.0975937
C	3.0465987	5.6576266	2.3420150
C	0.9891732	4.3604645	1.8489191
H	0.4099370	5.2966588	1.8573134
C	0.3460908	3.1693377	1.5346011
C	3.8541175	-1.4031728	0.5371551
C	4.7496552	-1.7404653	1.5450285
H	5.3657466	-2.6451505	1.4344577
C	4.8580953	-0.9821661	2.7450144
C	5.7036954	-1.4077762	3.8123394
C	4.0688271	0.2136272	2.9077623
C	4.1156443	0.8910295	4.1617982
C	3.2316520	0.6480313	1.8180739
C	3.1128814	-0.1933908	0.7079898
O	0.4293357	0.7795213	1.3876768
O	2.2260448	0.1620484	-0.3131243
P	0.6463405	-0.1275298	0.0232526
O	-0.1515713	0.4659747	-1.1472739
O	0.3838773	-1.5718385	0.4431350
C	4.4232807	5.7208658	2.4900905
C	5.1982286	4.5358651	2.3810225
H	2.4348240	6.5721917	2.3927778
H	4.9179756	6.6870596	2.6724526
H	5.2028992	2.4036884	2.0702185
H	6.2944296	4.5896424	2.4652761
C	4.9330775	0.4392406	5.1879257
C	5.7470369	-0.7106518	5.0097448
H	3.4780644	1.7725416	4.3155801
H	4.9424592	0.9716811	6.1512480
H	6.3952650	-1.0569749	5.8291372

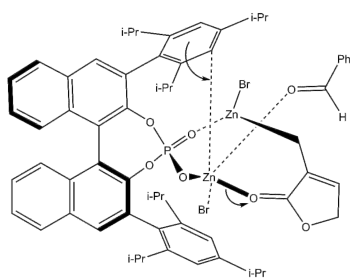
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C	-1.3900057	3.6585632	-0.2172019
C	-1.0772887	3.1454552	1.0730649
C	-2.7375375	3.6804959	-0.6215164
C	-2.1055960	2.6195006	1.8989844
C	-3.4379775	2.6664273	1.4454159
C	-3.7811168	3.2123085	0.1950512
C	-1.7981774	2.0506576	3.2827172
H	-4.2336156	2.2855374	2.1052291
C	-2.2467769	0.5880375	3.4169072
H	-3.3527191	0.4895215	3.4065669
H	-1.8737385	0.1385557	4.3590053
H	-1.8386843	-0.0152778	2.5821697
C	-2.3889720	2.9321557	4.3972482
H	-0.6975795	2.0581603	3.4121720
H	-3.4973513	2.9703955	4.3401704
H	-2.0141272	3.9729565	4.3238177
H	-2.1161569	2.5378141	5.3979466
C	-5.2270283	3.4082548	-0.2508778
C	-6.1591961	2.2323358	0.0711973
H	-7.1706482	2.4132607	-0.3471220
H	-6.2834096	2.0983409	1.1669517
H	-5.7690756	1.2843498	-0.3453483
C	-5.7766394	4.7270629	0.3293832
H	-5.2036932	3.5183680	-1.3582036
H	-6.8062354	4.9278541	-0.0341597
H	-5.1360903	5.5870198	0.0492136
H	-5.8075625	4.6825974	1.4384351
C	-0.3226716	4.2074186	-1.1649493
C	-0.3776108	3.5595707	-2.5581767
H	0.4458737	3.9456244	-3.1936866
H	-1.3280511	3.7781930	-3.0879585
H	-0.2683239	2.4612865	-2.4933350
C	-0.4106538	5.7424844	-1.2599713
H	0.6674432	3.9566800	-0.7338598
H	0.3954606	6.1423941	-1.9092063
H	-0.3175914	6.2224530	-0.2647626
H	-1.3820236	6.0609864	-1.6935342
H	2.1069438	-5.5633361	-3.8163419
H	6.0811892	-1.1434532	-3.6516953
H	3.3507468	-5.4662719	2.4044709
C	2.6413824	-4.6591760	-4.1840063
H	4.2652580	1.4768147	-3.2280567
H	1.3492354	-4.5339960	-5.9556214
H	0.8713199	-4.9178575	1.8969943
C	3.0106073	-3.8367755	-2.9561500
C	6.0460908	-0.6201921	-2.6729852
C	1.6797515	-3.8938515	-5.1113784
H	2.1667787	-2.9965344	-5.5464514
C	3.6111850	-2.5725337	-3.0811518
C	3.6309847	-5.1248471	1.3864806
H	4.5647156	-5.7215868	-4.2844354
C	2.7415729	-4.3072362	-1.6616864
C	3.8918997	-5.1374533	-4.9439412
H	3.6140039	-5.7759486	-5.8083495
H	2.2655841	-5.2949836	-1.5518869
C	3.7949721	0.4745162	-3.1544417
H	6.5562989	0.3579494	-2.7950770
H	6.6294798	-1.2251258	-1.9494698
C	3.9180145	-1.7754567	-1.9657799
C	1.1991632	-4.7120146	0.8559717
C	3.0126404	-3.5458633	-0.5087032
H	4.6532307	-4.7016375	1.4402548
H	3.6773970	-6.0159364	0.7250335
C	4.5944624	-0.4250225	-2.1953978
C	3.6115254	-2.2624068	-0.6633416
C	2.6108566	-4.0997631	0.8576868
H	2.7539405	0.6064849	-2.8007332
H	0.4760181	-4.0251366	0.3740457
H	3.7584339	0.0529016	-4.1806534
H	0.7792173	-3.5444165	-4.5666088

H	1.1534909	-5.6747343	0.3051337	H	-4.6950701	3.4670778	1.7600946
H	4.4733005	-4.2768158	-5.3363788	C	-2.9363098	2.5162794	0.9483828
H	4.6483844	0.1001834	-1.2207975	C	-1.2092944	-1.6329802	-2.8268820
H	2.5845420	-3.2500981	1.5702133	C	-1.5913817	-1.4610226	-4.1518197
H	3.8399606	-2.1837328	-4.0861413	H	-1.2186716	-2.1615252	-4.9141757
Zn	-1.7789622	-0.2513708	-2.0055771	C	-2.4112542	-0.3729067	-4.5633567
Br	-1.7095253	0.3201793	-4.2599084	C	-2.6983719	-0.1504904	-5.9436011
Zn	-0.3916468	-2.2829455	2.1736174	C	-2.9232016	0.5472547	-3.5778886
Br	1.0716833	-1.9333313	3.9424313	C	-3.6363205	1.6953209	-4.0350251
H	-2.9890565	4.0912435	-1.6133749	C	-2.6526394	0.2995948	-2.1821930
C	-7.5052655	-3.3340317	-1.9794237	C	-1.7631185	-0.7343955	-1.8651149
C	-6.2294077	-2.7657826	-2.0153117	O	-1.0729404	1.5359577	-0.1812436
C	-5.8464140	-1.9660318	-3.1187702	O	-1.4187303	-0.9609995	-0.5309522
C	-6.7525544	-1.7443598	-4.1791949	P	-0.3922329	0.0883055	0.1967010
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C	-8.4045308	-3.1107178	-3.0413239	O	1.0074948	0.1527674	-0.4200751
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C	-4.5162423	-1.3457838	-3.1624569	C	-6.9939083	0.9241535	-1.7091876
H	-6.4449907	-1.1187144	-5.0324374	H	-6.9568557	3.1945560	0.8659748
H	-8.7376175	-2.1496953	-4.9654212	H	-8.5596651	2.0526163	-0.6771522
H	-9.4086867	-3.5611399	-3.0101009	H	-5.2740323	-0.0534975	-2.5652904
O	-3.6701038	-1.5140199	-2.2769842	H	-7.7019541	0.3908046	-2.3616997
H	-5.5036517	-2.9256992	-1.2032391	C	-3.8789515	1.8970409	-5.3866197
H	-4.2705580	-0.6909826	-4.0402752	C	-3.4235522	0.9588117	-6.3510929
C	-4.5085241	-2.1782108	2.2366057	H	-3.9787588	2.4400471	-3.3037251
C	-3.3056071	-2.2885859	1.5944109	H	-4.4207693	2.7976792	-5.7136715
C	-3.2995533	-1.1954496	0.5938088	H	-3.6287020	1.1256005	-7.4195663
O	-4.4620724	-0.5184218	0.6036348	H	-2.3105003	-0.8689673	-6.6828235
C	-5.2906832	-1.0457277	1.6580361	C	-2.0208609	2.1362102	3.2579056
O	-2.3708583	-0.8861084	-0.1575344	C	-1.9550059	2.8428439	2.0276480
C	-2.1559046	-3.1838161	1.7479680	C	-0.9251047	2.2455000	4.1609222
H	-6.2657422	-1.3451247	1.2121744	C	-0.8520096	3.7021082	1.7521370
H	-5.4902654	-0.2135962	2.3708678	C	0.2027777	3.7917209	2.6780972
H	-1.9012710	-3.6334144	0.7636372	C	0.2010410	3.0726876	3.8855480
H	-2.3601266	-3.9922713	2.4755554	H	-1.0116607	1.7903051	5.1622354
H	-4.8755993	-2.8090674	3.0572588	C	-0.8432982	4.5560647	0.4890322
				H	1.0587668	4.4385746	2.4472328
				C	0.5558803	4.8448221	-0.0653340
				H	1.1403032	5.5275922	0.5855943
				H	0.4795361	5.3181499	-1.0638499
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				C	-1.6288811	5.8578846	0.7507896
				H	-1.3896701	3.9969879	-0.2965905
				H	-1.1419562	6.4610597	1.5452875
				H	-2.6678654	5.6443573	1.0737679
				H	-1.6748874	6.4741789	-0.1702097
				C	1.3116529	3.1982298	4.9213863
				C	2.6332370	3.7339097	4.3569927
				H	3.4288646	3.6600481	5.1251210
				H	2.5516407	4.8063373	4.0813107
				H	2.9677768	3.1761274	3.4604047
				C	0.8260836	4.0552218	6.1091471
				H	1.4904860	2.1694120	5.3111808
				H	1.6047924	4.0996304	6.8974801
				H	-0.0969773	3.6447251	6.5652864
				H	0.6111767	5.0934950	5.7802099
				C	-3.2371602	1.3082570	3.6641948
				C	-2.9019610	-0.1238919	4.1080226
				H	-3.8348432	-0.6698407	4.3553745
				H	-2.2544695	-0.1562792	5.0083115
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				C	-4.0336229	2.0649338	4.7462090
				H	-3.8889927	1.2219583	2.7738162
				H	-4.9626633	1.5137074	4.9976787
				H	-4.3170284	3.0823478	4.4075345
				H	-3.4420359	2.1734957	5.6793470
				H	3.5908871	-5.4692234	-1.5386442
				H	-2.2974198	-6.1313936	-1.5743285
				H	2.2036403	-0.8651536	-5.6319196
				C	2.5763945	-5.8378123	-1.2656499
				H	-3.3568322	-4.0676086	0.6204725

7.9 Interconversion of Complexes 14 - Mechanism 2

7.9.1 Pathway 14j-ma \leftrightarrow 14j-mi

TS1; COSMO



Energy (Hartree) = -11970.03154154

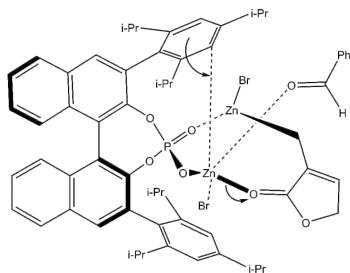
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Zn	1.8280178	1.6459107	-1.5311212
Br	0.3398210	2.2373768	-3.2721884
C	-2.4481564	1.7048320	-0.1233445
C	-3.2597996	1.1287722	-1.1026904
C	-4.6856933	1.3425092	-0.9923375
C	-5.6330193	0.6747533	-1.8254915
C	-5.1878813	2.2445687	0.0194821
C	-6.5910011	2.4943179	0.0985694
C	-4.2900115	2.8193844	0.9671086

H	3.3609509	-6.8783118	0.4965059
H	3.2044052	0.1266830	-3.4726135
C	1.5924254	-4.7375356	-1.6460976
C	-2.7919445	-5.1857186	-1.8806149
C	2.5787528	-6.1328407	0.2443216
H	1.6063322	-6.5505136	0.5783865
C	0.2403376	-4.7984319	-1.2659279
C	1.8645475	-1.7585885	-5.0677011
H	2.3574896	-6.9139965	-3.1730076
C	2.0062902	-3.6339647	-2.4110293
C	2.3141649	-7.1165797	-2.0838637
H	3.0625499	-7.9013488	-1.8472696
H	3.0637042	-3.5723794	-2.7173802
C	-2.2861886	-4.0253573	0.3315469
H	-3.8645026	-5.2640450	-1.6065055
H	-2.7237567	-5.1132920	-2.9852206
C	-0.6868905	-3.8059396	-1.6308171
C	2.9613612	-0.8428160	-2.9881975
C	1.1242051	-2.6030057	-2.7893023
H	0.9289151	-2.1202407	-5.5374599
H	2.6296864	-2.5542070	-5.1912626
C	-2.1436307	-3.9656762	-1.2001048
C	-0.2441355	-2.6998603	-2.4086730
C	1.6619610	-1.4135053	-3.5810879
H	-1.8364083	-3.1310224	0.8054604
H	2.8799935	-0.6865971	-1.8928742
H	-1.7932477	-4.9263343	0.7531763
H	2.7713171	-5.2168046	0.8382768
H	3.8336597	-1.5101758	-3.1501903
H	1.3083051	-7.5295272	-1.8587979
H	-2.6998548	-3.0717257	-1.5475402
H	0.9062012	-0.6036364	-3.5240673
H	-0.1107862	-5.6529601	-0.6657391
C	3.9734189	-2.4983267	0.6203331
C	3.3353591	-1.4138149	1.2281856
C	3.9010695	-0.8283407	2.3865172
C	5.1081100	-1.3336885	2.9214669
C	5.7335832	-2.4308372	2.3180056
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H	3.5348931	-2.9462585	-0.2837143
H	2.4116517	-0.9896328	0.8074530
C	3.2497044	0.3065374	3.0336507
H	5.5492999	-0.8570464	3.8107177
H	6.6685594	-2.8329299	2.7358937
H	5.6606471	-3.8721193	0.6904246
O	2.1336489	0.7440214	2.6960753
H	3.7877256	0.7643898	3.9004366
C	5.5597072	0.8754686	-1.4060952
C	4.7054703	1.6910117	-0.7247898
C	5.1038166	1.6068005	0.7105797
O	6.1749704	0.7595466	0.8363859
C	6.5132726	0.2322985	-0.4528767
O	4.6175656	2.1641541	1.6833630
C	3.5863696	2.5438063	-1.1535005
H	6.4117637	-0.8772326	-0.4136657
H	7.5823430	0.4633293	-0.6612818
H	3.8022533	3.0424056	-2.1205672
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H	5.5728244	0.6849662	-2.4878950

number of imaginary frequencies: 1

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Br	0.6411749	-0.8059116	5.3440522
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C	-2.4475286	1.7073188	-0.1222059
C	-3.2584486	1.1302781	-1.1017147
C	-4.6841486	1.3467129	-0.9947573
C	-5.6304770	0.6789937	-1.8286969
C	-5.1875131	2.2518220	0.0134468
C	-6.5900479	2.5035715	0.0878261
C	-4.2904591	2.8273453	0.9609697
H	-4.6953799	3.4773571	1.7522826
C	-2.9372953	2.5224422	0.9462956
C	-1.2074740	-1.6352875	-2.8178567
C	-1.5912993	-1.4672383	-4.1426035
H	-1.2178443	-2.1704568	-4.9020361
C	-2.4109576	-0.3808640	-4.5576237
C	-2.6990541	-0.1622603	-5.9377310
C	-2.9210014	0.5427533	-3.5747804
C	-3.6323631	1.6903308	-4.0350762
C	-2.6505762	0.2984011	-2.1784914
C	-1.7614599	-0.7349770	-1.8579368
O	-1.0734196	1.5378880	-0.1762995
O	-1.4181265	-0.9589336	-0.5235260
P	-0.3910892	0.0907947	0.2041718
O	-0.5335446	-0.2511500	1.6952000
O	1.0087738	0.1550800	-0.4109272
C	-7.4773467	1.8644943	-0.7643316
C	-6.9907545	0.9311368	-1.7167739
H	-6.9567447	3.2062263	0.8526659
H	-8.5571961	2.0642563	-0.6916134
H	-5.2695212	-0.0505977	-2.5660290
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C	-3.4231931	0.9458745	-6.3481143
H	-3.9712263	2.4382409	-3.3055932
H	-4.4157161	2.7884133	-5.7160553
H	-3.6281796	1.1097926	-7.4169687
H	-2.3111997	-0.8827852	-6.6748780
C	-2.0255581	2.1465396	3.2578174
C	-1.9575253	2.8506245	2.0262956
C	-0.9311949	2.2557686	4.1611190
C	-0.8521505	3.7062096	1.7491221
C	0.2022981	3.7937056	2.6752959
C	0.1975225	3.0775492	3.8845276
H	-1.0156801	1.7967792	5.1606663
C	-0.8408004	4.5560917	0.4828796
H	1.0622073	4.4344150	2.4420679
C	0.5592515	4.8521769	-0.0648468
H	1.1352066	5.5431611	0.5852617
H	0.4859506	5.3176734	-1.0671022
H	1.1497853	3.9224871	-0.1820961
C	-1.6367601	5.8535042	0.7335070
H	-1.3770733	3.9901892	-0.3048154
H	-1.1600156	6.4637514	1.5287615
H	-2.6764875	5.6346457	1.0500997
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C	1.3096130	3.1988318	4.9194183
C	2.6338259	3.7265033	4.3536959
H	3.4300146	3.6505664	5.1210856
H	2.5592724	4.7993033	4.0771337
H	2.9674780	3.1670199	3.4579212
C	0.8300843	4.0593228	6.1068359
H	1.4820587	2.1690613	5.3099398
H	1.6089017	4.1007155	6.8952277
H	-0.0947470	3.6546939	6.5644829
H	0.6200615	5.0987098	5.7782653
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TS1

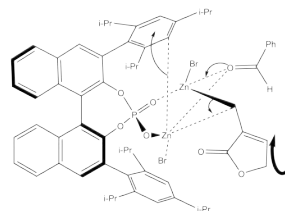


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H	-2.2892334	-6.1308373	-1.5567665
H	2.1939203	-0.8536287	-5.6292425
C	2.5844331	-5.8430805	-1.2833923
H	-3.3332555	-4.0667255	0.6476856
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H	3.1972349	0.1337072	-3.4701328
C	1.6001707	-4.7391075	-1.6523310
C	-2.7847550	-5.1842658	-1.8583923
C	2.5970845	-6.1462972	0.2248272
H	1.6265864	-6.5644862	0.5633628
C	0.2512143	-4.7988074	-1.2626394
C	1.8597828	-1.7500414	-5.0672014
H	2.3504398	-6.9077359	-3.1950438
C	2.0097719	-3.6344046	-2.4173723
C	2.3150152	-7.1166672	-2.1070451
H	3.0625781	-7.9051289	-1.8803640
H	3.0650553	-3.5731600	-2.7314439
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H	-3.8555826	-5.2630600	-1.5779343
H	-2.7230086	-5.1112819	-2.9631438
C	-0.6778065	-3.8060125	-1.6208124
C	2.9600077	-0.8383552	-2.9880467
C	1.1265379	-2.6021303	-2.7884556
H	0.9237142	-2.1118216	-5.5355578
H	2.6253649	-2.5443030	-5.1966437
C	-2.1317049	-3.9653261	-1.1807888
C	-0.2396190	-2.6999669	-2.4008156
C	1.6603667	-1.4101845	-3.5792449
H	-1.8113751	-3.1317724	0.8237111
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H	-1.7698776	-4.9260340	0.7709076
H	2.7933657	-5.2343341	0.8234171
H	3.8339671	-1.5028385	-3.1546130
H	1.3096368	-7.5284144	-1.8785259
H	-2.6893577	-3.0709043	-1.5245598
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C	3.9602199	-2.5130996	0.6152360
C	3.3254750	-1.4295715	1.2286406
C	3.8974226	-0.8451133	2.3835186
C	5.1081442	-1.3492469	2.9090427
C	5.7311632	-2.4446502	2.3005798
C	5.1574394	-3.0247202	1.1542479
H	3.5137501	-2.9606331	-0.2850956
H	2.3989330	-1.0055441	0.8139766
C	3.2463646	0.2896657	3.0347453
H	5.5557467	-0.8704576	3.7938428
H	6.6697142	-2.8453664	2.7118494
H	5.6469897	-3.8868464	0.6740667
O	2.1305868	0.7255286	2.6991326
H	3.7843078	0.7442575	3.9035736
C	5.5573072	0.8942499	-1.3997593
C	4.6975701	1.6981631	-0.7117139
C	5.0866749	1.5909387	0.7259989
O	6.1603352	0.7440474	0.8446160
C	6.5060384	0.2383364	-0.4488194
O	4.5887303	2.1267485	1.7032291
C	3.5779505	2.5525445	-1.1302747
H	6.4062348	-0.8723389	-0.4264079
H	7.5768040	0.4738643	-0.6467294
H	3.7922820	3.0650184	-2.0902349
H	3.3841389	3.3199083	-0.3533026

H 5.5747044 0.7196812 -2.4841714

TS2; COSMO



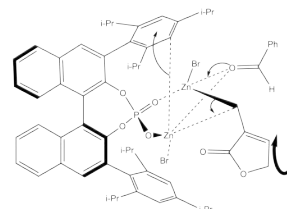
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Br	4.7123548	1.1641696	1.3510344
Zn	-0.3539859	3.0146608	1.8426649
Br	-2.0398418	4.5642164	2.2425361
C	-1.3734675	-1.9520259	1.5243332
C	-2.1836331	-2.5386842	0.5514575
C	-2.2825481	-3.9792367	0.5425051
C	-2.9603705	-4.7096605	-0.4794197
C	-1.6353557	-4.7234602	1.5993052
C	-1.7616872	-6.1453185	1.6269303
C	-0.8201371	-4.0446483	2.5517957
H	-0.2868893	-4.6378722	3.3101572
C	-0.6183344	-2.6697843	2.4994868
C	-2.5369195	-0.0973663	-2.3925739
C	-3.8807154	-0.2473394	-2.7136496
H	-4.2758114	0.2409574	-3.6174719
C	-4.7643425	-1.0185456	-1.9044699
C	-6.1599014	-1.0904199	-2.1951981
C	-4.2431570	-1.7427761	-0.7695961
C	-5.1595365	-2.4645433	0.0531069
C	-2.8299774	-1.6817493	-0.4851472
C	-2.0561873	-0.7916089	-1.2422942
O	-1.2979126	-0.5628010	1.5597286
O	-0.7054957	-0.5992533	-0.9216151
P	-0.3838234	0.2177446	0.4617047
O	1.1222368	-0.0176880	0.7112527
O	-0.8861019	1.6628994	0.4537770
C	-2.4607927	-6.8206349	0.6376951
C	-3.0485275	-6.0946755	-0.4322789
H	-1.2737318	-6.6988508	2.4445406
H	-2.5452742	-7.9175776	0.6693731
H	-3.4138030	-4.1646433	-1.3185799
H	-3.5749799	-6.6336531	-1.2347800
C	-6.5144153	-2.4990599	-0.2466201
C	-7.0199897	-1.8184518	-1.3867151
H	-4.7817798	-2.9862689	0.9436895
H	-7.2031830	-3.0532504	0.4090611
H	-8.0954100	-1.8587552	-1.6174241
H	-6.5431651	-0.5421448	-3.0700439
C	1.8067437	-2.2358578	2.9899605
C	0.4392416	-1.9619528	3.2887935
C	2.8028128	-1.5531498	3.7127658
C	0.1086388	-0.9703383	4.2553336
C	1.1464876	-0.2991841	4.9307301
C	2.5034081	-0.5950952	4.6953944
H	3.8618126	-1.7704354	3.5008492

C	-1.3405462	-0.6614271	4.6311835
H	0.8840304	0.4733807	5.6704240
C	-1.7091279	0.8171742	4.4174239
H	-1.1031853	1.4979691	5.0466781
H	-2.7784914	0.9931311	4.6538361
H	-1.5638185	1.1082793	3.3573852
C	-1.6303590	-1.1017445	6.0794837
H	-1.9962674	-1.2689431	3.9739352
H	-1.0233869	-0.5209146	6.8045618
H	-1.3976265	-2.1760260	6.2277584
H	-2.6991309	-0.9415154	6.3312274
C	3.6208522	0.0498802	5.5084398
C	3.6987731	1.5736034	5.3181433
H	4.5322820	1.9975781	5.9157342
H	2.7617210	2.0671018	5.6459139
H	3.8779570	1.8319937	4.2554370
C	3.4953239	-0.3187644	6.9986617
H	4.5742928	-0.3825029	5.1329678
H	4.3536994	0.0820343	7.5767690
H	3.4641427	-1.4178613	7.1432664
H	2.5686193	0.1061115	7.4379123
C	2.2425338	-3.2351992	1.9153442
C	3.2520461	-2.6361164	0.9192370
H	3.4743196	-3.3668221	0.1136250
H	4.2149733	-2.3711378	1.4015908
H	2.8487036	-1.7163491	0.4560926
C	2.7989501	-4.5234623	2.5510828
H	1.3445812	-3.5142522	1.3284937
H	3.0716555	-5.2640585	1.7706316
H	2.0615777	-4.9970387	3.2302708
H	3.7099231	-4.3094592	3.1484603
H	1.6681276	3.4556136	-5.4750425
H	-0.4021048	-1.8721868	-6.4492174
H	-4.1516600	3.9641038	-2.0997224
C	1.0193131	2.7747396	-6.0740040
H	0.3094633	-3.3677348	-3.7859582
H	2.5897014	2.5323207	-7.5701186
H	-2.0224997	4.5275983	-0.7716347
C	0.1660714	1.9968056	-5.0737598
C	-1.2187875	-2.1096953	-5.7359942
C	1.9325264	1.8996548	-6.9399178
H	1.3418340	1.2560285	-7.6249151
C	0.0301753	0.6009082	-5.1090882
C	-3.5560080	3.3845452	-2.8348163
H	-0.5047835	4.3481868	-6.3698127
C	-0.5589782	2.6981911	-4.0894040
C	0.1288882	3.6633605	-6.9674286
H	0.7462173	4.2797542	-7.6532031
H	-0.4516997	3.7932258	-4.0340217
C	0.3848312	-2.2606568	-3.7641812
H	-1.3506806	-3.2112560	-5.7426852
H	-2.1500447	-1.6497672	-6.1244433
C	-0.8266394	-0.0907806	-4.2287549
C	-1.4564451	4.0700384	-1.6071259
C	-1.4358350	2.0601311	-3.1935978
H	-4.1828490	2.5447306	-3.1937993
H	-3.3469952	4.0440106	-3.7035770
C	-0.9018969	-1.6151152	-4.3141434
C	-1.5825910	0.6471247	-3.2797314
C	-2.2431469	2.8891194	-2.1966757
H	0.5709769	-1.9468663	-2.7181090
H	-0.4808360	3.7391355	-1.1994621
H	1.2683943	-1.9667869	-4.3691460
H	2.5778965	1.2400265	-6.3275682
H	-1.2693405	4.8658431	-2.3584968
H	-0.5464642	3.0352422	-7.5853334
H	-1.7376110	-1.9477530	-3.6655367
H	-2.5054903	2.2249300	-1.3499074
H	0.6000162	0.0185194	-5.8470292
C	3.6393304	-0.6087287	-2.8409439
C	2.9269454	0.3429783	-2.1082488

C	2.9672882	1.7055055	-2.4951698
C	3.7109942	2.0924521	-3.6363482
C	4.4467991	1.1382191	-4.3471971
C	4.4094621	-0.2109506	-3.9501643
H	3.5937434	-1.6681183	-2.5482353
H	2.2953318	0.0247407	-1.2665967
C	2.2905563	2.7466015	-1.7319188
H	3.7264842	3.1499426	-3.9431654
H	5.0465181	1.4412991	-5.2179870
H	4.9787444	-0.9629815	-4.5176986
O	1.9270855	2.6689347	-0.5411049
H	2.1046000	3.7122919	-2.2636597
C	1.7162515	5.4310133	3.3514465
C	1.4097564	4.1322160	3.6011092
C	0.8500183	4.0750779	4.9866454
O	0.8223318	5.3441468	5.5015415
O	1.3294147	6.2655675	4.5290938
O	0.4821315	3.1081484	5.6293986
C	1.4661750	2.9200015	2.7431362
H	2.1758440	6.8306627	4.9800068
H	0.5281698	6.9984041	4.2796780
H	1.5711351	2.0199049	3.3865764
H	2.3789568	3.0629174	2.1101413
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T52

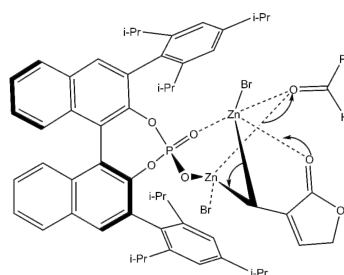


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Br	4.7127750	1.1895248	1.3276800
Zn	-0.3728297	3.0387380	1.8445102
Br	-2.0393058	4.6005019	2.2213971
C	-1.3725069	-1.9480615	1.5266709
C	-2.1791477	-2.5348197	0.5508001
C	-2.2780880	-3.9752660	0.5405485
C	-2.9548740	-4.7051085	-0.4821677
C	-1.6327425	-4.7200542	1.5978652
C	-1.7597986	-6.1413775	1.6238671
C	-0.8191413	-4.0413935	2.5515068
H	-0.2852573	-4.6340512	3.3098689
C	-0.6173717	-2.6666383	2.5016133
C	-2.5213155	-0.0873202	-2.3888385
C	-3.8640651	-0.2359485	-2.7141205
H	-4.2547536	0.2561094	-3.6178505
C	-4.7508513	-1.0086343	-1.9105393
C	-6.1452075	-1.0793802	-2.2049022
C	-4.2331695	-1.7359670	-0.7764220
C	-5.1521278	-2.4597725	0.0411792
C	-2.8211169	-1.6763208	-0.4871364
C	-2.0434138	-0.7849546	-1.2392644
O	-1.3002026	-0.5599376	1.5650019
O	-0.6946737	-0.5938360	-0.9128955
P	-0.3828208	0.2258180	0.4743641

O	1.1215886	-0.0108178	0.7345204	H	-1.3391022	-3.1916287	-5.7446806
O	-0.8845077	1.6691446	0.4580532	H	-2.1400196	-1.6296513	-6.1201338
C	-2.4577390	-6.8161145	0.6341037	C	-0.8125315	-0.0736783	-4.2260269
C	-3.0438712	-6.0896995	-0.4356061	C	-1.4414295	4.0825635	-1.5977907
H	-1.2729016	-6.6952995	2.4418386	C	-1.4248155	2.0739152	-3.1858970
H	-2.5426501	-7.9129811	0.6655598	H	-4.1734389	2.5546386	-3.1709800
H	-3.4076622	-4.1585954	-1.3206235	H	-3.3432393	4.0555204	-3.6841738
H	-3.5703336	-6.6278904	-1.2385814	C	-0.8862171	-1.5979509	-4.3140152
C	-6.5056465	-2.4931397	-0.2625895	C	-1.5675177	0.6606587	-3.2736355
C	-7.0076914	-1.8091878	-1.4015443	C	-2.2285531	2.9005679	-2.1843393
H	-4.7758690	-2.9837091	0.9309356	H	0.5894033	-1.9318656	-2.7220379
H	-7.1962976	-3.0489388	0.3896349	H	-0.4631738	3.7533286	-1.1948829
H	-8.0824531	-1.8478762	-1.6352973	H	1.2841741	-1.9488784	-4.3745983
H	-6.5259005	-0.5276787	-3.0787168	H	2.5773237	1.2754246	-6.3447506
C	1.8084983	-2.2333715	2.9839711	H	-1.2604090	4.8803955	-2.3488609
C	0.4423766	-1.9595058	3.2882088	H	-0.5676108	3.0479985	-7.5799999
C	2.8068316	-1.5469350	3.6991695	H	-1.7197325	-1.9319043	-3.6633795
C	0.1151150	-0.9658206	4.2535794	H	-2.4854977	2.2339268	-1.3361173
C	1.1552177	-0.2910197	4.9216654	H	0.6067073	0.0410554	-5.8502767
C	2.5111816	-0.5862134	4.6800590	C	3.6416158	-0.6865665	-2.7807435
H	3.8652122	-1.7629046	3.4829504	C	2.9268471	0.2797133	-2.0693819
C	-1.3329963	-0.6602113	4.6360757	C	2.9546688	1.6306453	-2.4931368
H	0.8955054	0.4843179	5.6592575	C	3.6882500	1.9907717	-3.6487161
C	-1.7091061	0.8167139	4.4239217	C	4.4261926	1.0234955	-4.3387627
H	-1.1049513	1.5000996	5.0518056	C	4.4011054	-0.3144221	-3.9049848
H	-2.7779635	0.9877958	4.6654370	H	3.6051143	-1.7366575	-2.4554714
H	-1.5718368	1.1094701	3.3633442	H	2.3047191	-0.0186410	-1.2137374
C	-1.6125253	-1.1000659	6.0865298	C	2.2738597	2.6870426	-1.7514410
H	-1.9897826	-1.2715439	3.9831073	H	3.6924672	3.0392991	-3.9857269
H	-1.0034181	-0.5158564	6.8067409	H	5.0177969	1.3073157	-5.2215912
H	-1.3747934	-2.1730654	6.2353958	H	4.9727977	-1.0773075	-4.4555155
H	-2.6801044	-0.9429686	6.3449787	O	1.9158674	2.6380312	-0.5601603
C	3.6327805	0.0594952	5.4866724	H	2.0802450	3.6374480	-2.3100100
C	3.7101046	1.5830754	5.2969517	C	1.6546394	5.4503742	3.3681058
H	4.5472530	2.0059971	5.8900813	C	1.3869060	4.1406584	3.6007939
H	2.7754443	2.0763058	5.6310471	C	0.8364671	4.0476050	4.9908908
H	3.8858015	1.8421389	4.2338907	O	0.7742642	5.3092967	5.5217949
C	3.5144228	-0.3104678	6.9770720	C	1.2446288	6.2557673	4.5598287
H	4.5842135	-0.3727650	5.1057165	O	0.5047043	3.0602072	5.6179998
H	4.3751329	0.0900512	7.5518196	H	1.4612174	2.9429325	2.7255352
H	3.4835504	-1.4095002	7.1211062	C	2.0726506	6.8461793	5.0141386
H	2.5898487	0.1140608	7.4205845	H	0.4163339	6.9619400	4.3195386
C	2.2411289	-3.2358860	1.9109313	H	1.5860351	2.0381505	3.3600767
C	3.2444182	-2.6377352	0.9081190	H	2.3646401	3.1110245	2.0845101
H	3.4656300	-3.3707284	0.1039493	H	2.0495329	5.8947622	2.4438856
H	4.2089991	-2.3668296	1.3834877				
H	2.8358743	-1.7202864	0.4452256				
C	2.8034924	-4.5204222	2.5485230				
H	1.3412904	-3.5194535	1.3290777				
H	3.0744655	-5.2642811	1.7705367				
H	2.0707083	-4.9925067	3.2334916				
H	3.7160681	-4.3024712	3.1416855				
H	1.6589400	3.4871456	-5.4870503				
H	-0.3941869	-1.8511412	-6.4518639				
H	-4.1369514	3.9717126	-2.0749965				
C	1.0102591	2.8003619	-6.0803517				
H	0.3273009	-3.3509184	-3.7911556				
H	2.5716952	2.5673048	-7.5888165				
H	-2.0029065	4.5378033	-0.7580782				
C	0.1689492	2.0172731	-5.0736545				
C	-1.2076785	-2.0900884	-5.7355209				
C	1.9237253	1.9314591	-6.9522963				
H	1.3323074	1.2837407	-7.6325270				
C	0.0388103	0.6210929	-5.1090140				
C	-3.5454124	3.3946394	-2.8149179				
H	-0.5278464	4.3614410	-6.3672638				
C	-0.5540239	2.7148177	-4.0855964				
C	0.1077125	3.6818114	-6.9683958				
H	0.7145796	4.3025052	-7.6595775				
H	-0.4526291	3.8105353	-4.0301816				
C	0.4018171	-2.2438465	-3.7682847				

TS3; COSMO

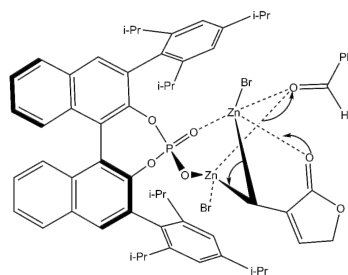


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Br	3.3076741	-0.5482394	3.6830564
Zn	-0.6086984	1.7128002	2.1603577
Br	-0.9799023	3.8064214	3.1144949
C	-0.7543674	-2.4628832	-1.3651199
C	-0.8019826	-2.2268566	-2.7446769
C	-0.3545473	-3.2810971	-3.6232070
C	-0.1957364	-3.1038897	-5.0309550
C	-0.0174650	-4.5656867	-3.0556766
C	0.3811101	-5.6284443	-3.9219541
C	-0.0181442	-4.7348210	-1.6413393

H	0.2867469	-5.7068710	-1.2244840	H	2.3201464	7.3723563	0.7634934
C	-0.3142795	-3.6874708	-0.7757386	H	-4.6474189	2.5980247	0.1230399
C	-1.1270054	1.5890262	-3.0835604	C	0.2003577	4.9798113	-0.7105843
C	-2.0430047	1.6957972	-4.1237795	C	2.1256331	3.5131068	-4.4146030
H	-2.3482678	2.6943848	-4.4706857	C	2.0843724	6.5502618	0.0581551
C	-2.6613683	0.5514457	-4.7039396	H	2.3715842	6.8926824	-0.9583378
C	-3.6688645	0.6912936	-5.7059074	C	1.0861487	4.3157438	-1.5746215
C	-2.3218067	-0.7670316	-4.2226867	C	-3.9249515	3.9772638	-2.1314914
C	-3.0740733	-4.1735422	-4.7135422	H	-1.3422227	7.2209999	-0.1469325
C	-1.2686559	-0.9018318	-3.2439571	C	-1.1205316	4.4956303	-0.6353548
C	-0.7198812	0.2710198	-2.7114527	C	-0.2576356	7.4237944	-0.2435221
O	-1.1734615	-1.4597415	-0.4940555	H	-0.0151781	8.2840427	0.4140143
O	0.2959115	0.1683344	-1.7566734	H	-1.8195834	4.9794223	0.0632188
P	-0.1587577	-0.1978992	-0.2274610	C	2.9260952	2.0254616	-2.5089553
O	1.1260039	-0.6307709	0.5018949	H	2.8270720	3.0129117	-5.1144041
O	-1.0287519	0.8966277	0.4056024	H	1.2460122	3.8566065	-4.9960778
C	0.4876458	-5.4319441	-5.2905599	C	0.6843651	3.2129693	-2.3572356
C	0.2139473	-4.1522593	-5.8436979	C	-3.5861326	2.9204194	0.1354774
H	0.6223409	-6.6062005	-3.4760004	C	-1.5806265	3.4180668	-1.4076699
H	0.8022426	-6.2580818	-5.9462917	H	-3.5943946	4.0375697	-3.1875714
H	-0.3949587	-2.1176892	-5.4723494	H	-3.8759816	5.0037679	-1.7108010
H	0.3327401	-3.9874746	-6.9255438	C	1.7066630	2.5565523	-3.2828057
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H	3.4720101	-5.6255732	1.2159315				
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H	-4.9872089	3.6561265	-2.1222713				
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TS3



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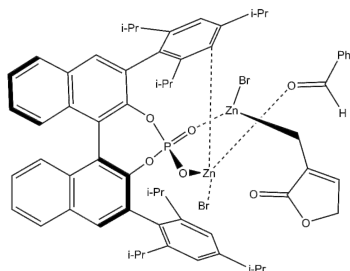
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C	-0.8072279	-2.2316015	-2.7516959
C	-0.3585530	-3.2858840	-3.6293424
C	-0.1965498	-3.1082903	-5.0364052
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C	0.3748593	-5.6329323	-3.9282119
C	-0.0286879	-4.7403887	-1.6478813
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H	3.4654025	-5.6311389	1.2049604
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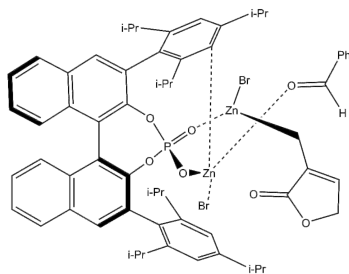
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C	-2.0639374	-2.9331264	6.1018276
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C	-4.3316394	-0.5919702	1.6093657
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H	3.0384973	-3.8907679	5.3016986
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H	-3.2189056	-5.6547191	-1.8600119
H	-4.0800169	-4.3236114	-2.7037873
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C	-2.1303812	-3.7496002	-1.8612007
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C	3.8664165	1.2309168	-1.4341472
H	5.4415193	1.8409093	-3.5262015
H	4.7399412	2.0028684	-5.9337106
H	2.3444027	1.6163186	-6.5575635
O	3.0824589	0.9529333	-0.5058962
H	4.9610793	1.3386176	-1.2329810
C	0.7239749	4.8634768	-2.9961649
C	1.2088670	4.4984166	-1.7755823
C	2.6757916	4.2841373	-1.9552503
O	3.0110259	4.5190305	-3.2651576
C	1.8335359	4.8837178	-3.9955922
O	3.5184512	3.9578346	-1.1337952
C	0.5709668	4.3310896	-0.4592348
H	1.6923123	4.1482314	-4.8210984
H	1.9992826	5.8814612	-4.4616488
H	-0.1348369	5.1604331	-0.2458265
H	1.3519580	4.3221186	0.3284190
H	-0.3167259	5.1082276	-3.2494721

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Energy (Hartree) = -11970.01909369

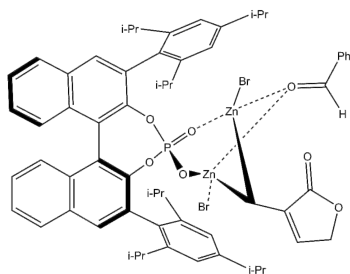
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Br	-2.7143160	2.6941862	0.8428574
C	-0.8655184	-0.5670813	2.8177148
C	-2.1014363	-1.2102144	2.7227588
C	-2.4886547	-2.0708144	3.8174552
C	-3.6438601	-2.9073612	3.7684814
C	-1.6654522	-2.1176868	5.0044537
C	-2.0711333	-2.9328539	6.1030372
C	-0.4319591	-1.4029702	5.0403799
H	0.2039620	-1.4819991	5.9360624
C	0.0081112	-0.6737256	3.9454365
C	-3.1567777	-1.0850867	-0.9747800
C	-4.5149549	-0.8172931	-0.8534897
H	-5.1348266	-0.7729518	-1.7614343
C	-5.1205837	-0.5412909	0.4038108
C	-6.4923979	-0.1591219	0.4912897
C	-4.3250127	-0.5974581	1.6050090
C	-4.9280767	-0.1876427	2.8311572
C	-2.9470778	-1.0152383	1.5112815
C	-2.4021211	-1.1905825	0.2331196
O	-0.4430648	0.2656394	1.7950637
O	-1.0550294	-1.5343513	0.1032034
P	0.0647389	-0.3645213	0.3590533
O	1.3784671	-1.1478165	0.5128925
O	-0.0154466	0.8113595	-0.6157413
C	-3.2194821	-3.7063681	6.0335262
C	-4.0000125	-3.7039953	4.8477431
H	-1.4401194	-2.9483770	7.0057111
H	-3.5169461	-4.3347134	6.8867352

H	-4.2538956	-2.9200955	2.8550911
H	-4.8938294	-4.3427306	4.7801722
C	-6.2589760	0.2015153	2.8798993
C	-7.0566507	0.1994675	1.7052679
H	-4.3193068	-0.1612104	3.7449489
H	-6.6959620	0.5253019	3.8368025
H	-8.1129579	0.5041525	1.7575278
H	-7.0890009	-0.1313955	-0.4340776
C	2.4696588	-0.9622675	3.5287439
C	1.3740556	-0.0931226	3.7702308
C	3.6920991	-0.3969548	3.0678664
C	1.5326954	1.3183848	3.6387429
C	2.7572395	1.8342724	3.1794958
C	3.8523799	1.0045547	2.8776500
H	4.5812012	-1.0439287	2.9798818
C	0.3963458	2.2509802	4.0462566
H	2.8635968	2.9188929	3.0497070
C	0.4131550	3.6155582	3.3513558
H	1.2660976	4.2482267	3.6744431
H	-0.5189044	4.1685662	3.5787977
H	0.4631080	3.5056369	2.2509933
C	0.3906156	2.4028753	5.5817996
H	-0.5563278	1.7611050	3.7599570
H	1.3296940	2.8771865	5.9355424
H	0.2933353	1.4207816	6.0865625
H	-0.4586709	3.0389334	5.9043832
C	5.2077668	1.5514651	2.4464812
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H	6.1355385	3.2065627	1.3786984
H	4.8776671	3.7240471	2.5263492
H	4.4101677	2.9857747	0.9615455
C	6.1756492	1.5465062	3.6481684
H	5.6106774	0.8295671	1.6987405
H	7.1852938	1.8803251	3.3336936
H	6.2742472	0.5368203	4.0948819
H	5.8185839	2.2359320	4.4416347
C	2.3981517	-2.4649279	3.7877308
C	2.8613216	-3.3298634	2.6054073
H	2.7535410	-4.4039923	2.8588042
H	3.9242380	-3.1620701	2.3356621
H	2.2423254	-3.1357271	1.7065587
C	3.1789444	-2.7990870	5.0746393
H	1.3357236	-2.7164183	3.9709763
H	3.0749169	-3.8751060	5.3226867
H	2.8132611	-2.2087827	5.9394577
H	4.2615894	-2.5841296	4.9561994
H	-0.5759169	-0.6071153	-6.6771369
H	-2.6639305	-5.1222675	-3.4923798
H	-4.5543629	2.6462701	-3.0467407
C	-0.6203604	-1.6295787	-6.2382624
H	-0.8409222	-5.2276737	-0.8708935
H	1.2950767	-2.1848748	-7.1532926
H	-2.1313155	3.3356703	-2.5059195
C	-1.2661357	-1.4906717	-4.8649312
C	-3.0548570	-4.7655628	-2.5164670
C	0.8215831	-2.1602462	-6.1499175
H	0.8476835	-3.1938710	-5.7468701
C	-1.3771697	-2.5892986	-3.9954504
C	-4.1963363	1.6610941	-3.4103655
H	-2.5082403	-2.0914970	-7.2696713
C	-1.7799554	-0.2592496	-4.4275347
C	-1.4809949	-2.4971372	-7.1750588
H	-1.0348524	-2.5520622	-8.1898254
H	-1.7108559	0.6103939	-5.1022038
C	-0.7292506	-4.3610503	-1.5548249
H	-3.1830868	-5.6527066	-1.8621569
H	-4.0558857	-4.3244221	-2.6981044
C	-1.9833038	-2.4872646	-2.7311311
C	-1.8185454	2.3959351	-3.0079052
C	-2.3747387	-0.0930390	-3.1621489
H	-4.9843630	0.9141991	-3.1919471

H	-4.0902738	1.7187136	-4.5145852
C	-2.1029857	-3.7425022	-1.8689842
C	-2.4939376	-1.2278169	-2.3100797
C	-2.8585503	1.2936472	-2.7432735
H	-0.0642369	-3.6219410	-1.0673238
H	-0.8135773	2.1108096	-2.6348860
H	-0.2247544	-4.7279728	-2.4730800
H	1.4468940	-1.5280788	-5.4882357
H	-1.7038998	2.6270411	-4.0881252
H	-1.5656397	-3.5343382	-6.7886584
H	-2.5592790	-3.4476819	-0.9026726
H	-3.0223344	1.2773083	-1.6466420
H	-0.9832007	-3.5677673	-4.3138266
C	1.6827265	1.2098023	-4.5253095
C	2.0755566	1.1103919	-3.1878189
C	3.4329787	1.3216269	-2.8445997
C	4.3806209	1.6371717	-3.8434910
C	3.9800234	1.7323928	-5.1805850
C	2.6322623	1.5176521	-5.5200324
H	0.6306125	1.0365378	-4.7931431
H	1.3544735	0.8663223	-2.3912688
C	3.8666440	1.1979703	-1.4564487
H	5.4292031	1.8147216	-3.5582307
H	4.7146643	1.9774220	-5.9620261
H	2.3167045	1.5844962	-6.5731932
O	3.0842516	0.9232223	-0.5279933
H	4.9626291	1.2990669	-1.2583539
C	0.7468217	4.8621688	-2.9713775
C	1.2392591	4.4804475	-1.7590316
C	2.7000983	4.2353332	-1.9596050
O	3.0230713	4.4727499	-3.2732794
C	1.8454133	4.8642858	-3.9845887
O	3.5432851	3.8802774	-1.1528492
C	0.6164720	4.3138544	-0.4368845
H	1.6789484	4.1352288	-4.8118702
H	2.0261034	5.8608459	-4.4491501
H	-0.0712484	5.1536307	-0.2065681
H	1.4084179	4.2841243	0.3391151
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C	-4.6102617	-2.2686772	-2.0454941
C	-5.9546233	-2.6431659	-2.3471679
C	-3.9625871	-2.8342392	-0.8854783
C	-4.7301374	-3.6860073	-0.0347598
C	-2.5860868	-2.4891031	-0.6162342
C	-1.9946581	-1.5032650	-1.4162168
O	-1.2411884	-0.9028356	1.2780622
O	-0.6680933	-1.1361302	-1.1749382
P	-0.3747647	-0.1561197	0.1023240
O	1.1423743	-0.2383085	0.3511611
O	-1.0068749	1.2355132	-0.0471513
C	-1.4244480	-7.3433808	1.0751714
C	-2.0505199	-6.8415792	-0.0971787
H	-0.3739020	-6.8360805	2.8996818
H	-1.3432488	-8.4296565	1.2328799
H	-2.6509558	-5.1028794	-1.2200546
H	-2.4383516	-7.5421438	-0.8524375
C	-6.0435145	-4.0131565	-0.3437788
C	-6.6580095	-3.5052652	-1.5195843
H	-4.2733589	-4.0791222	0.8837408
H	-6.6146248	-4.6670469	0.3328551
H	-7.6966776	-3.7795666	-1.7591263
H	-6.4304176	-2.2133949	-3.2426703
C	2.0104155	-1.9701871	2.9450724
C	0.6114821	-1.8545798	3.2040232
C	2.8931203	-1.1078395	3.6215856
C	0.1348637	-0.8547754	4.0962493
C	1.0643901	-0.0152699	4.7431236
C	2.4519800	-0.1372395	4.5367880
H	3.9746286	-1.1941130	3.4337017
C	-1.3495309	-0.7023290	4.4242840
O	0.6898690	0.7466309	5.4454368
C	-1.8906468	0.6947754	4.0677265
H	-1.3493872	1.5059685	4.5978457
H	-2.9633333	0.7736749	4.3400770
H	-1.8084677	0.8797703	2.9789319
C	-1.6197050	-1.0510853	5.9006727
H	-1.9061056	-1.4401890	3.8102111
H	-1.1165366	-0.3355728	6.5838945
H	-1.2530262	-2.0681562	6.1480053
H	-2.7070660	-1.0136780	6.1183597
C	3.4603026	0.6962129	5.3180792
C	3.2412670	2.2074731	5.1562965
H	4.0119373	2.7770925	5.7153736
H	2.2506127	2.5191896	5.5448806
H	3.3085689	2.5020290	4.0902127
C	3.4628175	0.2859005	6.8030428
H	4.4612098	0.4575542	4.8970995
H	4.2448092	0.8391082	7.3634276
H	3.6540186	-0.7997707	6.9228951
H	2.4850700	0.5108895	7.2785458
C	2.5999963	-3.0054146	1.9836336
C	3.5630355	-2.3942754	0.9501015
H	3.9247220	-3.1828544	0.2579509
H	4.4530810	-1.9309055	1.4222559
H	3.0517232	-1.6152074	0.3546988
C	3.2870189	-4.1417064	2.7662624
H	1.7626876	-3.4525533	1.4120651
H	3.6655699	-4.9228048	2.0747324
H	2.5936255	-4.6259964	3.4829913
H	4.1504303	-3.7565244	3.3483229
H	0.0056694	4.6401169	-3.9026283
H	0.0758678	-0.6737191	-6.4327155
H	-5.9862967	2.1845162	-2.2777937
C	-0.2319615	3.9942455	-4.7809295
H	1.6168251	-2.1943304	-4.0901357
H	1.4822777	4.7664890	-5.8912745
H	-4.6299199	2.9791023	-0.2932187
C	-0.8233433	2.7082122	-4.2057460
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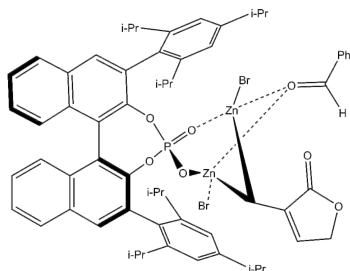


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Br	4.4159084	1.4974195	1.2947036
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Br	-0.3476339	5.0462455	-0.6656454
C	-1.1273253	-2.2860308	1.4027474
C	-1.8066250	-3.1070294	0.4941836
C	-1.6756944	-4.5366670	0.6520190
C	-2.1722615	-5.4740166	-0.3036071
C	-0.9824289	-5.0491763	1.8106833
C	-0.8938675	-6.4610585	2.0041289
C	-0.3278104	-4.1468756	2.6973144
H	0.2488065	-4.5578235	3.5399496
C	-0.3197530	-2.7742899	2.4751042
C	-2.6578507	-0.8406660	-2.4948220
C	-3.9296080	-1.2922989	-2.8278279
H	-4.4558452	-0.8373319	-3.6804588

H	0.8637902	3.2083555	-6.5134360
C	-0.3055374	1.4307523	-4.4762005
C	-5.0577172	2.1074187	-2.8807027
H	-2.1946861	4.9713958	-5.0641535
C	-1.9525269	2.7879294	-3.3674585
C	-1.2709222	4.7502753	-5.6337577
H	-0.8573853	5.7149499	-5.9935067
H	-2.3538289	3.7813780	-3.1165336
C	1.2119724	-1.1821486	-3.8824847
H	-0.0572213	-2.4163451	-6.0366925
H	-1.5279961	-1.3863764	-6.0761977
C	-0.8820656	0.2592249	-3.9427103
C	-3.7099009	2.9437544	-0.9120693
C	-2.5801286	1.6542253	-2.8285135
H	-5.2019595	1.3042804	-3.6309159
H	-4.9324827	3.0604470	-3.4365760
C	-0.2668236	-1.0925949	-4.2981102
C	-2.0355866	0.3668950	-3.1254422
C	-3.8371751	1.8414951	-1.9762019
H	1.3291545	-0.9822867	-2.7999015
H	-2.8517359	2.7510817	-0.2424224
H	1.8412876	-0.4544436	-4.4364448
H	1.8310246	3.2452843	-5.0138462
H	-3.5733971	3.9503230	-1.3572009
H	-1.5580204	4.1478272	-6.5212881
H	-0.8159066	-1.8716332	-3.7305703
H	-4.0201209	0.8925693	-1.4332032
H	0.5753627	1.3266589	-5.1265263
C	4.8840533	-0.0168350	-2.7545924
C	3.8118128	0.6526208	-2.1630720
C	3.4586671	1.9509317	-2.6148710
C	4.1962633	2.5669749	-3.6570823
C	5.2729853	1.8917031	-4.2397755
C	5.6127109	0.6013514	-3.7898019
H	5.1582089	-1.0252058	-2.4108906
H	3.2244236	0.1856660	-1.3606742
C	2.3419883	2.6544195	-2.0171508
C	3.9227423	3.5786471	-3.9945649
H	5.8520248	2.3658512	-5.0458567
H	6.4575829	0.0690520	-4.2535078
O	1.7275961	2.2219469	-1.0165908
H	2.0150800	3.6251655	-2.4630561
C	2.2587732	4.7124218	2.2613900
C	1.3306759	3.8536554	2.7404500
C	0.8763590	4.3754961	4.0627941
O	1.5608832	5.5383397	4.3284445
C	2.4536371	5.8212913	3.2439775
O	0.0615391	3.9062008	4.8348413
C	0.7746423	2.5920721	2.1793509
H	3.4950571	5.8702583	3.6347148
H	2.2065960	6.8200981	2.8192789
H	-0.3380085	2.6087264	2.2895796
H	0.9513598	1.7628123	2.9190823
H	2.8083675	4.6334841	1.3131132

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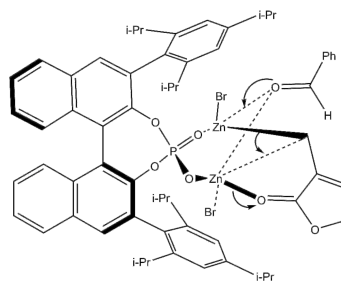


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Br	4.3843493	1.5436408	1.2943824
Zn	0.0661310	2.9016234	0.1023722

Br	-0.2987595	5.0332521	-0.7368226
C	-1.1437022	-2.2803395	1.4115719
C	-1.8250602	-3.1030346	0.5060042
C	-1.6972643	-4.5323672	0.6683283
C	-2.1991648	-5.4716720	-0.2822663
C	-1.0016026	-5.0429370	1.8262490
C	-0.9168104	-6.4540297	2.0235010
C	-0.3408109	-4.1391879	2.7064337
H	0.2412547	-4.5475765	3.5466209
C	-0.3312336	-2.7674295	2.4809970
C	-2.6587184	-0.8426202	-2.4917565
C	-3.9316612	-1.2895895	-2.8260965
H	-4.4531650	-0.8325598	-3.6805281
C	-4.6188284	-2.2608609	-2.0436729
C	-5.9636177	-2.6306285	-2.3470704
C	-3.9765407	-2.8263697	-0.8808626
C	-4.7495692	-3.6730818	-0.0304853
C	-2.5996740	-2.4863688	-0.6085621
C	-2.0012236	-1.5056854	-1.4098957
O	-1.2568541	-0.8979368	1.2844093
O	-0.6748980	-1.1426837	-1.1648762
P	-0.3888760	-0.1544620	0.1081888
O	1.1274106	-0.2309014	0.3638150
O	-1.0222144	1.2348090	-0.0546129
C	-1.4531682	-7.3379366	1.1001685
C	-2.0814232	-6.8384455	-0.0712494
H	-0.3946578	-6.8273514	2.9184871
H	-1.3747961	-8.4237983	1.2617610
H	-2.6797690	-5.1013547	-1.1979095
H	-2.4742748	-7.5402268	-0.8227062
C	-6.0628820	-3.9958725	-0.3422662
C	-6.6723535	-3.4879349	-1.5199856
H	-4.2953824	-4.0656341	0.8894290
H	-6.6380311	-4.6462217	0.3342689
H	-7.7115443	-3.7582201	-1.7615693
H	-6.4355467	-2.2003666	-3.2443684
C	2.0039487	-1.9627855	2.9184396
C	0.6091262	-1.8475716	3.1977530
C	2.8944287	-1.0957440	3.5773051
C	0.1443413	-0.8452037	4.0929657
C	1.0816448	0.0000603	4.7216456
C	2.4660613	-0.1212453	4.4946545
H	3.9731517	-1.1803652	3.3735417
C	-1.3354629	-0.6984707	4.4434590
H	0.7158332	0.7665110	5.4234426
C	-1.8915035	0.6933665	4.0899432
H	-1.3482869	1.5115287	4.6070178
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H	-1.0705004	-0.3198664	6.5970327
H	-1.2003349	-2.0552111	6.1722321
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C	3.4907878	0.7032737	5.2640374
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H	2.2734563	2.5028972	5.6209904
H	3.2623712	2.5527611	4.1186075
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H	4.4770665	0.4974627	4.7939275
H	4.3517672	0.7762751	7.2833156
H	3.7710072	-0.8534327	6.7972429
H	2.5956124	0.4195299	7.2501372
C	2.5820597	-3.0016524	1.9538235
C	3.5271456	-2.3938382	0.9016277
H	3.8883057	-3.1873970	0.2148332
H	4.4181099	-1.9152715	1.3566445
H	2.9991115	-1.6280979	0.3035798
C	3.2840831	-4.1306429	2.7334502
H	1.7381329	-3.4555677	1.3975911

H	3.6545473	-4.9160512	2.0424752
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H	0.0077115	4.6301759	-3.9252282
H	0.1001635	-0.7038813	-6.4116530
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C	-0.2233627	3.9766693	-4.7996759
H	1.6315504	-2.2021592	-4.0449397
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C	-0.2947572	1.4152936	-4.4745801
C	-5.0506924	2.1189191	-2.9052441
H	-2.1862098	4.9457906	-5.1021697
C	-1.9463559	2.7798345	-3.3835354
C	-1.2589822	4.7226623	-5.6648796
H	-0.8470379	5.6857200	-6.0307334
H	-2.3471476	3.7751891	-3.1396786
C	1.2234722	-1.1889110	-3.8493054
H	-0.0306278	-2.4432537	-6.0021855
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H	1.8412619	3.2270875	-5.0169416
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H	0.5884346	1.3061722	-5.1210279
C	4.9431748	0.0215806	-2.7228315
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C	5.3080930	1.9263218	-4.2166972
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H	3.4353727	5.8548165	3.6714232
H	2.1115295	6.8206239	2.9337868
H	-0.3979778	2.6301587	2.2497077
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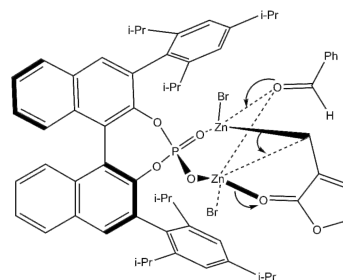
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Br	-3.3834886	1.7817716	1.4953109
C	-0.8836249	-2.1805968	1.7152718
C	-1.9079601	-2.6942235	0.9222621
C	-2.1770395	-4.1106927	1.0051549
C	-3.1018067	-4.7732218	0.1428292
C	-1.4606088	-4.9040899	1.9773254
C	-1.7440088	-6.2990716	2.0833328
C	-0.4556013	-4.2961371	2.7854260
H	0.0920218	-4.9163197	3.5114720
C	-0.1248249	-2.9553789	2.6448390
C	-2.6038570	-0.2905082	-1.9831260
C	-3.9957335	-0.2823507	-1.9878043
H	-4.5208147	0.2601077	-2.7889061
C	-4.7614124	-0.9225659	-0.9758020
C	-6.1836230	-0.8109509	-0.9395985
C	-4.0871845	-1.6885713	0.0419224
C	-4.8703606	-2.2686992	1.0839720
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C	-1.9587928	-1.0270214	-0.9464792
O	-0.5898805	-0.8180873	1.6368770
O	-0.5573077	-1.0142241	-0.9241060
P	0.1785913	-0.2238234	0.3133057
O	1.6398720	-0.7370447	0.2275743
O	-0.0402316	1.2839245	0.3376358
C	-2.6707774	-6.9050866	1.2483060
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H	-1.1989518	-6.8895397	2.8365145
H	-2.8762806	-7.9826144	1.3383777
H	-3.6242536	-4.1920568	-0.6294338
H	-4.0571448	-6.6228205	-0.4191749
C	-6.2507370	-2.1265301	1.1021756
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H	-4.3662673	-2.8171098	1.8918971
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H	-8.0129983	-1.3005942	0.1014385
H	-6.6855323	-0.2276938	-1.7275000
C	2.3329886	-2.4465770	2.8769849
C	1.0012320	-2.2606232	3.3371852
C	3.3367833	-1.5911619	3.3797334
C	0.7115803	-1.3003862	4.3445940
C	1.7446973	-0.4644997	4.8047617
C	3.0607264	-0.5735213	4.3178251
H	4.3810361	-1.7404666	3.0665292
C	-0.6725491	-1.2392916	4.9900178
H	1.5185440	0.2873274	5.5778266
C	-1.3289797	0.1475830	4.9516928
H	-0.7267806	0.9124728	5.4833486
H	-2.3272940	0.1155148	5.4332079
H	-1.4801271	0.4919448	3.9105466
C	-0.5904352	-1.7805038	6.4316755
H	-1.3323618	-1.9281017	4.4231352
H	0.0493940	-1.1330366	7.0671713
H	-0.1614202	-2.8028685	6.4548896

7.9.2 Pathway 14j-ma ↔ 14d-mi

TS1; COSMO

H	-1.5985948	-1.8173112	6.8935200	O	3.2451066	1.6225838	-0.5710168
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C	3.8869882	1.8115361	4.4352272	C	1.9299688	3.7173724	1.4703476
H	4.7305602	2.4685646	4.7294043	C	1.3542583	3.6503680	2.6956669
H	2.9763803	2.2002129	4.9348251	C	2.1387127	4.5599172	3.5911789
H	3.7465998	1.9211055	3.3401564	O	3.1712182	5.1149693	2.8615940
C	4.4103162	0.1903904	6.3227523	C	3.1222305	4.6186839	1.5209202
H	5.0971003	0.0416546	4.2824243	O	1.9702928	4.8152556	4.7667720
H	5.2633961	0.8202896	6.6485182	C	0.2346040	2.8271322	3.2168334
H	4.6365962	-0.8618362	6.5893429	H	4.0702861	4.0731924	1.3028225
H	3.5221279	0.5053438	6.9093557	H	3.0596909	5.4772703	0.8142583
C	2.7092133	-3.6050623	1.9525302	H	-0.2142625	3.3303182	4.0985181
C	3.6763458	-3.2424589	0.8153694	H	0.6633524	1.8772551	3.6134234
H	3.9395092	-4.1495723	0.2340196	H	1.5937830	3.1847842	0.5736828
H	4.6273207	-2.8031784	1.1794409				
H	3.2028497	-2.5366291	0.1024997				
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H	3.4840979	-5.6503202	2.1709705				
H	2.5742890	-5.0613447	3.6033831				
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H	-0.4446223	3.4837169	-6.5058042				
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C	-0.3936609	2.3867014	-6.6884087				
H	0.5993607	-3.3376500	-3.7094526				
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H	-1.9031358	4.2125532	-0.6667938				
C	-0.8411750	1.7043343	-5.4005864				
C	-1.6434132	-2.5895550	-5.1685056				
C	1.0517142	2.0438074	-7.0855165				
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C	-0.6706757	0.3218660	-5.2050748				
C	-3.8258709	3.4281418	-2.5280726				
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C	-1.4756871	2.4339123	-4.3797978				
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H	-1.5854939	3.5251684	-4.4969452				
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H	-1.5696281	-3.6889453	-5.0381510				
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C	-1.1752565	-0.3454104	-4.0729566				
C	-1.4946641	3.6732942	-1.5472233				
C	-1.9637455	1.8234047	-3.2077748				
H	-4.5985201	2.7212728	-2.8929454				
H	-3.6278273	4.1583107	-3.3413448				
C	-0.9981859	-1.8600737	-3.9761705				
C	-1.8615230	0.4093519	-3.0793906				
C	-2.5469525	2.6922412	-2.0968041				
H	0.9156304	-1.7672135	-2.9064011				
H	-0.5869700	3.1302589	-1.2191140				
H	1.0848307	-1.9204411	-4.6913806				
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H	-1.3768622	0.9813225	-8.0582144				
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H	4.3419298	6.0336021	-2.4790634				
H	4.2908469	3.8617946	-1.1966975				
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H	0.9799522	2.4945556	-3.6592949				
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TS1

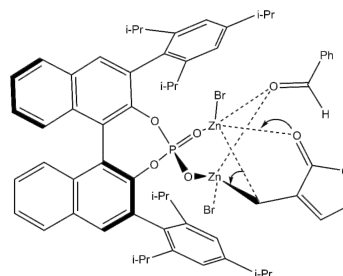


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Br	-3.3765254	1.8138387	1.4805875
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C	-1.9067220	-2.6889273	0.9220213
C	-2.1750477	-4.1055806	1.0039883
C	-3.0976516	-4.7683304	0.1399140
C	-1.4603756	-4.8988278	1.9771471
C	-1.7434535	-6.2935133	2.0816593
C	-0.4576979	-4.2899401	2.7868741
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C	-0.1267748	-2.9492030	2.6476871
C	-2.5985877	-0.2885647	-1.9860186
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C	-6.1801311	-0.8172556	-0.9535107
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C	-4.8699908	-2.2684272	1.0754945
C	-2.6488807	-1.7929317	-0.0060645
C	-1.9546305	-1.0223318	-0.9468833
O	-0.5916806	-0.8120623	1.6396415
O	-0.5533624	-1.0078145	-0.9213364
P	0.1795953	-0.2166243	0.3185010
O	1.6408510	-0.7330295	0.2379713
O	-0.0347216	1.2908182	0.3396924
C	-2.6678316	-6.8997663	1.2450491
C	-3.3375575	-6.1302767	0.2574845
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H	-2.8727634	-7.9774089	1.3344473
H	-3.6189927	-4.1864121	-0.6323830
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H	-4.3665164	-2.8138282	1.8856468
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H	-8.0112283	-1.3103569	0.0814902	H	1.1049286	-1.9002817	-4.6878290
H	-6.6807691	-0.2353391	-1.7430960	H	1.7507297	2.2934362	-6.2925817
C	2.3311217	-2.4439624	2.8818108	H	-1.2108344	4.4422838	-2.3070112
C	0.9994418	-2.2562801	3.3413796	H	-1.3938139	0.9736565	-8.0588878
C	3.3359614	-1.5910927	3.3859920	H	-1.5054480	-2.2006976	-3.0628057
C	0.7106453	-1.2964517	4.3492497	H	-2.8194693	2.0288427	-1.2555530
C	1.7453838	-0.4639867	4.8114336	H	-0.1509810	-0.2608794	-5.9810954
C	3.0617240	-0.5751511	4.3261906	C	3.5963014	5.2421478	-2.7460657
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H	-1.3346455	-1.9194835	4.4236836	H	0.9632228	2.4844815	-3.6621978
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H	-1.6046796	-1.8103885	6.8941741	O	3.2327564	1.6233904	-0.5721495
C	4.1722068	0.3400540	4.8238181	H	1.8104910	1.0417676	-1.9360602
C	3.8965314	1.8064097	4.4534080	C	1.9474733	3.7114030	1.4782123
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H	3.5230279	0.4924973	6.9220303	H	3.1002034	5.4619678	0.8355811
C	2.7064523	-3.6034831	1.9579676	H	-0.2001233	3.3318896	4.1017393
C	3.6735589	-3.2432618	0.8199898	H	0.6639804	1.8729831	3.6118491
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H	4.2252997	-4.4586884	3.2977774				
H	-0.4726187	3.4883047	-6.5205246				
H	-1.1243785	-2.3343341	-6.1230839				
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C	-0.4136690	2.3907586	-6.6996904				
H	0.6289469	-3.3174814	-3.7018570				
H	1.3306903	2.6368311	-8.0024744				
H	-1.9186713	4.2171300	-0.6740543				
C	-0.8493719	1.7096451	-5.4070557				
C	-1.6200216	-2.5891157	-5.1631459				
C	1.0323271	2.0589906	-7.1038120				
H	1.1486966	0.9843099	-7.3544732				
C	-0.6683253	0.3292171	-5.2082100				
C	-3.8389169	3.4209011	-2.5302659				
H	-2.4354626	2.3428117	-7.5668215				
C	-1.4864383	2.4369700	-4.3866350				
C	-1.3984693	2.0616115	-7.8384417				
H	-1.1257021	2.5985397	-8.7706471				
H	-1.6053715	3.5270910	-4.5059853				
C	0.5072447	-2.2196917	-3.8081662				
H	-1.5389806	-3.6875974	-5.0301540				
H	-2.6943233	-2.3334757	-5.2616456				
C	-1.1668866	-0.3388396	-4.0740637				
C	-1.5074226	3.6809205	-1.5546611				
C	-1.9682736	1.8264405	-3.2121796				
H	-4.6082192	2.7092607	-2.8924189				
H	-3.6486547	4.1519020	-3.3447032				
C	-0.9791135	-1.8519088	-3.9734091				
C	-1.8573670	0.4132886	-3.0816895				
C	-2.5546068	2.6933350	-2.1016414				
H	0.9333392	-1.7435282	-2.9032097				
H	-0.5961677	3.1437004	-1.2265218				

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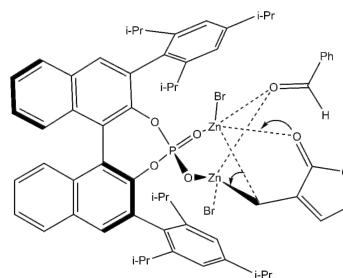


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Br	3.7542041	-0.9365086	-3.3914282
Zn	1.1376423	2.5540832	-1.6472988
Br	0.7859429	4.4955383	-2.8607763
C	0.6373365	-0.8273354	2.4558407
C	-0.5897239	-1.1666052	3.0332243
C	-0.6575105	-2.3673532	3.8328822
C	-1.8835091	-2.9065012	4.3279447
C	0.5645956	-3.0775027	4.1246987
C	0.5188429	-4.2380428	4.9550979
C	1.7833055	-2.6521103	3.5247631
H	2.7000256	-3.2285857	3.7209064
C	1.8349561	-1.5824815	2.6376759
C	-3.3706356	0.6835404	1.1369436
C	-4.2089251	1.0399014	2.1887073
H	-5.1689650	1.5275507	1.9624389
C	-3.8454506	0.8404359	3.5491882
C	-4.6733320	1.3099795	4.6134300
C	-2.5992783	0.1846413	3.8587908
C	-2.2068431	0.0929419	5.2286109
C	-1.7899325	-0.3245315	2.7777086

C	-2.1651344	-0.0073095	1.4651160	C	-7.0259076	1.9388551	-3.9575633
O	0.7130854	0.3302677	1.6810325	H	-7.5697465	2.3195843	-4.8469502
O	-1.3650623	-0.4343060	0.3999296	H	-4.2837443	3.7745444	-2.2564789
P	0.0779571	0.3075729	0.1665344	C	-3.3186505	-2.3070194	-1.6407015
O	0.8826276	-0.6147722	-0.7701908	H	-5.6837198	-3.0592853	-0.3645378
O	-0.0825281	1.7785437	-0.2494760	H	-6.3290653	-1.4117031	-0.0597411
C	-0.6861724	-4.7132801	5.4497978	C	-4.2189093	0.0192971	-1.1584137
C	-1.8971311	-4.0496372	5.1156929	C	-2.2236237	4.4309618	-0.5168047
H	1.4620426	-4.7610620	5.1782130	C	-3.7357934	2.3896335	-0.6807824
H	-0.7093831	-5.6130362	6.0832910	H	-5.0451368	3.6901087	1.4311494
H	-2.8302196	-2.4112422	4.0726817	H	-4.9545698	4.8233024	0.0496043
H	-2.8567314	-4.4475481	5.4796424	C	-4.2424014	-1.4541643	-0.7544584
C	-3.0236308	0.5788783	6.2402214	C	-3.7503005	1.0270744	-0.2711515
C	-4.2757389	1.1776532	5.9351166	C	-3.2052307	3.5062691	0.2183767
H	-1.2374693	-0.3593078	5.4798468	H	-2.2813365	-1.9184915	-1.6272193
H	-2.6943898	0.5048098	7.2878990	H	-1.4088562	3.8600861	-0.9971688
H	-4.9179787	1.5511046	6.7471992	H	-3.6654687	-2.3210073	-2.6942318
H	-5.6277583	1.7980280	4.3607394	H	-3.8866235	1.7650119	-5.5170774
C	3.3756215	-2.2185950	0.7610464	H	-2.7222156	5.0308505	-1.3061108
C	3.0556725	-1.3114406	1.8146405	H	-7.2488123	0.8552679	-3.8625502
C	4.5479144	-1.9912436	0.0164945	H	-3.8543142	-1.5220647	0.2819310
C	3.8895926	-0.1900106	2.0722159	H	-2.6424573	3.0256641	1.0444375
C	5.0470927	-0.0053964	1.2874054	H	-5.1263346	-0.3793601	-3.0824938
C	5.4080941	-0.9079195	0.2683727	C	-0.3092912	-2.8969984	-4.6563356
H	4.8131873	-2.6906933	-0.7909111	C	0.0828736	-1.6692317	-4.1208206
C	3.5957589	0.7801618	3.2156504	C	-0.8184937	-0.5742182	-4.1487323
H	5.6917276	0.8640874	1.4912696	C	-2.1038673	-0.7284430	-4.7214372
C	3.2934468	2.2055187	2.7175321	C	-2.4833642	-1.9570099	-5.2702459
H	4.1291104	2.6259956	2.1205865	C	-1.5881097	-3.0411391	-5.2324591
H	3.1144642	2.8837203	3.5773275	H	0.3848675	-3.7501929	-4.6308248
H	2.3798788	2.2140830	2.0909395	H	1.0867588	-1.5425096	-3.6891900
C	4.7388055	0.7765657	4.2483615	C	-0.4684769	0.7129042	-3.5789794
H	2.6879548	0.4112792	3.7372208	H	-2.8004854	0.1207115	-4.7197563
H	5.6796665	1.1739010	3.8141104	H	-3.4810727	-2.0772651	-5.7183065
H	4.9444340	-0.2482006	4.6193759	H	-1.8888958	-4.0121809	-5.6553379
H	4.4792605	1.4135241	5.1189781	O	0.6435377	0.9807503	-3.0757062
C	6.7183771	-0.7823316	-0.4993930	H	-1.2533017	1.5100244	-3.5896196
C	6.8953872	0.5824845	-1.1798058	C	4.2832419	2.9221123	-3.0732174
H	7.8393427	0.6077357	-1.7621468	C	4.1219798	2.7427351	-1.7423412
H	6.9396568	1.4062282	-0.4392653	C	5.2270166	3.4718107	-1.0544136
H	6.0587475	0.7838022	-1.8778904	O	6.0207037	4.0589469	-2.0110769
C	7.9104224	-1.1073049	0.4213689	C	5.4953108	3.7621438	-3.3105793
H	6.6881431	-1.5521672	-1.3009118	O	5.4633270	3.5687241	0.1356429
H	8.8640390	-1.0877163	-0.1460161	C	3.0984991	1.9818426	-0.9711757
H	7.8036631	-2.1094829	0.8838534	H	6.2738603	3.2324258	-3.9046756
H	7.9907921	-0.3639119	1.2422224	H	5.2605598	4.7147550	-3.8362225
C	2.5351423	-3.4615440	0.4552720	H	2.7642382	2.5987097	-0.1019845
C	2.1903148	-3.6246452	-1.0350093	H	3.6300913	1.2000638	-0.3600465
H	1.5708409	-4.5337711	-1.1806701	H	3.6497484	2.5247688	-3.8784453
H	3.0930688	-3.7311416	-1.6701196				
H	1.6133702	-2.7566038	-1.4036991				
C	3.2385339	-4.7257153	0.9886558				
H	1.5729859	-3.3586982	0.9959140				
H	2.6078549	-5.6244630	0.8270459				
H	3.4565569	-4.6514323	2.0727365				
H	4.2042968	-4.8901119	0.4662275				
H	-5.3546374	3.2777381	-4.1890608				
H	-6.1366510	-2.0056511	-1.7386620				
H	-3.9559479	5.1113011	1.5103637				
C	-5.5097929	2.1808852	-4.0923438				
H	-3.2956640	-3.3570722	-1.2824795				
H	-5.5051738	1.8973690	-6.2633561				
H	-1.7612550	5.1466817	0.1934360				
C	-4.7919904	1.7506228	-2.8161039				
C	-5.6774952	-2.0107976	-0.7279099				
C	-4.9600627	1.5290680	-5.3702956				
H	-5.0771549	0.4247934	-5.3501340				
C	-4.7272309	0.4020383	-2.4150877				
C	-4.3551208	4.3230380	0.8391154				
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C	-4.2606614	2.7174525	-1.9456982				

TS2

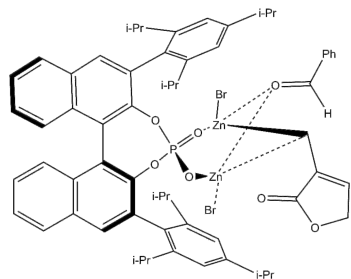


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number of imaginary frequencies: 1

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Br	3.7294057	-0.9632889	-3.4000417
Zn	1.1058387	2.5226701	-1.6743457
Br	0.7432596	4.4651008	-2.8692198
C	0.6324782	-0.8342460	2.4571648
C	-0.5917539	-1.1760074	3.0398130

C	-0.6522330	-2.3730507	3.8453793	H	-5.2742996	3.3254932	-4.1812513
C	-1.8743015	-2.9142317	4.3471769	H	-6.1466207	-1.9655012	-1.7711839
C	0.5733520	-3.0767908	4.1372508	H	-3.9646992	5.1019880	1.5495624
C	0.5338051	-4.2327045	4.9735845	C	-5.4437409	2.2298565	-4.0942879
C	1.7883092	-2.6487259	3.5322101	H	-3.3247982	-3.3512447	-1.2874873
H	2.7086344	-3.2195553	3.7279924	H	-5.4110092	1.9621155	-6.2681963
C	1.8338951	-1.5833835	2.6400330	H	-1.7488770	5.1441841	0.2716090
C	-3.3751446	0.6748919	1.1474202	C	-4.7480802	1.7828286	-2.8115677
C	-4.2117434	1.0319764	2.1998189	C	-5.6983347	-1.9802506	-0.7556674
H	-5.1689998	1.5250175	1.9735375	C	-4.8836416	1.5818575	-5.3695182
C	-3.8482582	0.8300062	3.5596341	H	-5.0146398	0.4789861	-5.3595431
C	-4.6737347	1.3000603	4.6248960	C	-4.7023343	0.4312533	-2.4188409
C	-2.6023895	0.1730834	3.8675557	C	-4.3538860	4.3197954	0.8657371
C	-2.2086440	0.0817240	5.2367759	H	-7.3787718	2.5082869	-3.0869599
C	-1.7949413	-0.3376984	2.7857909	C	-4.2201678	2.7385086	-1.9274790
C	-2.1724780	-0.0220379	1.4735498	C	-6.9641977	2.0051255	-3.9831189
O	0.7028386	0.3187489	1.6769434	H	-7.4921595	2.3984925	-4.8765427
O	-1.3775725	-0.4535655	0.4073772	H	-4.2284802	3.7978143	-2.2309599
P	0.0644752	0.2899182	0.1644552	C	-3.3322557	-2.2996399	-1.6414367
O	0.8659348	-0.6362897	-0.7716975	H	-5.7214075	-3.0302069	-0.3974464
O	-0.1027831	1.7568647	-0.2594323	H	-6.3508255	-1.3766109	-0.0928884
C	-0.6672217	-4.7098176	5.4746734	C	-4.2128809	0.0353754	-1.1589298
C	-1.8811393	-4.0526527	5.1410535	C	-2.2003304	4.4360647	-0.4527111
H	1.4796869	-4.7510253	5.1962727	C	-3.7154837	2.3982372	-0.6579858
H	-0.6847901	-5.6061822	6.1130449	H	-5.0553461	3.6843200	1.4413225
H	-2.8230005	-2.4228619	4.0921190	H	-4.9395041	4.8276418	0.0708694
H	-2.8381059	-4.4517506	5.5104553	C	-4.2569500	-1.4398546	-0.7631944
C	-3.0236266	0.5681619	6.2489922	C	-3.7452949	1.0324699	-0.2595801
C	-4.2751382	1.1676635	5.9456830	C	-3.1949243	3.5061732	0.2577056
H	-1.2392333	-0.3712357	5.4858907	H	-2.2908714	-1.9234670	-1.6133307
H	-2.6929029	0.4939469	7.2961267	H	-1.3780974	3.8702216	-0.9251952
H	-4.9160775	1.5420197	6.7582998	H	-3.6663280	-2.3666701	-2.6992344
H	-5.6276507	1.7895595	4.3731202	H	-3.8052161	1.8048487	-5.4989433
C	3.3735332	-2.2180862	0.7624998	H	-2.6833886	5.0453539	-1.2443497
C	3.0513955	-1.3090900	1.8135483	H	-7.2015186	0.9238763	-3.8982179
C	4.5409952	-1.9851960	0.0125867	H	-3.8818145	-1.5162540	0.2773793
C	3.8782151	-0.1808170	2.0637788	H	-2.6465887	3.0179234	1.0887666
C	5.0309507	0.0091077	1.2734770	H	-5.1031317	-0.3419121	-3.0949647
C	5.3945169	-0.8951460	0.2570452	C	-0.2826852	-2.9475230	-4.6778676
H	4.8074893	-2.6847407	-0.7942885	C	0.0904036	-1.7138422	-4.1418255
C	3.5822883	0.7912503	3.2051145	C	-0.8286586	-0.6343090	-4.1683205
H	5.6684086	0.8856093	1.4696897	C	-2.1111735	-0.8082596	-4.7405694
C	3.2669369	2.2130979	2.7049357	C	-2.4707438	-2.0426032	-5.2899439
H	4.0959834	2.6402870	2.1036627	C	-1.5585927	-3.1122305	-5.2530536
H	3.0867311	2.8917028	3.5640521	H	0.4268268	-3.7879633	-4.6520345
H	2.3489634	2.2129796	2.0848372	H	1.0938722	-1.5711783	-3.7131164
C	4.7305734	0.7988587	4.2319043	C	-0.4953531	0.6583811	-3.5956037
H	2.6800799	0.4164746	3.7323891	H	-2.8216565	0.0293507	-4.7367860
H	5.6660031	1.2021040	3.7919051	H	-3.4667722	-2.1779976	-5.7375235
H	4.9462167	-0.2230525	4.6047556	H	-1.8442749	-4.0878324	-5.6762347
H	4.4714816	1.4366500	5.1019755	O	0.6115721	0.9359590	-3.0915726
C	6.7016900	-0.7649802	-0.5152018	H	-1.2899588	1.4467512	-3.6038655
C	6.8696639	0.5974715	-1.2023275	C	4.2463675	2.9190102	-3.0803519
H	7.8118365	0.6244243	-1.7874257	C	4.0844049	2.7343156	-1.7513294
H	6.9120418	1.4259415	-0.4671004	C	5.1828101	3.4702962	-1.0556046
H	6.0307203	0.7899218	-1.8999853	O	5.9720524	4.0701712	-2.0108842
C	7.8974163	-1.0798925	0.4041298	C	5.4519793	3.7734726	-3.3089244
H	6.6730812	-1.5381997	-1.3135892	O	5.4149033	3.5567183	0.1336330
H	8.8499847	-1.0575295	-0.1648239	C	3.0662001	1.9640900	-0.9835688
H	7.7969808	-2.0802608	0.8715948	H	6.2368276	3.2537420	-3.9047535
H	7.9757721	-0.3330576	1.2218270	H	5.2069608	4.7255713	-3.8321036
C	2.5409477	-3.4685286	0.4652575	H	2.7289892	2.5770195	-0.1117968
C	2.1899278	-3.6400910	-1.0225957	H	3.6039006	1.1856337	-0.3733804
H	1.5765380	-4.5544240	-1.1616526	H	3.6172773	2.5176162	-3.8869831
H	3.0896265	-3.7413786	-1.6627721				
H	1.6045030	-2.7776528	-1.3909993				
C	3.2565247	-4.7250396	1.0001102				
H	1.5806061	-3.3713854	1.0101775				
H	2.6327278	-5.6297925	0.8456483				
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H	4.2213059	-4.8840625	0.4745346				

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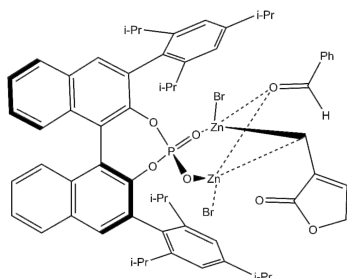
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Br	2.1298411	-0.3461748	4.8134877
Zn	-1.7905994	1.2606365	2.6719903
Br	-3.4338456	2.6207985	3.5631172
C	-0.5207569	-2.3142680	-0.9236962
C	-0.5320453	-2.0616179	-2.2968688
C	0.0916880	-3.0242194	-3.1734692
C	0.2824333	-2.7983440	-4.5704098
C	0.5720933	-4.2641130	-2.6119120
C	1.1498145	-5.2447092	-3.4738052
C	0.5160950	-4.4655796	-1.2035780
H	0.9087743	-5.4052052	-0.7865327
C	0.0364265	-3.4896436	-0.3374539
C	-1.0374636	1.6824905	-2.9436275
C	-1.9244425	1.6443214	-4.0151541
H	-2.1786398	2.5836379	-4.5292775
C	-2.5241670	0.4338518	-4.4610981
C	-3.5058549	0.4279291	-5.4973930
C	-2.1331146	-0.8124112	-3.8510912
C	-2.7863426	-2.0088738	-4.2753609
C	-1.1252783	-0.8005960	-2.8193384
C	-0.6873293	0.4393882	-2.3354865
O	-1.1273001	-1.3888230	-0.0753354
O	0.1983949	0.4796891	-1.2503391
P	-0.3907110	0.0484527	0.2193815
O	0.8298331	-0.1226439	1.1437249
O	-1.5055826	0.9966947	0.6961784
C	1.2893222	-5.0060071	-4.8326043
C	0.8666576	-3.7642986	-5.3785110
H	1.5002253	-6.1906524	-3.0318446
H	1.7422776	-5.7674290	-5.4856467
H	-0.0316970	-1.8410033	-5.0083371
H	1.0073902	-3.5629644	-6.4514839
C	-3.7516724	-1.9794878	-5.2722694
C	-4.1070842	-0.7550129	-5.8999558
H	-2.5277675	-2.9612542	-3.7916903
H	-4.2503963	-2.9129507	-5.5745822
H	-4.8689087	-0.7468748	-6.6942615
H	-3.7868070	1.3863898	-5.9614303
C	1.4434217	-3.3794563	1.7430477
C	0.1707988	-3.6212955	1.1479035
C	1.5721748	-3.5475381	3.1344477
C	-0.9397918	-3.9958901	1.9501654
C	-0.7567266	-4.1385137	3.3411085
C	0.4962331	-3.9390952	3.9515922
H	2.5507399	-3.3754497	3.6072777
C	-2.3075044	-4.2853765	1.3332301
H	-1.6206258	-4.4224992	3.9623311
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H	-2.9855226	-5.8202108	2.7629627
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C	0.6093974	-5.7037108	5.7434149
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H	0.8387824	-5.9067291	6.8100795
H	1.3099990	-6.2957911	5.1203108
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H	4.3928055	-1.6878320	0.8263171
H	3.9944214	-2.2127907	2.4872874
H	2.9745489	-0.9899646	1.6653021
C	3.5251011	-4.2953063	0.6583812
H	2.3216694	-2.6612354	-0.0751819
H	4.3947914	-4.0643703	0.0088075
H	2.9387578	-5.0982929	0.1702267
H	3.9127796	-4.7008770	1.6164108
H	0.3887852	7.5763107	-1.3518696
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C	1.0884207	7.0537018	-2.0406608
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C	0.9846016	7.7421711	-3.4159697
H	1.2655812	8.8135375	-3.3462982
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C	2.9431137	1.8499804	-2.8267857
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C	2.0577315	3.0145670	1.5970982
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O	-3.0272400	-1.0595378	6.9970248
C	-2.1747504	0.0559585	7.2817545
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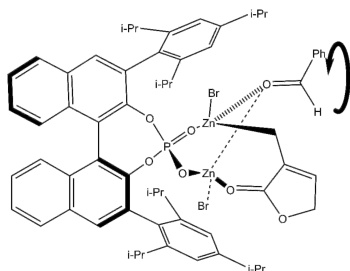
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H	0.8938266	-5.3988658	-0.7762250
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P	-0.3919671	0.0625614	0.2197563
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H	-2.5439756	-2.9515237	-3.7776438
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H	-1.5993956	-4.4277169	3.9760985
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C	2.6693146	-2.9804052	0.9044401
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H	4.3754623	-1.6280562	0.8192735
H	4.0065705	-2.1837764	2.4764272
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C	3.5175568	-4.2394465	0.6319448
H	2.3028861	-2.6000704	-0.0715536
H	4.3834616	-3.9979153	-0.0187692
H	2.9313328	-5.0370912	0.1355763
H	3.9105751	-4.6576638	1.5821566
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H	-4.6742143	3.9987693	-1.8477246
C	1.1232945	7.0425694	-2.0256611
H	3.5060723	1.0261146	-3.3730232
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C	2.5470723	7.1687919	-1.4603806
H	3.2950446	6.6863125	-2.1242368
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C	1.7515198	2.2879546	-3.7424407
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O	-3.0481959	-1.1346164	6.9621199	C	-1.0773113	2.0583656	3.9055976
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H	-1.5387353	-0.2315381	8.0709028	H	-0.8661075	0.1495128	4.9571690
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				H	-0.8917833	2.4691531	6.0531186
				C	-5.3750051	3.1555688	1.3929235
				C	-6.0646342	2.1704372	2.3441345
				H	-7.1535046	2.1315069	2.1370527
				H	-5.9455183	2.4776651	3.4041292
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				C	-5.9379908	4.5786996	1.5855771
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				H	3.5350390	-6.7164513	-3.1662706
				C	1.9971750	-4.7021037	-0.5620453
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7.9.3 Pathway 14d-ma ↔ 14j-mi

TS1; COSMO



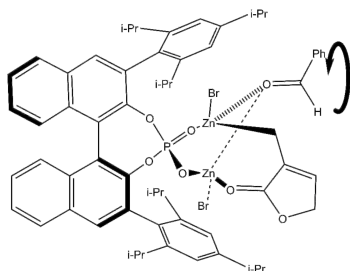
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C	2.5968132	4.6094735	1.6475584
C	3.2779860	5.8643385	1.6508834
C	1.1814056	4.5410436	1.7849770
H	0.6169468	5.4762010	1.9231094
C	0.4875856	3.3395175	1.6848892
C	3.6513001	-1.4336392	0.4303937
C	4.7598158	-1.6567506	1.2401981
H	5.2957761	-2.6148411	1.1608258
C	5.1735280	-0.7196054	2.2285620
C	6.2536624	-1.0144104	3.1147547
C	4.4468320	0.5178783	2.3855009
C	4.7914543	1.3643836	3.4827945
C	3.3883947	0.8280475	1.4525116
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C	3.1067239	-2.4564063	-1.8380589
C	0.8947684	-4.0283452	2.1895289
C	2.4816535	-3.6454910	0.2301712
H	3.2300313	-4.8393921	3.4360058
H	3.0740894	-5.8126294	1.9385344
C	3.7117756	-1.2689470	-2.5844094
C	3.0743992	-2.5230296	-0.4181157
C	2.3428870	-3.7483990	1.7505216
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H	0.2074820	-3.2652320	1.7799749
H	2.3510748	-1.2807529	-4.3219743
H	-0.5173657	-5.1280809	-2.8440978
H	0.5366918	-5.0201124	1.8452583
H	2.9147055	-5.6896193	-4.4956892
H	4.0171703	-0.5152065	-1.8309511
H	2.6219026	-2.7661296	2.1814916
H	2.6465327	-3.4914563	-3.6803776
Zn	-1.5707753	0.7629559	-2.3537762
Br	-1.0143265	0.9843600	-4.5980644
Zn	-1.9826808	-1.8966197	0.1092817
Br	-2.1148199	-4.1992627	-0.4060063
H	-3.6238809	4.1975565	-0.3918440
C	-5.3661164	-2.8787333	-4.4272107
C	-4.3491920	-2.3364263	-3.6415721
C	-3.0146814	-2.7866030	-3.8030290
C	-2.7166230	-3.7810909	-4.7655821
C	-3.7400991	-4.3196613	-5.5528429
C	-5.0620651	-3.8713617	-5.3818154
H	-6.4038189	-2.5333051	-4.3059003
C	-1.9446226	-2.2160894	-3.0044788
H	-1.6783281	-4.1205205	-4.8911046
H	-3.5112915	-5.0908621	-6.3030932
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O	-2.1290629	-1.2698195	-2.1967660
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H	-0.9157759	-2.6261306	-3.1468837
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C	-4.3859285	-0.1689448	-0.0840923
O	-4.3660373	0.7046387	-1.2795666
C	-5.5951498	0.8091618	-1.8236439
C	-6.5100953	0.0010660	-1.0564609
O	-3.4235697	1.3241348	-1.8019411
C	-3.1943285	-0.4069539	0.7315313
H	-6.9770567	-0.7330152	-1.7513355
H	-7.3208866	0.6626140	-0.6768273
H	-3.4683751	-0.6597735	1.7749279
H	-2.5593291	0.5015285	0.7506978
H	-6.0884907	-1.2655556	0.7964190

C	4.7524837	3.4893960	1.2428701
C	2.5956020	4.5976126	1.6702094
C	3.2810079	5.8495515	1.6829198
C	1.1786956	4.5329438	1.7880238
H	0.6137172	5.4691064	1.9170353
C	0.4827414	3.3336280	1.6799364
C	3.6607628	-1.4373091	0.4451920
C	4.7587503	-1.6637307	1.2679137
H	5.2982823	-2.6195145	1.1852166
C	5.1568877	-0.7345935	2.2696415
C	6.2256117	-1.0327839	3.1676269
C	4.4267851	0.5007445	2.4249821
C	4.7576279	1.3418277	3.5302913
C	3.3789576	0.8149417	1.4817263
C	3.0206804	-0.1649383	0.5481301
O	0.5598813	0.9290495	1.5476171
O	2.0114127	0.1103768	-0.3690357
P	0.4474949	0.1151756	0.1215371
O	-0.3019483	0.9681938	-0.9105029
O	-0.0707612	-1.2864398	0.4405581
C	4.6505832	5.9151449	1.4795275
C	5.3861557	4.7240602	1.2402119
H	2.6930382	6.7677515	1.8390794
H	5.1657157	6.8877654	1.4839449
H	5.3325145	2.5771515	1.0473994
H	6.4678693	4.7795129	1.0444735
C	5.7895481	1.0132321	4.3984140
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H	4.1771892	2.2591402	3.6978342
H	6.0192157	1.6775036	5.2455039
H	7.3667829	-0.4198082	4.8975545
H	6.7798409	-1.9741457	3.0274112
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C	-1.0111541	3.2917101	1.6152697
C	-3.0844662	3.7877989	0.4390363
C	-1.7651779	2.6738300	2.6489361
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C	-3.8544314	3.1963688	1.4564021
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H	-3.7393584	2.1783540	3.3670753
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H	-0.9151596	0.1773586	4.9616134
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H	-0.0091203	2.1519535	3.7649595
H	-2.5534390	2.8680465	5.3581488
H	-1.1791119	3.9651895	5.0237632
H	-0.9375337	2.5042519	6.0398338
C	-5.3777554	3.2111622	1.3472647
C	-6.0881482	2.2433238	2.3010531
H	-7.1774924	2.2234268	2.0928355
H	-5.9669704	2.5537379	3.3597692
H	-5.7001461	1.2101178	2.2024864
C	-5.9171518	4.6444184	1.5311837
H	-5.6218939	2.9007048	0.3044941
H	-7.0167700	4.6797718	1.3846234
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H	-5.6952337	5.0123378	2.5546558
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H	-0.7696724	4.6645215	-2.8128037
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H	0.1357962	4.5205653	-0.4451457
H	-0.7119654	6.6707074	-1.3402164
H	-1.0969551	6.5471338	0.4097784
H	-2.3774400	6.2802325	-0.8076769
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H	4.8565464	-2.3516015	-4.1059406

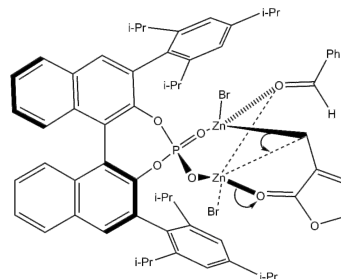
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number of imaginary frequencies: 1

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H	4.3800501	-4.6377571	2.0125962
C	1.6057521	-5.8028256	-2.8780340
H	3.2154300	0.3700435	-3.9689479
H	-0.1084498	-6.2729348	-4.1747608
H	0.8334490	-4.0994964	3.2355489
C	2.1194864	-4.6455105	-2.0308480
C	5.0604264	-1.6146992	-3.3009627
C	0.2981953	-5.4193927	-3.5920727
H	0.4753752	-4.5806275	-4.3002102
C	2.6610150	-3.4878082	-2.6169902
C	3.3236025	-4.8622232	2.2633769
H	3.5972322	-6.6067174	-3.3477366
C	2.0406001	-4.6961475	-0.6313104
C	2.6614965	-6.3208107	-3.8687603
H	2.2862933	-7.2096011	-4.4172567
H	1.5820662	-5.5812399	-0.1622523
C	2.7646888	-0.5301857	-3.5031270
H	5.7964836	-2.0713702	-2.6084616
H	5.5334089	-0.7277094	-3.7711383
C	3.1545944	-2.4194002	-1.8468318
C	0.9122746	-4.0828344	2.1286062
C	2.5124961	-3.6556131	0.1888349
H	3.2408880	-4.9278791	3.3681874
H	3.0904743	-5.8649059	1.8476958
C	3.7691928	-1.2171677	-2.5611670
C	3.1042838	-2.5160331	-0.4292034
C	2.3633028	-3.7950995	1.7052215
H	1.8553233	-0.2033565	-2.9633933
H	0.2297724	-3.3055356	1.7386610
H	2.4452964	-1.2005333	-4.3280947
H	-0.4690733	-5.1018848	-2.8569320
H	0.5503996	-5.0619085	1.7538449
H	2.9217220	-5.5514843	-4.6254576
H	4.0572191	-0.4752268	-1.7893969
H	2.6417268	-2.8246179	2.1623742
H	2.7200177	-3.4159838	-3.7151083
Zn	-1.5422809	0.7417181	-2.3840814
Br	-0.9777623	0.9046136	-4.6191635
Zn	-1.9727140	-1.9073405	0.1050251
Br	-2.0954977	-4.1935579	-0.4537800
H	-3.6029393	4.2095147	-0.4377411
C	-5.4948125	-3.0153099	-4.2807750
C	-4.4629099	-2.4212316	-3.5535980
C	-3.1290985	-2.8627324	-3.7311075
C	-2.8462141	-3.8996988	-4.6503659
C	-3.8847125	-4.4917139	-5.3772837
C	-5.2068515	-4.0520782	-5.1910049
H	-6.5328338	-2.6746185	-4.1477657
C	-2.0423279	-2.2337774	-2.9946592
H	-1.8079705	-4.2352036	-4.7854124
H	-3.6667077	-5.2988396	-6.0922667
H	-6.0237764	-4.5194098	-5.7623542
O	-2.2247588	-1.2641455	-2.2177384
H	-4.6577335	-1.6093947	-2.8396233
H	-1.0079856	-2.6137543	-3.1738384
C	-5.6608280	-0.5805050	0.0460950
C	-4.3619362	-0.1621405	-0.0590998
C	-4.3303718	0.7172398	-1.2544161
O	-5.5628013	0.8364220	-1.7957765
C	-6.4839959	0.0399350	-1.0295874
O	-3.3833762	1.3253561	-1.7726241
C	-3.1740904	-0.4172615	0.7537335
H	-6.9640826	-0.6854391	-1.7257896
H	-7.2842617	0.7119664	-0.6441527
H	-3.4483738	-0.6784762	1.7948896
H	-2.5294405	0.4839915	0.7784766
H	-6.0740363	-1.2424427	0.8187833



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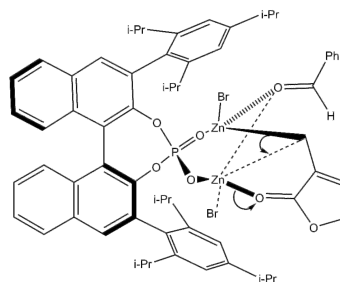
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C	4.3090657	3.4477955	1.5219248
C	2.1285418	4.5329179	1.8939005
C	2.8022725	5.7907336	1.9455096
C	0.7094223	4.4544116	1.9777877
H	0.1350848	5.3832436	2.1169253
C	0.0267533	3.2506042	1.8343213
C	3.2794841	-1.4747046	0.6131234
C	4.3349437	-1.7167548	1.4837453
H	4.8954647	-2.6598288	1.3986115
C	4.6807339	-0.8045746	2.5209286
C	5.7073281	-1.1158381	3.4629289
C	3.9446414	0.4292488	2.6583016
C	4.2234776	1.2557996	3.7890457
C	2.9414331	0.7577917	1.6721956
C	2.6259713	-0.2079833	0.7095021
O	0.1331162	0.8540969	1.6332864
O	1.6567663	0.0803625	-0.2520473
P	0.0751659	0.0690510	0.1885508
O	-0.6252418	0.9400772	-0.8757307
O	-0.4679588	-1.3241756	0.4926308
C	4.1776233	5.8700005	1.7866919
C	4.9319311	4.6879837	1.5569356
H	2.2024198	6.7019988	2.0970873
H	4.6840595	6.8466291	1.8211008
H	4.9037401	2.5428320	1.3352497
H	6.0192923	4.7555408	1.3996754
C	5.2139784	0.9147223	4.7001524
C	5.9776765	-0.2708685	4.5287595
H	3.6363395	2.1714065	3.9427603
H	5.4039474	1.5670727	5.5661816
H	6.7667005	-0.5259206	5.2525700
H	6.2683575	-2.0550246	3.3357189
C	-2.1469460	3.8186198	0.6773750
C	-1.4659928	3.1918795	1.7644444
C	-3.5516779	3.7652138	0.6423862
C	-2.2124111	2.5139081	2.7679073
C	-3.6181580	2.4960694	2.6817227
C	-4.3124981	3.1214709	1.6340343
C	-1.5520613	1.8538710	3.9776001
H	-4.1838510	1.9802784	3.4718294
C	-1.9100468	0.3613251	4.0928161
H	-2.9943013	0.2119588	4.2788280
H	-1.3621356	-0.1042023	4.9378964
H	-1.6360775	-0.1841234	3.1687683
C	-1.8884805	2.6215633	5.2703755
H	-0.4537431	1.9180718	3.8465299
H	-2.9772180	2.5952610	5.4862882
H	-1.5867774	3.6861120	5.1950075
H	-1.3624475	2.1752135	6.1396535
C	-5.8353064	3.1868161	1.5754334
C	-6.5425650	2.0193884	2.2776141
H	-7.6337448	2.0545002	2.0815164
H	-6.4121471	2.0643126	3.3790096

TS2; COSMO

H	-6.1578219	1.0379736	1.9356536
C	-6.3271107	4.5368420	2.1366668
H	-6.1148544	3.1540482	0.4983401
H	-7.4294772	4.6287885	2.0455008
H	-5.8644265	5.3900158	1.6011703
H	-6.0618107	4.6299931	3.2107435
C	-1.4241086	4.5782606	-0.4383124
C	-1.7369278	4.0312993	-1.8416530
H	-1.2659392	4.6638392	-2.6216720
H	-2.8235204	3.9881633	-2.0565495
H	-1.3103007	3.0166399	-1.9714780
C	-1.7313815	6.0861350	-0.3518387
H	-0.3341004	4.4535509	-0.2867749
H	-1.1519844	6.6496090	-1.1120979
H	-1.4780130	6.4964160	0.6470874
H	-2.8081211	6.2892543	-0.5297730
H	0.3965630	-5.7771011	-2.9436603
H	5.2023715	-2.3858508	-3.6907976
H	3.7222504	-4.3921497	2.0860380
C	1.4732694	-5.5818914	-3.1559451
H	3.8534810	0.4924503	-3.6114027
H	1.1431175	-6.0516661	-5.2631183
H	0.0427731	-4.2679932	2.9331808
C	1.8973277	-4.4501877	-2.2226972
C	5.3424370	-1.7262611	-2.8086788
C	1.6091257	-5.2557114	-4.6479601
H	2.6754603	-5.1906939	-4.9513304
C	2.6977255	-3.3747272	-2.6398661
C	2.6770700	-4.7365014	2.2096292
H	2.1358527	-7.1548453	-1.7556924
C	1.5337471	-4.5117986	-0.8625025
C	2.2546377	-6.8688913	-2.8198621
H	1.9085219	-7.7184852	-3.4446502
H	0.8825632	-5.3349025	-0.5280293
C	3.2378947	-0.3741816	-3.2927840
H	5.8982312	-2.3043013	-2.0425840
H	5.9786948	-0.8738637	-3.1256109
C	3.1405707	-2.3832143	-1.7411016
C	0.2322572	-4.2532508	1.8402021
C	1.9873135	-3.5771824	0.0826546
H	2.4800990	-4.8462103	3.2964634
H	2.6008997	-5.7425814	1.7457850
C	3.9936420	-1.2273062	-2.2590947
C	2.8031904	-2.4988318	-0.3701162
C	1.6625485	-3.7689401	1.5650809
H	2.2931082	0.0152599	-2.8636495
H	-0.5185644	-3.5951501	1.3692333
H	2.9929959	-0.9620194	-4.2019698
H	1.1260767	-4.2966921	-4.9114507
H	0.0570460	-5.2831921	1.4665145
H	3.3386656	-6.7220883	-3.0099925
H	4.2219837	-0.5679808	-1.3964858
H	1.7729757	-2.7805873	2.0579901
H	2.9858665	-3.2916125	-3.6983989
Zn	-2.3112979	0.7685887	-1.8177801
Br	-2.4482541	0.7434634	-4.1482845
Zn	-2.1610098	-2.0072790	-0.4257382
Br	-2.9523148	-4.2339229	-0.3488201
H	-4.0814341	4.2409046	-0.1986498
C	0.5755827	-1.5741754	-6.1276697
C	0.0293836	-1.6418235	-4.8443539
C	-0.9749985	-2.5996899	-4.5621114
C	-1.4300281	-3.4770219	-5.5744752
C	-0.8894954	-3.3930978	-6.8627224
C	0.1142497	-2.4454413	-7.1351121
H	1.3609945	-0.8375918	-6.3541483
C	-1.5565905	-2.6904392	-3.2347221
H	-2.2078019	-4.2206146	-5.3390705
H	-1.2407518	-4.0692878	-7.6561304
H	0.5457142	-2.3851349	-8.1463172
O	-1.2826958	-1.8936426	-2.3145386

H	0.3622430	-0.9735183	-4.0388461
H	-2.2859314	-3.5172214	-3.0397746
C	-6.0045317	-0.9500427	-0.0025089
C	-4.7952010	-0.3357169	-0.1574073
C	-5.0414662	0.8109696	-1.0452628
O	-6.3394963	0.9328595	-1.3521263
C	-7.0446181	-0.1787318	-0.7481797
O	-4.1861188	1.5989931	-1.4897593
C	-3.4346299	-0.5490422	0.3320257
H	-7.5360728	-0.7446833	-1.5697554
H	-7.8429672	0.2342416	-0.0931278
H	-3.4404695	-1.1415891	1.2723965
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TS2

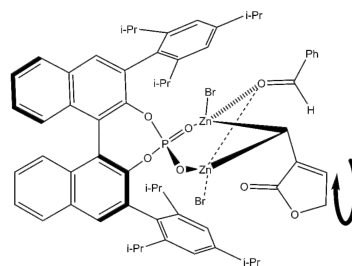


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C	4.3385366	3.4890515	1.5049119
C	2.1518156	4.5590617	1.8822007
C	2.8177733	5.8204579	1.9339276
C	0.7333775	4.4709937	1.9653982
H	0.1519434	5.3955901	2.1029830
C	0.0585350	3.2632348	1.8202813
C	3.3006973	-1.4651162	0.6336947
C	4.3480494	-1.7061346	1.5140364
H	4.8903982	-2.6614427	1.4505652
C	4.7032031	-0.7820505	2.5368366
C	5.7235608	-1.0903356	3.4857990
C	3.9810755	0.4617413	2.6535601
C	4.2671642	1.3014227	3.7725983
C	2.9851272	0.7868560	1.6590800
C	2.6660716	-0.1860769	0.7043016
O	0.1814000	0.8672098	1.6236767
O	1.7024931	0.1025756	-0.2624763
P	0.1211772	0.0855254	0.1764778
O	-0.5916832	0.9450003	-0.8873047
O	-0.4053731	-1.3151411	0.4801523
C	4.1918329	5.9091430	1.7733959
C	4.9532415	4.7327807	1.5414319
H	2.2118331	6.7275656	2.0862636
H	4.6915137	6.8891928	1.8078370
H	4.9374542	2.5871867	1.3169888
H	6.0398496	4.8075705	1.3826631
C	5.2514275	0.9628635	4.6906543
C	6.0015186	-0.2332644	4.5391427
H	3.6898150	2.2254340	3.9108166
H	5.4470809	1.6264323	5.5467770
H	6.7862157	-0.4864762	5.2681902
H	6.2736452	-2.0378870	3.3739573
C	-2.1200592	3.8153947	0.6671729
C	-1.4335235	3.1928036	1.7525936

C	-3.5231495	3.7395239	0.6270600	H	1.8292655	-2.7140437	2.1575460
C	-2.1728590	2.4990535	2.7503538	H	2.8625085	-3.3925789	-3.6219109
C	-3.5774252	2.4550714	2.6562061	Zn	-2.3146494	0.7691962	-1.7683310
C	-4.2769605	3.0720092	1.6075693	Br	-2.6269294	0.7532384	-4.0766982
C	-1.5062783	1.8481055	3.9615178	Zn	-2.0395765	-2.0630606	-0.4680725
H	-4.1375857	1.9209352	3.4382349	Br	-2.7696787	-4.2959896	-0.4801111
C	-1.8561313	0.3549851	4.0885168	H	-4.0579948	4.2054273	-0.2157529
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H	-1.5853961	-0.1950249	3.1661427	C	-0.9727391	-2.3900684	-4.6686015
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H	-1.3127144	2.1886512	6.1211638	C	-1.5057859	-2.5777540	-3.3288934
C	-5.7995634	3.0889749	1.5254089	H	-2.2173297	-3.9602467	-5.5231104
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H	-7.5658160	1.8764350	1.9532372	H	0.4492677	-1.9165353	-8.2682628
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H	-6.0575583	3.0865110	0.4427557	C	-5.8922754	-1.1830527	-0.1660122
H	-7.4523308	4.4561831	2.0183507	C	-4.7302130	-0.4727700	-0.2438145
H	-5.9068572	5.2861443	1.6328898	C	-5.0398106	0.7238831	-1.0473820
H	-6.1065792	4.4613816	3.2084614	O	-6.3405011	0.7729021	-1.3767388
C	-1.4066273	4.5831276	-0.4489437	C	-6.9708233	-0.4278514	-0.8775429
C	-1.7278799	4.0421802	-1.8526638	O	-4.2345896	1.6038286	-1.3891429
H	-1.2599394	4.6764443	-2.6331909	C	-3.3650145	-0.6156009	0.2551612
H	-2.8150591	4.0033707	-2.0659175	H	-7.4071936	-0.9626271	-1.7505047
H	-1.3056613	3.0269924	-1.9907038	H	-7.8095304	-0.1239957	-0.2117164
C	-1.7180562	6.0892820	-0.3506736	H	-3.3449787	-1.2291732	1.1826812
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C	1.7685880	-4.4723966	-2.0901125				
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H	2.1241499	-7.1577195	-1.6294457				
C	1.4435041	-4.4909934	-0.7199538				
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H	5.9855849	-1.0966949	-3.1371376				
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C	2.7885950	-2.5084179	-0.3109167				
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H	2.3435446	-0.0413246	-2.8863113				
H	-0.5131189	-3.4540892	1.5559015				
H	2.9937636	-1.0863332	-4.1997885				
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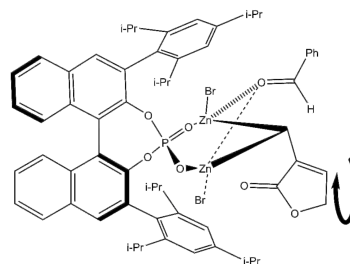


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C	2.0914025	4.5950366	2.2774952
C	2.7545503	5.8547735	2.3869283
C	0.6692023	4.5149374	2.2654421
H	0.0857792	5.4433637	2.3600437
C	0.0028607	3.3123808	2.0578802
C	3.3034230	-1.3896836	0.9236683
C	4.3606736	-1.6331552	1.7922844
H	4.9214584	-2.5760782	1.7052762
C	4.6888334	-0.7342017	2.8466651
C	5.7107473	-1.0524208	3.7916229
C	3.9326282	0.4852568	3.0056740
C	4.1858134	1.2868172	4.1599751
C	2.9351673	0.8250327	2.0164750
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O	1.6758853	0.1532342	0.0677686
P	0.0905121	0.1362177	0.4758833

O	-0.6166646	0.9166122	-0.6449507	H	5.5590076	-0.6663492	-3.1099355
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C	4.9059338	4.7731998	2.0694939	C	2.0849813	-3.5512172	0.5057349
H	2.1420731	6.7593789	2.5269439	H	2.7665979	-4.9399628	3.6366681
H	4.6330836	6.9237200	2.3718781	H	2.6645676	-5.8097254	2.0704177
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C	5.1712715	0.9381295	5.0736215	C	1.8843276	-3.7584064	2.0087078
C	5.9560854	-0.2302184	4.8809225	H	1.8685824	0.0169012	-2.4941352
H	3.5817905	2.1883074	4.3302746	H	-0.2671793	-3.3423002	2.0427195
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H	6.7413318	-0.4907938	5.6068241	H	0.9378107	-4.3214021	-4.4790575
H	6.2872985	-1.9797240	3.6480264	H	0.1176434	-5.0896466	1.9764283
C	-1.9826453	3.7848363	0.5810973	H	3.0163328	-6.8551366	-2.5221542
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C	-3.3536136	3.6376025	0.3058811	H	2.1232415	-2.8009076	2.5140084
C	-2.3342512	2.5417065	2.6818182	H	2.6232124	-3.1967411	-3.3585102
C	-3.7028767	2.4438188	2.3646683	Zn	-2.2815824	0.2825844	-1.5076290
C	-4.2409854	2.9914633	1.1884629	Br	-3.0412811	1.2022137	-3.4981352
C	-1.8460044	1.9546708	4.0047974	Zn	-1.7022165	-2.2070940	-0.3806752
H	-4.3701014	1.9305866	3.0726722	Br	-2.1169689	-4.5051474	-0.4909764
C	-2.1925716	0.4614767	4.1439271	H	-3.7573032	4.0534133	-0.6316429
H	-3.2892370	0.2991942	4.2001571	C	-0.0637891	-0.0156761	-6.1090398
H	-1.7499733	0.0449874	5.0722723	C	-0.3221697	-0.4761210	-4.8162407
H	-1.7999502	-0.1204679	3.2870165	C	-0.7428035	-1.8177737	-4.6214341
C	-2.3827872	2.7726919	5.1950448	C	-0.9082934	-2.6815196	-5.7352975
H	-0.7409500	2.0408890	4.0292665	C	-0.6537579	-2.2098170	-7.0254832
H	-3.4912109	2.7335627	5.2433782	C	-0.2293958	-0.8791187	-7.2090635
H	-2.0880956	3.8388253	5.1147859	H	0.2630605	1.0226149	-6.2663643
H	-1.9887512	2.3774955	6.1544521	C	-1.0168972	-2.3256675	-3.2965511
C	-5.7314070	2.9725324	0.8726769	H	-1.2427959	-3.7183770	-5.5745589
C	-6.5172308	1.8836007	1.6107156	H	-0.7838506	-2.8730499	-7.8932394
H	-7.5600498	1.8474409	1.2370089	H	-0.0249587	-0.5096702	-8.2258985
H	-6.5635183	2.0718249	2.7044539	O	-0.9984663	-1.6097275	-2.2639083
H	-6.0721425	0.8822720	1.4466864	H	-0.2022297	0.1806518	-3.9447411
C	-6.3426930	4.3645599	1.1339533	H	-1.2675422	-3.4090122	-3.1841538
H	-5.8180764	2.7563009	-0.2120460	C	-4.8253639	-2.5115557	-2.0489258
H	-7.4140227	4.3849734	0.8448281	C	-4.6331732	-1.3664228	-1.3468313
H	-5.8185771	5.1547234	0.5592560	C	-5.7167343	-0.4169486	-1.7507285
H	-6.2730658	4.6301938	2.2102982	O	-6.5095677	-1.0286570	-2.6884337
C	-1.1134028	4.5658688	-0.4067318	C	-6.0165020	-2.3483920	-2.9381306
C	-1.2343836	4.0675625	-1.8546483	O	-5.9349111	0.7060753	-1.3437362
H	-0.5652742	4.6547479	-2.5173205	C	-3.5914276	-0.9459938	-0.3729156
H	-2.2642418	4.1659368	-2.2538368	H	-5.7577706	-2.4383762	-4.0180051
H	-0.9487734	3.0019438	-1.9330434	H	-6.8261759	-3.0832717	-2.7281846
C	-1.4229301	6.0733580	-0.3136650	H	-3.5483864	-1.6501180	0.4948625
H	-0.0548473	4.4256567	-0.1113967	H	-3.9047301	-0.0014801	0.1343935
H	-0.7507898	6.6554789	-0.9779715	H	-4.2228505	-3.4302998	-1.9974682
H	-1.3005239	6.4564081	0.7200179				
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H	0.1726922	-5.6488490	-2.4387553				
H	4.8104230	-2.2262405	-3.5728093				
H	3.9201334	-4.5604445	2.3155874				
C	1.2587624	-5.5521765	-2.6742534				
H	3.3189634	0.5831076	-3.3863712				
H	0.9135478	-6.0884279	-4.7621532				
H	0.3520347	-4.1847102	3.5001453				
C	1.7817609	-4.4282848	-1.7815868				
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C	1.3987636	-5.2817422	-4.1764476				
H	2.4653091	-5.2465644	-4.4834173				
C	2.4630478	-3.3037022	-2.2755685				
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H	1.7947350	-7.1529822	-1.2474063				
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C	1.9258733	-6.8959404	-2.3168197				
H	1.4946711	-7.7223587	-2.9187476				
H	1.0305684	-5.3707571	0.0160052				
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TS3

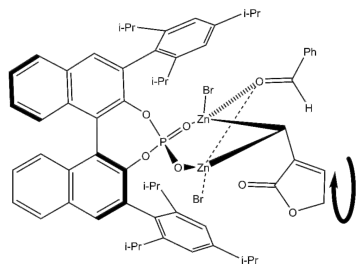


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C	2.0842866	4.5876313	2.2611141
C	2.7470704	5.8474917	2.3651061

C	0.6625712	4.5059813	2.2483809	H	0.9390509	-6.1067836	-4.7672212
H	0.0773214	5.4338561	2.3364286	H	0.3366811	-4.1953775	3.4887133
C	-0.0039126	3.3025972	2.0471134	C	1.7908313	-4.4393428	-1.7856402
C	3.2991517	-1.3973375	0.9219139	C	5.0125914	-1.5514327	-2.7139824
C	4.3577143	-1.6384720	1.7892149	C	1.4191496	-5.2979698	-4.1799949
H	4.9186807	-2.5811516	1.7009439	H	2.4867492	-5.2613686	-4.4829241
C	4.6865722	-0.7387807	2.8423361	C	2.4732126	-3.3150269	-2.2779485
C	5.7099124	-1.0537697	3.7860970	C	2.8598697	-4.8216542	2.5391803
C	3.9292572	0.4797988	3.0008121	H	1.8086016	-7.1623500	-1.2468735
C	4.1837371	1.2834130	4.1530985	C	1.5933953	-4.5236998	-0.3934893
C	2.9300289	0.8176332	2.0130407	C	1.9426464	-6.9074349	-2.3161910
C	2.6345022	-0.1381558	1.0331493	H	1.5160707	-7.7367928	-2.9173770
O	0.1155526	0.9062835	1.9126897	H	1.0285675	-5.3782513	0.0086163
O	1.6686615	0.1418678	0.0669390	C	2.7991705	-0.3246293	-3.0034205
P	0.0838976	0.1245281	0.4790678	H	5.6724752	-2.0868804	-2.0017934
O	-0.6288071	0.9040387	-0.6382918	H	5.5672293	-0.6726766	-3.1034595
O	-0.4514123	-1.2813787	0.8125042	C	2.9661830	-2.3051672	-1.4261574
C	4.1272218	5.9384578	2.2730194	C	0.4304823	-4.1301274	2.3852557
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H	2.1337857	6.7523541	2.4997542	H	2.7556048	-4.9381023	3.6378640
H	4.6243386	6.9175731	2.3474669	H	2.6670692	-5.8104559	2.0725287
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H	5.9909929	4.8425563	1.9467931	C	2.7897753	-2.4376660	-0.0261932
C	5.1710655	0.9375305	5.0650835	C	1.8739218	-3.7642605	2.0037651
C	5.9563998	-0.2299140	4.8731986	H	1.8743290	0.0077678	-2.4933347
H	3.5787832	2.1845325	4.3214758	H	-0.2810354	-3.3642085	2.0258767
H	5.3411946	1.5720251	5.9482010	H	2.5102684	-0.9354969	-3.8844096
H	6.7430687	-0.4887199	5.5981110	H	0.9589209	-4.3382565	-4.4860361
H	6.2868417	-1.9809447	3.6432163	H	0.1158156	-5.1086058	1.9688045
C	-1.9881763	3.7711042	0.5671059	H	3.0337561	-6.8643693	-2.5165539
C	-1.4731176	3.2203000	1.7801458	H	3.9754779	-0.4287147	-1.2100629
C	-3.3601091	3.6289731	0.2951269	H	2.1043439	-2.8041650	2.5082046
C	-2.3424982	2.5415313	2.6749513	H	2.6400206	-3.2098487	-3.3601004
C	-3.7122219	2.4508066	2.3615188	Zn	-2.2979252	0.2714403	-1.4955721
C	-4.2501880	2.9958058	1.1841924	Br	-3.0619992	1.1661562	-3.4903286
C	-1.8542740	1.9583330	3.9996295	Zn	-1.6949157	-2.2231458	-0.3855101
H	-4.3815687	1.9465310	3.0739415	Br	-2.0974056	-4.5170614	-0.5463405
C	-2.2095627	0.4682757	4.1475843	H	-3.7632437	4.0391701	-0.6450349
H	-3.3068675	0.3124789	4.2088199	C	-0.0702700	0.0501815	-6.0811456
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H	-1.8228177	-0.1205409	3.2927571	C	-0.7066669	-1.7857768	-4.6169031
C	-2.3813526	2.7870836	5.1865606	C	-0.8425245	-2.6399736	-5.7410642
H	-0.7485978	2.0368757	4.0201743	C	-0.5933999	-2.1478179	-7.0243748
H	-3.4897699	2.7569947	5.2384774	C	-0.2050578	-0.8041237	-7.1909939
H	-2.0800138	3.8505273	5.0984359	H	0.2254284	1.0998827	-6.2233666
H	-1.9877326	2.3955669	6.1476276	H	-0.9794661	-2.3109654	-3.2965485
C	-5.7422459	2.9927361	0.8764934	C	-1.1493512	-3.6872969	-5.5930816
C	-6.5375773	1.9195216	1.6268348	H	-0.6999889	-2.8048107	-7.9001304
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H	-7.4062503	4.4266779	0.8508150	C	-4.6428632	-1.3853973	-1.3122770
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C	-1.1169747	4.5430983	-0.4262916	C	-6.0533496	-2.3444170	-2.8902536
C	-1.2422822	4.0392923	-1.8718798	O	-5.9353934	0.6894484	-1.2650696
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H	-2.2718464	4.1378522	-2.2713909	H	-5.8091742	-2.4230597	-3.9751302
H	-0.9591749	2.9729222	-1.9464438	H	-6.8613710	-3.0817778	-2.6787545
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H	-1.2958323	6.4401338	0.6917066				
H	-2.4657394	6.2648747	-0.6463915				
H	0.1869204	-5.6645304	-2.4459182				
H	4.8213556	-2.2324079	-3.5697190				
H	3.9131587	-4.5540214	2.3220924				
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TS4; COSMO



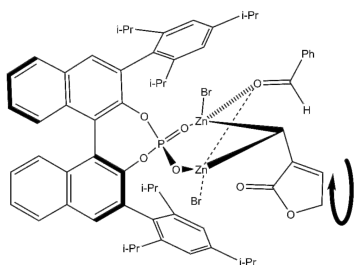
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H	4.9608351	2.6078077	1.6967739
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H	5.5888213	1.5869207	5.7913151
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H	0.2062923	-5.7466609	-2.3685005
H	4.5622676	-2.0576484	-3.7357075
H	4.2247572	-4.7253783	2.0571975
C	1.2597960	-5.5795774	-2.6945107
H	2.9226242	0.6652736	-3.4219294
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C	1.2474213	-5.2557942	-4.1923862
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H	1.2780486	-5.4988252	0.0099026
C	2.4755150	-0.2697875	-3.0256734
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H	5.2431517	-0.4572136	-3.3058563
C	2.8588849	-2.2548022	-1.4858597
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C	2.2451443	-3.6245299	0.4687304
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H	2.9398818	-5.9568937	1.8875502
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C	2.8217435	-2.4386774	-0.0794286
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H	1.5641718	0.0012406	-2.4584233
H	0.0565555	-3.4357288	2.2445349
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H	0.7036514	-4.3172285	-4.4159961
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H	3.0955986	-6.7791354	-2.7448466
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Br	-1.9248356	-4.6884148	-0.2655511
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C	-1.0139564	-1.5655071	-4.3022665
C	-1.0192230	-2.3175608	-5.5044586
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C	-1.1722925	-2.2483488	-3.0353738
H	-1.1556017	-3.4093531	-5.4636014
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H	-6.2630269	-2.6002600	-3.0266658
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TS4



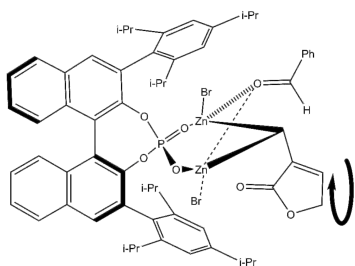
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O	1.6260875	0.1069962	0.1178732
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H	2.2002643	6.7533197	2.2769392
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C	2.2455581	-3.6245942	0.4693061
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H	2.9383084	-5.9598818	1.8829320
C	3.4796242	-1.0126591	-2.1235680
C	2.8230815	-2.4388895	-0.0778305
C	2.1804594	-3.8979041	1.9738094
H	1.5667684	0.0052748	-2.4526896
H	0.0580368	-3.4357941	2.2477970
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H	0.7043094	-4.3128257	-4.4157014
H	0.3757460	-5.1794911	2.0018995
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C	-0.8647624	-0.1423514	-4.3414682
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C	-1.0121583	-2.3006245	-5.5076918
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H	-1.1347368	-3.3942493	-5.4693558
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H	-3.3808928	-1.9634922	1.1886092
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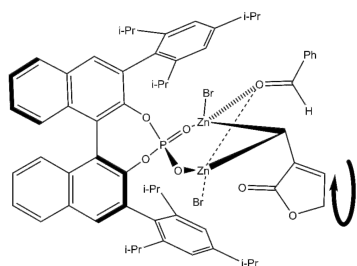
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C	2.2629612	4.5817777	1.9618369
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C	0.1803785	3.2824573	1.8082142
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C	4.8718921	-0.7746828	2.5455733
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C	4.1469597	0.4632162	2.7122436
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C	3.1209646	0.8061528	1.7548131
C	2.7850018	-0.1534430	0.7916837
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P	0.2345782	0.0646866	0.3411061

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O	-0.2190923	-1.3529040	0.7153947
C	4.2986328	5.9433019	1.9083234
C	5.0724000	4.7701602	1.7014734
H	2.3048321	6.7520301	2.1534070
H	4.7918344	6.9262023	1.9536794
H	5.0765975	2.6252256	1.4851734
H	6.1625224	4.8499327	1.5714581
C	5.4685174	0.9228805	4.7265370
C	6.2224345	-0.2639617	4.5243421
H	3.8759102	2.1919664	4.0210582
H	5.6824815	1.5656511	5.5940617
H	7.0282839	-0.5294455	5.2254302
H	6.4724051	-2.0399604	3.3105848
C	-1.7603033	3.6028044	0.2388183
C	-1.2857266	3.1804163	1.5178594
C	-3.1153357	3.3996219	-0.0806623
C	-2.1871667	2.5915292	2.4419451
C	-3.5441342	2.4496089	2.0845184
C	-4.0362651	2.8269879	0.8215283
C	-1.7447314	2.1202022	3.8254642
H	-4.2269243	2.0001964	2.8189446
C	-2.0147024	0.6185280	4.0405155
H	-3.0921291	0.3665102	3.9553272
H	-1.6772729	0.3066694	5.0503637
H	-1.4613523	0.0098798	3.2989977
C	-2.3956324	2.9753285	4.9291895
H	-0.6482414	2.2753644	3.8980924
H	-3.4992689	2.8569243	4.9342622
H	-2.1727753	4.0526880	4.7892680
H	-2.0227767	2.6726233	5.9294210
C	-5.4830745	2.5703997	0.3929510
C	-6.4044704	2.1410535	1.5416855
H	-7.4177198	1.9110828	1.1554939
H	-6.5080124	2.9502676	2.2953078
H	-6.0418192	1.2394704	2.0711491
C	-6.0913657	3.7633293	-0.3665002
H	-5.4283094	1.7234275	-0.3328309
H	-7.1324313	3.5340781	-0.6720404
H	-5.5283708	4.0080213	-1.2880925
H	-6.1147143	4.6702709	0.2736395
C	-0.8630913	4.3006006	-0.7858750
C	-0.9690756	3.7240203	-2.2076582
H	-0.2691775	4.2581732	-2.8828817
H	-1.9865695	3.8285394	-2.6362000
H	-0.7068939	2.6496126	-2.2146171
C	-1.1512333	5.8154721	-0.7882981
H	0.1880880	4.1606174	-0.4646195
H	-0.4626584	6.3467954	-1.4776384
H	-1.0358364	6.2586979	0.2214177
H	-2.1906724	6.0185755	-1.1214547
H	-0.1917750	-5.5383609	-2.3705585
H	4.6179964	-2.4691763	-3.8404555
H	4.0202006	-4.5744871	2.0836173
C	0.8769814	-5.5240972	-2.6902738
H	3.2750707	0.4223244	-3.6912064
H	0.3332938	-6.0465612	-4.7396335
H	0.5456466	-4.1336019	3.5043473
C	1.5468501	-4.4341803	-1.8555296
C	4.8857118	-1.7639527	-3.0257283
C	0.9210300	-5.2754400	-4.2019240
H	1.9605199	-5.3224253	-4.5895092
C	2.2567501	-3.3589605	-2.4142209
C	2.9806198	-4.8164829	2.3817797
H	1.3984767	-7.1506463	-1.2882144
C	1.4643308	-4.4992797	-0.4508802
H	1.4679245	-6.9113220	-2.3673745
H	0.9325076	-7.7073708	-2.9248559
H	0.8814405	-5.3134950	0.0053760
C	2.7240771	-0.4370491	-3.2559746
H	5.5559340	-2.3016108	-2.3246445

H	5.4594917	-0.9290643	-3.4790752
C	2.8756578	-2.3737527	-1.6170668
C	0.5609950	-4.0871080	2.3961035
C	2.0814854	-3.5607648	0.3904159
H	2.9555986	-4.9176521	3.4867074
H	2.7328492	-5.8061574	1.9434805
C	3.6307043	-1.2382116	-2.3045557
C	2.8047803	-2.4818974	-0.2052455
C	1.9777941	-3.7457770	1.9059230
H	1.8414084	-0.0408496	-2.7176770
H	-0.1668915	-3.3200920	2.0740616
H	2.3612367	-1.0590143	-4.1009426
H	0.5131173	-4.2837328	-4.4791418
H	0.2071023	-5.0691589	2.0214983
H	2.5400881	-6.9539003	-2.6532015
H	3.9788780	-0.5399437	-1.5160754
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H	2.3411582	-3.2714556	-3.5073595
Zn	-2.4521991	0.2942546	-1.1108754
Br	-3.7124996	1.0352429	-2.9223324
Zn	-1.8431693	-2.1914902	-0.0933239
Br	-2.4351858	-4.4246718	-0.2930126
H	-3.4641761	3.7001973	-1.0782628
C	-0.4427236	0.3705258	-5.7244070
C	-0.7164986	-0.2215494	-4.4903408
C	-1.0748635	-1.5934211	-4.4343497
C	-1.1616377	-2.3562094	-5.6255454
C	-0.8908844	-1.7537859	-6.8580434
C	-0.5300103	-0.3936764	-6.9047036
H	-0.1615614	1.4328938	-5.7726771
C	-1.3570438	-2.2231370	-3.1593265
H	-1.4489825	-3.4178544	-5.5728127
H	-0.9592910	-2.3392161	-7.7867642
H	-0.3130354	0.0778393	-7.8756964
O	-1.4004044	-1.5825061	-2.0862377
H	-0.6512536	0.3525505	-3.5557029
H	-1.5491747	-3.3239141	-3.1303826
C	-5.4573934	-1.4681057	-0.6406801
C	-4.6998855	-1.1624704	0.4379104
C	-5.5512731	-1.3499076	1.6505049
O	-6.7968403	-1.7692804	1.2473428
C	-6.8233802	-1.8662234	-0.1809387
O	-5.2666346	-1.1672081	2.8193264
C	-3.2913971	-0.6993828	0.5686775
H	-7.6226584	-1.1987085	-0.5755298
H	-7.0852899	-2.9086964	-0.4708559
H	-2.8778014	-1.1124894	1.5227158
H	-3.2908416	0.3725593	0.9078485
H	-5.1532011	-1.4249233	-1.6961583

C	0.8398127	4.4935910	1.9639308
H	0.2512026	5.4216932	2.0239106
C	0.1801970	3.2804763	1.8081133
C	3.4035076	-1.4368095	0.6832743
C	4.4839080	-1.6877947	1.5204653
H	5.0131841	-2.6491344	1.4398591
C	4.8750499	-0.7730283	2.5396483
C	5.9254417	-1.0951153	3.4507843
C	4.1510067	0.4652291	2.7061006
C	4.4637472	1.2799242	3.8358647
C	3.1234122	0.8076438	1.7503576
C	2.7858676	-0.1523523	0.7881258
O	0.3132035	0.8816152	1.7619448
O	1.7944584	0.1429770	-0.1491374
P	0.2352774	0.0648184	0.3405480
O	-0.5683962	0.8226123	-0.7324572
O	-0.2176554	-1.3532947	0.7123573
C	4.2958024	5.9454414	1.9030926
C	5.0701928	4.7735405	1.6951999
H	2.3019877	6.7518874	2.1505771
H	4.7878800	6.9288825	1.9479672
H	5.0759480	2.6286473	1.4788734
H	6.1600469	4.8543451	1.5639562
C	5.4772904	0.9273206	4.7161131
C	6.2300414	-0.2596616	4.5141703
H	3.8835646	2.1956974	4.0122306
H	5.6935055	1.5714448	5.5820083
H	7.0374067	-0.5244760	5.2136935
H	6.4762200	-2.0373089	3.3030520
C	-1.7602293	3.5985273	0.2385796
C	-1.2857892	3.1767083	1.5177381
C	-3.1143300	3.3924598	-0.0820785
C	-2.1866935	2.5855364	2.4408127
C	-3.5429190	2.4413327	2.0822514
C	-4.0347984	2.8182483	0.8192611
C	-1.7446265	2.1133444	3.8241150
H	-4.2253207	1.9897223	2.8156208
C	-2.0125775	0.6109787	4.0377050
H	-3.0893365	0.3561843	3.9523630
H	-1.6750226	0.2987171	5.0472763
H	-1.4571303	0.0038566	3.2966867
C	-2.3975648	2.9668247	4.9278512
H	-0.6483699	2.2703116	3.8975389
H	-3.5009186	2.8471400	4.9320137
H	-2.1763596	4.0445580	4.7890415
H	-2.0255936	2.6639586	5.9283081
C	-5.4811681	2.5601535	0.3901699
C	-6.4023747	2.1306409	1.5391092
H	-7.4157238	1.9003992	1.1534080
H	-6.5064961	2.9403085	2.2920860
H	-6.0404863	1.2292749	2.0692772
C	-6.0898904	3.7526103	-0.3695104
H	-5.4256039	1.7132924	-0.3356906
H	-7.1306916	3.5229586	-0.6755090
H	-5.5271835	3.9973631	-1.2911388
H	-6.1140816	4.6595793	0.2703816
C	-0.8638373	4.2988450	-0.7852733
C	-0.9662444	3.7219207	-2.2071657
H	-0.2668726	4.2579965	-2.8814994
H	-1.9831880	3.8223951	-2.6377883
H	-0.7004906	2.6484749	-2.2130788
C	-1.1565773	5.8127487	-0.7881172
H	0.1874295	4.1621422	-0.4628945
H	-0.4690666	6.3467332	-1.4764630
H	-1.0442312	6.2562855	0.2216983
H	-2.1962157	6.0128827	-1.1219861
H	-0.2058461	-5.5368710	-2.3560137
H	4.6110626	-2.4838153	-3.8407780
H	4.0155623	-4.5745339	2.0845900
C	0.8625115	-5.5262852	-2.6774601
H	3.2776600	0.4136994	-3.6956439

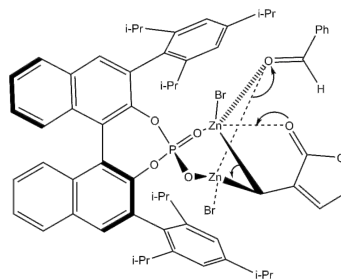
TS5



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C	3.0535913	3.3837193	1.8095689
C	4.4647963	3.5254756	1.6488507
C	2.2617110	4.5822463	1.9590047
C	2.9182419	5.8479310	2.0233539

H	0.3162758	-6.0554119	-4.7249025
H	0.5453335	-4.1214404	3.5130539
C	1.5361278	-4.4350006	-1.8477189
C	4.8813448	-1.7776977	-3.0277997
C	0.9058536	-5.2835068	-4.1901041
H	1.9447867	-5.3344924	-4.5785212
C	2.2480106	-3.3632704	-2.4102332
C	2.9760172	-4.8128349	2.3856217
H	1.3824372	-7.1488069	-1.2710978
C	1.4551860	-4.4962250	-0.4431682
C	1.4508299	-6.9136209	-2.3509790
H	0.9130513	-7.7108311	-2.9045112
H	0.8693494	-5.3066980	0.0157594
C	2.7242205	-0.4431291	-3.2585614
H	5.5496467	-2.3166156	-2.3261790
H	5.4582199	-0.9460945	-3.4832372
C	2.8704741	-2.3778522	-1.6164348
C	0.5584986	-4.0769219	2.4048454
C	2.0763258	-3.5578908	0.3949082
H	2.9535013	-4.9127801	3.4906294
H	2.7248823	-5.8023018	1.9491261
C	3.6286639	-1.2462780	-2.3069735
C	2.8013542	-2.4824508	-0.2045307
C	1.9750516	-3.7399433	1.9109013
H	1.8441641	-0.0424275	-2.7194277
H	-0.1681068	-3.3086139	2.0838000
H	2.3581160	-1.0647128	-4.1025094
H	0.5008894	-4.2914732	-4.4707573
H	0.2002159	-5.0583207	2.0330645
H	2.5225133	-6.9595676	-2.6375188
H	3.9796593	-0.5478429	-1.5199101
H	2.2598841	-2.7788995	2.3849014
H	2.3321444	-3.2792173	-3.5037144
Zn	-2.4532641	0.2948687	-1.1092247
Br	-3.7080335	1.0305451	-2.9247917
Zn	-1.8407456	-2.1928007	-0.0979039
Br	-2.4229405	-4.4240453	-0.3178961
H	-3.4628687	3.6914439	-1.0802130
C	-0.4401056	0.3978858	-5.7133462
C	-0.7139211	-0.2020497	-4.4829076
C	-1.0613321	-1.5764021	-4.4349166
C	-1.1374393	-2.3334014	-5.6297986
C	-0.8667571	-1.7233910	-6.8583626
C	-0.5164191	-0.3605663	-6.8971677
H	-0.1681587	1.4628912	-5.7541426
C	-1.3440792	-2.2127672	-3.1615593
H	-1.4156357	-3.3978069	-5.5828211
H	-0.9270084	-2.3049603	-7.7901267
H	-0.2994678	0.1172558	-7.8651545
O	-1.3933144	-1.5753738	-2.0891701
H	-0.6570843	0.3681833	-3.5454401
H	-1.5309257	-3.3151015	-3.1343310
C	-5.4574278	-1.4673691	-0.6423954
C	-4.6995685	-1.1656153	0.4359105
C	-5.5497951	-1.3542129	1.6515342
O	-6.7971690	-1.7733207	1.2466177
C	-6.8234909	-1.8666471	-0.1793162
O	-5.2620284	-1.1693847	2.8166490
C	-3.2913702	-0.7038923	0.5677383
H	-7.6235461	-1.1982631	-0.5724489
H	-7.0856369	-2.9088722	-0.4719624
H	-2.8794903	-1.1190629	1.5220612
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H	-5.1540621	-1.4188124	-1.6979840



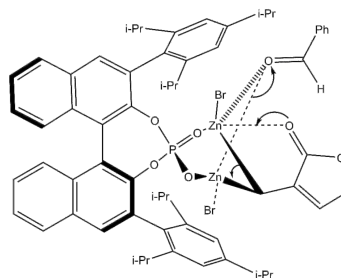
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C	4.2775164	3.6169564	1.2665561
C	2.0917243	4.6882579	1.6425051
C	2.7542873	5.9528315	1.6653461
C	0.6740009	4.5981259	1.7399694
H	0.0928780	5.5226264	1.8801037
C	0.0017146	3.3886578	1.6009781
C	3.3286665	-1.3964198	0.7254415
C	4.3873160	-1.5448724	1.6115253
H	4.9521915	-2.4893847	1.6233262
C	4.7177543	-0.5333801	2.5579656
C	5.7452350	-0.7453946	3.5262032
C	3.9554356	0.6925712	2.5884585
C	4.2046354	1.6062874	3.6574986
C	2.9528993	0.9229385	1.5695523
C	2.6618651	-0.1330250	0.6986521
O	0.1246609	0.9927183	1.4249086
O	1.7166724	0.0372312	-0.3072226
P	0.1152195	0.1331114	0.0258919
O	-0.4833593	0.8801887	-1.1704499
O	-0.4832703	-1.2183572	0.4611921
C	4.1270371	6.0420055	1.4888735
C	4.8893257	4.8632424	1.2695495
H	2.1473026	6.8612641	1.8050853
H	4.6241264	7.0239841	1.4985285
H	4.8774172	2.7133547	1.0894937
H	5.9735410	4.9377933	1.0947264
C	5.1960274	1.3610312	4.5982583
C	5.9907270	0.1864857	4.5232180
H	3.5935562	2.5147441	3.7425641
H	5.3602209	2.0818882	5.4138072
H	6.7811322	0.0077184	5.2680602
H	6.3258470	-1.6800479	3.4769729
C	-2.1901857	3.8959092	0.4527363
C	-1.4904763	3.3027092	1.5450033
C	-3.5888103	3.7574887	0.3929753
C	-2.2143687	2.6082758	2.5536090
C	-3.6139499	2.5028743	2.4428189
C	-4.3233430	3.0512508	1.3628125
C	-1.5322294	2.0008402	3.7782970
H	-4.1590128	1.9506224	3.2220875
C	-1.8778264	0.5138759	3.9710360
H	-2.9550168	0.3651756	4.1935619
H	-1.3056723	0.0921248	4.8229353
H	-1.6275388	-0.0741547	3.0659695
C	-1.8534217	2.8284798	5.0380571
H	-0.4364121	2.0659684	3.6270905
H	-2.9396918	2.8063796	5.2673717
H	-1.5596869	3.8899612	4.9075783
H	-1.3134923	2.4273136	5.9208436
C	-5.8374964	2.9275424	1.2187705
C	-6.4476376	1.7570820	2.0006009
H	-7.5121366	1.6193419	1.7215387
H	-6.4181059	1.9339667	3.0961910

TS6; COSMO

H	-5.9156420	0.8064414	1.7966803	H	-0.2193437	-0.0924269	-4.0589335
C	-6.5261023	4.2557782	1.5905779	H	-1.2905079	-3.6200942	-2.9902030
H	-6.0308072	2.7430633	0.1371495	C	-5.9294708	-0.4828504	-0.9711265
H	-7.6211047	4.1998239	1.4182268	C	-4.6822648	-0.5976695	-0.4235737
H	-6.1274204	5.1014281	0.9949015	C	-4.6952824	-1.8629859	0.3359001
H	-6.3594670	4.4924138	2.6624745	O	-5.9164660	-2.4223904	0.3329143
C	-1.4840489	4.6676833	-0.6629255	C	-6.7763310	-1.6234976	-0.5102651
C	-1.7829653	4.0954708	-2.0566935	O	-3.7443460	-2.4014965	0.9339572
H	-1.2493630	4.6737976	-2.8390593	C	-3.4563280	0.1903915	-0.4498673
H	-2.8630031	4.1213751	-2.3077918	H	-7.6584264	-1.3095871	0.0911047
H	-1.4463012	3.0441992	-2.1323191	H	-7.1436237	-2.2824305	-1.3281399
C	-1.8198685	6.1692217	-0.5836519	H	-2.9290435	0.0978147	0.5209015
H	-0.3921725	4.5650432	-0.5075775	H	-3.6772895	1.2721764	-0.5759418
H	-1.2533600	6.7398756	-1.3484747	H	-6.2951595	0.3219614	-1.6228225
H	-1.5738065	6.5906179	0.4126839				
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H	0.1912493	-5.8632741	-2.3291664				
H	4.9489966	-2.7037352	-3.6135095				
H	3.8460812	-4.3512578	2.4539131				
C	1.2902810	-5.8403668	-2.5180801				
H	3.5275702	0.1451778	-3.7450883				
H	1.0204364	-6.5691753	-4.5575244				
H	0.2386474	-3.8692583	3.4723519				
C	1.8233357	-4.6556751	-1.7149023				
C	5.1378926	-1.9439239	-2.8262669				
C	1.5114690	-5.7263078	-4.0303547				
H	2.5917214	-5.7609801	-4.2858003				
C	2.5441735	-3.5977704	-2.2931826				
C	2.7869018	-4.5960562	2.6692865				
H	1.6731400	-7.3143889	-0.9158845				
C	1.5834048	-4.5990888	-0.3271344				
C	1.8701973	-7.1705652	-1.9964381				
H	1.4270454	-8.0322416	-2.5372029				
H	0.9850940	-5.3965677	0.1379108				
C	2.9663489	-0.6980535	-3.2915519				
H	5.7689255	-2.4182557	-2.0472967				
H	5.7216325	-1.1207971	-3.2882715				
C	3.0412608	-2.5226228	-1.5285967				
C	0.3663175	-3.9266558	2.3719359				
C	2.0718169	-3.5624693	0.4835305				
H	2.6513628	-4.5915038	3.7708746				
H	2.6043448	-5.6298520	2.3074077				
C	3.8214507	-1.4129758	-2.2300276				
C	2.8279756	-2.5188259	-0.1278331				
C	1.8199351	-3.6041649	1.9925419				
H	2.0413056	-0.2898345	-2.8403060				
H	-0.3314158	-3.2020463	1.9124969				
H	2.6762801	-1.3846409	-4.1141890				
H	1.1020554	-4.7849277	-4.4470177				
H	0.0575343	-4.9429221	2.0537471				
H	2.9703220	-7.2017327	-2.1453012				
H	4.0937087	-0.6580873	-1.4640702				
H	2.0396202	-2.5943167	2.3952417				
H	2.7371503	-3.5991752	-3.3759107				
Zn	-2.1974474	0.3191743	-2.0625667				
Br	-2.9795551	1.1280092	-4.1183136				
Zn	-1.8935698	-2.3936560	-0.1822110				
Br	-2.0475553	-4.6998949	-0.6259547				
H	-4.1284378	4.1942897	-0.4639244				
C	0.1052585	-0.5391848	-6.1580342				
C	-0.2802351	-0.8496297	-4.8516874				
C	-0.7370059	-2.1569913	-4.5459033				
C	-0.7878991	-3.1460558	-5.5628230				
C	-0.4092507	-2.8246532	-6.8688479				
C	0.0345697	-1.5209124	-7.1642409				
H	0.4561014	0.4753302	-6.3970393				
C	-1.1360341	-2.5353146	-3.2075423				
H	-1.1397973	-4.1594721	-5.3148785				
H	-0.4600162	-3.5846813	-7.6623663				
H	0.3353910	-1.2687037	-8.1928688				
O	-1.3573420	-1.7275431	-2.2697986				

TS6

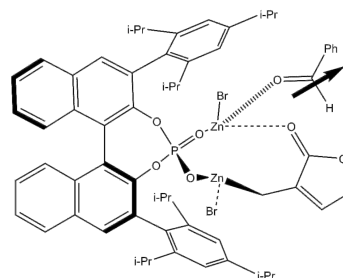


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number of imaginary frequencies: 1

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C	2.9071631	3.5073473	1.5208306
C	4.3120197	3.6346057	1.3047901
C	2.1331751	4.7113174	1.7001121
C	2.8019981	5.9718099	1.7313035
C	0.7151794	4.6271551	1.7971688
H	0.1380497	5.5528833	1.9461246
C	0.0374154	3.4227997	1.6470026
C	3.3435717	-1.3731699	0.7350395
C	4.4079689	-1.5282286	1.6125248
H	4.9677495	-2.4758486	1.6171009
C	4.7482099	-0.5224270	2.5610805
C	5.7819807	-0.7412486	3.5202729
C	3.9899713	0.7056751	2.6024800
C	4.2523645	1.6143485	3.6723995
C	2.9797025	0.9438194	1.5925674
C	2.6791967	-0.1083201	0.7196406
O	0.1492305	1.0279379	1.4580874
O	1.7270936	0.0654749	-0.2771286
P	0.1267544	0.1695475	0.0588571
O	-0.4627838	0.9188273	-1.1389873
O	-0.4847032	-1.1753663	0.4996122
C	4.1737466	6.0571018	1.5497380
C	4.9292797	4.8776614	1.3160388
H	2.1992864	6.8815634	1.8805537
H	4.6747128	7.0369500	1.5656261
H	4.9063050	2.7297254	1.1164209
H	6.0128219	4.9487860	1.1361801
C	5.2500826	1.3619549	4.6037990
C	6.0390595	0.1851269	4.5185866
H	3.6453786	2.5245762	3.7650938
H	5.4240442	2.0797017	5.4199684
H	6.8348692	0.0005287	5.2561188
H	6.3587023	-1.6777859	3.4626153
C	-2.1535082	3.9218333	0.4940749
C	-1.4544341	3.3345480	1.5894263

C	-3.5472629	3.7532321	0.4157192	H	2.0923012	-2.5787772	2.4240276
C	-2.1763329	2.6231009	2.5877573	H	2.6761914	-3.5562302	-3.3649049
C	-3.5714998	2.4891453	2.4584740	Zn	-2.1649019	0.4065622	0.4065622
C	-4.2782410	3.0254118	1.3709382	Br	-2.8798823	1.2124652	-4.1481072
C	-1.4988696	2.0259713	3.8202265	Zn	-1.9007219	-2.3521414	-0.1252860
H	-4.1145680	1.9231593	3.2291254	Br	-2.0295106	-4.6649088	-0.5226190
C	-1.8072417	0.5287546	3.9996923	H	-4.0851914	4.1868413	-0.4440461
H	-2.8845534	0.3508611	4.1990146	C	-0.0023140	-0.6838918	-6.1799574
H	-1.2432457	0.1190147	4.8626810	C	-0.3669288	-0.9394237	-4.8552252
H	-1.5241586	-0.0492097	3.0985764	C	-0.8801106	-2.2128884	-4.5019507
C	-1.8656476	2.8345685	5.0797606	C	-1.0059602	-3.2242692	-5.4898325
H	-0.4025322	2.1225597	3.6879087	C	-0.6473674	-2.9575477	-6.8130483
H	-2.9544470	2.7799519	5.2898408	C	-0.1485287	-1.6856838	-7.1559467
H	-1.6008753	3.9049932	4.9628578	H	0.3870644	0.3070763	-6.4549551
H	-1.3306289	2.4418971	5.9692447	C	-1.2641782	-2.5386342	-3.1447277
C	-5.7836247	2.8493674	1.1949401	H	-1.3992885	-4.2123355	-5.2039192
C	-6.3650452	1.6495509	1.9534721	H	-0.7572388	-3.7347032	-7.5837305
H	-7.4191240	1.4765678	1.6556241	H	0.1352790	-1.4756851	-8.1988844
H	-6.3605151	1.8148187	3.0511861	O	-1.4227629	-1.7014792	-2.2206340
H	-5.7942994	0.7209564	1.7512095	H	-0.2473163	-0.1655174	-4.0861547
C	-6.5299933	4.1480914	1.5587020	H	-1.4661306	-3.6100001	-2.8968542
H	-5.9474553	2.6650660	0.1083177	C	-5.8450264	-0.5756821	-1.3006306
H	-7.6180945	4.0528618	1.3615263	C	-4.6716152	-0.5911666	-0.5981305
H	-6.1497525	5.0118806	0.9774888	C	-4.6957087	-1.8420744	0.1904667
H	-6.3962957	4.3847469	2.6349752	O	-5.8732211	-2.4778173	0.0610008
C	-1.4516811	4.7197918	-0.6056609	C	-6.6674058	-1.7606521	-0.9065106
C	-1.6982655	4.1392410	-2.0064440	O	-3.7869623	-2.3095798	0.9009745
H	-1.1730105	4.7397148	-2.7773328	C	-3.4919581	0.2581339	-0.5237709
H	-2.7727340	4.1225541	-2.2812628	H	-7.6392971	-1.4968085	-0.4321476
H	-1.3166285	3.1031973	-2.0765391	H	-6.8821612	-2.4650654	-1.7416305
C	-1.8427383	6.2079776	-0.5304396	H	-3.0275750	0.1809418	0.4793403
H	-0.3605283	4.6565406	-0.4265226	H	-3.7519784	1.3283803	-0.6678958
H	-1.2799715	6.8009767	-1.2808193	H	-6.1687259	0.1786583	-2.0301145
H	-1.6348475	6.6341404	0.4725364				
H	-2.9249315	6.3516207	-0.7323649				
H	0.1434334	-5.8228495	-2.2753860				
H	4.8935903	-2.6682350	-3.6291494				
H	3.8720932	-4.3622460	2.4431465				
C	1.2376970	-5.7968222	-2.4901309				
H	3.4764280	0.1855327	-3.7336268				
H	0.9230326	-6.5150293	-4.5276016				
H	0.2870387	-3.8332603	3.5198593				
C	1.7875105	-4.6161080	-1.6927722				
C	5.0943595	-1.9104290	-2.8430445				
C	1.4234906	-5.6736974	-4.0065516				
H	2.4975642	-5.7054491	-4.2870344				
C	2.5013042	-3.5583167	-2.2790516				
C	2.8128775	-4.5922038	2.6740950				
H	1.6615447	-7.2782706	-0.9060051				
C	1.5730831	-4.5657276	-0.3010298				
C	1.8322768	-7.1286166	-1.9899697				
H	1.3785726	-7.9888543	-2.5242866				
H	0.9784036	-5.3622154	0.1702125				
C	2.9192983	-0.6576764	-3.2751217				
H	5.7340777	-2.3886275	-2.0739434				
H	5.6744083	-1.0880064	-3.3109294				
C	3.0153295	-2.4888335	-1.5186657				
C	0.3976107	-3.8836566	2.4172812				
C	2.0793756	-3.5350966	0.5058359				
H	2.6951719	-4.5923187	3.7776532				
H	2.6102843	-5.6211663	2.3095758				
C	3.7872297	-1.3783196	-2.2278911				
C	2.8271853	-2.4910566	-0.1143607				
C	1.8505125	-3.5822568	2.0183303				
H	2.0025125	-0.2469826	-2.8092122				
H	-0.2945741	-3.1446655	1.9730247				
H	2.6168649	-1.3408997	-4.0963859				
H	1.0032589	-4.7307065	-4.4088302				
H	0.0659416	-4.8914616	2.0957511				
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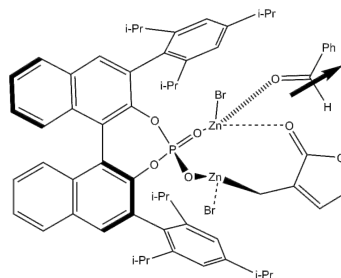


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C	2.3670995	5.4260076	-1.8117007
C	-0.0306799	5.7138407	-1.3265065
C	0.0048061	6.9393855	-2.0580032
C	-1.2525441	5.2133929	-0.7905923
H	-2.1696428	5.8107665	-0.9124276
C	-1.3243379	3.9729823	-0.1668314
C	3.7233548	0.8937760	0.0224620
C	4.8160320	1.5952858	0.5187056
H	5.7651267	1.0641783	0.6860182
C	4.7324376	2.9727582	0.8688249
C	5.8371411	3.6452171	1.4736190
C	3.4998765	3.6912200	0.6499702
C	3.4139752	5.0359510	1.1224102
C	2.4007317	3.0136154	-0.0001165
C	2.5298288	1.6388557	-0.2350481
O	-0.1708184	2.0904399	0.7592143
O	1.4721756	0.9451090	-0.8104743
P	0.1414476	0.6191209	0.0948835

O	-0.9203104	0.1629529	-0.8909690	H	4.8143950	0.4317266	-4.4675627
O	0.4892899	-0.2540342	1.3052530	C	3.6839782	-1.0992873	-1.5388349
C	1.1781988	7.3856255	-2.6476562	C	3.0540902	-1.7181676	3.2878935
C	2.3632720	6.6103764	-2.5363023	C	3.9024435	-1.4787704	0.8859002
H	-0.9278602	7.5163055	-2.1606735	H	5.5568429	-0.6876393	3.8625931
H	1.1894030	8.3283009	-3.2157878	H	5.7908526	-2.1646395	2.8720500
H	3.2898239	4.8335398	-1.7401079	C	3.5808788	-0.1953912	-2.7658188
H	3.2860862	6.9477365	-3.0325327	C	3.7699641	-0.5835669	-0.2171006
C	4.4992475	5.6552744	1.7276665	C	4.0124281	-0.9925789	2.3319213
C	5.7292864	4.9635785	1.8898620	H	1.4050630	-0.4180702	-3.0078889
H	2.4673586	5.5828460	1.0153544	H	2.0054281	-1.6029165	2.9634394
H	4.4017570	6.6899623	2.0903959	H	2.3619680	-1.5265205	-4.0350081
H	6.5858986	5.4682019	2.3621847	H	2.5324461	-5.0651621	-2.4508732
H	6.7745942	3.0860267	1.6207133	H	3.2704835	-2.8044255	3.3600806
C	-3.5455278	2.9231813	-0.7518300	H	6.1929294	-4.8446756	-1.3926510
C	-2.6071235	3.3237678	0.2435218	H	3.4913825	0.8513240	-2.4125561
C	-4.6662526	2.1676739	-0.3557735	H	3.7285646	0.0788863	2.3476191
C	-2.8493459	3.0110328	1.6122459	H	3.6916642	-2.8748018	-2.7661948
C	-3.9881187	2.2605650	1.9491597	Zn	-2.2876896	-0.7500470	-2.0150544
C	-4.8984296	1.8040456	0.9811435	Br	-1.4047031	-1.3458669	-4.1140486
C	-1.9461806	3.5142639	2.7376581	Zn	-0.5451257	-1.4563826	2.4468408
H	-4.1628246	2.0164549	3.0082656	Br	-0.6656129	-1.4608801	4.7501675
C	-1.4676354	2.3899109	3.6718724	H	-5.3798794	1.8264285	-1.1237640
H	-2.3078458	1.9024419	4.2077348	C	-0.4240962	-4.5807791	-2.4332240
H	-0.7782672	2.7923044	4.4421586	C	-0.0928489	-3.9942992	-1.2091344
H	-0.9232712	1.6051963	3.1131645	C	0.3947210	-4.7999083	-0.1511696
C	-2.6553039	4.6355821	3.5228701	C	0.5655227	-6.1909407	-0.3368438
H	-1.0453970	3.9674745	2.2768066	C	0.2170008	-6.7772782	-1.5606425
H	-3.5712622	4.2574007	4.0236817	C	-0.2785299	-5.9728223	-2.6032026
H	-2.9572065	5.4672130	2.8539445	H	-0.7947386	-3.9436887	-3.2521228
H	-1.9876288	5.0487396	4.3072684	C	0.6617805	-4.2056353	1.1595180
C	-6.1138758	0.9671026	1.3609225	H	0.9557638	-6.8070575	0.4889944
C	-5.7718958	-0.1572387	2.3533779	H	0.3369999	-7.8609890	-1.7078874
H	-6.6415427	-0.8306845	2.4964737	H	-0.5449906	-6.4329017	-3.5672924
H	-5.5022882	0.2465631	3.3512842	O	0.3009567	-3.0635790	1.4525680
H	-4.9126576	-0.7619853	2.0009771	H	-0.1932509	-2.9085812	-1.0534836
C	-7.2489281	1.8598408	1.8983048	H	1.1884980	-4.8448659	1.9162666
H	-6.4776108	0.4903750	0.4233064	C	-3.9336771	-3.9029598	-0.6286664
H	-8.1526497	1.2589603	2.1314744	C	-3.6553236	-2.5889964	-0.3625139
H	-7.5321440	2.6388274	1.1619733	C	-2.7830562	-2.6103192	0.8294286
H	-6.9340673	2.3758859	2.8297505	O	-2.5654240	-3.8661577	1.2572376
C	-3.3617313	3.2279246	-2.2406341	C	-3.2585531	-4.7766921	0.3740774
C	-2.9023484	1.9844708	-3.0198915	O	-2.2805008	-1.6265564	1.3965169
H	-2.7690507	2.1994715	-4.0997626	C	-3.9533634	-1.3259418	-1.0425204
H	-3.6559732	1.1679631	-2.9480343	H	-3.9515073	-5.3885290	0.9924815
H	-1.9228557	1.6282547	-2.6401405	H	-2.4982637	-5.4613425	-0.0654748
C	-4.6174063	3.8546945	-2.8696900	H	-4.1299580	-0.5063496	-0.3192834
H	-2.5471578	3.9701942	-2.3389133	H	-4.7952054	-1.4095130	-1.7551486
H	-4.4160269	4.1519626	-3.9193090	H	-4.5394921	-4.2949076	-1.4564850
H	-4.9393901	4.7574573	-2.3117031				
H	-5.4727176	3.1477207	-2.8871227				
H	3.4458653	-5.3919918	-0.0936800				
H	5.0276588	-1.2889177	-4.0175290				
H	6.1745460	-0.5611739	2.1824502				
C	4.0624615	-4.8973531	-0.8788967				
H	2.2483979	0.2057374	-4.4573279				
H	3.5820276	-6.5067159	-2.2741489				
H	3.1301765	-1.2983786	4.3111930				
C	3.9039852	-3.3935340	-0.6722000				
C	4.8687134	-0.2689742	-3.6086055				
C	3.5675737	-5.3986292	-2.2404194				
H	4.2158305	-5.0371880	-3.0658512				
C	3.7505548	-2.4921152	-1.7369603				
C	5.4642712	-1.1037163	2.8380015				
H	5.8828715	-5.0103617	0.3624786				
C	3.9664567	-2.8598191	0.6286229				
C	5.5270958	-5.3184012	-0.6410881				
H	5.6439145	-6.4190465	-0.7251177				
H	4.0774123	-3.5533937	1.4788904				
C	2.3310443	-0.5026771	-3.6072744				
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TS7

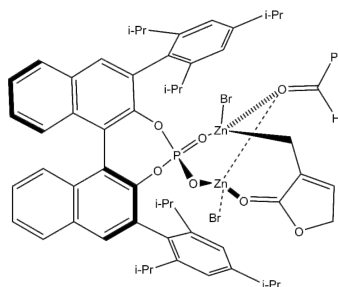


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number of imaginary frequencies: 1

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C	2.3643554	5.4202198	-1.8115744
C	-0.0317063	5.7122546	-1.3233438
C	0.0056990	6.9372285	-2.0547457

C	-1.2534179	5.2133756	-0.7863752	H	3.5971590	-6.5129264	-2.2732101
H	-2.1708007	5.8105194	-0.9077159	H	3.1375393	-1.3092000	4.3177634
C	-1.3266472	3.9733992	-0.1624571	C	3.9048537	-3.3978572	-0.6697905
C	3.7179321	0.8883260	0.0266786	C	4.8521279	-0.2677880	-3.6039075
C	4.8125836	1.5902187	0.5170943	C	3.5715776	-5.4050846	-2.2364020
H	5.7614660	1.0578693	0.6810932	H	4.2093645	-5.0365532	-3.0666318
C	4.7320479	2.9683703	0.8638507	C	3.7441041	-2.4966109	-1.7332039
C	5.8389359	3.6415191	1.4626328	C	5.4691709	-1.0934263	2.8343160
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C	2.3976649	3.0095713	0.0022165	C	5.5439923	-5.3089406	-0.6546735
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O	-0.1771059	2.0931802	0.7665740	H	4.0872307	-3.5580798	1.4807439
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O	-0.9246495	0.1461060	-0.8616967	H	4.7940676	0.4325159	-4.4627905
O	0.4909384	-0.2399730	1.3363089	C	3.6740415	-1.1042631	-1.5341602
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H	-0.9261238	7.5157174	-2.1562716	H	5.5620794	-0.6794071	3.8595933
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C	-1.9557347	3.5074179	2.7419336	Zn	-0.5263309	-1.4543690	2.4795030
H	-4.1767418	2.0179194	3.0028816	Br	-0.6423458	-1.5194153	4.7704878
C	-1.4811555	2.3788772	3.6733817	H	-5.3826041	1.8354779	-1.1322052
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H	-0.7919887	2.7764671	4.4459881	C	-0.0855876	-3.9881073	-1.2274993
H	-0.9358500	1.5950646	3.1146481	C	0.4013215	-4.7887337	-0.1661931
C	-2.6650253	4.6272652	3.5288909	C	0.5667049	-6.1810036	-0.3447060
H	-1.0531897	3.9606759	2.2845840	C	0.2146153	-6.7732563	-1.5643409
H	-3.5831448	4.2497755	4.0259808	C	-0.2808562	-5.9728873	-2.6100974
H	-2.9641123	5.4616441	2.8623924	H	-0.7935852	-3.9420050	-3.2664952
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C	-5.8021059	-0.1398810	2.3491146	H	0.3324716	-7.8579873	-1.7063108
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H	-7.5374470	2.6611412	1.1336451	C	-2.7666160	-2.6065589	0.8403163
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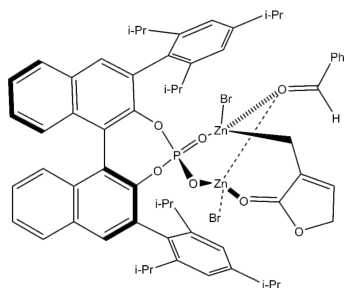
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C	2.2057283	4.5696608	2.0326099
C	2.7899947	5.8686798	2.1303970
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H	0.1525440	5.2984418	1.9919805
C	0.2086809	3.1583355	1.7610345
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C	4.9257448	-1.4764528	1.7930452
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C	5.1030303	-0.5675251	2.8767862
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O	0.2249919	-1.5411211	0.6249485
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H	6.1038788	5.0345732	1.9442098
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C	-1.5671496	1.8960556	3.8147855
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H	1.3976779	-4.6053819	3.2202387
C	2.4278548	-4.0764427	-2.1145130
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C	3.5338499	0.0747064	-3.0354107
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C	2.9217680	-3.5371089	0.2397786
H	3.8545475	-5.3119356	3.0978240
H	3.6720156	-5.9638863	1.4363532
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C	2.8308026	-3.9528161	1.7080771
H	2.5506882	0.3406971	-2.6026225
H	0.6769414	-3.6105637	1.9062614
H	3.3433065	-0.4649005	-3.9859605
H	-0.2643757	-4.4752969	-2.2411309
H	1.0937303	-5.3195429	1.6111092
H	2.3258743	-4.0650372	-5.0247489
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C	-4.1624952	-1.6152427	-5.7633624
C	-3.2886372	-1.6667296	-4.6752378
C	-3.4456219	-2.6806366	-3.6961324
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C	-5.3586391	-3.5764612	-4.9266610
C	-5.1982145	-2.5611872	-5.8881289
H	-4.0348899	-0.8321057	-6.5253211
C	-2.6222631	-2.8013889	-2.5075230
H	-4.5900421	-4.4351141	-3.0818729
H	-6.1643488	-4.3179656	-5.0328357
H	-5.8841558	-2.5099257	-6.7477911
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H	-2.4680041	-0.9378258	-4.5982778
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H	-6.3266142	-1.7516156	-2.3776186
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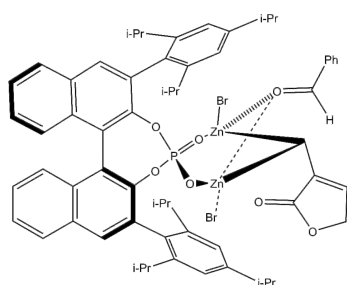
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H	5.5559689	-2.3724559	1.7237895
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C	3.2883013	0.8582098	1.9479369
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P	0.6001894	-0.0880698	0.2902068
O	-0.1515671	0.5962611	-0.8612802
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C	5.0202266	4.8979177	2.0096875
H	2.1341982	6.7450548	2.2154813
H	4.6179934	7.0398861	2.2093119
H	5.1456306	2.7550773	1.8205047
H	6.1121540	5.0293004	1.9654180
C	5.3310036	1.1170474	5.1264864
C	6.1996665	0.0033313	4.9827740
H	3.7099145	2.2618368	4.2835355
H	5.4062384	1.7581973	6.0180401
H	6.9551397	-0.2079522	5.7548339
H	6.7243472	-1.7125848	3.7714430
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H	-5.7977023	0.5969675	1.5530732
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H	-5.5873728	2.2181236	-0.3902855
H	-7.2613471	3.9104046	0.3962007
H	-5.6894307	4.6917671	0.0204939
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C	-1.0562379	3.5742593	-2.1895514
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C	-1.3249023	5.6897863	-0.8162730
H	0.1065210	4.1191882	-0.4826868
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H	4.8852202	-4.7128294	1.7496328
C	1.6789403	-4.9497988	-3.1270687
H	4.0429206	1.0302004	-3.2917169
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H	1.3838988	-6.1123335	3.2111599
C	2.4085081	-4.0648942	-2.1234242
C	5.7064052	-1.1422193	-2.6716388
C	0.2120011	-4.4855469	-3.2389636
H	0.1651364	-3.4457652	-3.6270960
C	3.0599275	-2.8808538	-2.5074534
C	3.8573153	-5.0426250	2.0049621
H	3.4144217	-5.3036027	-4.4320763
C	2.3650684	-4.3772303	-0.7542682
C	2.3461938	-5.0163558	-4.5074195
H	1.8340725	-5.7599635	-5.1516539
H	1.8620789	-5.3066507	-0.4418029
C	3.5099716	0.0919710	-3.0333983
H	6.3303106	-1.7026831	-1.9460213
H	6.2709280	-0.2409377	-2.9896975
C	3.6151330	-1.9977316	-1.5655007
C	1.4052003	-4.3955566	2.1231323
C	2.9022469	-3.5304026	0.2316187
H	3.8400528	-5.3165122	3.0805208
H	3.6518015	-5.9620566	1.4175834
C	4.3476313	-0.7511620	-2.0584192
C	3.5157509	-2.3124023	-0.1823967
C	2.8131571	-3.9511659	1.6986655
H	2.5308696	0.3631463	-2.5950885
H	0.6602174	-3.6073624	1.9093010
H	3.3112832	-0.4438091	-3.9843056
H	-0.2801458	-4.5018264	-2.2455164
H	1.0717287	-5.3144092	1.5993151
H	2.2931320	-4.0411927	-5.0347109
H	4.5663459	-0.1159801	-1.1754403
H	3.0659913	-3.0673351	2.3176657

H	3.1250319	-2.6204069	-3.5742692	O	-0.4643697	-1.2676987	0.4426764
Zn	-1.1135219	0.0442836	-2.4539924	C	3.6549680	6.2791810	1.3645395
Br	-0.1470577	0.2374420	-4.5510956	C	4.5087822	5.1692979	1.1242721
Zn	-1.6362734	-2.2102654	0.3007757	H	1.6287834	6.9267083	1.7699717
Br	-2.0442409	-4.5197092	0.4932525	H	4.0634749	7.3009929	1.3416154
H	-3.5875402	3.6135606	-0.9332869	H	4.6784805	3.0237202	0.9667757
C	-4.1788215	-1.6328852	-5.7442718	H	5.5738635	5.3368713	0.9025227
C	-3.3029164	-1.6686924	-4.6564344	C	5.2959022	1.5824090	4.3961175
C	-3.4306523	-2.6948968	-3.6872381	C	6.1284899	0.4381074	4.2745942
C	-4.4393994	-3.6836990	-3.8392325	H	3.6074191	2.6766842	3.6305813
C	-5.3185097	-3.6328125	-4.9251354	H	5.4795128	2.3091348	5.2022233
C	-5.1869805	-2.6055471	-5.8781374	H	6.9644702	0.2891261	4.9748944
H	-4.0716289	-0.8391222	-6.4983697	H	6.4789989	-1.4123733	3.2055036
C	-2.5983611	-2.8065812	-2.5003883	C	-2.5091248	3.5133739	0.7090135
H	-4.5233015	-4.4844145	-3.0869717	C	-1.6856324	3.0281313	1.7678195
H	-6.1023295	-4.3966153	-5.0384549	C	-3.8799911	3.1938966	0.7200108
H	-5.8739745	-2.5669373	-6.7377520	C	-2.2616309	2.2468704	2.8108651
O	-1.7625480	-1.9763566	-2.0613393	C	-3.6393985	1.9666442	2.7739594
H	-2.5015357	-0.9187075	-4.5740889	C	-4.4697077	2.4226584	1.7357688
H	-2.7401517	-3.7290672	-1.8837030	C	-1.4505259	1.7443039	4.0049834
C	-5.3069805	-1.3410875	-0.4705796	H	-4.0776462	1.3718465	3.5903570
C	-4.0833801	-0.7191144	-0.4429772	C	-1.5684011	0.2211194	4.1950417
C	-4.0026848	0.0207365	-1.7271623	H	-2.6008378	-0.0781730	4.4721657
O	-5.1608402	-0.0657377	-2.4109977	H	-0.8971215	-0.1207934	5.0098079
C	-6.0491885	-0.9480332	-1.7006258	H	-1.2872314	-0.3183317	3.2695305
O	-3.0507591	0.6458449	-2.2222570	C	-1.8427331	2.5058848	5.2857835
C	-3.0025827	-0.7091223	0.5315450	H	-0.3821385	1.9705728	3.8155410
H	-6.2838337	-1.7936913	-2.3882180	H	-2.9055605	2.3262008	5.5515711
H	-6.9978030	-0.4022027	-1.4962290	H	-1.7088568	3.5995697	5.1597591
H	-3.3825018	-0.8671582	1.5595810	H	-1.2199737	2.1791837	6.1445133
H	-2.4469635	0.2468832	0.4929175	C	-5.9695367	2.1553926	1.7211338
H	-5.7210196	-1.9988534	0.3053123	C	-6.3386031	0.7185081	2.1210250
				H	-7.4261370	0.5461674	1.9865047
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				H	-5.7973471	-0.0281324	1.5060645
				C	-6.7034433	3.1826084	2.6054177
				H	-6.3032762	2.3059084	0.6726498
				H	-7.8026703	3.0354769	2.5574352
				H	-6.4806178	4.2204865	2.2853702
				H	-6.3919655	3.0841496	3.6670201
				C	-1.9793283	4.3920078	-0.4255810
				C	-2.3310584	3.8534815	-1.8213267
				H	-1.9634713	4.5443102	-2.6078493
				H	-3.4220844	3.7265864	-1.9719439
				H	-1.8521177	2.8726009	-1.9996099
				C	-2.4732983	5.8419344	-0.2512969
				H	-0.8733731	4.4060633	-0.3593062
				H	-2.0385221	6.5028228	-1.0297327
				H	-2.1984002	6.2526765	0.7418969
				H	-3.5786400	5.8985811	-0.3377654
				H	0.0883844	-5.6220591	-2.4417287
				H	5.1316410	-2.8898145	-3.6205171
				H	3.7089343	-3.6710989	2.5102069
				C	1.1947952	-5.6750240	-2.5737539
				H	4.1179760	0.1083950	-3.7313287
				H	0.9777085	-6.4733225	-4.5936050
				H	0.0140268	-3.6261169	3.3081007
				C	1.7692577	-4.4968808	-1.7884678
				C	5.3879873	-2.1923401	-2.7956008
				C	1.4986885	-5.6436013	-4.0753078
				H	2.5851889	-5.7590688	-4.2724478
				C	2.6462903	-3.5505716	-2.3437333
				C	2.6898052	-4.0676012	2.6780409
				H	1.4010244	-7.1005907	-0.8973660
				C	1.4306819	-4.3580056	-0.4259276
				C	1.6600719	-7.0165979	-1.9710101
				H	1.1885506	-7.8701784	-2.5002930
				H	0.7294004	-5.0806307	0.0162752
				C	3.4282891	-0.6484950	-3.3031174
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				H	6.1020322	-1.4462670	-3.2016583

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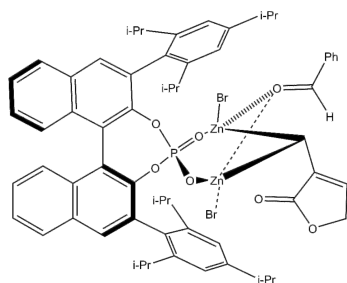


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C	2.6318851	3.6243352	1.4353899
C	4.0098222	3.8742199	1.1608406
C	1.7554234	4.7552740	1.6317423
C	2.3051340	6.0727478	1.6075834
C	0.3570153	4.5458223	1.8109509
H	-0.2929917	5.4199029	1.9690120
C	-0.2111347	3.2784272	1.7399609
C	3.3298713	-1.2372387	0.6148084
C	4.4354290	-1.3478423	1.4481804
H	5.0379395	-2.2686094	1.4231892
C	4.7789792	-0.3277392	2.3800853
C	5.8655572	-0.5014750	3.2895131
C	3.9726292	0.8672283	2.4576523
C	4.2458785	1.7910487	3.5121993
C	2.9113098	1.0599650	1.4950319
C	2.6246180	0.0059718	0.6182295
O	0.1143433	0.9063428	1.5552824
O	1.6251131	0.1672250	-0.3440344
P	0.0471594	0.1423788	0.1087453
O	-0.7045001	0.9502682	-0.9651449

C	3.1805148	-2.4901224	-1.5797439
C	0.2282624	-3.8318029	2.2396559
C	1.9484321	-3.3344570	0.3820001
H	2.4786168	-4.0121143	3.7661510
H	2.6927744	-5.1381666	2.3839738
C	4.1365334	-1.4951457	-2.2333541
C	2.8270496	-2.3797917	-0.2145621
C	1.6209919	-3.2948648	1.8763792
H	2.5600432	-0.1163111	-2.8688298
H	-0.5669208	-3.3596289	1.6356417
H	3.0585975	-1.2764261	-4.1407164
H	1.1778493	-4.6954545	-4.5497249
H	0.1549156	-4.9301392	2.0985767
H	2.7617037	-7.1226286	-2.0614842
H	4.4796818	-0.7997759	-1.4393012
H	1.6580597	-2.2311611	2.1939961
H	2.9366409	-3.6296723	-3.4018572
Zn	-2.3617668	0.2114335	-1.8167104
Br	-3.0264359	0.7125247	-3.9835748
Zn	-1.7937386	-2.2176724	-0.6838027
Br	-2.3925423	-4.4594969	-0.8238434
H	-4.5183866	3.5419528	-0.1061355
C	0.8448961	0.5799978	-5.6496325
C	0.2938816	-0.0841110	-4.5522760
C	0.0507231	-1.4805743	-4.6275334
C	0.3616168	-2.1936761	-5.8126967
C	0.9138714	-1.5210240	-6.9063602
C	1.1554556	-0.1360834	-6.8217282
H	1.0378513	1.6614212	-5.5959285
C	-0.5215077	-2.1871638	-3.5021058
H	0.1561018	-3.2739218	-5.8683870
H	1.1558785	-2.0692632	-7.8287000
H	1.5925415	0.3927886	-7.6828540
O	-0.8896558	-1.6047863	-2.4554983
H	0.0580387	0.4531304	-3.6233002
H	-0.6517557	-3.2933543	-3.5759556
C	-5.5361357	-2.1873572	-1.1172916
C	-4.8259388	-1.0517680	-0.9042408
C	-5.6354911	0.0845155	-1.4330180
O	-6.8116254	-0.4066091	-1.9330841
C	-6.8283135	-1.8330650	-1.7840050
O	-5.3592075	1.2707902	-1.4333184
C	-3.4966241	-0.7846406	-0.3111708
H	-6.9389391	-2.2963363	-2.7904704
H	-7.7220732	-2.1204976	-1.1855062
H	-3.3168088	-1.4475545	0.5676934
H	-3.4896691	0.2240686	0.1703942
H	-5.2359000	-3.2149666	-0.8674530

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C	2.0816714	2.2978781	1.5369222
C	2.6399014	3.6269550	1.4848019
C	4.0196797	3.8755176	1.2196350
C	1.7640118	4.7588314	1.6768995
C	2.3163501	6.0748003	1.6585411
C	0.3642336	4.5510170	1.8443901
H	-0.2869720	5.4255376	1.9949272

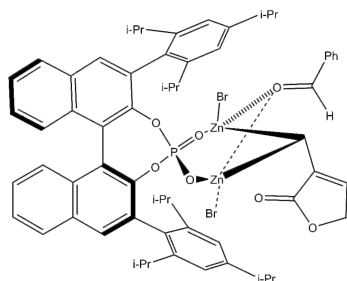
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C	4.4325969	-1.3479167	1.4647589
H	5.0324809	-2.2701257	1.4305958
C	4.7784392	-0.3370917	2.4054483
C	5.8640889	-0.5195634	3.3134797
C	3.9749243	0.8588850	2.4922178
C	4.2508444	1.7743586	3.5529878
C	2.9140657	1.0616776	1.5316336
C	2.6246660	0.0158497	0.6456063
O	0.1195752	0.9118058	1.5933197
O	1.6257894	0.1865110	-0.3138533
P	0.0491233	0.1524280	0.1437567
O	-0.7130729	0.9594761	-0.9211092
O	-0.4508708	-1.2628070	0.4759854
C	3.6676545	6.2798252	1.4257481
C	4.5209050	5.1694170	1.1894934
H	1.6398716	6.9293698	1.8170567
H	4.0776762	7.3010754	1.4076255
H	4.6874819	3.0237848	1.0288164
H	5.5877928	5.3354099	0.9756027
C	5.3005294	1.5570110	4.4344912
C	6.1296616	0.4117839	4.3049168
H	3.6142795	2.6606161	3.6762434
H	5.4863352	2.2777810	5.2453495
H	6.9652651	0.2553407	5.0039538
H	6.4750346	-1.4315171	3.2229748
C	-2.4903435	3.5237198	0.7107357
C	-1.6808870	3.0383482	1.7804222
C	-3.8616382	3.2076210	0.7061640
C	-2.2709553	2.2600796	2.8171797
C	-3.6488864	1.9836089	2.7644133
C	-4.4657536	2.4409291	1.7166927
C	-1.4751232	1.7581921	4.0217418
H	-4.0981298	1.3917692	3.5769284
C	-1.5991802	0.2360538	4.2146439
H	-2.6351869	-0.0604524	4.4811938
H	-0.9384279	-0.1060547	5.0377899
H	-1.3090300	-0.3071200	3.2942026
C	-1.8791814	2.5250664	5.2954875
H	-0.4040001	1.9806093	3.8434595
H	-2.9456395	2.3508978	5.5496729
H	-1.7406783	3.6177233	5.1673318
H	-1.2681094	2.1993729	6.1629013
C	-5.9669359	2.1830940	1.6853417
C	-6.3533507	0.7568920	2.1056206
H	-7.4395696	0.5895169	1.9554744
H	-6.1400924	0.5667325	3.1784870
H	-5.8073539	-0.0056826	1.5148865
C	-6.7051001	3.2317737	2.5402298
H	-6.2843493	2.3164905	0.6295045
H	-7.8047837	3.0932256	2.4795682
H	-6.4688488	4.2616307	2.2050000
H	-6.4091052	3.1514067	3.6076405
C	-1.9459735	4.4002032	-0.4188330
C	-2.2804015	3.8619019	-1.8191606
H	-1.9133381	4.5586988	-2.6005729
H	-3.3682972	3.7240393	-1.9820697
H	-1.7880087	2.8876823	-1.9970115
C	-2.4416748	5.8502527	-0.2503857
H	-0.8409030	4.4138823	-0.3389683
H	-1.9961041	6.5121479	-1.0217810
H	-2.1820884	6.2602811	0.7471960
H	-3.5455058	5.9081566	-0.3520976
H	0.1344880	-5.6239977	-2.4655743
H	5.1361430	-2.8014173	-3.6181226
H	3.7160436	-3.6820234	2.5158869
C	1.2417817	-5.6615565	-2.5957117
H	4.0499598	0.1761324	-3.7159702
H	1.0374545	-6.4439399	-4.6240506
H	0.0146617	-3.6627250	3.2908795

C	1.7986829	-4.4813419	-1.8013376
C	5.3765554	-2.0997889	-2.7920292
C	1.5492403	-5.6144146	-4.0960803
H	2.6371802	-5.7198103	-4.2911553
C	2.6590587	-3.5162038	-2.3492339
C	2.6988699	-4.0883150	2.6708105
H	1.4629854	-7.0963400	-0.9302480
C	1.4578435	-4.3583292	-0.4382435
C	1.7237832	-7.0010460	-2.0022926
H	1.2657237	-7.8576439	-2.5384924
H	0.7650365	-5.0930735	-0.0027887
C	3.3799663	-0.6001518	-3.2911376
H	5.9133194	-2.6749663	-2.0106100
H	6.0728941	-1.3367295	-3.1972319
C	3.1771137	-2.4543530	-1.5769181
C	0.2383296	-3.8610252	2.2230807
C	1.9624740	-3.3355325	0.3786732
H	2.4803286	-4.0487147	3.7580695
H	2.7124176	-5.1547585	2.3628945
C	4.1097009	-1.4345973	-2.2260244
C	2.8283619	-2.3641811	-0.2092317
C	1.6300628	-3.3128787	1.8722134
H	2.4993543	-0.0922476	-2.8525098
H	-0.5565692	-3.3919213	1.6164237
H	3.0262354	-1.2323798	-4.1322696
H	1.2237764	-4.6637863	-4.5622199
H	0.1724033	-4.9588985	2.0756629
H	2.8269424	-7.0912680	-2.0892965
H	4.4371764	-0.7350828	-1.4290640
H	1.6598864	-2.2523354	2.2005801
H	2.9492216	-3.5808973	-3.4083631
Zn	-2.3830571	0.2452838	-1.7622154
Br	-2.9852104	0.6856003	-3.9540027
Zn	-1.7407615	-2.2117826	-0.6972951
Br	-2.3434907	-4.4454625	-0.9070169
H	-4.4891784	3.5538693	-0.1290327
C	0.7734243	0.4692745	-5.7870465
C	0.2673845	-0.1577869	-4.6465203
C	-0.0003134	-1.5505934	-4.6741397
C	0.2331539	-2.2961793	-5.8557709
C	0.7415917	-1.6610402	-6.9922674
C	1.0126700	-0.2798729	-6.9541403
H	0.9819773	1.5490096	-5.7710785
C	-0.5339701	-2.2134046	-3.5010893
H	0.0045041	-3.3731681	-5.8731087
H	0.9251036	-2.2353180	-7.9123387
H	1.4137686	0.2199290	-7.8495710
O	-0.8084207	-1.5951529	-2.4496361
H	0.0759439	0.4044094	-3.7223148
H	-0.7246868	-3.3137623	-3.5462749
C	-5.5199666	-2.2043472	-1.0966875
C	-4.7982019	-1.0794504	-0.8695082
C	-5.5841576	0.0710788	-1.4059759
O	-6.7652058	-0.3988233	-1.9127883
C	-6.8007437	-1.8235914	-1.7750560
O	-5.2774269	1.2489523	-1.4050199
C	-3.4735066	-0.8236895	-0.2665719
H	-6.9067120	-2.2767027	-2.7872580
H	-7.7056112	-2.1048203	-1.1893364
H	-3.2806233	-1.5234291	0.5796130
H	-3.4708698	0.1666355	0.2513339
H	-5.2314270	-3.2370946	-0.8542621

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C	3.0129067	3.3896597	2.1534660
C	4.4275041	3.4992735	1.9963748
C	2.2511400	4.6054717	2.3191508
C	2.9383872	5.8538142	2.4074089
C	0.8273070	4.5545138	2.3091697
H	0.2627763	5.4971265	2.3743391
C	0.1383100	3.3618498	2.1237273
C	3.3314164	-1.3845955	0.9182018
C	4.4237299	-1.6440621	1.7384251
H	4.9737369	-2.5897290	1.6167307
C	4.7995896	-0.7623410	2.7912743
C	5.8565851	-1.0996905	3.6900841
C	4.0577649	0.4587303	2.9983436
C	4.3619303	1.2427856	4.1522335
C	3.0222730	0.8178326	2.0566275
C	2.6778754	-0.1248207	1.0788132
O	0.2044916	0.9597722	2.0638184
O	1.6668188	0.1686802	0.1630149
P	0.1043017	0.1522424	0.6485507
O	-0.6616897	0.9030277	-0.4518057
O	-0.4175314	-1.2470889	1.0323978
C	4.3188067	5.9188456	2.2921333
C	5.0640546	4.7314220	2.0642014
H	2.3441748	6.7705647	2.5471118
H	4.8353217	6.8887612	2.3545940
H	5.0185285	2.5924544	1.8095792
H	6.1556311	4.7872113	1.9339702
C	5.3809230	0.8755650	5.0207193
C	6.1501341	-0.2944388	4.7801345
H	3.7702157	2.1450452	4.3584658
H	5.5893339	1.4943013	5.9068603
H	6.9620869	-0.5698376	5.4702761
H	6.4213616	-2.0279903	3.5106660
C	-1.7466594	3.7885600	0.5185659
C	-1.3181208	3.2965252	1.7897308
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C	-3.5881809	2.5315396	2.2425695
C	-4.0390659	3.0035316	0.9984136
C	-1.8437522	2.1350394	4.0291922
H	-4.3023237	2.0521665	2.9275921
C	-2.2232632	0.6574196	4.2324759
H	-3.3240147	0.5143180	4.2410385
H	-1.8361933	0.2871740	5.2041014
H	-1.7984957	0.0218067	3.4306030
C	-2.4331047	3.0268863	5.1387838
H	-0.7398685	2.2073752	4.1093342
H	-3.5430310	3.0067734	5.1225486
H	-2.1150074	4.0822746	5.0169310
H	-2.1031873	2.6807473	6.1404090
C	-5.4958150	2.9222958	0.5551890
C	-6.3687403	2.0081177	1.4201534
H	-7.3761188	1.9108659	0.9702666
H	-6.4936981	2.4089139	2.4486511
H	-5.9486512	0.9854900	1.4928749
C	-6.1120872	4.3335734	0.4680002
H	-5.4873376	2.4898303	-0.4688604
H	-7.1490753	4.2843102	0.0764135
H	-5.5286614	4.9983945	-0.1999599
H	-6.1462372	4.8103170	1.4706948
C	-0.8088006	4.5198004	-0.4444607
C	-0.8367642	3.9644634	-1.8769791
H	-0.0950886	4.5007000	-2.5047512
H	-1.8282024	4.0827962	-2.3588636
H	-0.5904910	2.8860222	-1.8877054
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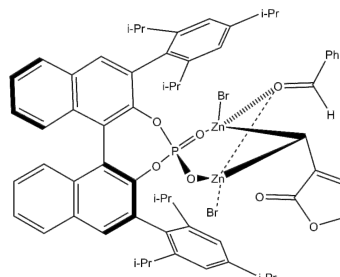
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H	-0.0006348	-5.6045105	-2.2881014
H	4.5061153	-2.1064414	-3.6750542
H	4.0793638	-4.7700121	2.1241846
C	1.0619563	-5.4941229	-2.6099104
H	2.9512072	0.6697383	-3.3712154
H	0.5555605	-5.9815696	-4.6766088
H	0.6634066	-4.2578244	3.6540182
C	1.6500150	-4.3901437	-1.7327012
C	4.7364304	-1.4187373	-2.8343423
C	1.0753649	-5.1822728	-4.1107903
H	2.1128291	-5.1216216	-4.5018145
C	2.2539442	-3.2327637	-2.2508957
C	3.0373119	-4.9790299	2.4412755
H	1.7198807	-7.1320990	-1.2784547
C	1.6002099	-4.5242978	-0.3316087
C	1.7612913	-6.8432301	-2.3469423
H	1.2847615	-7.6547472	-2.9346949
H	1.1023798	-5.4070832	0.0977839
C	2.4776521	-0.2508688	-2.9720143
H	5.4588165	-1.9330338	-2.1683886
H	5.2366705	-0.5240201	-3.2596138
C	2.8052043	-2.2360723	-1.4199664
C	0.6548686	-4.1117494	2.5540239
C	2.1496194	-3.5732506	0.5431510
H	3.0371390	-5.1332037	3.5403257
H	2.7314421	-5.9346710	1.9657298
C	3.4602678	-1.0192863	-2.0701474
C	2.7699997	-2.4130934	-0.0124604
C	2.0809177	-3.8358592	2.0494523
H	1.5731528	0.0463244	-2.4064146
H	-0.0148482	-3.2619554	2.3228302
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H	0.2148221	-5.0221131	2.0988073
H	2.8308446	-6.7901384	-2.6403267
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H	2.4284962	-2.9212130	2.5687858
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Zn	-2.3801030	0.3005743	-1.2197660
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H	-3.4223263	3.9673437	-0.8378675
C	-0.7247414	-0.0567742	-5.9960805
C	-0.8047694	-0.4985529	-4.6734682
C	-1.2032207	-1.8338375	-4.4042503
C	-1.5229403	-2.7114830	-5.4730498
C	-1.4495614	-2.2572372	-6.7920171
C	-1.0479640	-0.9317909	-7.0506729
H	-0.4157969	0.9766922	-6.2108113
C	-1.2945419	-2.3263780	-3.0487302
H	-1.8318626	-3.7456383	-5.2536200
H	-1.7014413	-2.9306219	-7.6244404
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O	-1.1532137	-1.5987411	-2.0324708
H	-0.5569756	0.1681793	-3.8371131
H	-1.4981622	-3.4141110	-2.8950904
C	-4.5707239	-2.6404662	-2.0461797
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O	-6.1963741	0.3194842	-1.2212909
C	-3.6722975	-1.0402617	-0.2011531
H	-5.3527845	-2.5552977	-4.0775069
H	-6.4146344	-3.4289014	-2.9230898
H	-3.6212100	-1.7741549	0.6417470
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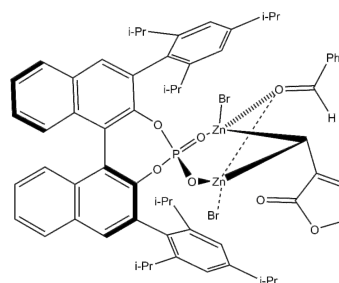


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C	4.4149100	3.4823248	1.9791472
C	2.2382496	4.5919222	2.2839239
C	2.9259487	5.8401755	2.3618607
C	0.8148993	4.5403136	2.2707128
H	0.2490780	5.4829316	2.3233268
C	0.1252867	3.3463292	2.0970143
C	3.3209658	-1.4012584	0.9192353
C	4.4112842	-1.6580879	1.7427074
H	4.9613729	-2.6039011	1.6225496
C	4.7849831	-0.7745541	2.7942811
C	5.8402546	-1.1079510	3.6958569
C	4.0431800	0.4471676	2.9956837
C	4.3468748	1.2362800	4.1459598
C	3.0085280	0.8026961	2.0522886
C	2.6646120	-0.1426036	1.0768021
O	0.1924452	0.9431704	2.0631773
O	1.6523559	0.1465504	0.1616785
P	0.0906473	0.1289121	0.6522068
O	-0.6809678	0.8760711	-0.4469121
O	-0.4255771	-1.2718182	1.0374889
C	4.3062470	5.9038915	2.2511032
C	5.0514895	4.7144334	2.0377742
H	2.3313081	6.7582874	2.4901540
H	4.8226647	6.8742625	2.3059586
H	5.0054301	2.5730403	1.8037172
H	6.1435643	4.7682940	1.9113684
C	5.3648537	0.8728123	5.0164465
C	6.1331482	-0.2984462	4.7822328
H	3.7551883	2.1398799	4.3458909
H	5.5729709	1.4957801	5.8996158
H	6.9441651	-0.5714134	5.4743558
H	6.4046093	-2.0373857	3.5210834
C	-1.7602228	3.7629178	0.4893065
C	-1.3313202	3.2825365	1.7647232
C	-3.1093189	3.6011596	0.1319439
C	-2.2613447	2.6607597	2.6370775
C	-3.6084534	2.5552701	2.2397709
C	-4.0619666	3.0219858	0.9947482
C	-1.8580158	2.1483171	4.0177803
H	-4.3260389	2.0974495	2.9357264
C	-2.2447514	0.6738869	4.2298937
H	-3.3461519	0.5358309	4.2365893
H	-1.8620999	0.3072423	5.2045550
H	-1.8200152	0.0308148	3.4341460
C	-2.4381256	3.0497664	5.1241549

H	-0.7534425	2.2141741	4.0938535	C	-1.3024159	-2.1547780	-6.8114649
H	-3.5480551	3.0369542	5.1124194	C	-0.9579975	-0.8063502	-7.0289902
H	-2.1150245	4.1024949	4.9944439	H	-0.4439902	1.1093529	-6.1270441
H	-2.1070051	2.7083080	6.1269517	C	-1.2431532	-2.3019404	-3.0637297
C	-5.5250831	2.9696101	0.5689052	H	-1.6566398	-3.6946973	-5.3173999
C	-6.4144181	2.1106536	1.4723317	H	-1.5009324	-2.8188787	-7.6655982
H	-7.4293674	2.0304161	1.0369417	H	-0.8867917	-0.4233409	-8.0588345
H	-6.5137794	2.5472153	2.4891142	O	-1.1451432	-1.5874274	-2.0368477
H	-6.0268470	1.0776434	1.5681835	H	-0.6025012	0.2360020	-3.7787414
C	-6.1004194	4.3951931	0.4440127	H	-1.4243341	-3.3972151	-2.9302279
H	-5.5420378	2.5047708	-0.4407531	C	-4.6337248	-2.6492319	-1.9732467
H	-7.1429110	4.3636760	0.0660149	C	-4.6200536	-1.5524376	-1.1743297
H	-5.5072841	5.0222746	-0.2510944	C	-5.8283606	-0.7363795	-1.5274983
H	-6.1082911	4.9045824	1.4309549	O	-6.4947689	-1.3652614	-2.5511515
C	-0.8190617	4.4718498	-0.4874706	C	-5.8107274	-2.5685643	-2.8944845
C	-0.8546796	3.8956137	-1.9117068	O	-6.2284321	0.2867333	-1.0168694
H	-0.1174290	4.4233925	-2.5516998	C	-3.6693944	-1.0812832	-0.1327116
H	-1.8486528	4.0035583	-2.3904886	H	-5.5048805	-2.5182948	-3.9656635
H	-0.6048044	2.8180716	-1.9070907	H	-6.5110783	-3.4286250	-2.7893372
C	-1.1101554	5.9856070	-0.4983268	H	-3.5995527	-1.8193883	0.7054174
H	0.2168817	4.3370096	-0.1190025	H	-4.0935046	-0.1929994	0.3928939
H	-0.3925460	6.5215297	-1.1538805	H	-3.9252356	-3.4902039	-1.9549227
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H	-2.1335364	6.1892575	-0.8772874				
H	0.0556838	-5.6549085	-2.3109342				
H	4.5288528	-2.1018026	-3.6684091				
H	4.0735905	-4.7883202	2.1284903				
C	1.1169063	-5.5258849	-2.6300216				
H	2.9517613	0.6621021	-3.3640698				
H	0.6218131	-6.0128390	-4.7004658				
H	0.6415801	-4.2986350	3.6269827				
C	1.6840654	-4.4151554	-1.7481272				
C	4.7487118	-1.4153385	-2.8240092				
C	1.1285165	-5.2085126	-4.1296479				
H	2.1654355	-5.1320550	-4.5192682				
C	2.2810496	-3.2515924	-2.2596974				
C	3.0296503	-5.0009569	2.4366230				
H	1.8025198	-7.1544983	-1.3025871				
C	1.6213127	-4.5507876	-0.3481942				
C	1.8397569	-6.8629659	-2.3703068				
H	1.3792252	-7.6822502	-2.9600797				
H	1.1254103	-5.4374751	0.0752853				
C	2.4822525	-0.2621846	-2.9686529				
H	5.4704387	-1.9276483	-2.1561697				
H	5.2457964	-0.5161452	-3.2434234				
C	2.8155480	-2.2510774	-1.4227804				
C	0.6424230	-4.1442865	2.5282141				
C	2.1539301	-3.5963057	0.5326233				
H	3.0208385	-5.1567319	3.5353126				
H	2.7327005	-5.9575160	1.9576267				
C	3.4658032	-1.0276619	-2.0654934				
C	2.7696637	-2.4306828	-0.0160893				
C	2.0721032	-3.8612848	2.0378251				
H	1.5750868	0.0295104	-2.4047651				
H	-0.0267006	-3.2936330	2.2996255				
H	2.1676644	-0.8717621	-3.8418497				
H	0.6187316	-4.2540007	-4.3661598				
H	0.2065326	-5.0514074	2.0628543				
H	2.9087388	-6.7900463	-2.6608505				
H	3.7683973	-0.3383764	-1.2514394				
H	2.4108217	-2.9459036	2.5618012				
H	2.3469631	-3.1074407	-3.3480893				
Zn	-2.4190704	0.2857558	-1.1801603				
Br	-3.3298491	1.2952581	-3.0621650				
Zn	-1.6966555	-2.2283108	-0.1122757				
Br	-2.0410546	-4.5366722	-0.2071017				
H	-3.4409306	3.9467238	-0.8597838				
C	-0.7046585	0.0562355	-5.9466817				
C	-0.7951212	-0.4211157	-4.6368631				
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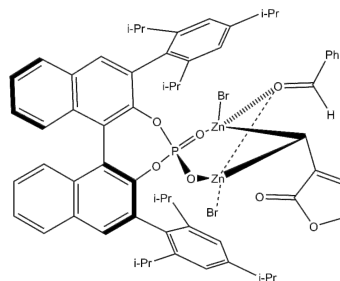


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C	4.2645918	3.5851077	1.8801607
C	2.0174081	4.5634214	2.1284742
C	2.6278422	5.8495251	2.2372828
C	0.5999952	4.4282497	2.0791987
H	-0.0200852	5.3360571	2.1323489
C	-0.0136821	3.1969427	1.8794030
C	3.4142678	-1.3815536	0.7801348
C	4.4737870	-1.6122283	1.6494800
H	5.0450920	-2.5489092	1.5652101
C	4.7924722	-0.7081481	2.7032261
C	5.8217439	-1.0128738	3.6446204
C	4.0164586	0.4982070	2.8704310
C	4.2577191	1.2980456	4.0283137
C	3.0110232	0.8244905	1.8859228
C	2.7424824	-0.1252182	0.8923800
O	0.2038852	0.8015894	1.8055749
O	1.7708881	0.1542188	-0.0720120
P	0.2004841	0.0136969	0.3662603
O	-0.5987668	0.7690745	-0.7124228
O	-0.2137349	-1.4282304	0.6916548
C	4.0052576	5.9942455	2.1676604
C	4.8258101	4.8519602	1.9680977
H	1.9775289	6.7303018	2.3573506
H	4.4624743	6.9923752	2.2460673
H	4.9123764	2.7129442	1.7169466
H	5.9162678	4.9713000	1.8768518
C	5.2516265	0.9622940	4.9376855
C	6.0557741	-0.1914694	4.7371163

H	3.6380492	2.1878845	4.2040517	H	-0.1403940	-3.4362117	1.9908408
H	5.4124703	1.5934527	5.8249965	H	2.5771170	-0.9122420	-4.0310942
H	6.8471678	-0.4421198	5.4598354	H	0.8279140	-4.1858005	-4.5665775
H	6.4135247	-1.9297475	3.4960307	H	0.3112213	-5.1661235	1.9132329
C	-1.9117724	3.5314489	0.2633052	H	2.8442344	-6.8447136	-2.7125538
C	-1.4638528	3.0591408	1.5319626	H	4.0709611	-0.4272031	-1.3662857
C	-3.2574701	3.3275648	-0.1017825	H	2.2492608	-2.8062931	2.3969612
C	-2.3778770	2.3975993	2.3965891	H	2.5827358	-3.1452516	-3.4935788
C	-3.7141307	2.2298735	1.9853736	Zn	-2.4515614	0.1643035	-1.1380693
C	-4.1850215	2.6775004	0.7341095	Br	-3.7048132	0.8720130	-2.9626473
C	-1.9711116	1.8945589	3.7805376	Zn	-1.7702036	-2.3192490	-0.1964417
H	-4.4057220	1.7056599	2.6596938	Br	-2.2703821	-4.5733741	-0.4479882
C	-2.2220821	0.3845751	3.9522088	H	-3.5844191	3.6896598	-1.0849715
H	-3.2921924	0.1230636	3.8176346	C	-0.1501249	0.6691352	-5.5098690
H	-1.9197206	0.0562437	4.9679340	C	-0.4927410	-0.0386200	-4.3569010
H	-1.6292732	-0.1978896	3.2200742	C	-0.7687290	-1.4281058	-4.4417745
C	-2.6754045	2.7108734	4.8812774	C	-0.7025219	-2.0921214	-5.6922222
H	-0.8809319	2.0665385	3.8953815	C	-0.3634624	-1.3743345	-6.8433468
H	-3.7759875	2.5723393	4.8423445	C	-0.0859752	0.0029146	-6.7496306
H	-2.4681429	3.7950946	4.7739132	H	0.0693531	1.7453434	-5.4485771
H	-2.3314881	2.3914907	5.8868126	C	-1.1175268	-2.1768163	-3.2510261
C	-5.6291112	2.4176911	0.2942922	H	-0.9281513	-3.1682125	-5.7511760
C	-6.6354310	2.5384647	1.4522790	H	-0.3138077	-1.8827880	-7.8174401
H	-7.6641884	2.3506960	1.0833702	H	0.1854196	0.5655457	-7.6562786
H	-6.6102917	3.5570333	1.8934827	O	-1.2998465	-1.6306905	-2.1409190
H	-6.4435043	1.8028533	2.2564565	H	-0.5390725	0.4574241	-3.3775833
C	-6.0694138	3.2760900	-0.9001634	H	-1.2317269	-3.2857140	-3.3259540
H	-5.6512453	1.3572609	-0.0556600	C	-5.3248648	-1.8481320	-0.7958618
H	-7.1244278	3.0543788	-1.1584471	C	-4.7102690	-1.2924517	0.2735192
H	-5.4614720	3.0726924	-1.8033165	C	-5.7503415	-1.0732297	1.3223036
H	-5.9986473	4.3592263	-0.6652819	O	-6.9623790	-1.4916509	0.8265704
C	-1.0007915	4.2738210	-0.7173042	C	-6.7817249	-1.9995101	-0.5015213
C	-1.0488214	3.7101854	-2.1482622	O	-5.6315694	-0.6013823	2.4383826
H	-0.3377646	4.2632402	-2.7963499	C	-3.2892465	-0.9066203	0.4968638
H	-2.0545636	3.7992077	-2.6070528	H	-7.4206313	-1.4169088	-1.2029900
H	-0.7672596	2.6406049	-2.1554944	H	-7.1244434	-3.0579282	-0.5363746
C	-1.3250367	5.7808880	-0.7110264	H	-2.9143187	-1.4325861	1.4121050
H	0.0430166	4.1553104	-0.3650832	H	-3.2634184	0.1235595	0.9421905
H	-0.6294641	6.3365798	-1.3737108	H	-4.8608435	-2.1374566	-1.7489016
H	-1.2488065	6.2137745	0.3068604				
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H	0.0676338	-5.5040710	-2.5183722				
H	4.8545467	-2.2801734	-3.7084672				
H	4.0932533	-4.5149214	2.1181798				
C	1.1485748	-5.4556221	-2.7904355				
H	3.4442501	0.5752366	-3.5481848				
H	0.7093699	-5.9460952	-4.8722703				
H	0.5585013	-4.2516499	3.4271237				
C	1.7539370	-4.3689987	-1.9033275				
C	5.0704196	-1.5920375	-2.8642337				
C	1.2516045	-5.1718624	-4.2930275				
H	2.3079621	-5.1811640	-4.6350397				
C	2.4561695	-3.2617283	-2.4072258				
C	3.0551907	-4.8066999	2.3736862				
H	1.6497439	-7.1019053	-1.4034534				
C	1.6189241	-4.4726668	-0.5048434				
C	1.7600637	-6.8352290	-2.4727397				
H	1.2695947	-7.6303331	-3.0713652				
H	1.0444467	-5.3155986	-0.0922371				
C	2.8925925	-0.3046898	-3.1571108				
H	5.7205080	-2.1340637	-2.1477026				
H	5.6450497	-0.7332351	-3.2692537				
C	3.0152253	-2.2806787	-1.5618592				
C	0.6087628	-4.1786827	2.3213455				
C	2.1746275	-3.5385145	0.3829415				
H	2.9966533	-4.9366712	3.4743478				
H	2.8633359	-5.7939739	1.9030948				
C	3.7732029	-1.1115578	-2.1871597				
C	2.8875186	-2.4244372	-0.1574887				
C	2.0252137	-3.7660384	1.8887340				
H	1.9805471	0.0614605	-2.6476298				

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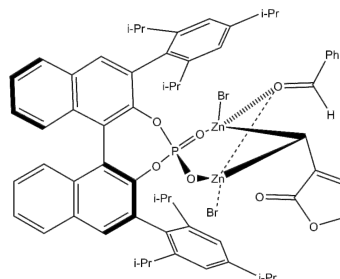


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C	4.2680342	3.5829696	1.9047601
C	2.0210036	4.5635759	2.1405749
C	2.6326150	5.8486594	2.2484874
C	0.6039721	4.4291721	2.0846445
H	-0.0165118	5.3372118	2.1290255
C	-0.0104336	3.1979882	1.8880542
C	3.4102369	-1.3801087	0.7890850
C	4.4687013	-1.6157087	1.6581694
H	5.0366213	-2.5541030	1.5702084
C	4.7899228	-0.7161217	2.7146120
C	5.8183176	-1.0251347	3.6548550
C	4.0173149	0.4917650	2.8852000
C	4.2618529	1.2884249	4.0442670

C	3.0118150	0.8230165	1.9028738	C	1.7832251	-6.8188521	-2.4963539
C	2.7407436	-0.1229749	0.9062728	H	1.2982828	-7.6150578	-3.0980116
O	0.2059893	0.8024529	1.8279170	H	1.0486827	-5.3139839	-0.1080001
O	1.7680127	0.1599280	-0.0548078	C	2.8732276	-0.2790667	-3.1397719
P	0.1991070	0.0155547	0.3885767	H	5.7134146	-2.0988282	-2.1475207
O	-0.6042937	0.7709250	-0.6867779	H	5.6288329	-0.6918517	-3.2604916
O	-0.2112370	-1.4277246	0.7118959	C	3.0102642	-2.2647032	-1.5579453
C	4.0099364	5.9922004	2.1852845	C	0.6064674	-4.1885045	2.3112601
C	4.8298998	4.8490685	1.9926307	C	2.1748414	-3.5377005	0.3787127
H	1.9824445	6.7302786	2.3629712	H	2.9932564	-4.9626494	3.4584466
H	4.4674503	6.9901534	2.2634832	H	2.8575412	-5.8067288	1.8806121
H	4.9148634	2.7092301	1.7470463	C	3.7606823	-1.0874102	-2.1771381
H	5.9208970	4.9668553	1.9065319	C	2.8841140	-2.4179624	-0.1544722
C	5.2555215	0.9483791	4.9516012	C	2.0243467	-3.7763482	1.8826485
C	6.0556759	-0.2070140	4.7484143	H	1.9606672	0.0788256	-2.6254064
H	3.6444296	2.1795640	4.2208107	H	-0.1391335	-3.4381370	1.9913512
H	5.4189368	1.5775416	5.8397888	H	2.5599737	-0.8821860	-4.0177056
H	6.8467662	-0.4616920	5.4699707	H	0.8326722	-4.1625590	-4.5723408
H	6.4070942	-1.9435749	3.5040861	H	0.3024386	-5.1690624	1.8918383
C	-1.8958429	3.5178475	0.2546746	H	2.8671170	-6.8186589	-2.7367677
C	-1.4582842	3.0589739	1.5315994	H	4.0558631	-0.4064894	-1.3525956
C	-3.2379248	3.3076499	-0.1198084	H	2.2508304	-2.8214760	2.3988337
C	-2.3789733	2.4057138	2.3952288	H	2.5844253	-3.1204049	-3.4946150
C	-3.7122680	2.2348281	1.9763108	Zn	-2.4646466	0.1807385	-1.0937063
C	-4.1729544	2.6687576	0.7165848	Br	-3.6990793	0.8246046	-2.9501428
C	-1.9823052	1.9150638	3.7864625	Zn	-1.7534821	-2.3186061	-0.2035052
H	-4.4098678	1.7194280	2.6511165	Br	-2.2530097	-4.5608121	-0.5234885
C	-2.2347997	0.4066519	3.9692155	H	-3.5576391	3.6595714	-1.1090247
H	-3.3036468	0.1433481	3.8284935	C	-0.2058062	0.6584595	-5.5463686
H	-1.9409252	0.0871690	4.9901815	C	-0.5189540	-0.0431257	-4.3809191
H	-1.6342060	-0.1819150	3.2484860	C	-0.7830486	-1.4349497	-4.4495248
C	-2.6950558	2.7413033	4.8741089	C	-0.7369500	-2.1072987	-5.6952570
H	-0.8928907	2.0883671	3.9074560	C	-0.4264044	-1.3963527	-6.8585316
H	-3.7950844	2.6021904	4.8280916	C	-0.1593737	-0.0163512	-6.7812514
H	-2.4877871	3.8245204	4.7583344	H	0.0013224	1.7376120	-5.4956642
H	-2.3592769	2.4315940	5.8853493	C	-1.1074400	-2.1727331	-3.2421111
C	-5.6164035	2.4136657	0.2718287	H	-0.9526550	-3.1862052	-5.7401939
C	-6.6267858	2.5551493	1.4238611	H	-0.3913944	-1.9121265	-7.8294910
H	-7.6558164	2.3766258	1.0514190	H	0.0883850	0.5412059	-7.6978626
H	-6.5918943	3.5769110	1.8566231	O	-1.2558553	-1.6125667	-2.1371356
H	-6.4488389	1.8229960	2.2342032	H	-0.5563125	0.4600965	-3.4049845
C	-6.0434987	3.2623379	-0.9343063	H	-1.2362094	-3.2820639	-3.3018031
H	-5.6455394	1.3497722	-0.0668676	C	-5.3120217	-1.8782584	-0.7582937
H	-7.0993809	3.0477110	-1.1947206	C	-4.7015061	-1.3039782	0.3024420
H	-5.4347520	3.0429695	-1.8331264	C	-5.7480689	-1.0479973	1.3392739
H	-5.9646912	4.3472922	-0.7109877	O	-6.9612953	-1.4675831	0.8414221
C	-0.9789842	4.2546475	-0.7248179	C	-6.7738503	-2.0066884	-0.4696848
C	-1.0103360	3.6779091	-2.1511709	O	-5.6304425	-0.5490258	2.4410531
H	-0.3029344	4.2352979	-2.7996516	C	-3.2790472	-0.9269829	0.5288983
H	-2.0139219	3.7475406	-2.6179135	H	-7.3992756	-1.4332070	-1.1915538
H	-0.7127430	2.6127569	-2.1457219	H	-7.1283384	-3.0623904	-0.4848199
C	-1.3111134	5.7598849	-0.7349305	H	-2.8993314	-1.4792981	1.4268602
H	0.0621871	4.1450896	-0.3620054	H	-3.2497983	0.0908313	1.0011892
H	-0.6119955	6.3145490	-1.3947105	H	-4.8406322	-2.1929721	-1.6994503
H	-1.2484032	6.2015286	0.2800313				
H	-2.3418068	5.9359452	-1.1078016				
H	0.0805417	-5.5001085	-2.5308544				
H	4.8469117	-2.2406412	-3.7070789				
H	4.0901900	-4.5334890	2.1050394				
C	1.1606512	-5.4422990	-2.8045196				
H	3.4186395	0.6068980	-3.5258918				
H	0.7217331	-5.9224432	-4.8895877				
H	0.5559719	-4.2744514	3.4159599				
C	1.7593952	-4.3565663	-1.9121974				
C	5.0593519	-1.5558691	-2.8593743				
C	1.2601083	-5.1489293	-4.3055142				
H	2.3158837	-5.1514229	-4.6493927				
C	2.4565786	-3.2433961	-2.4091021				
C	3.0513422	-4.8237429	2.3589482				
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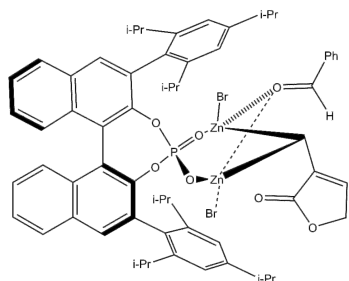


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C	4.2815983	3.5726104	2.0548608	H	3.8948823	-4.5233614	2.2758802
C	2.0477504	4.5948715	2.2417255	C	1.1177521	-5.3995474	-2.7469753
C	2.6808540	5.8661256	2.3886593	H	3.5637038	0.5761297	-3.4252107
C	0.6295771	4.4908033	2.1475686	H	0.7451256	-5.8827440	-4.8433877
H	0.0270795	5.4104362	2.1989256	H	0.3162826	-4.1557505	3.4380048
C	-0.0008439	3.2753829	1.9090270	C	1.7166435	-4.3267936	-1.8389240
C	3.3573168	-1.3798467	0.9014791	C	5.1255486	-1.6229018	-2.6894748
C	4.3761774	-1.6389720	1.8103398	C	1.2849698	-5.1214440	-4.2448914
H	4.9243930	-2.5909923	1.7476130	H	2.3530137	-5.1598711	-4.5461861
C	4.6786257	-0.7432792	2.8760750	C	2.4630944	-3.2377745	-2.3180105
C	5.6627291	-1.0760992	3.8554530	C	2.8396448	-4.7863902	2.4887459
C	3.9289404	0.4832461	3.0157581	H	1.5236388	-7.0548058	-1.3398348
C	4.1462335	1.2742588	4.1843702	C	1.5273051	-4.4236379	-0.4463184
C	2.9709553	0.8368504	1.9935742	C	1.6812992	-6.7935587	-2.4044957
C	2.7172251	-0.1052883	0.9890820	H	1.1936910	-7.5772377	-3.0202758
O	0.1668778	0.8824034	1.7937626	H	0.9153833	-5.2497496	-0.0540425
O	1.7950087	0.2002980	-0.0141835	C	2.9836420	-0.2941544	-3.0540775
P	0.2038048	0.1028846	0.3512074	H	5.7415551	-2.1761256	-1.9517291
O	-0.5166360	0.8812398	-0.7656230	H	5.7295744	-0.7761166	-3.0767118
O	-0.2696087	-1.3244843	0.6584318	C	3.0149954	-2.2690490	-1.4541731
C	4.0625520	5.9826397	2.3665479	C	0.4150812	-4.0932207	2.3349560
C	4.8656372	4.8260544	2.1787586	C	2.0741398	-3.5022833	0.4602269
H	2.0453804	6.7588155	2.4998295	H	2.7319364	-4.9111302	3.5862785
H	4.5373310	6.9698139	2.4737990	H	2.6408078	-5.7697614	2.0129309
H	4.9159171	2.6887526	1.9017294	C	3.8167917	-1.1164456	-2.0549497
H	5.9607630	4.9235654	2.1255333	C	2.8357837	-2.4084919	-0.0548717
C	5.0953596	0.9112542	5.1304147	C	1.8587108	-3.7203783	1.9593863
C	5.8763727	-0.2626514	4.9579958	H	2.0609157	0.0872554	-2.5755808
H	3.5435729	2.1794362	4.3393281	H	-0.3015547	-3.3359789	1.9680205
H	5.2380494	1.5365441	6.0249679	H	2.6888358	-0.8966451	-3.9387320
H	6.6325922	-0.5350639	5.7099066	H	0.8979661	-4.1254787	-4.5362031
H	6.2351470	-2.0082596	3.7276319	H	0.1097102	-5.0762877	1.9221412
C	-1.8488385	3.6287509	0.2364305	H	2.7732233	-6.8312829	-2.6030030
C	-1.4442193	3.1593145	1.5245600	H	4.1012096	-0.4366681	-1.2256560
C	-3.1754978	3.4084464	-0.1741026	H	2.0880557	-2.7651226	2.4737952
C	-2.3831527	2.5059307	2.3645960	H	2.6302491	-3.1257988	-3.3993123
C	-3.7121336	2.3505495	1.9194188	Zn	-2.3190576	0.3163176	-1.3823661
C	-4.1317741	2.7775151	0.6485145	Br	-3.4260748	1.1685718	-3.2470576
C	-2.0122487	1.9746565	3.7473584	Zn	-1.8086561	-2.1621018	-0.2883006
H	-4.4293088	1.8519045	2.5870491	Br	-2.3675021	-4.3999361	-0.5420761
C	-2.2806721	0.4631479	3.8778999	H	-3.4795819	3.7362807	-1.1799141
H	-3.3552862	0.2157827	3.7511785	C	0.0200737	0.4701616	-5.7743865
H	-1.9743338	0.1005048	4.8805353	C	-0.3434919	-0.1332684	-4.5695948
H	-1.7059619	-0.1077182	3.1229842	C	-0.7288986	-1.4991125	-4.5567028
C	-2.7285216	2.7738917	4.8525055	C	-0.7513069	-2.2444635	-5.7624451
H	-0.9229270	2.1314831	3.8879275	C	-0.3927151	-1.6299916	-6.9659884
H	-3.8303459	2.6546371	4.7884241	C	-0.0054171	-0.2763161	-6.9690920
H	-2.5020372	3.8569237	4.7775361	H	0.3245499	1.5269872	-5.7901598
H	-2.4117227	2.4238243	5.8566301	C	-1.0988401	-2.1445132	-3.3142026
C	-5.5507827	2.5675668	0.1234578	H	-1.0593671	-3.3013820	-5.7437169
C	-6.4176756	1.6560360	1.0000966	H	-0.4119972	-2.2011489	-7.9058039
H	-7.3888909	1.4570267	0.5043576	H	0.2822215	0.2044758	-7.9168688
H	-6.6377935	2.1242108	1.9823443	O	-1.2107748	-1.5213479	-2.2336019
H	-5.9352877	0.6777801	1.1947486	H	-0.3254850	0.4267977	-3.6243778
C	-6.2552870	3.9180570	-0.1144629	H	-1.2961195	-3.2441301	-3.3143407
H	-5.4327156	2.0748658	-0.8703583	C	-5.4261717	-1.4445732	-1.2749685
H	-7.2568633	3.7645580	-0.5662228	C	-4.6644747	-1.3786302	-0.1572953
H	-5.6742317	4.5735946	-0.7929779	C	-5.3530673	-2.1762594	0.9020820
H	-6.3913774	4.4604335	0.8447539	O	-6.5014273	-2.7080996	0.3710957
C	-0.9042847	4.3878239	-0.6979520	C	-6.6261731	-2.2930416	-0.9947191
C	-0.9054961	3.8707320	-2.1456999	C	-5.0167040	-2.3469955	2.0578838
H	-0.1697254	4.4413059	-2.7491790	O	-3.3782070	-0.7072745	0.1594028
H	-1.8932527	3.9807053	-2.6374533	H	-7.5879731	-1.7457489	-1.1188122
H	-0.6275216	2.8006847	-2.1807905	H	-6.6705000	-3.1968460	-1.6437565
C	-1.2250993	5.8955671	-0.6556306	H	-3.0707654	-1.0130437	1.1890274
H	0.1268337	4.2549025	-0.3149783	H	-3.5496134	0.3821427	0.3686980
H	-0.5049976	6.4691369	-1.2754270	H	-5.2234078	-0.9682647	-2.2454476
H	-1.1851432	6.2969503	0.3771220				
H	-2.2448899	6.0925378	-1.0482042				
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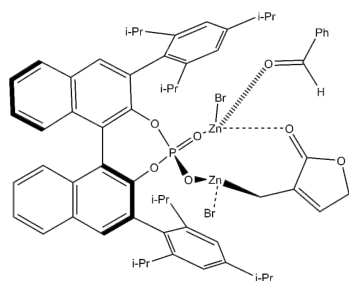
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C	4.2832281	3.5736695	2.0778809
C	2.0488148	4.5943325	2.2597722
C	2.6814282	5.8647610	2.4112481
C	0.6312720	4.4893389	2.1610070
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C	0.0017560	3.2743116	1.9196268
C	3.3588554	-1.3762905	0.9032492
C	4.3765914	-1.6391533	1.8120348
H	4.9218387	-2.5926639	1.7462192
C	4.6801476	-0.7476515	2.8805744
C	5.6630932	-1.0839524	3.8592385
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O	1.7991757	0.2081137	-0.0070870
P	0.2078670	0.1055607	0.3583181
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O	-0.2611414	-1.3235384	0.6614142
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C	4.8662780	4.8265574	2.2070386
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H	4.9173734	2.6897098	1.9253893
H	5.9615424	4.9242243	2.1581375
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H	3.5482549	2.1715085	4.3510068
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H	6.6336564	-0.5501537	5.7148063
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C	-1.4400957	3.1572321	1.5299679
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C	2.8371680	-2.4020839	-0.0560393
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Br	-2.3454458	-4.3929546	-0.6040891
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C	-0.7425798	-1.5112318	-4.5659920
C	-0.7796254	-2.2669539	-5.7637480
C	-0.4458040	-1.6617699	-6.9789503
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C	-1.0918227	-2.1443839	-3.3081573
H	-1.0770263	-3.3266330	-5.7289617
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O	-1.1820231	-1.5086746	-2.2361019

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C	-4.6607811	-1.3622887	-0.1409022
C	-5.4059292	-2.0723665	0.9455844
O	-6.5553984	-2.6019176	0.4077173
C	-6.6233012	-2.2682237	-0.9801897
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C	-3.3630008	-0.7128043	0.1750393
H	-7.5647616	-1.7036126	-1.1712131
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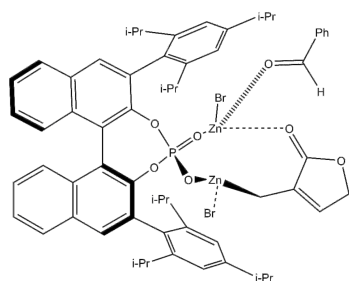
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C	0.6006156	4.6345566	2.4354709
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C	3.9584723	0.7254669	2.8785834
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O	0.1067243	1.0677507	1.7963787
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P	0.0878125	0.3013635	0.3435625
O	-0.5991410	1.0988568	-0.7495561
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H	2.0399000	6.8977704	2.7578153
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C	5.2280675	1.2310238	4.9176693
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H	0.4184894	-3.6906568	3.7765856
C	1.7046369	-4.4839753	-1.4977066
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C	2.5912999	-5.5847073	-3.7841651
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H	1.4164017	-7.8796196	-2.2822318
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C	2.8667735	-2.3146561	-1.3886911
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C	3.5493618	-1.1752766	-2.1400676
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C	-0.9145774	-1.1992998	-6.4141923
C	-0.8470862	-1.4535136	-5.0422249
C	-1.2233537	-2.7244281	-4.5457522
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H	3.5948627	2.4260218	4.1869586
H	5.4058200	1.8716271	5.7733261
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H	-7.7524188	3.0743379	1.7682202
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C	1.7144951	-4.5012965	-1.5042852
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H	1.4847794	-7.9032308	-2.2808031
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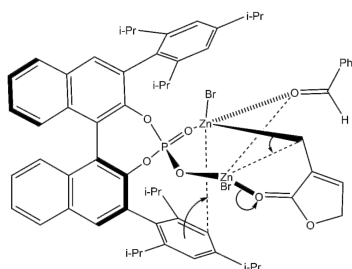
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C	2.8101149	3.5863950	2.0476000
C	4.2110508	3.7607363	1.8400463
C	2.0158376	4.7521736	2.3512587
C	2.6627081	6.0144047	2.5109798
C	0.5990848	4.6338419	2.4372023
H	0.0053794	5.5297392	2.6770845
C	-0.0556779	3.4374229	2.1653120
C	3.2867148	-1.2158228	0.8577637
C	4.3739212	-1.4214641	1.6978744
H	4.9310099	-2.3683474	1.6294886
C	4.7263330	-0.4886605	2.7131828
C	5.7793432	-0.7706843	3.6343999
C	3.9507803	0.7187527	2.8689036
C	4.2148580	1.5376273	4.0087240
C	2.9266576	1.0244641	1.8930565
C	2.6253747	0.0483848	0.9341153
O	0.0942620	1.0679080	1.8063966
O	1.6645684	0.3109117	-0.0337313
P	0.0670074	0.2973837	0.3552801
O	-0.6315147	1.0915387	-0.7323441

C	2.8521086	-2.3193138	-1.3964630
C	0.4620077	-3.7201603	2.6606899
C	2.0576125	-3.3940120	0.6740456
H	2.8038693	-4.5207246	3.8948288
H	2.6115357	-5.5266860	2.4222113
C	3.5231866	-1.1730631	-2.1478841
C	2.7332394	-2.3220185	0.0150678
C	1.9037028	-3.4588834	2.1961442
H	1.6493996	-0.1245485	-2.6281952
H	-0.2213928	-2.9323021	2.2922189
H	2.2360449	-1.2003868	-3.9381617
H	0.8168661	-4.7050339	-4.1876548
H	0.0704737	-4.6966341	2.3110665
H	2.9916290	-6.9644065	-2.0085103
H	3.8127120	-0.4074236	-1.3993270
H	2.1953070	-2.4720039	2.6069433
H	2.4829838	-3.4153291	-3.2189472
Zn	-1.6589536	1.6251310	-2.3532273
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Br	-2.1450708	-4.6203641	0.0065558
H	-4.0319438	4.2223809	-0.1779269
C	-0.9369734	-1.1782049	-6.3910119
C	-0.8526826	-1.4372671	-5.0205113
C	-1.1943077	-2.7178260	-4.5266030
C	-1.6139817	-3.7365535	-5.4161560
C	-1.6912113	-3.4719952	-6.7882652
C	-1.3535319	-2.1934857	-7.2730847
H	-0.6803764	-0.1740055	-6.7610811
C	-1.1689698	-2.9872767	-3.0928212
H	-1.8757298	-4.7305758	-5.0193749
H	-2.0139661	-4.2592683	-7.4859306
H	-1.4171860	-1.9877315	-8.3530586
O	-0.8625943	-2.1276467	-2.2471681
H	-0.5339413	-0.6433384	-4.3274593
H	-1.4754181	-4.0088561	-2.7503330
C	-4.6377060	-0.3333917	-3.7482406
C	-4.0413909	0.1288496	-2.6059881
C	-3.6412061	-1.0809522	-1.8538316
C	-3.9818889	-2.2047229	-2.5223122
O	-4.6309856	-1.8262415	-3.7541803
O	-3.0397014	-1.1209808	-0.7725920
C	-3.6578182	1.4543740	-2.1222702
H	-5.6414037	-2.2928415	-3.7627300
H	-4.0456334	-2.2691956	-4.5923424
H	-3.7832493	1.5472969	-1.0260116
H	-4.1787646	2.2755588	-2.6492351
H	-5.0425261	0.2712601	-4.5705720

C	2.6300717	4.7284876	1.6972704
C	3.3418717	5.9634983	1.7772203
C	1.2085908	4.6939032	1.7709750
H	0.6616271	5.6362329	1.9276651
C	0.4918115	3.5170364	1.5844889
C	3.5918613	-1.3519580	0.4810755
C	4.6501971	-1.5966333	1.3481723
H	5.1522879	-2.5759667	1.3173532
C	5.0386247	-0.6554242	2.3437162
C	6.0608336	-0.9698897	3.2894179
C	4.3339931	0.6005091	2.4532256
C	4.6345622	1.4411034	3.5676839
C	3.3390797	0.9335361	1.4570920
C	3.0008186	-0.0522496	0.5237794
O	0.5071868	1.1327386	1.3197722
O	2.0657985	0.2351183	-0.4647798
P	0.4732373	0.3490003	-0.1239685
O	-0.1177245	1.1661664	-1.2763330
O	-0.1701714	-1.0108258	0.2180580
C	4.7191859	6.0043424	1.6222072
C	5.4368708	4.8052096	1.3669572
H	2.7691193	6.8890973	1.9454183
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H	5.3430347	2.6672095	1.0996137
H	6.5256077	4.8425763	1.2094774
C	5.6195042	1.0964193	4.4836295
C	6.3560201	-0.1087247	4.3352902
H	4.0687941	2.3721390	3.7057350
H	5.8253813	1.7621379	5.3357047
H	7.1417596	-0.3665859	5.0616050
H	6.5967062	-1.9261268	3.1823772
C	-1.6347537	4.1308480	0.3723108
C	-1.0009688	3.4962555	1.4812443
C	-3.0369390	4.0649002	0.2698375
C	-1.7895046	2.8251936	2.4575010
C	-3.1896957	2.8083537	2.3134839
C	-3.8376445	3.4124066	1.2231389
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H	-3.7902886	2.2933501	3.0783504
C	-1.5506669	0.6600212	3.7761646
H	-2.6407801	0.5241801	3.9404513
H	-1.0281830	0.1785831	4.6282061
H	-1.2629488	0.1186705	2.8534230
C	-1.5451140	2.9089229	4.9711562
H	-0.0718203	2.2037352	3.5849938
H	-2.6408446	2.8935409	5.1493433
H	-1.2300015	3.9706321	4.9158845
H	-1.0540331	2.4493049	5.8538011
C	-5.3547178	3.4181930	1.0710063
C	-6.0434766	2.1692427	1.6391680
H	-7.1234727	2.1750880	1.3882167
H	-5.9686325	2.1268884	2.7460358
H	-5.6009748	1.2364407	1.2353016
C	-5.9455693	4.7034914	1.6845831
H	-5.5610938	3.4469956	-0.0225429
H	-7.0427296	4.7542857	1.5251818
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H	-5.7558356	4.7354399	2.7781945
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H	-0.5661052	4.9748419	-2.8646051
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H	-0.8590965	3.3316184	-2.2305099
C	-1.1243837	6.4118073	-0.5774468
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H	-0.5111325	6.9773587	-1.3091374
H	-0.8855331	6.7911312	0.4373351
H	-2.1904099	6.6498961	-0.7763918
H	0.6338617	-6.3168542	-1.9350713
H	4.7377760	-2.6120100	-3.9732945
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7.9.4 Pathway 14d-ma ↔ 14d-mi

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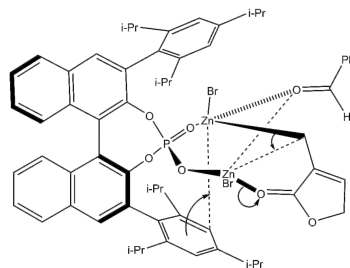


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C	4.7765102	3.5856963	1.3062349

C	1.0075713	-5.5668604	-2.6661017
H	3.3525385	0.2740338	-4.0301039
H	-0.7537509	-5.8043678	-3.9656920
H	0.6959711	-3.6189833	3.4428861
C	1.6965958	-4.4728896	-1.8605952
C	4.9934159	-1.8417259	-3.2155753
C	-0.2149552	-5.0074807	-3.4118737
H	0.0844290	-4.2325213	-4.1492090
C	2.3602850	-3.4074110	-2.4948457
C	2.9872251	-4.7783214	2.3793154
H	2.8473303	-6.7013838	-3.0761577
C	1.6684102	-4.4846350	-0.4576813
C	1.9761908	-6.2848444	-3.6211311
H	1.4659834	-7.1190368	-4.1457492
H	1.1282956	-5.2994646	0.0502941
C	2.8142191	-0.5678959	-3.5481506
H	5.5542955	-1.0344492	-3.7308960
H	5.6710975	-2.3133687	-2.4751812
C	2.9952089	-2.3831515	-1.7714734
C	0.7258563	-3.6160800	2.3333382
C	2.2872395	-3.4865399	0.3185691
H	4.0517887	-4.7264688	2.0717800
H	2.5791235	-5.7388141	2.0005608
C	3.7281204	-1.2835618	-2.5369236
C	2.9716408	-2.4295612	-0.3500724
C	2.1832790	-3.5795424	1.8426150
H	1.9109554	-0.1550936	-3.0572017
H	0.1676015	-2.7317215	1.9705386
H	2.4851433	-1.2525696	-4.3578997
H	-0.9253444	-4.5471342	-2.6984830
H	0.1847029	-4.5174311	1.9803493
H	2.3658871	-5.5943003	-4.3982641
H	4.0642347	-0.5249859	-1.8017984
H	2.6359729	-2.6642237	2.2708006
H	2.3923007	-3.3741536	-3.5958371
Zn	-1.9298870	0.6906545	-2.0416578
Br	-2.3769862	1.4869167	-4.1893337
Zn	-1.7350755	-1.8815622	-0.5314520
Br	-2.2659659	-4.0901032	-0.0052533
H	-3.5293352	4.5396774	-0.5949852
C	-4.3828072	-4.5047554	-4.0617782
C	-3.4941956	-3.5992635	-3.4810710
C	-2.7140007	-2.7538408	-4.3101064
C	-2.8479765	-2.8252722	-5.7216733
C	-3.7408086	-3.7339345	-6.2947359
C	-4.5070903	-4.5726095	-5.4632348
H	-4.9893699	-5.1597069	-3.4192062
C	-1.7869550	-1.7786453	-3.7851499
H	-2.2512561	-2.1503570	-6.3552296
H	-3.8497666	-3.7892058	-7.3878716
H	-5.2143562	-5.2862655	-5.9137296
O	-1.5327260	-1.5467089	-2.5718868
H	-3.3838384	-3.5546722	-2.3889763
H	-1.2574854	-1.1452681	-4.5329673
C	-4.2027698	-1.3275198	1.2472023
C	-3.9603073	-0.7232341	0.0479308
C	-4.8564242	-1.3775188	-0.9611558
O	-5.6013251	-2.3367176	-0.3260432
C	-5.2339804	-2.3925649	1.0593198
O	-4.9348349	-1.1587485	-2.1546293
C	-3.0555729	0.3763980	-0.3376221
H	-4.8344951	-3.4090004	1.2760484
H	-6.1416192	-2.2318180	1.6833617
H	-2.5201274	0.7903740	0.5370755
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TS1



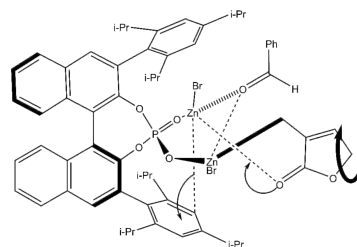
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C	4.7767898	3.5871695	1.3102424
C	2.6293228	4.7293320	1.6952471
C	3.3405602	5.9643613	1.7738178
C	1.2079758	4.6934912	1.7673420
H	0.6596885	5.6355795	1.9207500
C	0.4922905	3.5158116	1.5830753
C	3.5939157	-1.3508168	0.4849708
C	4.6512714	-1.5956320	1.3529170
H	5.1525318	-2.5753868	1.3224121
C	5.0395665	-0.6547041	2.3485975
C	6.0608985	-0.9685648	3.2949040
C	4.3352976	0.6013285	2.4574731
C	4.6356667	1.4421212	3.5715445
C	3.3410515	0.9345505	1.4609510
C	3.0032828	-0.0508978	0.5271100
O	0.5096060	1.1315614	1.3223858
O	2.0695115	0.2358615	-0.4618182
P	0.4765278	0.3480907	-0.1224192
O	-0.1176627	1.1634391	-1.2730116
O	-0.1617535	-1.0144764	0.2198161
C	4.7176752	6.0057658	1.6211608
C	5.4361828	4.8068574	1.3697236
H	2.7670278	6.8899955	1.9390276
H	5.2526489	6.9660640	1.6753053
H	5.3438005	2.6683751	1.1067565
H	6.5251540	4.8444291	1.2142437
C	5.6199496	1.0975930	4.4877303
C	6.3559236	-0.1074308	4.3402667
H	4.0700967	2.3733872	3.7085172
H	5.8257112	1.7636423	5.3395224
H	7.1412524	-0.3653211	5.0669661
H	6.5964567	-1.9250304	3.1885681
C	-1.6325165	4.1248005	0.3658513
C	-1.0001419	3.4935206	1.4773184
C	-3.0342736	4.0564312	0.2613717
C	-1.7893048	2.8233870	2.4533728
C	-3.1889117	2.8041397	2.3068612
C	-3.8357073	3.4049851	1.2143957
C	-1.1752632	2.1524606	3.6812904
H	-3.7901218	2.2899599	3.0717957
C	-1.5486081	0.6616128	3.7777713
H	-2.6386742	0.5242404	3.9416563
H	-1.0261348	0.1828638	4.6312652
H	-1.2590976	0.1186253	2.8566254
C	-1.5481180	2.9137839	4.9671276
H	-0.0724899	2.2070300	3.5844295
H	-2.6439310	2.8977025	5.1443336
H	-1.2346811	3.9756803	4.9091965
H	-1.0574760	2.4574800	5.8517113
C	-5.3525679	3.4085225	1.0597886
C	-6.0407123	2.1589606	1.6273413
H	-7.1203368	2.1631287	1.3749019

H	-5.9678695	2.1175230	2.7343746
H	-5.5963685	1.2264661	1.2248926
C	-5.9464831	4.6935139	1.6709078
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H	-7.0434338	4.7429428	1.5096880
H	-5.4905262	5.6005539	1.2260716
H	-5.7585369	4.7270459	2.7646432
C	-0.8566299	4.8907425	-0.7065069
C	-1.1408669	4.3812715	-2.1271213
H	-0.5579192	4.9616866	-2.8712855
H	-2.2101510	4.4696782	-2.4084360
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C	-1.1240682	6.4037775	-0.5885402
H	0.2237562	4.7295760	-0.5234052
H	-0.5106148	6.9686769	-1.3204641
H	-0.8880118	6.7861868	0.4257269
H	-2.1899799	6.6399749	-0.7898896
H	0.6262017	-6.3068813	-1.9354978
H	4.7402912	-2.6113486	-3.9699510
H	2.9487775	-4.8138231	3.4878836
C	1.0032721	-5.5581345	-2.6660634
H	3.3633027	0.2794760	-4.0229551
H	-0.7575197	-5.7915674	-3.9673682
H	0.6955110	-3.6162500	3.4454846
C	1.6944668	-4.4664069	-1.8592848
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C	2.3611280	-3.4022963	-2.4921596
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H	2.8403742	-6.6976848	-3.0729485
C	1.6653216	-4.4790070	-0.4566829
C	1.9712114	-6.2792935	-3.6193039
H	1.4598135	-7.1123074	-4.1446195
H	1.1225570	-5.2925838	0.0503279
C	2.8223757	-0.5612787	-3.5421544
H	5.5612332	-1.0366295	-3.7255479
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C	0.7249300	-3.6121891	2.3359949
C	2.2861891	-3.4832798	0.3206026
H	4.0484524	-4.7289230	2.0711872
H	2.5742041	-5.7379989	1.9991750
C	3.7339699	-1.2816995	-2.5322259
C	2.9733537	-2.4275568	-0.3469038
C	2.1821809	-3.5778180	1.8445525
H	1.9207940	-0.1455569	-3.0509060
H	0.1683577	-2.7262623	1.9747517
H	2.4912413	-1.2435182	-4.3532272
H	-0.9269127	-4.5336945	-2.7007845
H	0.1813286	-4.5117925	1.9825610
H	2.3642988	-5.5902919	-4.3959971
H	4.0721233	-0.5251531	-1.7959350
H	2.6369533	-2.6640010	2.2737751
H	2.3943850	-3.3685476	-3.5931177
Zn	-1.9291173	0.6825357	-2.0390622
Br	-2.3750742	1.4712808	-4.1879416
Zn	-1.7228435	-1.8899599	-0.5308066
Br	-2.2543620	-4.0989743	-0.0108428
H	-3.5256142	4.5281122	-0.6057206
C	-4.4061630	-4.4761420	-4.0563429
C	-3.5055191	-3.5812938	-3.4775761
C	-2.7236779	-2.7396033	-4.3077775
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H	-5.0144392	-5.1273767	-3.4117302
C	-1.7851465	-1.7736514	-3.7832444
H	-2.2704424	-2.1302646	-6.3523370
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O	-1.5231601	-1.5508470	-2.5711502
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C	-4.1900914	-1.3437194	1.2528445
C	-3.9528033	-0.7391202	0.0531239
C	-4.8459481	-1.4008434	-0.9556718
O	-5.5851071	-2.3641872	-0.3171278
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O	-4.9235307	-1.1854946	-2.1479861
C	-3.0535907	0.3635685	-0.3345821
H	-4.8075702	-3.4298076	1.2820821
H	-6.1231421	-2.2614669	1.6917523
H	-2.5220346	0.7840496	0.5393792
H	-3.6992284	1.1808404	-0.7401334
H	-3.7111969	-1.1116883	2.2142780

TS2; COSMO

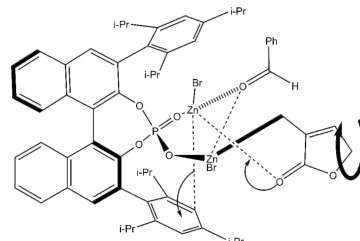


Energy (Hartree) = -11970.01103186

C	0.2453651	3.3048926	-0.1630926
C	1.4955627	3.6450020	-0.6986467
C	1.5547804	4.7163780	-1.6619174
C	2.7301875	5.0150880	-2.4147317
C	0.3699808	5.5028401	-1.9013294
C	0.4266328	6.5842881	-2.8316948
C	-0.8366018	5.1747793	-1.2217638
H	-1.7229660	5.8058932	-1.3841655
C	-0.9436284	4.0636334	-0.3909475
C	3.8287443	0.7679435	0.2888193
C	4.9697322	1.4483090	0.6912007
H	5.8398890	0.8821073	1.0567932
C	5.0132995	2.8716028	0.7187446
C	6.1614278	3.5598444	1.2144351
C	3.8484700	3.6272602	0.3208272
C	3.8662480	5.0403563	0.5265780
C	2.7115959	2.9258667	-0.2326399
C	2.7406972	1.5285309	-0.2348452
O	0.1490483	2.2052153	0.6925024
O	1.6870117	0.8168076	-0.7934954
P	0.2383482	0.7173748	0.0004777
O	-0.8156966	0.4808849	-1.0619055
O	0.3525113	-0.2551222	1.1948083
C	1.5922899	6.8635998	-3.5292183
C	2.7475199	6.0610176	-3.3274166
H	-0.4826242	7.1835135	-2.9964480
H	1.6208581	7.6949478	-4.2499686
H	3.6276674	4.3962580	-2.2742649
H	3.6626445	6.2659672	-3.9037745
C	4.9910069	5.6785640	1.0315395
C	6.1579255	4.9386494	1.3604611
H	2.9707881	5.6293916	0.2879127
H	4.9740848	6.7685659	1.1835850
H	7.0466380	5.4576748	1.7505133
H	7.0454434	2.9682258	1.5000872
C	-3.3403836	3.2747919	-0.5613851
C	-2.2441358	3.6907838	0.2473688

C	-4.5736379	3.0036863	0.0612544	H	3.0608703	0.8504540	2.5980796
C	-2.4016524	3.7924855	1.6587824	H	3.8448534	-3.7391071	-1.0666695
C	-3.6582416	3.5145096	2.2245989	Zn	-2.1066582	-1.0416447	-1.5305296
C	-4.7642257	3.1300421	1.4471713	Br	-1.4325673	-1.3958462	-3.7652958
C	-1.2688653	4.2406637	2.5821870	Zn	0.5882537	-2.1673867	1.3579281
H	-3.7795813	3.6126528	3.3148169	Br	-0.1508680	-3.6639989	2.9759374
C	-0.9212944	3.1627339	3.6252822	H	-5.4284501	2.6863254	-0.5578015
H	-1.7684883	2.9783508	4.3183172	C	-2.0811720	-5.3244321	-3.4283670
H	-0.0516265	3.4798975	4.2378443	C	-1.5311986	-4.4693710	-2.4724008
H	-0.6644704	2.2048410	3.1326129	C	-0.1234573	-4.3415259	-2.3654789
C	-1.5931184	5.5916696	3.2470112	C	0.7183159	-5.0629509	-3.2495738
H	-0.3633937	4.4013452	1.9633334	C	0.1627151	-5.9076773	-4.2143896
H	-2.4850733	5.5176807	3.9035649	C	-1.2361099	-6.0406091	-4.2981588
H	-1.7992811	6.3735844	2.4878232	H	-3.1731662	-5.4230737	-3.5133562
H	-0.7435574	5.9350419	3.8733712	C	0.5094490	-3.5009559	-1.3729399
C	-6.1418027	2.9280734	2.0657227	H	1.8115865	-4.9523209	-3.1705518
C	-6.1212541	2.0349879	3.3160394	H	0.8137908	-6.4660507	-4.9028148
H	-7.1554870	1.8572756	3.6775838	H	-1.6748685	-6.7079491	-5.0559747
H	-5.5661167	2.5157972	4.1491671	O	-0.0898165	-2.8139962	-0.5093829
H	-5.6553578	1.0540246	3.1044782	H	-2.1779193	-3.8810295	-1.8080092
C	-6.7937077	4.2934904	2.3615766	H	1.6213921	-3.4917815	-1.3806685
H	-6.7640626	2.4172756	1.2979453	C	-3.2290478	-3.5601519	0.8764466
H	-7.8221323	4.1641150	2.7589716	C	-3.6672512	-2.2781299	0.8165316
H	-6.8515604	4.9231758	1.4503058	C	-4.4272548	-2.0354680	2.0873240
H	-6.2055404	4.8530724	3.1194620	O	-4.4286470	-3.1885907	2.8379221
C	-3.2297976	3.1215410	-2.0792557	C	-3.7005441	-4.2041722	2.1405731
C	-3.7734822	1.7730515	-2.5750470	O	-4.9781993	-1.0214738	2.4677219
H	-3.5381117	1.6205064	-3.6471785	C	-3.5895953	-1.2129930	-0.2184109
H	-4.8725329	1.6871930	-2.4513892	H	-4.3730371	-5.0738776	1.9596916
H	-3.3101662	0.9410392	-2.0119440	H	-2.8578022	-4.5498871	2.7787998
C	-3.9298762	4.2802510	-2.8152360	H	-3.6774029	-0.2266702	0.2895960
H	-2.1526295	3.1470974	-2.3412284	H	-4.5085673	-1.2834941	-0.8472057
H	-3.8081252	4.1796876	-3.9137517	H	-2.6074167	-4.0898809	0.1439933
H	-3.5255852	5.2676164	-2.5157631				
H	-5.0176703	4.2870466	-2.5932618				
H	2.7390120	-5.0219447	2.3673082				
H	5.5338168	-2.8502707	-2.4485664				
H	4.5087352	0.5072074	4.6057033				
C	3.1418071	-4.9601639	1.3339599				
H	3.3366427	-1.0771364	-3.9557738				
H	2.1235457	-6.7998123	0.7470175				
H	2.0290529	0.3238205	4.7805582				
C	3.2365604	-3.4763271	0.9991396				
C	5.5529113	-1.7425587	-2.3737975				
C	2.1727345	-5.7381381	0.4313534				
H	2.4902065	-5.7284293	-0.6323198				
C	3.6363010	-3.0099889	-0.2666386				
C	4.5128614	-0.2296679	3.7769636				
H	5.2310940	-5.0569615	2.0218337				
C	3.0215823	-2.5131911	2.0180221				
C	4.5477459	-5.5899703	1.3306731				
H	4.4984482	-6.6524135	1.6454452				
H	2.7699253	-2.8722710	3.0272491				
C	3.0845473	-1.5078034	-2.9656480				
H	5.8374199	-1.3474801	-3.3702113				
H	6.3494849	-1.4663142	-1.6537030				
C	3.8113467	-1.6357278	-0.5370502				
C	1.9992140	-0.4205516	3.9595627				
C	3.2517452	-1.1315851	1.8142899				
H	5.3802689	-0.0068991	3.1255569				
H	4.6704571	-1.2370847	4.2158835				
C	4.1873826	-1.1787494	-1.9426797				
C	3.6429309	-0.6983610	0.5141544				
C	3.1776832	-0.1746766	3.0039954				
H	2.1029700	-1.0936015	-2.6603193				
H	1.0262640	-0.3052704	3.4452722				
H	2.9750298	-2.6036630	-3.1111422				
H	1.1452733	-5.3284022	0.5060160				
H	2.0310375	-1.4242770	4.4307565				
H	4.9994970	-5.5578301	0.3171137				
H	4.2832148	-0.0741043	-1.9090165				

TS2

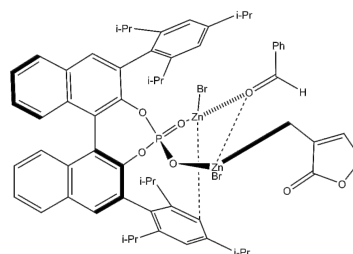


Energy (Hartree) = -11969.99547707
number of imaginary frequencies: 2

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C	1.5537886	4.7136577	-1.6644835
C	2.7297982	5.0100506	-2.4166963
C	0.3705119	5.5016565	-1.9052685
C	0.4301569	6.5814512	-2.8366382
C	-0.8364618	5.1763355	-1.2255927
H	-1.7227195	5.8073974	-1.3886006
C	-0.9465197	4.0669459	-0.3931559
C	3.8166299	0.7618988	0.2934939
C	4.9582586	1.4406976	0.6964818
H	5.8260454	0.8718988	1.0640557
C	5.0060736	2.8634832	0.7215638
C	6.1546233	3.5506830	1.2164257
C	3.8435589	3.6203860	0.3200059
C	3.8648169	5.0338946	0.5217249
C	2.7053042	2.9209902	-0.2330809
C	2.7298802	1.5230746	-0.2322349
O	0.1429140	2.2070464	0.6903998
O	1.6780045	0.8111758	-0.7896648

P	0.2216909	0.7212778	-0.0070310	H	5.8030644	-1.3296206	-3.3856860
O	-0.8278358	0.4926239	-1.0731117	H	6.3292352	-1.4434896	-1.6735415
O	0.3246639	-0.2543439	1.1885947	C	3.8025719	-1.6399055	-0.5349018
C	1.5962386	6.8587741	-3.5332260	C	1.9779144	-0.4322119	3.9524439
C	2.7496502	6.0551083	-3.3296981	C	3.2515341	-1.1418467	1.8195125
H	-0.4784579	7.1811080	-3.0031912	H	5.3648865	-0.0043850	3.1491041
H	1.6262275	7.6892528	-4.2548358	H	4.6525417	-1.2367007	4.2346608
H	3.6256790	4.3895148	-2.2742154	C	4.1615988	-1.1791817	-1.9441915
H	3.6656420	6.2581092	-3.9052799	C	3.6334780	-0.7047128	0.5177999
C	4.9903236	5.6706554	1.0255307	C	3.1647521	-0.1835179	3.0079082
C	6.1546743	4.9293826	1.3581136	H	2.0706734	-1.1115157	-2.6468973
H	2.9706672	5.6232654	0.2795659	H	1.0096437	-0.3180169	3.4294370
H	4.9757206	6.7611441	1.1738797	H	2.9514142	-2.6151813	-3.1015741
H	7.0442700	5.4472195	1.7475955	H	1.1828167	-5.3476485	0.5216209
H	7.0368510	2.9577672	1.5050656	H	2.0052244	-1.4358946	4.4238208
C	-3.3443061	3.2824181	-0.5624938	H	5.0384026	-5.5523914	0.3183459
C	-2.2471614	3.6966820	0.2455519	H	4.2460198	-0.0736120	-1.9104005
C	-4.5770087	3.0131592	0.0614920	H	3.0474621	0.8405538	2.5994743
C	-2.4030563	3.7978969	1.6570745	H	3.8533909	-3.7423729	-1.0636057
C	-3.6590860	3.5210720	2.2233554	Zn	-2.1221004	-1.0335857	-1.5445996
C	-4.7666057	3.1392241	1.4472706	Br	-1.4486656	-0.3180169	-3.7628619
C	-1.2688986	4.2437598	2.5799733	Zn	0.5202209	-2.1621784	1.3548866
H	-3.7797139	3.6170210	3.3137801	Br	-0.1167050	-3.7065390	2.9586022
C	-0.9226257	3.1651891	3.6227540	H	-5.4326795	2.6962912	-0.5565998
H	-1.7692125	2.9817122	4.3165178	C	-2.0655484	-5.3137795	-3.4744450
H	-0.0519750	3.4802430	4.2350788	C	-1.5265046	-4.4639717	-2.5063673
H	-0.6695018	2.2060914	3.1307871	C	-0.1200320	-4.3568238	-2.3668903
C	-1.5904396	5.5953654	3.2445731	C	0.7307568	-5.0899836	-3.2317251
H	-0.3633259	4.4033118	1.9608324	C	0.1865129	-5.9274143	-4.2084428
H	-2.4827993	5.5237584	3.9006109	C	-1.2119067	-6.0415193	-4.3235878
H	-1.7957795	6.3773652	2.4855173	H	-3.1566001	-5.3953365	-3.5851180
H	-0.7408858	5.9377923	3.8714479	C	0.4993689	-3.5183240	-1.3632096
C	-6.1427773	2.9394862	2.0691624	H	1.8229675	-4.9904926	-3.1273101
C	-6.1235863	2.0305714	3.3079601	H	0.8449658	-6.4946312	-4.8825956
H	-7.1578170	1.8527455	3.6690030	H	-1.6421725	-6.7030491	-5.0914106
H	-5.5664164	2.4998353	4.1463778	O	-0.1145260	-2.8188282	-0.5219199
H	-5.6621444	1.0495927	3.0878061	H	-2.1785904	-3.8687599	-1.8536865
C	-6.7825521	4.3063228	2.3838143	H	1.6114415	-3.5201590	-1.3436126
H	-6.7717201	2.4424483	1.2976726	C	-3.2238741	-3.5374060	0.8704138
H	-7.8100438	4.1803948	2.7844792	C	-3.6583770	-2.2544394	0.8221198
H	-6.8386561	4.9484766	1.4812896	C	-4.4106218	-2.0150824	2.1019774
H	-6.1872063	4.8521286	3.1459411	O	-4.4104048	-3.1759791	2.8432872
C	-3.2347231	3.1292351	-2.0805754	C	-3.6887670	-4.1851768	2.1373404
C	-3.7778899	1.7808275	-2.5768963	O	-4.9514756	-1.0012437	2.4879793
H	-3.5414120	1.6263855	-3.6483900	C	-3.5811170	-1.1812427	-0.2038119
H	-4.8769766	1.6942815	-2.4539273	H	-4.3615728	-5.0558186	1.9568545
H	-3.3147651	0.9494387	-2.0130284	H	-2.8400502	-4.5343417	2.7666212
C	-3.9356229	4.2877648	-2.8157842	H	-3.6421900	-0.1987979	0.3155419
H	-2.1578734	3.1544571	-2.3437653	H	-4.5164757	-1.2274477	-0.8104598
H	-3.8140049	4.1888798	-3.9144229	H	-2.6079103	-4.0620639	0.1289890
H	-3.5331690	5.2755355	-2.5152673				
H	-5.0233156	4.2944828	-2.5938503				
H	2.7796292	-5.0352446	2.3765303				
H	5.5232444	-2.8351432	-2.4622353				
H	4.4791527	0.5065839	4.6210577				
C	3.1794101	-4.9700066	1.3421316				
H	3.2920131	-1.0866007	-3.9509029				
H	2.1657184	-6.8159161	0.7632158				
H	1.9966244	0.3122879	4.7736777				
C	3.2597901	-3.4848780	1.0075717				
C	5.5295814	-1.7272305	-2.3871443				
C	2.2109924	-5.7548014	0.4447949				
H	2.5251543	-5.7473624	-0.6200838				
C	3.6442600	-3.0152932	-0.2616129				
C	4.4927517	-0.2308669	3.7929289				
H	5.2719135	-5.0531836	2.0215064				
C	3.0399211	-2.5244803	2.0250444				
C	4.5892867	-5.5902634	1.3329436				
H	4.5513527	-6.6538801	1.6455915				
H	2.7808262	-2.8839332	3.0319971				
C	3.0534321	-1.5182166	-2.9578412				

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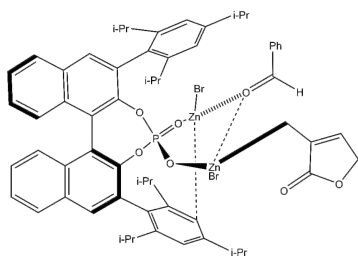


Energy (Hartree) = -11970.03810749

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C	4.1046076	3.7896551	1.6339591
C	1.8429507	4.7512652	1.7997692
C	2.4371237	6.0451513	1.9042450

C	0.4294299	4.5886530	1.7670748	H	0.4492227	-6.2280634	-4.2318530
H	-0.2077900	5.4794309	1.8723433	H	0.0619323	-3.6462177	3.4780782
C	-0.1679455	3.3503186	1.5569315	C	2.0126474	-4.5346025	-1.5925770
C	3.3969092	-1.2465887	0.8915593	C	5.6147517	-2.0668658	-2.3769247
C	4.3627449	-1.4002286	1.8769704	C	0.7456849	-5.3302382	-3.6526584
H	4.9333719	-2.3394584	1.9358517	H	1.3295185	-4.6741009	-4.3319386
C	4.5767199	-0.4032215	2.8711738	C	2.8973468	-3.5730257	-2.1038222
C	5.5080220	-0.6150836	3.9320680	C	2.6189544	-4.3402820	2.8077555
C	3.7799629	0.8010889	2.8550522	H	3.3300896	-6.9327615	-1.8850324
C	3.8967383	1.6946101	3.9628128	C	1.5724842	-4.3806824	-0.2516291
C	2.8836033	1.0335331	1.7443767	C	2.7604575	-6.6231553	-2.7843252
C	2.7223118	0.0094701	0.8062642	H	2.4178151	-7.5388283	-3.3079876
O	0.0834281	0.9655581	1.3354594	H	0.9381895	-5.1692203	0.1828001
O	1.8970665	0.2133615	-0.2924360	C	3.5838707	-0.7226111	-3.1356095
P	0.2577555	0.1618075	-0.0950275	H	6.2919549	-1.7287471	-2.7825629
O	-0.3365400	0.9210575	-1.2676801	H	6.1211016	-2.5483931	-1.5158422
O	-0.2164816	-1.2660999	0.2309305	C	3.3512155	-2.4852160	-1.3307983
C	3.8146201	6.2011187	1.8687805	C	0.2206097	-3.6620943	2.3810014
C	4.6514360	5.0629699	1.7159830	C	2.0539157	-3.3401524	0.5863167
H	1.7758922	6.9211868	1.9956883	H	3.6896257	-4.1168971	2.6338328
H	4.2607863	7.2046401	1.9414368	H	2.4321645	-5.3792481	2.4645502
H	4.7633963	2.9191311	1.5073622	C	4.2689385	-1.4452969	-1.9616421
H	5.7429799	5.1916022	1.6560326	C	2.9466573	-2.3803517	0.0249112
C	4.7956039	1.4490880	4.9920105	C	1.6929804	-3.3478986	2.0724526
C	5.6253440	0.2965809	4.9701021	H	2.6219551	-0.2690205	-2.8281102
H	3.2574900	2.5866265	4.0037093	H	-0.4561155	-2.9063673	1.9379212
H	4.8603744	2.1531148	5.8356534	H	3.3887070	-1.4174459	-3.9797241
H	6.3418040	0.1189282	5.7864650	H	-0.1827884	-4.8000761	-3.3632817
H	6.1176139	-1.5323409	3.9201831	H	-0.0917334	-4.6637067	2.0216401
C	-2.2909537	3.7521924	0.2470266	H	3.4608323	-6.0915600	-3.4619904
C	-1.6498927	3.2105925	1.3983077	H	4.4845762	-0.6833070	-1.1846100
C	-3.6875991	3.6148307	0.1252178	H	1.8984370	-2.3329748	2.4675273
C	-2.4210516	2.5489969	2.3963526	H	3.2387385	-3.6599176	-3.1472989
C	-3.8140041	2.4529096	2.2278841	Zn	-1.5197495	0.6959974	-2.9150914
C	-4.4709883	2.9728996	1.0981299	Br	0.0237623	1.1255031	-4.6522826
C	-1.7915869	1.9727423	3.6643126	Zn	-0.2523312	-2.9112448	-0.8354000
H	-4.4068998	1.9480957	3.0075781	Br	-1.9962721	-4.4488604	-0.7555497
C	-2.0243827	0.4558224	3.7884120	H	-4.1910438	4.0277035	-0.7639047
H	-3.1042573	0.2142008	3.8785214	C	-3.3967603	-2.8605420	-4.7791583
H	-1.5199396	0.0576250	4.6929671	C	-2.2696940	-2.5923322	-3.9973879
H	-1.6178556	-0.0797494	2.9086224	C	-1.0307194	-2.3056937	-4.6186582
C	-2.2802683	2.7259311	4.9156577	C	-0.9351222	-2.2888911	-6.0326644
H	-0.6959924	2.1313209	3.6025657	C	-2.0604617	-2.5721905	-6.8102249
H	-3.3735555	2.6023585	5.0631406	C	-3.2898660	-2.8549064	-6.1824537
H	-2.0728227	3.8124761	4.8369325	H	-4.3560759	-3.0502802	-4.2773059
H	-1.7739040	2.3435262	5.8260509	C	0.1644642	-2.0064690	-3.8444889
C	-5.9826068	2.8661610	0.9393189	H	0.0265309	-2.0381838	-6.5067536
C	-6.4686623	1.4063340	0.9439682	H	-1.9904267	-2.5614135	-7.9081334
H	-7.5610883	1.3555205	0.7581799	H	-4.1793072	-3.0644288	-6.7968447
H	-6.2778660	0.9195179	1.9236444	O	0.2621587	-2.0475615	-2.5983422
H	-5.9561695	0.8088430	0.1642861	H	-2.3487706	-2.6070625	-2.9013799
C	-6.7136096	3.7035181	2.0051543	H	1.0782744	-1.7412007	-4.4254491
H	-6.2306483	3.2974130	-0.0554234	C	-3.2478647	-0.1842582	0.0375177
H	-7.8118229	3.6697108	1.8494701	C	-3.6545937	-0.3792173	-1.2447594
H	-6.3928480	4.7644988	1.9755462	C	-4.4922006	-1.6192102	-1.2428834
H	-6.5075387	3.3181473	3.0259453	O	-4.5603080	-2.1082782	0.0390259
C	-1.5224623	4.5075249	-0.8385462	C	-3.7703600	-1.2827167	0.9022572
C	-1.8595575	4.0356495	-2.2596269	O	-5.0692684	-2.1618541	-2.1689786
H	-1.2056274	4.5305790	-3.0049169	C	-3.4413971	0.4225463	-2.4719436
H	-2.9117845	4.2436269	-2.5419185	H	-2.9558871	-1.9044465	1.3402425
H	-1.6956066	2.9452683	-2.3540117	H	-4.4076477	-0.9198237	1.7393660
C	-1.7490754	6.0271456	-0.7136266	H	-3.8173384	1.4588361	-2.3267296
H	-0.4427698	4.3094580	-0.6847422	H	-3.9905357	-0.0268322	-3.3228459
H	-1.1493489	6.5776348	-1.4676428	H	-2.6458306	0.6486075	0.4215640
H	-1.4695075	6.4062332	0.2894931				
H	-2.8174312	6.2806977	-0.8773752				
H	0.8836292	-6.3293424	-1.7595837				
H	5.4822216	-2.8370621	-3.1654742				
H	2.4340130	-4.3031501	3.9006050				
C	1.5588140	-5.7351913	-2.4122859				
H	4.2356976	0.0866071	-3.5230362				

int1



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C	4.1233195	3.7879877	1.6650497
C	1.8626885	4.7508927	1.8265494
C	2.4582202	6.0438277	1.9293739
C	0.4494563	4.5897480	1.7860246
H	-0.1893929	5.4819259	1.8747518
C	-0.1482274	3.3507858	1.5799202
C	3.4102888	-1.2450203	0.8988811
C	4.3832427	-1.4014576	1.8767441
H	4.9543787	-2.3409978	1.9264232
C	4.6042554	-0.4098680	2.8743453
C	5.5431012	-0.6251056	3.9272629
C	3.8070846	0.7939880	2.8691195
C	3.9321932	1.6828459	3.9794776
C	2.9021963	1.0312172	1.7666769
C	2.7334457	0.0112130	0.8245505
O	0.1010619	0.9640931	1.3808087
O	1.8975677	0.2176186	-0.2639001
P	0.2612803	0.1450388	-0.0437493
O	-0.3704453	0.8694724	-1.2145177
O	-0.1788974	-1.2878812	0.3151735
C	3.8352852	6.1991220	1.8964354
C	4.6709350	5.0605299	1.7464592
H	1.7972920	6.9204457	2.0172768
H	4.2817700	7.2025017	1.9681720
H	4.7809611	2.9165626	1.5400968
H	5.7626250	5.1879239	1.6875695
C	4.8389736	1.4338078	5.0002211
C	5.6683947	0.2820073	4.9676312
H	3.2928858	2.5743883	4.0271590
H	4.9101952	2.1348301	5.8457754
H	6.3912153	0.1011597	5.7775901
H	6.1527796	-1.5421979	3.9071372
C	-2.2403840	3.7711721	0.2315441
C	-1.6252150	3.2130112	1.3888641
C	-3.6291515	3.6073956	0.0624651
C	-2.4176391	2.5294642	2.3548897
C	-3.8029581	2.4178244	2.1437727
C	-4.4324186	2.9372214	0.9986538
C	-1.8211572	1.9551626	3.6397787
H	-4.4122589	1.8987129	2.9006485
C	-2.0615636	0.4401383	3.7695560
H	-3.1438527	0.2011770	3.8349257
H	-1.5818621	0.0475919	4.6898153
H	-1.6347864	-0.1047489	2.9052906
C	-2.3381236	2.7190958	4.8732477
H	-0.7238905	2.1097049	3.6040982
H	-3.4356054	2.6029402	4.9922808
H	-2.1237974	3.8039495	4.7924347
H	-1.8586272	2.3409487	5.7998395
C	-5.9388179	2.8280060	0.7973783
C	-6.4598505	1.3882444	0.9376691
H	-7.5449620	1.3413506	0.7136076
H	-6.3230932	1.0034797	1.9702339

H	-5.9345008	0.6997157	0.2475683
C	-6.6826801	3.7879089	1.7455622
H	-6.1459828	3.1574627	-0.2447698
H	-7.7771976	3.7559792	1.5652213
H	-6.3400771	4.8338341	1.6124872
H	-6.5069689	3.5108304	2.8063609
C	-1.4672952	4.5796413	-0.8123812
C	-1.5856609	4.0060770	-2.2322615
H	-1.0436922	4.6409339	-2.9619599
H	-2.6372632	3.9244681	-2.5760379
H	-1.1153944	3.0050431	-2.2768981
C	-1.8913634	6.0605945	-0.7715419
H	-0.3924227	4.5369096	-0.5489382
H	-1.2799256	6.6639215	-1.4738319
H	-1.7735272	6.4903428	0.2442127
H	-2.9560279	6.1846315	-1.0598203
H	0.8986671	-6.3195540	-1.7698885
H	5.4498262	-2.7657997	-3.1961490
H	2.5266113	-4.3708092	3.8870534
C	1.5597015	-5.7132598	-2.4260637
H	4.1571469	0.1446598	-3.5236870
H	0.4216945	-6.1944183	-4.2318507
H	0.1468187	-3.7155615	3.5131433
C	2.0179040	-4.5192628	-1.5984874
C	5.5792805	-1.9966147	-2.4060691
C	0.7217306	-5.3013404	-3.6471651
H	1.2880409	-4.6333063	-4.3298564
C	2.8797726	-3.5395129	-2.1142745
C	2.6915121	-4.3904705	2.7905082
H	3.3481878	-6.9042648	-1.9425587
C	1.6071060	-4.3902990	-0.2474803
C	2.7611918	-6.5879865	-2.8281703
H	2.4188493	-7.4999497	-3.3585217
H	0.9787536	-5.1843994	0.1850016
C	3.5215720	-0.6761031	-3.1338563
H	6.2410686	-1.2067899	-2.8164483
H	6.1026783	-2.4750060	-1.5535936
C	3.3355891	-2.4561018	-1.3370035
C	0.2865499	-3.7051697	2.4133315
C	2.0901271	-3.3553517	0.5937023
H	3.7593831	-4.1654890	2.6014870
H	2.4994150	-5.4245229	2.4356023
C	4.2289410	-1.3974957	-1.9728552
C	2.9585760	-2.3754155	0.0283528
C	1.7541241	-3.3871100	2.0857122
H	2.5575296	-0.2357576	-2.8147023
H	-0.3948846	-2.9371096	2.0004136
H	3.3274525	-1.3668835	-3.9817298
H	-0.2055709	-4.7823027	-3.3355998
H	-0.0376293	-4.6959025	2.0350490
H	3.4478483	-6.0429404	-3.5091917
H	4.4422497	-0.6374526	-1.1933717
H	1.9662211	-2.3787038	2.4934770
H	3.1999143	-3.6072334	-3.1659587
Zn	-1.5890471	0.7248532	-2.8587350
Br	-0.0397436	1.0964806	-4.5994563
Zn	-0.2845748	-2.8983893	-0.7902172
Br	-1.9680434	-4.4877028	-0.6955255
H	-4.1112498	4.0298381	-0.8347219
C	-3.4602126	-2.8703224	-4.6901729
C	-2.3264028	-2.5906010	-3.9214657
C	-1.0985212	-2.2885364	-4.5556931
C	-1.0203578	-2.2671230	-5.9703573
C	-2.1503329	-2.5629635	-6.7351480
C	-3.3687243	-2.8612831	-6.0936884
H	-4.4114732	-3.0661112	-4.1754538
C	0.1044660	-1.9812843	-3.7946516
H	-0.0687621	-1.9973778	-6.4542395
H	-2.0935557	-2.5469450	-7.8338330
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O	0.2219305	-2.0341378	-2.5507531

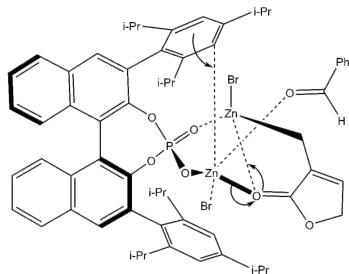
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C	-3.2633860	-0.3030977	0.0958614
C	-3.6997524	-0.3913521	-1.1881462
C	-4.5653740	-1.6131019	-1.2629126
O	-4.6239935	-2.1912072	-0.0173217
C	-3.8050846	-1.4478170	0.8882645
O	-5.1629106	-2.0718551	-2.2182198
C	-3.4987413	0.4946949	-2.3571842
H	-3.0037986	-2.1196095	1.2749082
H	-4.4244756	-1.1244590	1.7558225
H	-3.8180304	1.5314531	-2.1129503
H	-4.1015900	0.1355041	-3.2146266
H	-2.6392133	0.4877779	0.5289514

H	-3.7880714	-6.5621542	4.3713280
H	-4.3088186	-3.7472281	1.1151170
H	-4.9790390	-5.8286261	2.2789076
C	-6.5554797	-0.8771903	1.9277792
C	-7.2050516	-0.5111923	0.7183274
H	-4.7084411	-1.4563572	2.8807486
H	-7.1277109	-0.9086420	2.8675628
H	-8.2797095	-0.2733012	0.7228581
H	-6.9654309	-0.1280192	-1.3995266
C	2.1285107	-1.6083273	3.5352689
C	0.8437814	-1.0921488	3.8660622
C	3.2590352	-0.8123064	3.8032696
C	0.7222794	0.1751956	4.4990601
C	1.8850639	0.9244154	4.7505477
C	3.1633848	0.4600437	4.3933648
H	4.2590205	-1.1909737	3.5414255
C	-0.6311241	0.7019651	4.9745380
H	1.7867072	1.9057527	5.2420909
C	-0.9668686	2.0968897	4.4277873
H	-0.2424282	2.8635718	4.7737425
H	-1.9742189	2.4165065	4.7638817
H	-0.9751672	2.1074662	3.3213103
C	-0.7032073	0.6678953	6.5135946
H	-1.4116308	0.0086812	4.5995354
H	0.0409840	1.3572960	6.9650172
H	-0.4979948	-0.3497213	6.9042995
H	-1.7085429	0.9775264	6.8671075
C	4.4131642	1.2882030	4.6666599
C	4.3872900	2.6346611	3.9226132
H	5.3138089	3.2119426	4.1236794
H	3.5269704	3.2574155	4.2452107
H	4.3038521	2.4877030	2.8276696
C	4.6355944	1.4873556	6.1771850
H	5.2745939	0.7072947	4.2704285
H	5.5849868	2.0292874	6.3689218
H	4.6789926	0.5162670	6.7108084
H	3.8139172	2.0820951	6.6288806
C	2.3085446	-3.0213318	2.9780652
C	3.3663500	-3.1436141	1.8704342
H	3.4572327	-4.2000500	1.5449076
H	4.3719674	-2.8140872	2.2011645
H	3.0822935	-2.5475411	0.9826269
C	2.6340834	-3.9954924	4.1300721
H	1.3390212	-3.3322356	2.5369707
H	2.6918386	-5.0406687	3.7612226
H	1.8690034	-3.9554394	4.9304398
H	3.6106416	-3.7412971	4.5934398
H	0.2688251	1.1273247	-6.7425081
H	-1.8559053	-4.0951047	-4.9967310
H	-4.2914037	3.3290529	-3.0103894
C	0.1231010	0.0300829	-6.6370135
H	-0.3501026	-4.7173501	-2.2487673
H	2.0783845	-0.3435026	-7.5495260
H	-1.9823571	3.9335862	-2.0819371
C	-0.6360306	-0.1863631	-5.3334918
C	-2.3866744	-3.9999112	-4.0263154
C	1.5163387	-0.6187846	-6.6333439
H	1.4540286	-1.7265510	-6.6057062
C	-0.7471902	-1.4581166	-4.7458072
C	-3.8459708	2.4669669	-3.5484676
H	-1.6992824	0.0707986	-7.8689210
C	-1.2751066	0.8855748	-4.6899817
C	-0.7158001	-0.4401135	-7.8408362
H	-0.1915112	-0.2355578	-8.7977729
H	-1.1931985	1.8904654	-5.1342853
C	-0.2316930	-3.7098755	-2.6989746
H	-2.5158698	-5.0216470	-3.6125579
H	-3.3932372	-3.5832023	-4.2339415
C	-1.4884991	-1.6786233	-3.5710503
C	-1.5554886	3.1116012	-2.6907767
C	-1.9941795	0.7326870	-3.4891359

7.10 Interconversion of Complexes 14 - Mechanism 3

7.10.1 Pathway 14j-ma ↔ 14d-mi

TS1; COSMO

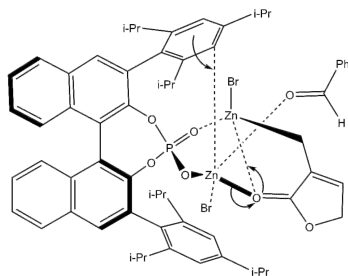


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Zn	-0.3085313	2.8030346	0.7887195
Br	-2.6174024	3.1850070	0.8845075
C	-1.1502638	-1.3853482	2.3585104
C	-2.3005997	-2.0175017	1.8789791
C	-2.7128129	-3.2433283	2.5201766
C	-3.7810433	-4.0533147	2.0288745
C	-1.9946869	-3.6969378	3.6883630
C	-2.4148374	-4.8931351	4.3442687
C	-0.8582305	-2.9696024	4.1468664
H	-0.3227585	-3.3303200	5.0381567
C	-0.3942282	-1.8417027	3.4825699
C	-2.9432686	-0.7857966	-1.7016562
C	-4.3208132	-0.5962810	-1.6788459
H	-4.8380982	-0.3071932	-2.6059767
C	-5.0816218	-0.7275301	-0.4822876
C	-6.4784988	-0.4346180	-0.4604059
C	-4.4304167	-1.1407200	0.7375408
C	-5.2022404	-1.1860642	1.9368425
C	-3.0240567	-1.4545077	0.7032947
C	-2.3287322	-1.2040796	-0.4836316
O	-0.7149631	-0.2183003	1.7362761
O	-0.9476387	-1.4174686	-0.5119349
P	-0.0182091	-0.3094392	0.2490672
O	1.3700158	-1.0009842	0.3454727
O	-0.0444620	1.0905811	-0.3377287
C	-3.4778547	-5.6392552	3.8579280
C	-4.1543143	-5.2205915	2.6811807
H	-1.8653116	-5.2204178	5.2410311

H	-4.6193891	1.6763038	-3.6234556
H	-3.6072543	2.7965435	-4.5821968
C	-1.6064721	-3.1079260	-3.0425181
C	-2.1275006	-0.5739521	-2.9388297
C	-2.5822831	1.9736889	-2.8192936
H	0.3086835	-3.0706759	-1.9738706
H	-0.6324031	2.7699145	-2.1849528
H	0.4013461	-3.8236656	-3.6040447
H	2.1092700	-0.2891213	-5.7558615
H	-1.2742140	3.5381958	-3.6772283
H	-0.9074427	-1.5325422	-7.7852602
H	-2.1950606	-3.0790345	-2.1037352
H	-2.8704044	1.6979377	-1.7844675
H	-0.2565426	-2.3180912	-5.2287906
C	1.7333591	3.0946656	-5.2575643
C	1.9611750	2.3380322	-4.1065542
C	3.2881922	1.9679830	-3.7734538
C	4.3710261	2.3489224	-4.6035314
C	4.1284002	3.0859166	-5.7670285
C	2.8105227	3.4626939	-6.0876111
H	0.7107587	3.4087114	-5.5136159
H	1.1411689	2.0373282	-3.4403411
C	3.5595518	1.2287794	-2.5553495
H	5.3975233	2.0606027	-4.3262108
H	4.9622109	3.3796178	-6.4217562
H	2.6200550	4.0559939	-6.9954226
O	2.6583398	0.7851635	-1.8147361
H	4.6330672	1.0770422	-2.2724274
C	3.1142637	5.1336622	1.4339872
C	2.2735668	4.1527052	1.0106004
C	2.2509054	4.2310061	-0.4769896
O	3.1249306	5.1947514	-0.9023875
C	3.6937007	5.8407170	0.2482822
O	1.5500930	3.5950712	-1.2497945
C	1.4425037	3.1524588	1.7075206
H	3.4352512	6.9230733	0.2028339
H	4.8033773	5.7626617	0.1968816
H	1.3443712	3.3755366	2.7862144
H	1.9275472	2.1482487	1.6393081
H	3.3689389	5.3878978	2.4722588

TS1



Energy (Hartree) = -11969.99840653
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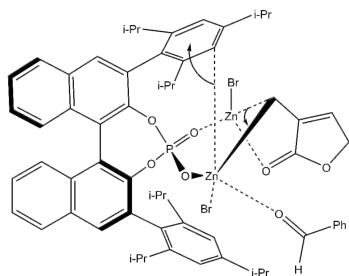
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Br	-2.7173080	3.1922835	0.8733357
C	-1.1811732	-1.3851027	2.3871897
C	-2.3209526	-2.0238542	1.8923925
C	-2.7292536	-3.2558156	2.5246544
C	-3.7869934	-4.0711869	2.0205944
C	-2.0187371	-3.7094953	3.6975367
C	-2.4376111	-4.9104688	4.3443817
C	-0.8874376	-2.9803259	4.1657401
H	-0.3503734	-3.3467164	5.0538005
C	-0.4253814	-1.8476721	3.5091481
C	-2.9202123	-0.7804624	-1.6912960

C	-4.3001360	-0.6095111	-1.6893537
H	-4.8048035	-0.3222630	-2.6238018
C	-5.0788326	-0.7550416	-0.5066879
C	-6.4788330	-0.4792617	-0.5060162
C	-4.4425453	-1.1649425	0.7216921
C	-5.2328695	-1.2239379	1.9079728
C	-3.0323343	-1.4621386	0.7087757
C	-2.3203747	-1.1978679	-0.4658388
O	-0.7533853	-0.2065069	1.7832072
O	-0.9360674	-1.3943146	-0.4725036
P	-0.0388415	-0.2698356	0.3042398
O	1.3564269	-0.9455353	0.4199750
O	-0.0921952	1.1300650	-0.2765970
C	-3.4909235	-5.6613998	3.8459900
C	-4.1586652	-5.2428222	2.6650268
H	-1.8937558	-5.2378983	5.2445262
H	-3.7997310	-6.5880845	4.3532770
H	-4.3078390	-3.7642284	1.1033317
H	-4.9757113	-5.8543820	2.2527090
C	-6.5890260	-0.9317871	1.8778152
C	-7.2232147	-0.5692704	0.6598701
H	-4.7502124	-1.4908302	2.8584263
H	-7.1755820	-0.9729330	2.8082547
H	-8.3003371	-0.3434360	0.6479075
H	-6.9535351	-0.1732257	-1.4514798
C	2.0956545	-1.6271972	3.5060441
C	0.8228076	-1.1050857	3.8714681
C	3.2334641	-0.8237207	3.7144049
C	0.7217645	0.1720988	4.4868139
C	1.8905075	0.9302736	4.6756542
C	3.1556965	0.4621856	4.2785302
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C	-0.6154878	0.6998120	5.0049307
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H	-0.2704668	2.8563980	4.7056047
H	-1.9929704	2.3880971	4.7993886
H	-1.0662293	2.0394813	3.3202269
C	-0.6149438	0.7225069	6.5458946
H	-1.4005940	-0.0193583	4.6930647
H	0.1359326	1.4406737	6.9372067
H	-0.3727097	-0.2754461	6.9645876
H	-1.6080666	1.0289554	6.9345946
C	4.4133467	1.2967581	4.4898206
C	4.3618014	2.6269342	3.7190545
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H	3.5130295	3.2583359	4.0544420
H	4.2445079	2.4582828	2.6303422
C	4.6869267	1.5271475	5.9872953
H	5.2608804	0.7082819	4.0756133
H	5.6423492	2.0718497	6.1359474
H	4.7473764	0.5675084	6.5391040
H	3.8815221	2.1314973	6.4549377
C	2.2582742	-3.0547595	2.9815148
C	3.2733928	-3.2114693	1.8390432
H	3.3546662	-4.2777224	1.5447175
H	4.2908694	-2.8700077	2.1172411
H	2.9498418	-2.6489733	0.9422776
C	2.6260232	-3.9918686	4.1512591
H	1.2738987	-3.3799312	2.5866634
H	2.6715695	-5.0484417	3.8147682
H	1.8898948	-3.9250570	4.9765808
H	3.6176273	-3.7232416	4.5722463
H	0.3152695	1.1892556	-6.6960874
H	-1.7546526	-4.0652561	-4.9795564
H	-4.3012021	3.3205151	-2.9557406
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H	-0.2494956	-4.6650754	-2.2224411
H	2.0835656	-0.2895412	-7.5659783
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C	-0.5969774	-0.1379354	-5.3050402

C	-2.2902878	-3.9805029	-4.0109351
C	1.5291056	-0.5818367	-6.6505313
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C	-0.6898647	-1.4115429	-4.7195116
C	-3.8485535	2.4684672	-3.5030453
H	-1.6922087	0.1994386	-7.8124679
C	-1.2513090	0.9233868	-4.6593060
C	-0.7190467	-0.3311677	-7.8139933
H	-0.2075084	-0.1156259	-8.7754637
H	-1.1830421	1.9305485	-5.1007603
C	-0.1467502	-3.6558065	-2.6721817
H	-2.4041143	-5.0051311	-3.5999803
H	-3.3024844	-3.5803152	-4.2225458
C	-1.4327709	-1.6453169	-3.5482852
C	-1.5634719	3.1441323	-2.6621162
C	-1.9716124	0.7584341	-3.4613266
H	-4.6116039	1.6680153	-3.5758976
H	-3.6234255	2.8058094	-4.5373509
C	-1.5297153	-3.0771167	-3.0224557
C	-2.0915138	-0.5522398	-2.9170885
C	-2.5727998	1.9898373	-2.7856555
H	0.3792542	-3.0081420	-1.9441341
H	-0.6289617	2.8161954	-2.1672183
H	0.4933116	-3.7585082	-3.5735953
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H	-1.2998364	3.5817776	-3.6488485
H	-0.9334285	-1.4200191	-7.7792677
H	-2.1234018	-3.0592876	-2.0867387
H	-2.8503538	1.7100939	-1.7489392
H	-0.1841369	-2.2633039	-5.2010416
C	1.7552595	3.0655115	-5.1494287
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C	3.2998211	1.8622362	-3.7170295
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C	4.1273110	2.9356966	-5.7399959
C	2.8201639	3.3793755	-6.0151841
H	0.7410766	3.4303094	-5.3677166
H	1.1708608	2.0367446	-3.3135510
C	3.5756496	1.1198108	-2.5012203
H	5.3907719	1.8487440	-4.3409586
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H	2.6296050	3.9828256	-6.9163369
O	2.6828417	0.7312223	-1.7231270
H	4.6501938	0.9168470	-2.2518738
C	3.0296315	5.2308635	1.4525432
C	2.1866839	4.2393960	1.0590661
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O	3.2047071	5.0846057	-0.8724703
C	3.7119696	5.8135088	0.2532081
O	1.6164387	3.4938042	-1.1920083
C	1.2837741	3.3288883	1.7887011
H	3.4940978	6.8948845	0.0953533
H	4.8200039	5.7019516	0.2887114
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H	1.7591981	2.3221442	1.8776491
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Br	5.1588471	-0.7033107	1.4493551
Zn	-0.6509456	1.5696266	2.4068113
Br	-2.9877174	1.4372526	2.5780666
C	-1.4191752	-2.5180569	0.6251546
C	-2.3544058	-2.7338514	-0.3915012
C	-2.6718025	-4.0994266	-0.7381861
C	-3.4841690	-4.4467865	-1.8599943
C	-2.1189138	-5.1706370	0.0574717
C	-2.4611182	-6.5212842	-0.2531875
C	-1.1920946	-4.8707128	1.0972751
H	-0.7479402	-5.7014673	1.6666520
C	-0.7869237	-3.5682305	1.3583599
C	-2.5670973	0.5103151	-2.4377732
C	-3.9334477	0.5816595	-2.6844471
H	-4.3221421	1.3910624	-3.3201056
C	-4.8559707	-0.3268018	-2.0928841
C	-6.2634721	-0.1717454	-2.2744450
C	-4.3658594	-1.3954120	-1.2567897
C	-5.3187752	-2.2157659	-0.5813430
C	-2.9412601	-1.5702323	-1.1120440
C	-2.1009164	-0.5938914	-1.6611258
O	-1.0877586	-1.2168574	0.9764442
O	-0.7197346	-0.7117410	-1.4937147
P	-0.1052911	-0.3428959	-0.0183683
O	1.3017427	-0.9976764	-0.0495726
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C	-3.2837670	-6.8200857	-1.3288459
C	-3.7827680	-5.7718107	-2.1473907
H	-2.0419186	-7.3256974	0.3716552
H	-3.5354999	-7.8661868	-1.5607844
H	-3.8710914	-3.6489417	-2.5083514
H	-4.4080029	-6.0109247	-3.0212305
C	-6.6819769	-2.0257996	-0.7614671
C	-7.1618652	-1.0072558	-1.6280787
H	-4.9622668	-2.9991872	0.1016145
H	-7.3967123	-2.6652053	-0.2211350
H	-8.2450483	-0.8710358	-1.7683998
H	-6.6224845	0.6418497	-2.9242765
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C	0.3426700	-3.2167943	2.2731039
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C	0.0938165	-2.5676604	3.5152420
C	1.1867199	-2.1651040	4.3044755
C	2.5170524	-2.3644116	3.8965497
H	3.7754863	-3.2109748	2.3551981
C	-1.3374783	-2.3835003	4.0160960
H	0.9920654	-1.6790572	5.2706841
C	-1.5185626	-1.2174425	4.9951823
H	-1.0087656	-1.3984960	5.9646871
H	-2.5951758	-1.0681773	5.2090813
H	-1.1423397	-0.2689287	4.5652777
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H	-1.9677866	-2.1543603	3.1319480
H	-1.2458611	-3.9823074	5.5174233
H	-1.7985415	-4.5388939	3.9046602
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C	3.7009807	-2.0193540	4.7904236
C	3.5854225	-0.6467026	5.4674620
H	4.5042639	-0.4224223	6.0463443
H	2.7319201	-0.6024808	6.1755860
H	3.4417596	0.1583945	4.7213429
C	3.9151904	-3.1383278	5.8292083
H	4.5957045	-1.9914109	4.1314068
H	4.8155028	-2.9368666	6.4460377
H	4.0462162	-4.1244449	5.3395911
H	3.0431177	-3.2147499	6.5122359
C	2.0002634	-4.2646015	0.5834551
C	3.1105591	-3.6702370	-0.2981597
H	3.3220163	-4.3484973	-1.1497624
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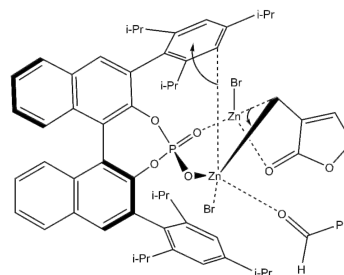
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Energy (Hartree) = -11970.02049097

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H	2.5076538	-6.3446155	0.0933460
H	1.5509615	-6.1711120	1.6021887
H	3.2851332	-5.7355594	1.5922943
H	0.9951998	5.5263187	-3.6461722
H	-0.2666812	0.5724748	-6.6382171
H	-4.5895023	4.2437513	-1.0094879
C	1.1397477	4.6487367	-4.3145385
H	0.8411111	-1.7931232	-4.8061477
H	3.2857212	5.0646417	-4.4888864
H	-2.7046820	4.1353529	0.7391581
C	0.1898646	3.5629887	-3.8237653
C	-0.9646133	-0.0654023	-6.0561162
C	2.6148995	4.2267980	-4.2070287
H	2.8448622	3.3763537	-4.8823391
C	0.2323823	2.2599520	-4.3492810
C	-3.8644870	4.0100366	-1.8163881
H	-0.2643876	5.4370492	-5.8137821
C	-0.7707882	3.8389890	-2.8372614
C	0.7865157	5.0901548	-5.7470963
H	1.4459538	5.9172794	-6.0838435
H	-0.8120985	4.8556399	-2.4159770
C	0.8259052	-0.7665402	-4.3847318
H	-0.9528889	-1.0780355	-6.5103829
H	-1.9837678	0.3546113	-6.1783857
C	-0.6499906	1.2522293	-3.9211347
C	-2.0040083	4.0470309	-0.1143503
C	-1.6678818	2.8655853	-2.3574035
H	-4.3985512	3.4345231	-2.5978362
H	-3.5424901	4.9701707	-2.2728228
C	-0.5622862	-0.1278202	-4.5706776
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C	-2.6537825	3.2424856	-1.2506300
H	1.0887438	-0.8311296	-3.3107299
H	-1.0977802	3.5442982	0.2683402
H	1.6164629	-0.1840762	-4.9029312
H	2.8690431	3.9168757	-3.1740642
H	-1.7310302	5.0764046	-0.4304559
H	0.9079489	4.2491815	-6.4619809
H	-1.2971026	-0.7877551	-4.0667887
H	-3.0222637	2.3009151	-0.7948083
H	0.9749060	2.0171591	-5.1264496
C	1.6705112	5.3412974	-0.5792105
C	1.9515260	3.9986607	-0.3180573
C	3.2973525	3.5558511	-0.3261867
C	4.3478294	4.4544948	-0.6331623
C	4.0536766	5.7941434	-0.9109935
C	2.7171430	6.2356881	-0.8747709
H	0.6305237	5.6955164	-0.5471496
H	1.1544735	3.2719532	-0.0973734
C	3.6087794	2.1782324	0.0307681
H	5.3885402	4.0931053	-0.6444750
H	4.8621083	6.5005065	-1.1513477
H	2.4877517	7.2923757	-1.0817393
O	2.7317584	1.3692788	0.3734874
H	4.6843586	1.8628034	0.0156064
C	3.2106989	2.8537648	3.3516337
C	1.9023004	2.4983125	3.2440292
C	1.1698835	3.7455884	2.8982994
O	2.0088813	4.8086008	2.8936297
C	3.3439284	4.3322349	3.1539649
O	-0.0195813	3.8386037	2.5933416
C	1.1239228	1.2389819	3.3351527
H	3.7454256	4.8577153	4.0487187
H	3.9782921	4.6142314	2.2842114
H	0.8941325	1.0178881	4.4008453
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H	4.0692831	2.1955918	3.5479216



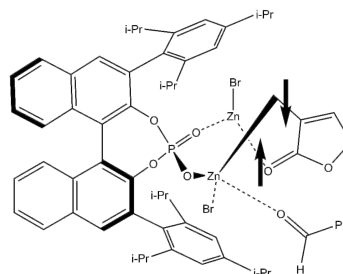
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Zn	-0.6480236	1.5832610	2.4054065
Br	-2.9724762	1.4354503	2.5712516
C	-1.4200982	-2.5190119	0.6251316
C	-2.3519868	-2.7362361	-0.3941922
C	-2.6697028	-4.1020145	-0.7391694
C	-3.4799429	-4.4501268	-1.8619225
C	-2.1206333	-5.1724987	0.0597061
C	-2.4645001	-6.5225017	-0.2495690
C	-1.1963015	-4.8712609	1.1009701
H	-0.7531258	-5.7009847	1.6727430
C	-0.7906169	-3.5689503	1.3612265
C	-2.5560404	0.5090586	-2.4381592
C	-3.9213836	0.5801982	-2.6892772
H	-4.3062021	1.3918104	-3.3243531
C	-4.8463575	-0.3284391	-2.1031245
C	-6.2527219	-0.1734743	-2.2892548
C	-4.3593392	-1.3974419	-1.2662696
C	-5.3146024	-2.2176534	-0.5945362
C	-2.9353116	-1.5727932	-1.1173538
C	-2.0921657	-0.5968236	-1.6629805
O	-1.0889265	-1.2184163	0.9759117
O	-0.7110234	-0.7165810	-1.4930086
P	-0.0999184	-0.3488885	-0.0157357
O	1.3026966	-1.0164305	-0.0385759
O	-0.2494505	1.1093462	0.3772096
C	-3.2849427	-6.8219905	-1.3259956
C	-3.7801530	-5.7747501	-2.1471428
H	-2.0480189	-7.3264094	0.3777394
H	-3.5379178	-7.8680990	-1.5562802
H	-3.8640790	-3.6519711	-2.5113580
H	-4.4042317	-6.0142203	-3.0216321
C	-6.6766000	-2.0275502	-0.7797846
C	-7.1532086	-1.0090168	-1.6471897
H	-4.9599409	-3.0002865	0.0900317
H	-7.3931093	-2.6666531	-0.2416242
H	-8.2357909	-0.8720619	-1.7908214
H	-6.6090580	0.6414430	-2.9388175
C	1.6728084	-3.4549647	1.8439205
C	0.3383248	-3.2169049	2.2763446
C	2.7336124	-2.9980016	2.6580358
C	0.0890749	-2.5635673	3.5161774
C	1.1821859	-2.1600248	4.3045089
C	2.5124384	-2.3603811	3.8980923
H	3.7716752	-3.2097532	2.3587563
C	-1.3420938	-2.3737662	4.0149607
H	0.9864843	-1.6707906	5.2688295
C	-1.5215988	-1.2054626	4.9913644
H	-1.0153724	-1.3860253	5.9630478
H	-2.5979491	-1.0510650	5.2012805
H	-1.1448541	-0.2580106	4.5601301
H	-1.8602860	-3.6901828	4.6294786
H	-1.9706235	-2.1428224	3.1301080
H	-1.2576763	-3.9713954	5.5185317

TS2

H	-1.8100762	-4.5280657	3.9059592	H	2.4631245	7.2677883	-1.0668052
H	-2.9160258	-3.5804020	4.9516702	O	2.7295382	1.3441814	0.3701689
C	3.6961424	-2.0166435	4.7927623	H	4.6795573	1.8372162	0.0100852
C	3.5852356	-0.6410210	5.4642996	C	3.2339413	2.8394116	3.3370277
H	4.5030771	-0.4188295	6.0455320	C	1.9212434	2.4981473	3.2388214
H	2.7300415	-0.5892571	6.1698495	C	1.1993136	3.7519837	2.8849888
H	3.4475675	0.1619159	4.7150882	O	2.0529203	4.8069259	2.8723551
C	3.9032912	-3.1325076	5.8360749	C	3.3803651	4.3170978	3.1301815
H	4.5921248	-1.9935584	4.1351936	O	0.0141998	3.8526967	2.5775122
H	4.8030840	-2.9336633	6.4544342	C	1.1291942	1.2498819	3.3371774
H	4.0301866	-4.1211395	5.3507932	H	3.7918441	4.8430682	4.0210664
H	3.0296364	-3.2033776	6.5174497	H	4.0148916	4.5889043	2.2566246
C	1.9966243	-4.2720044	0.5915793	H	0.8856736	1.0468059	4.4037288
C	3.1042354	-3.6801835	-0.2952557	H	1.7085699	0.3565676	3.0118455
H	3.3166460	-4.3631303	-1.1428428	H	4.0843674	2.1698762	3.5310410
H	4.0606489	-3.5302597	0.2464790				
H	2.7854374	-2.7152654	-0.7376098				
C	2.3521029	-5.7148335	1.0072475				
H	1.0786076	-4.3154936	-0.0274144				
H	2.5078042	-6.3546838	0.1143776				
H	1.5524405	-6.1727492	1.6226904				
H	3.2850463	-5.7348860	1.6085979				
H	0.9728480	5.5476424	-3.6479489				
H	-0.2583118	0.5870281	-6.6356719				
H	-4.5913926	4.2213317	-0.9861648				
C	1.1218094	4.6706314	-4.3165335				
H	0.8661309	-1.7755883	-4.8063888				
H	3.2641932	5.1050317	-4.5019413				
H	-2.6992431	4.1235427	0.7535712				
C	0.1834748	3.5771974	-3.8205555				
C	-0.9510149	-0.0554084	-6.0525040				
C	2.6012238	4.2623420	-4.2158359				
H	2.8356291	3.4135113	-4.8914647				
C	0.2349764	2.2746862	-4.3456392				
C	-3.8692841	3.9955520	-1.7975315				
H	-0.2965241	5.4442761	-5.8090870				
C	-0.7769672	3.8459988	-2.8322420				
C	0.7578917	5.1081395	-5.7474161				
H	1.4077852	5.9407180	-6.0892392				
H	-0.8266699	4.8627296	-2.4119323				
C	0.8457520	-0.7495055	-4.3842675				
H	-0.9349254	-1.0670506	-6.5086983				
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C	-0.6401218	1.2612482	-3.9169956				
C	-2.0033009	4.0433958	-0.1042468				
C	-1.6664264	2.8668261	-2.3503454				
H	-4.4035570	3.4187409	-2.5776584				
H	-3.5571636	4.9589612	-2.2538269				
C	-0.5456343	-0.1175528	-4.5680639				
C	-1.6054663	1.5611629	-2.9165427				
C	-2.6507251	3.2353168	-1.2391899				
H	1.1104100	-0.8146785	-3.3108525				
H	-1.0913763	3.5483381	0.2747231				
H	1.6334966	-0.1632053	-4.9024122				
H	2.8637001	3.9540590	-3.1845809				
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C	1.6544911	5.3119945	-0.5710757				
C	1.9408707	3.9684266	-0.3195763				
C	3.2874287	3.5299963	-0.3364306				
C	4.3329707	4.4329115	-0.6462269				
C	4.0336661	5.7727045	-0.9161257				
C	2.6962274	6.2102853	-0.8681841				
H	0.6130291	5.6597717	-0.5262113				
H	1.1467302	3.2387790	-0.0973924				
C	3.6026090	2.1525702	0.0236860				
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H	4.8383980	6.4823338	-1.1594157				

TS3; COSMO

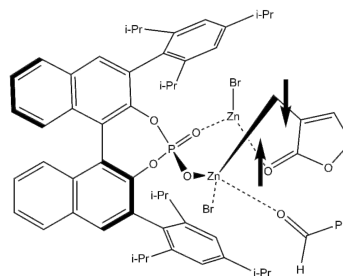


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Zn	0.0441364	1.4766318	2.2129623
Br	-1.3547046	0.9840136	3.9518261
C	-0.6436429	-2.6140386	1.0090559
C	-2.0371354	-2.7400917	0.9741008
C	-2.5959191	-4.0709011	0.9339102
C	-3.9855084	-4.3222388	0.7213402
C	-1.7159984	-5.2039698	1.0894084
C	-2.2657458	-6.5214143	1.0981040
C	-0.3113145	-4.9928385	1.1827316
H	0.3506813	-5.8644698	1.2983698
C	0.2493713	-3.7252355	1.0843950
C	-3.5147716	0.6289246	-0.1371269
C	-4.6199608	0.7195445	0.7031084
H	-5.3056760	1.5729075	0.5948874
C	-4.8569896	-0.2171489	1.7474554
C	-5.9314747	-0.0359859	2.6694744
C	-3.9642490	-1.3367943	1.9149278
C	-4.1471019	-2.1839155	3.0482378
C	-2.9049201	-1.5305762	0.9551798
C	-2.6923718	-0.5317766	0.0002500
O	-0.0718702	-1.3425218	1.0329466
O	-1.6245319	-0.6754393	-0.8937768
P	-0.1423961	-0.3471653	-0.2859653
O	0.8851354	-0.6624928	-1.3645795
O	-0.1023135	1.0720542	0.3337053
C	-3.6254611	-6.7274999	0.9210939
C	-4.4867510	-5.6166768	0.7143223
H	-1.5816799	-7.3744549	1.2298390
H	-4.0364000	-7.7485908	0.9220729
H	-4.6642979	-3.4752444	0.5514771
H	-5.5610202	-5.7828901	0.5411988
C	-5.1874378	-1.9676031	3.9410842
C	-6.0997142	-0.8964813	3.7434966
H	-3.4422750	-3.0090345	3.2200294
H	-5.3015589	-2.6282399	4.8140694

H	-6.9256685	-0.7408462	4.4542190	H	-2.2624747	0.2297670	-4.9066366
H	-6.6123580	0.8171737	2.5224501	H	0.0748491	4.3714434	-3.9626872
C	2.3958534	-3.6165264	-0.2299051	H	-1.4248126	5.0766598	1.0638870
C	1.7312967	-3.5155092	1.0258071	H	-3.5037749	4.5595635	-5.3684597
C	3.7883981	-3.4148119	-0.2674558	H	-3.7289590	-0.5376085	-2.2960193
C	2.4614153	-3.2252101	2.2069242	H	-2.7766349	2.3323792	1.4741596
C	3.8559424	-3.0520919	2.1156215	H	-2.7382385	2.3930454	-4.4250784
C	4.5403843	-3.1444720	0.8904355	C	3.7741601	6.0253903	-1.8774756
H	4.3142341	-3.4696453	-1.2321053	C	3.3493013	4.6948002	-1.8196600
C	1.7664050	-3.0982003	3.5620259	C	1.9924956	4.4027681	-1.5417811
H	4.4232526	-2.8326557	3.0343265	C	1.0717106	5.4516652	-1.3276948
C	1.7206918	-1.6366553	4.0429271	C	1.5029132	6.7835566	-1.3813017
H	2.7413110	-1.2155228	4.1583209	C	2.8519481	7.0687169	-1.6556712
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H	1.1675225	-1.0012320	3.3243904	H	4.0402118	3.8548464	-1.9935378
C	2.3942856	-4.0174579	4.6242263	C	1.5438723	3.0052978	-1.4574453
H	0.7154953	-3.4287017	3.4263432	H	0.0200562	5.2068819	-1.1171093
H	3.4360665	-3.7187004	4.8641821	H	0.7888588	7.6031849	-1.2107402
H	2.4175892	-5.0719164	4.2814830	H	3.1907385	8.1152971	-1.7012532
H	1.8134140	-3.9743488	5.5685202	O	2.3306362	2.0580170	-1.5414265
C	6.0494934	-2.9412868	0.8015034	H	0.4499596	2.8261338	-1.2904268
C	6.4310870	-1.4581260	0.9673200	C	4.8113330	2.2214356	1.1064115
H	7.5299069	-1.3233707	0.8850160	C	3.5856286	1.6497377	1.3426042
H	6.1184295	-1.0723434	1.9612327	C	2.7483702	2.7541344	1.8531649
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H	6.3484372	-3.2399991	-0.2267433	O	1.5623872	2.7465184	2.2531957
H	7.9125365	-3.7344253	1.6388227	C	3.0711291	0.3019004	1.1114852
H	6.5488876	-4.9029983	1.6644229	H	5.4624763	3.9894214	2.2385496
H	6.6046472	-3.5555141	2.8433539	H	4.9405246	4.3364327	0.5540386
C	1.6391886	-4.0164037	-1.4984481	H	2.1498759	0.1001945	1.6912154
C	2.1680399	-3.3651257	-2.7841874	H	3.8025355	-0.4845720	1.3723376
H	1.4846411	-3.5928183	-3.6275889	H	5.6969236	1.7160389	0.6991279
H	3.1707045	-3.7496795	-3.0632831				
H	2.2447637	-2.2671415	-2.6896213				
C	1.6330787	-5.5514097	-1.6548095				
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H	2.6699545	-5.9316425	-1.7687658				
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C	-2.0340051	4.9801125	-3.7888439				
H	-2.7567313	-1.4078859	-4.3893396				
H	-0.4801953	5.4862474	-5.2526078				
H	-1.3292874	3.9820942	2.4642115				
C	-2.4262922	3.8470536	-2.8487322				
C	-4.8834217	0.3407007	-3.8713579				
C	-0.7832288	4.6303562	-4.6149507				
H	-0.9701227	3.7646283	-5.2836849				
C	-2.7576055	2.5713969	-3.3380990				
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C	-3.2076382	5.3919830	-4.6963286				
H	-2.9293702	6.2556882	-5.3350196				
H	-2.2369014	5.0425607	-1.0596867				
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H	-5.2176683	-0.6350031	-4.2810270				
H	-5.6813135	0.7249512	-3.2037339				
C	-3.1295708	1.5134719	-2.4894299				
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H	-4.9224042	3.6238704	1.1778732				
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C	-3.5492048	0.1853846	-3.1164148				
C	-3.1518083	1.7305545	-1.0823295				
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TS3

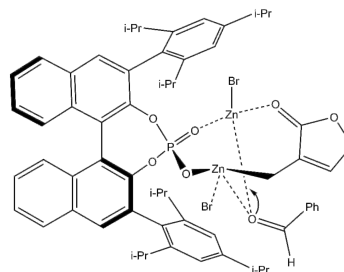


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Br	-1.3675214	0.9767959	3.9602857
C	-0.6402291	-2.6131212	1.0068231
C	-2.0336201	-2.7393363	0.9688921
C	-2.5924859	-4.0695541	0.9209104
C	-3.9821618	-4.3194942	0.7091767
C	-1.7124010	-5.2033771	1.0683306
C	-2.2625662	-6.5201325	1.0682686
C	-0.3081712	-4.9921442	1.1643389
H	0.3551006	-5.8635186	1.2744870
C	0.2533041	-3.7242654	1.0766047
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C	-4.6115071	0.7239652	0.7116692
H	-5.2954068	1.5790636	0.6056671
C	-4.8500602	-0.2155936	1.7526932
C	-5.9230868	-0.0367015	2.6761464
C	-3.9592920	-1.3373801	1.9151255
C	-4.1435697	-2.1891802	3.0444158

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C	-2.6855579	-0.5268299	0.0036825	C	-3.2471354	5.4099568	-4.6718617
O	-0.0699155	-1.3417554	1.0376838	H	-2.9811903	6.2766727	-5.3117141
O	-1.6187461	-0.6684185	-0.8903678	H	-2.2463428	5.0548181	-1.0473398
P	-0.1348291	-0.3447604	-0.2812836	C	-2.4452135	-0.3917102	-4.0111453
O	0.8922090	-0.6636493	-1.3573779	H	-5.2108587	-0.6283790	-4.2729221
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C	-3.6219546	-6.7252268	0.8918491	C	-3.1289926	1.5250608	-2.4802239
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H	-1.5782579	-7.3740220	1.1929583	C	-2.8027096	3.0199760	-0.5481810
H	-4.0325769	-7.7463689	0.8862610	H	-4.9145199	3.6274896	1.1977117
H	-4.6603942	-3.4706785	0.5469340	H	-3.9777078	5.1279392	0.9450456
H	-5.5578639	-5.7782953	0.5226507	C	-3.5440709	0.1963609	-3.1087966
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C	-6.0924177	-0.9009985	3.7462157	C	-2.7438906	3.3113286	0.9516020
H	-3.4397303	-3.0159845	3.2112847	H	-1.4924245	-0.5057809	-3.4588658
H	-5.2974237	-2.6385680	4.8085398	H	-0.5507331	3.5470595	0.8991129
H	-6.9171064	-0.7460744	4.4584323	H	-2.2569628	0.2474189	-4.8990296
H	-6.6017762	0.8189358	2.5336207	H	0.0481804	4.4034268	-3.9766805
C	2.4086926	-3.6085894	-0.2245639	H	-1.4193837	5.0850386	1.0726622
C	1.7355249	-3.5142059	1.0270902	H	-3.5471802	4.5781076	-5.3427087
C	3.8014600	-3.4076513	-0.2510249	H	-3.7204792	-0.5280746	-2.2890485
C	2.4573767	-3.2313633	2.2148926	H	-2.7657143	2.3387102	1.4843024
C	3.8524547	-3.0598642	2.1341606	H	-2.7505646	2.4098051	-4.4152193
C	4.5454130	-3.1457449	0.9136251	C	3.7736116	5.9942155	-1.9612029
H	4.3335152	-3.4538060	-1.2126069	C	3.3433829	4.6671436	-1.8706068
C	1.7531482	-3.1108629	3.5659502	C	1.9890181	4.3881548	-1.5708201
H	4.4137304	-2.8476525	3.0582400	C	1.0758411	5.4447567	-1.3680932
C	1.7070241	-1.6525757	4.0562547	C	1.5131786	6.7730652	-1.4543557
H	2.7276636	-1.2343948	4.1819049	C	2.8595578	7.0463291	-1.7501866
H	1.1789261	-1.5740636	5.0282831	H	4.8233971	6.2198033	-2.2038713
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C	6.4366719	-1.4612761	1.0088104	C	4.8009676	2.2030748	1.0953803
H	7.5361671	-1.3271036	0.9348716	C	3.5787517	1.6292486	1.3479061
H	6.1169761	-1.0773623	2.0013102	C	2.7415419	2.7351116	1.8587622
H	5.9616726	-0.8460626	0.2177817	O	3.4124976	3.8948162	1.8866350
C	6.8151975	-3.8414796	1.8272142	C	4.7520018	3.6567841	1.4087000
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H	6.5951591	-3.5668609	2.8802385	H	4.9099493	4.3153284	0.5240191
C	1.6618844	-4.0013141	-1.5011623	H	2.1402657	0.0837204	1.7016708
C	2.1995513	-3.3427440	-2.7796496	H	3.7939905	-0.5055273	1.3808930
H	1.5230465	-3.5671110	-3.6292984	H	5.6794021	1.6951237	0.6761558
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C	1.6597623	-5.5353926	-1.6658239				
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H	1.0928320	-5.8303905	-2.5731046				
H	1.2041136	-6.0508836	-0.7988385				
H	2.6979621	-5.9132474	-1.7738636				
H	-1.8063126	5.8757306	-3.1396492				
H	-4.7871644	1.0562341	-4.7116999				
H	-3.9121426	4.2854447	2.5294420				
C	-2.0619215	5.0005765	-3.7785845				
H	-2.7463136	-1.3919390	-4.3847448				
H	-0.5250231	5.5205525	-5.2563558				
H	-1.3180712	3.9876367	2.4712379				
C	-2.4396190	3.8627719	-2.8381166				
C	-4.8795476	0.3477210	-3.8620378				
C	-0.8177495	4.6611632	-4.6186154				
H	-1.0063519	3.7972637	-5.2890190				
C	-2.7661107	2.5865408	-3.3279669				
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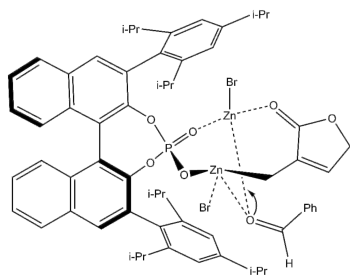


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Br	2.1739532	-2.0812967	-3.7899312
Zn	0.7046674	2.4821502	1.5636051
Br	-0.0734026	3.9156418	3.1493555
C	-0.2288600	-1.6631968	2.5577394
C	-1.5967013	-1.9436661	2.6466528

C	-1.9880869	-3.2118589	3.2144075	H	-2.5984277	3.5697900	-5.1785993
C	-3.3378401	-3.6771828	3.2152274	H	-4.8377759	-1.7303403	-3.8637526
C	-0.9710374	-4.0677640	3.7795291	H	-3.8300884	4.8948579	0.8604264
C	-1.3550130	-5.3065463	4.3760872	C	-3.1067349	2.5812100	-5.2428872
C	0.4005795	-3.6922644	3.6876364	H	-2.3304403	-3.2905872	-2.6195321
H	1.1643258	-4.3682639	4.1012072	H	-2.2981421	2.2742711	-7.2509534
C	0.8006561	-2.5315669	3.0369122	H	-1.3101634	4.7679337	0.4523333
C	-3.4088464	0.4087689	0.2008128	C	-3.0871800	1.9874037	-3.8390093
C	-4.5068498	0.7934996	0.9644010	C	-4.7801218	-1.9253794	-2.7723417
H	-5.2707910	1.4446222	0.5135007	C	-2.3529538	1.7374600	-6.2820411
C	-4.6555467	0.4075665	2.3265731	H	-2.8639407	0.7713027	-6.4737871
C	-5.7441820	0.8907371	3.1139511	C	-3.2038364	0.6072379	-3.6099515
C	-3.6708182	-0.4534452	2.9370690	C	-4.0114674	4.2155053	0.0020866
C	-3.7907058	-0.7346173	4.3315731	H	-5.0924805	3.4943700	-4.9679496
C	-2.5931531	-0.9626734	2.1249327	C	-2.9859478	2.8249340	-2.7133137
C	-2.4788155	-0.4860846	0.8130576	C	-4.5596123	2.8419564	-5.6887711
O	0.1715761	-0.4530049	1.9979593	H	-4.5896646	3.3291054	-6.6856283
O	-1.4071161	-0.9196886	0.0358216	H	-2.8608861	3.9088779	-2.8741701
P	0.0452458	-0.2326250	0.3596710	C	-2.2452430	-2.2003292	-2.8069225
O	1.0917758	-1.0089682	-0.4105224	H	-4.9086967	-3.0172127	-2.6214927
O	-0.0833535	1.3079659	0.2567782	H	-5.6363900	-1.4089279	-2.2922904
C	-2.6809608	-5.7128321	4.3887569	C	-3.2760314	0.0605600	-2.3140151
C	-3.6757218	-4.8959109	3.7879368	C	-1.5294543	4.1746257	-0.4583045
H	-0.5699204	-5.9439662	4.8124124	C	-3.0170490	2.3308566	-1.3950480
H	-2.9617873	-6.6736748	4.8463732	H	-4.9229049	3.6256411	0.2222198
H	-4.1171632	-3.0609321	2.7459905	H	-4.2274316	4.8425674	-0.8885582
H	-4.7232170	-5.2336851	3.7700809	C	-3.4383545	-1.4522222	-2.1822322
C	-4.8509265	-0.2329237	5.0740591	C	-3.2161271	0.9321672	-1.1904226
C	-5.8463640	0.5739768	4.4600718	C	-2.7887173	3.3124199	-0.2428280
H	-3.0234192	-1.3500022	4.8214339	H	-1.2807398	-1.8563159	-2.3860292
H	-4.9168257	-0.4580827	6.1494898	H	-0.6441643	3.5441842	-0.6784369
H	-6.6863238	0.9594371	5.0578558	H	-2.2027588	-2.0558343	-3.9066819
H	-6.4942206	1.5375126	2.6320441	H	-1.3174014	1.5134309	-5.9567835
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C	2.2309455	-2.1913651	2.7555326	H	-5.1226922	1.8875494	-5.7573168
C	4.2439908	-2.4942751	1.4249874	H	-3.4597359	-1.7037738	-1.1039350
C	2.8512199	-1.1030686	3.4251740	H	-2.6149463	2.7156534	0.6756736
C	4.1614766	-0.7378805	3.0695886	H	-3.2572220	-0.0777562	-4.4695995
C	4.8728548	-1.4094155	2.0604291	C	2.5310190	2.1240496	-6.2523297
H	4.7919055	-3.0290329	0.6323281	C	1.9915912	1.6120465	-5.0677078
C	2.1407593	-0.3645329	4.5564105	C	0.9995467	2.3498755	-4.3790454
H	4.6358196	0.1062133	3.5910572	C	0.5550245	3.5928032	-4.8861829
C	2.3359262	1.1556858	4.4971699	C	1.1128564	4.1079407	-6.0632948
H	3.3776545	1.4593250	4.7288794	C	2.0985420	3.3714675	-6.7451946
H	1.6687824	1.6737937	5.2142178	H	3.2907244	1.5480439	-6.8020526
H	2.1042298	1.5470476	3.4859061	H	2.3017348	0.6286942	-4.6758387
C	2.5714515	-0.9326795	5.9222585	C	0.4171718	1.8491717	-3.1280726
H	1.0532566	-0.5558778	4.4538054	H	-0.2295658	4.1479858	-4.3468946
H	3.6609288	-0.7913853	6.0823830	H	0.7749259	5.0777330	-6.4582927
H	2.3597898	-2.0193923	5.9871269	H	2.5291132	3.7693500	-7.6772024
H	2.0340108	-0.4265984	6.7511016	O	0.8430177	0.8898578	-2.4821359
C	6.2979506	-1.0227193	1.6793693	H	-0.4747588	2.4034944	-2.7383293
C	6.5622944	0.4893963	1.7379236	C	3.8619093	2.8133426	-2.3218678
H	7.5687433	0.7232783	1.3347636	C	3.6772819	1.8623067	-1.3465286
H	6.5331394	0.8718362	2.7796111	C	2.8913367	2.5462004	-0.3027933
H	5.8132209	1.0551965	1.1481632	O	2.5575918	3.7965722	-0.6654733
C	7.3135538	-1.7969397	2.5429522	C	3.1634837	4.0756912	-1.9503637
H	6.4411498	-1.3474499	0.6244034	O	2.5330382	2.0974079	0.8059569
H	8.3556469	-1.5701345	2.2350110	C	3.9812547	0.4369719	-1.2623842
H	7.1595990	-2.8918698	2.4618303	H	3.8276484	4.9584293	-1.8189916
H	7.2054233	-1.5214104	3.6132881	H	2.3528034	4.3665626	-2.6557979
C	2.3374999	-4.1197943	1.0366720	H	4.0881727	0.0887860	-0.2166770
C	2.5403417	-4.1068563	-0.4851098	H	4.8537358	0.1400483	-1.8740813
H	2.0316537	-4.9770036	-0.9483160	H	4.3894417	2.6804937	-3.2755382
H	3.6104928	-4.1681551	-0.7722202				
H	2.1147002	-3.1950444	-0.9418196				
C	2.8892812	-5.4218604	1.6516399				
H	1.2429578	-4.1025726	1.2145119				
H	2.4175575	-6.3102777	1.1826717				
H	2.7080078	-5.4731236	2.7442348				
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TS4



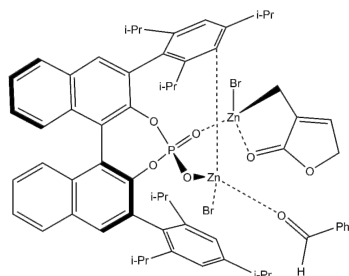
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Br	2.1815424	-2.0561270	-3.7996607
Zn	0.6962928	2.4876592	1.5708263
Br	-0.0791378	3.9219415	3.1508049
C	-0.2283134	-1.6591599	2.5601826
C	-1.5959317	-1.9407808	2.6481736
C	-1.9863943	-3.2093089	3.2154875
C	-3.3355949	-3.6751777	3.2165849
C	-0.9690416	-4.0647747	3.7802389
C	-1.3527718	-5.3031896	4.3762174
C	0.4019743	-3.6884536	3.6879290
H	1.1669248	-4.3642622	4.0995805
C	0.8017028	-2.5273998	3.0381407
C	-3.4061968	0.4094797	0.1995883
C	-4.5066025	0.7914300	0.9606748
H	-5.2698384	1.4416066	0.5072588
C	-4.6585597	0.4047994	2.3219738
C	-5.7498970	0.8843805	3.1068734
C	-3.6735513	-0.4541412	2.9345136
C	-3.7967691	-0.7364723	4.3282271
C	-2.5928684	-0.9610460	2.1251010
C	-2.4761624	-0.4842990	0.8134129
O	0.1725836	-0.4487318	2.0016332
O	-1.4035709	-0.9164045	0.0382808
P	0.0480668	-0.2287274	0.3633701
O	1.0946158	-1.0050530	-0.4061163
O	-0.0834874	1.3120091	0.2591562
C	-2.6778832	-5.7099060	4.3892928
C	-3.6726220	-4.8935305	3.7890928
H	-0.5671703	-5.9404532	4.8118492
H	-2.9579370	-6.6708131	4.8467497
H	-4.1146490	-3.0586344	2.7475589
H	-4.7199358	-5.2313903	3.7714296
C	-4.8600278	-0.2380921	5.0677199
C	-5.8552853	0.5665599	4.4519172
H	-3.0290941	-1.3505875	4.8188005
H	-4.9282960	-0.4642957	6.1427287
H	-6.6977546	0.9497830	5.0475002
H	-6.4997979	1.5301029	2.6233765
C	2.9365211	-2.9033895	1.7456260
C	2.2316353	-2.1876552	2.7547517
C	4.2425962	-2.4915008	1.4227508
C	2.8536011	-1.1011963	3.4253659
C	4.1640681	-0.7378584	3.0697239
C	4.8738207	-1.4093394	2.0597823
H	4.7885704	-3.0257268	0.6284167
C	2.1445975	-0.3627288	4.5576317
H	4.6397081	0.1050989	3.5917704
C	2.3394408	1.1575827	4.4990584
H	3.3813490	1.4614000	4.7297607
H	1.6733465	1.6763810	5.2164127
H	2.1064808	1.5498323	3.4887461
C	2.5760545	-0.9321727	5.9225016
H	1.0569541	-0.5537293	4.4556500
H	3.6656628	-0.7921396	6.0819886

H	2.3644374	-2.0187330	5.9864121
H	2.0398551	-0.4269761	6.7526363
C	6.3006523	-1.0269135	1.6808867
C	6.5707753	0.4839865	1.7410509
H	7.5787337	0.7148698	1.3400363
H	6.5417880	0.8657815	2.7828647
H	5.8251312	1.0534003	1.1508116
C	7.3120490	-1.8060971	2.5445984
H	6.4438194	-1.3503422	0.6254543
H	8.3557686	-1.5835554	2.2391044
H	7.1532659	-2.9000171	2.4626790
H	7.2030868	-1.5321003	3.6149958
C	2.3339830	-4.1137496	1.0322151
C	2.5358487	-4.1005134	-0.4897756
H	2.0257136	-4.9691109	-0.9535918
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C	2.8852690	-5.4167388	1.6456184
H	1.2395700	-4.0957521	1.2107746
H	2.4129322	-6.3044023	1.1761082
H	2.7054967	-5.4693335	2.7383320
H	3.9817757	-5.4920341	1.4878128
H	-2.6044356	3.5809012	-5.1754767
H	-4.8226189	-1.7284935	-3.8686842
H	-3.8329039	4.8910238	0.8699361
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H	-2.3094845	-3.2831243	-2.6246640
H	-2.3001761	2.2894953	-7.2507012
H	-1.3139775	4.7708538	0.4600453
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C	-4.7643087	-1.9248001	-2.7776021
C	-2.3506092	1.7518257	-6.2820344
H	-2.8565664	0.7833920	-6.4747762
C	-3.1953309	0.6133953	-3.6100000
C	-4.0137406	4.2143573	0.0095954
H	-5.0982219	3.4905731	-4.9610113
C	-2.9857385	2.8299300	-2.7103830
C	-4.5625029	2.8432464	-5.6840203
H	-4.5977847	3.3315266	-6.6801642
H	-2.8649165	3.9148042	-2.8693116
C	-2.2281854	-2.1926361	-2.8107742
H	-4.8897328	-3.0172268	-2.6292255
H	-5.6225294	-1.4118089	-2.2976369
C	-3.2671205	0.0644312	-2.3152055
C	-1.5326769	4.1801937	-0.4523710
C	-3.0159575	2.3342887	-1.3928800
H	-4.9237283	3.6222752	0.2289409
H	-4.2328655	4.8434816	-0.8788267
C	-3.4241169	-1.4490473	-2.1861392
C	-3.2113134	0.9348210	-1.1905947
C	-2.7896530	3.3143509	-0.2389348
H	-1.2645552	-1.8478041	-2.3891415
H	-0.6462137	3.5521113	-0.6743837
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H	-1.3136690	1.5315647	-5.9593220
H	-1.6555263	4.8972726	-1.2913010
H	-5.1204130	1.8860631	-5.7524487
H	-3.4456770	-1.7020354	-1.1082476
H	-2.6135213	2.7169028	0.6785818
H	-3.2445168	-0.0710682	-4.4702254
C	2.5111156	2.0935379	-6.2592089
C	1.9753899	1.5898113	-5.0690235
C	0.9960964	2.3405179	-4.3768675
C	0.5595786	3.5849827	-4.8861102
C	1.1143937	4.0910474	-6.0686107
C	2.0885123	3.3430735	-6.7539121
H	3.2597515	1.5064009	-6.8122981
H	2.2752330	0.6017140	-4.6782280
C	0.4173964	1.8484519	-3.1187657
H	-0.2185080	4.1466129	-4.3439727
H	0.7826010	5.0623305	-6.4656637

H	2.5167815	3.7337008	-7.6901891
O	0.8434172	0.8903109	-2.4736829
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C	3.8558892	2.8114804	-2.3203611
C	3.6749094	1.8621380	-1.3417491
C	2.8850479	2.5469091	-0.2993689
O	2.5465649	3.7963603	-0.6680101
C	3.1507523	4.0720805	-1.9526262
O	2.5278410	2.1022300	0.8090581
C	3.9807164	0.4404410	-1.2515134
H	3.8101261	4.9597056	-1.8241092
H	2.3380766	4.3558700	-2.6594975
H	4.0806922	0.0937064	-0.2047152
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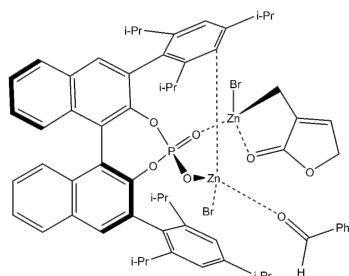
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Zn	-0.6565371	2.6109235	1.2923746
Br	-2.9764038	2.2870078	1.5532027
C	-1.3028906	-1.8064581	1.9367492
C	-2.4643373	-2.3054916	1.3401197
C	-2.9279374	-3.6098888	1.7614204
C	-4.0018583	-4.2951818	1.1162212
C	-2.2624201	-4.2775834	2.8568991
C	-2.7467467	-5.5430657	3.3055913
C	-1.0892709	-3.7019631	3.4264398
H	-0.5603410	-4.2477059	4.2231034
C	-0.5690014	-2.5104042	2.9443863
C	-2.9673050	-0.4725772	-1.9971309
C	-4.3511020	-0.3441363	-2.0242166
H	-4.8351304	0.0828029	-2.9150120
C	-5.1615306	-0.6845176	-0.9038768
C	-6.5661869	-0.4309198	-0.9060948
C	-4.5506464	-1.2529739	0.2724825
C	-5.3684644	-1.4731521	1.4203282
C	-3.1375015	-1.5393641	0.2545483
C	-2.3921431	-1.0807754	-0.8381274
O	-0.8217011	-0.5558597	1.5827376
O	-1.0129041	-1.2704984	-0.8492212
P	-0.0797843	-0.3291113	0.1196055
O	1.2821216	-1.0534482	0.0765530
O	-0.1655740	1.1635667	-0.1643505
C	-3.8196178	-6.1599363	2.6798370
C	-4.4365859	-5.5357170	1.5634011
H	-2.2360431	-6.0303161	4.1511468
H	-4.1798096	-7.1384961	3.0321139
H	-4.4853592	-3.8328460	0.2454746
H	-5.2642319	-6.0410488	1.0425926
C	-6.7280675	-1.1943178	1.3946216
C	-7.3387129	-0.6849615	0.2173681
H	-4.9053471	-1.8531217	2.3416682
H	-7.3356048	-1.3608706	2.2973154

H	-8.4189959	-0.4741070	0.2062428
H	-7.0215046	-0.0060343	-1.8145589
C	1.9340050	-2.5430955	2.7425990
C	0.7706381	-1.9491283	3.2931759
C	3.1659928	-1.8387214	2.8550218
C	0.8574580	-0.7353484	4.0338625
C	2.0910280	-0.0654168	4.1141418
C	3.2587642	-0.5844937	3.5221792
H	4.1011570	-2.3404688	2.5551402
C	-0.3547792	-0.2464032	4.8186582
H	2.1499045	0.8771597	4.6778656
C	-0.5722188	1.2688787	4.8035284
H	0.2779061	1.8279930	5.2460518
H	-1.4771336	1.5254997	5.3896131
H	-0.7367363	1.6337624	3.7727276
C	-0.2513712	-0.7947269	6.2583461
H	-1.2525041	-0.7076085	4.3589127
H	0.6374980	-0.3795821	6.7783650
H	-0.1615949	-1.9001157	6.2661376
H	-1.1518483	-0.5171790	6.8433891
C	4.6184481	0.0824517	3.6906415
C	4.5891425	1.5920749	3.4079231
H	5.6110071	2.0161826	3.4780428
H	3.9518033	2.1399741	4.1322018
H	4.1979362	1.7992655	2.3924796
C	5.1807049	-0.2227693	5.0926149
H	5.2965265	-0.3848244	2.9426242
H	6.2009586	0.1982968	5.2026109
H	5.2371785	-1.3143802	5.2770249
H	4.5398757	0.2224970	5.8821706
C	1.9131021	-3.9296380	2.1060782
C	2.6448124	-4.0284983	0.7596405
H	2.5540576	-5.0586329	0.3596968
H	3.7276856	-3.8022228	0.8388238
H	2.1975596	-3.3411353	0.0140283
C	2.4621765	-4.9558924	3.1189355
H	0.8527150	-4.1853890	1.9153743
H	2.3852409	-5.9832445	2.7080649
H	1.9043535	-4.9247555	4.0767987
H	3.5312344	-4.7605066	3.3461152
H	0.7688967	-2.7859557	-5.8241392
H	-1.3325087	-2.7597064	-5.8424416
H	-4.7241293	3.6077955	-2.8785507
C	0.8714306	1.6785200	-5.8631025
H	-0.1035042	-4.0906844	-3.1917707
H	3.0575293	1.8151081	-6.0277377
H	-2.7485475	4.2612798	-1.3224037
C	-0.1834170	1.1066924	-4.9243642
C	-1.9635711	-2.9451695	-4.9478552
C	2.2933751	1.3294690	-5.3857147
H	2.4714858	0.2343890	-5.4217707
C	-0.3024800	-0.2790812	-4.7172242
C	-4.0524066	2.9250137	-3.4391215
H	-0.3666204	1.5231045	-7.6744308
C	-1.0553785	1.9495351	-4.2185309
C	0.6450223	1.2391017	-7.3205219
H	1.3914589	1.7057066	-7.9966504
H	-0.9830803	3.0361171	-4.3849546
C	0.0275444	-3.0019258	-3.3622611
H	-2.0871742	-4.0433103	-4.8429144
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C	-1.2258130	-0.8224097	-3.8079791
C	-2.1098977	3.6634659	-2.0014289
C	-1.9946297	1.4625866	-3.2886225
H	-4.6603320	2.0755851	-3.8103681
H	-3.6748820	3.4734412	-4.3282826
C	-1.3253694	-2.3420736	-3.6815229
C	-2.0691847	0.0568441	-3.0697243
C	-2.8851935	2.4586729	-2.5480845
H	0.4770640	-2.5617805	-2.4509649
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H	0.7491740	-2.8858787	-4.1979258
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H	-1.7548838	4.3421154	-2.8060327
H	0.7411091	0.1380351	-7.4265260
H	-2.0093810	-2.5693179	-2.8391928
H	-3.3090707	1.9419577	-1.6639136
H	0.3537192	-0.9645035	-5.2773878
C	1.6480919	4.0933938	-2.6957373
C	1.9906414	3.1167242	-1.7576177
C	3.3501434	2.7466055	-1.6045955
C	4.3497428	3.3355450	-2.4177628
C	3.9955249	4.3118813	-3.3559158
C	2.6466804	4.6928485	-3.4879383
H	0.5969283	4.3918162	-2.8082467
H	1.2296764	2.6081028	-1.1452788
C	3.7377110	1.7335982	-0.6349962
H	5.3995881	3.0222947	-2.3025312
H	4.7657733	4.7768808	-3.9889954
H	2.3673761	5.4616420	-4.2247739
O	2.9510076	1.2481474	0.2022524
H	4.7938871	1.3630174	-0.6763006
C	2.9477701	4.6818183	1.3680303
C	1.6717823	4.2364490	1.5270094
C	0.8418361	5.0386693	0.5900948
O	1.5933581	5.9861362	-0.0253170
C	2.9652870	5.8056454	0.3778653
O	-0.3455486	4.8587012	0.3271366
C	0.9978718	3.1841989	2.3121356
H	3.3458065	6.7616114	0.8010597
H	3.5565036	5.5825941	-0.5393327
H	0.5660719	3.6331879	3.2349202
H	1.6854735	2.3741885	2.6185744
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int1



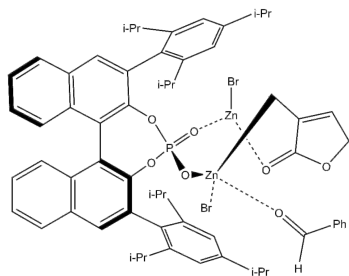
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Br	-2.9719926	2.2623833	1.5482520
C	-1.2962262	-1.8107111	1.9414282
C	-2.4558364	-2.3086224	1.3403427
C	-2.9221815	-3.6128751	1.7589367
C	-3.9940039	-4.2960360	1.1085397
C	-2.2628428	-4.2824352	2.8566747
C	-2.7515109	-5.5469079	3.3019312
C	-1.0924012	-3.7076704	3.4316767
H	-0.5663605	-4.2537317	4.2302239
C	-0.5690808	-2.5162242	2.9530024
C	-2.9502731	-0.4690593	-1.9935700
C	-4.3341395	-0.3431726	-2.0230703
H	-4.8147564	0.0870594	-2.9140321
C	-5.1474211	-0.6864830	-0.9064640
C	-6.5517207	-0.4339541	-0.9108844
C	-4.5386155	-1.2557019	0.2700893
C	-5.3582093	-1.4767710	1.4161202
C	-3.1253700	-1.5414097	0.2539510

C	-2.3769267	-1.0800585	-0.8354272
O	-0.8099338	-0.5620668	1.5907258
O	-0.9971539	-1.2701327	-0.8434665
P	-0.0652009	-0.3320009	0.1294222
O	1.2954481	-1.0629132	0.0924331
O	-0.1387032	1.1604118	-0.1527959
C	-3.8223399	-6.1613182	2.6715559
C	-4.4329412	-5.5354073	1.5532930
H	-2.2455477	-6.0354577	4.1496170
H	-4.1862130	-7.1390139	3.0222957
H	-4.4720753	-3.8311589	0.2363033
H	-5.2593548	-6.0386002	1.0286131
C	-6.7175318	-1.1993252	1.3875651
C	-7.3261510	-0.6901074	0.2099834
H	-4.8956717	-1.8547988	2.3383482
H	-7.3261816	-1.3655620	2.2894448
H	-8.4063608	-0.4794359	0.1970269
H	-7.0047671	-0.0065809	-1.8192268
C	1.9354449	-2.5515636	2.7707037
C	0.7679951	-1.9555188	3.3104240
C	3.1662323	-1.8480857	2.8911309
C	0.8490865	-0.7385170	4.0465221
C	2.0824502	-0.0694611	4.1329585
C	3.2543265	-0.5913655	3.5520159
H	4.1028494	-2.3470965	2.5918295
C	-0.3697599	-0.2445726	4.8183620
H	2.1361347	0.8772911	4.6902764
C	-0.5827482	1.2711518	4.8016826
H	0.2645206	1.8289339	5.2517209
H	-1.4922040	1.5307323	5.3789838
H	-0.7406115	1.6368811	3.7703393
C	-0.2842603	-0.7947612	6.2583951
H	-1.2641484	-0.7014604	4.3480795
H	0.6007793	-0.3848114	6.7889623
H	-0.1995041	-1.9004765	6.2664051
H	-1.1891911	-0.5140735	6.8349057
C	4.6120920	0.0791783	3.7230430
C	4.5847315	1.5813453	3.4024643
H	5.6044555	2.0100460	3.4785027
H	3.9337012	2.1467884	4.1007473
H	4.2098319	1.7609260	2.3756468
C	5.1584964	-0.1914434	5.1379008
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H	6.1774511	0.2320197	5.2510703
H	5.2129859	-1.2781179	5.3495876
H	4.5091439	0.2709896	5.9103951
C	1.9201639	-3.9383892	2.1337330
C	2.6414140	-4.0287071	0.7806506
H	2.5624989	-5.0602699	0.3818175
H	3.7217544	-3.7863520	0.8477672
H	2.1766442	-3.3495869	0.0383989
C	2.4841971	-4.9619758	3.1405470
H	0.8601416	-4.2016210	1.9514569
H	2.4115181	-5.9898359	2.7301670
H	1.9340747	-4.9355737	4.1030432
H	3.5537569	-4.7610812	3.3603160
H	0.7557494	2.8178574	-5.8239369
H	-1.3131578	-2.7390692	-5.8433551
H	-4.7263507	3.6097727	-2.8573270
C	0.8536628	1.7103625	-5.8776212
H	-0.0622417	-4.0665744	-3.1971421
H	3.0371996	1.8426722	-6.0829039
H	-2.7462762	4.2567530	-1.2943310
C	-0.1866983	1.1315325	-4.9271507
C	-1.9377746	-2.9303821	-4.9456201
C	2.2833651	1.3514387	-5.4329217
H	2.4583964	0.2567529	-5.4863526
C	-0.2932437	-0.2546792	-4.7188895
C	-4.0542232	2.9319002	-3.4229159
H	-0.4208701	1.5812492	-7.6648633
C	-1.0609156	1.9674480	-4.2165980

C	0.5964549	1.2893788	-7.3353377
H	1.3311893	1.7592270	-8.0220101
H	-0.9992442	3.0546315	-4.3839515
C	0.0608448	-2.9771037	-3.3685162
H	-2.0539674	-4.0294911	-4.8428007
H	-2.9392273	-2.4942980	-5.1365456
C	-1.2083719	-0.8051935	-3.8062729
C	-2.1120100	3.6677723	-1.9846428
C	-1.9920798	1.4738478	-3.2823529
H	-4.6607558	2.0834127	-3.7984782
H	-3.6804598	3.4854163	-4.3104187
C	-1.2973673	-2.3255502	-3.6814306
C	-2.0548834	0.0675206	-3.0643817
C	-2.8848324	2.4638099	-2.5361277
H	0.5130386	-2.5342948	-2.4600010
H	-1.2325266	3.3378550	-1.4036151
H	0.7783614	-2.8573411	-4.2071184
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H	-1.7658206	4.3559182	-2.7853385
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H	-1.9763177	-2.5582398	-2.8366039
H	-3.3063694	1.9438123	-1.6527633
H	0.3651096	-0.9352527	-5.2822844
C	1.6296295	4.0916213	-2.6890765
C	1.9785399	3.1054728	-1.7627579
C	3.3337772	2.7100128	-1.6455895
C	4.3220214	3.2800216	-2.4852593
C	3.9623217	4.2659459	-3.4106811
C	2.6182340	4.6741749	-3.5046801
H	0.5814031	4.4100552	-2.7685110
H	1.2241946	2.6078695	-1.1332167
C	3.7266325	1.6927506	-0.6806779
H	5.3679066	2.9441274	-2.4001121
H	4.7239053	4.7164001	-4.0645115
H	2.3348714	5.4514349	-4.2310615
O	2.9587524	1.2400575	0.1895054
H	4.7695936	1.2876689	-0.7543051
C	2.9648632	4.6486706	1.3610517
C	1.6825508	4.2242349	1.5243706
O	0.8633787	5.0301220	0.5774232
C	1.6315509	5.9649446	-0.0425567
C	2.9974669	5.7655054	0.3611894
O	-0.3209394	4.8578830	0.3086426
C	0.9925985	3.1888597	2.3147191
H	3.3942990	6.7188355	0.7773196
H	3.5850742	5.5270120	-0.5552495
H	0.5530041	3.6548475	3.2254641
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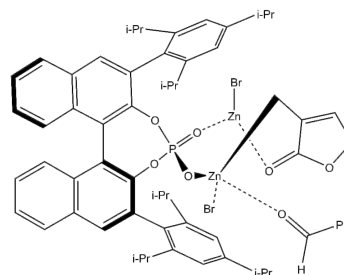


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Br	-4.2940764	-0.3181950	1.0676173
C	-0.0469432	-2.6969078	0.8297711
C	-0.5970413	-3.3505272	-0.2777189
C	-0.2791320	-4.7443299	-0.4732226

C	-0.6498720	-5.4666746	-1.6480885
C	0.4667338	-5.4405291	0.5471926
C	0.7504131	-6.8298090	0.3815598
C	0.9446006	-4.7211755	1.6788916
H	1.5134033	-5.2620324	2.4507495
C	0.7500766	-3.3518036	1.8166356
C	-1.7078654	-0.7081037	-2.8305892
C	-2.9362476	-1.2268552	-3.2280036
H	-3.4964926	-0.7192799	-4.0274940
C	-3.5198505	-2.3619607	-2.5993125
C	-4.8304724	-2.8072360	-2.9473819
C	-2.7920756	-3.0525477	-1.5639443
C	-3.4401130	-4.1231727	-0.8787394
C	-1.4609163	-2.6070543	-1.2345778
C	-0.9926019	-1.4311882	-1.8285818
O	-0.3314285	-1.3495856	1.0358662
O	0.2556640	-0.9282225	-1.4297838
P	0.2327859	-0.1710757	0.0225567
O	1.6472528	0.2889747	0.3607649
O	-0.8629175	0.9145506	0.0467172
C	0.3498995	-7.5079273	-0.7597397
C	-0.3423138	-6.8130668	-1.7878029
H	1.3110950	-7.3491503	1.1746377
H	0.5808122	-8.5774813	-0.8790078
H	-1.1788430	-4.9422759	-2.4558654
H	-0.6333765	-7.3450085	-2.7065105
C	-4.7243503	-4.5187886	-1.2257657
C	-5.4222987	-3.8678136	-2.2784635
H	-2.9162814	-4.6265405	-0.0544443
H	-5.2088341	-5.3394734	-0.6750101
H	-6.4377486	-4.1957047	-2.5484452
H	-5.3711390	-2.2765315	-3.7467668
C	2.6644282	-2.0144021	2.7616761
C	1.3648019	-2.5704142	2.9367224
C	3.2201111	-1.2688826	3.8185380
C	0.6616511	-2.3967745	4.1578011
C	1.2749062	-1.6610741	5.1905381
C	2.5505916	-1.0875553	5.0425088
H	4.2147139	-0.8157868	3.6932710
C	-0.7385636	-2.9797731	4.3529373
H	0.7341932	-1.5294626	6.1403567
C	-1.8337470	-1.9290714	4.0837282
H	-1.7459781	-1.0750459	4.7875607
H	-2.8437240	-2.3716043	4.2062635
H	-1.7695572	-1.5294561	3.0535801
C	-0.9279675	-3.6322967	5.7322119
H	-0.8648757	-3.7804226	3.5943659
H	-0.9200348	-2.8829538	6.5510482
H	-0.1310101	-4.3735163	5.9451060
H	-1.9059096	-4.1535868	5.7798954
C	3.1951377	-0.2691073	6.1564208
C	2.5762016	1.1388580	6.2414310
H	3.0785924	1.7445496	7.0244516
H	1.4965401	1.0838088	6.4978258
H	2.6817064	1.6694396	5.2734111
C	3.1556729	-0.9839186	7.5168618
H	4.2626449	-0.1379387	5.8745818
H	3.7158703	-0.4040778	8.2790970
H	3.6033467	-1.9966735	7.4566581
H	2.1161360	-1.0964676	7.8899370
C	3.4827887	-2.2979411	1.4998034
C	4.4596878	-1.1803983	1.1077943
H	4.9075873	-1.4072447	0.1187601
H	5.2970624	-1.0905431	1.8306243
H	3.9606481	-0.1967476	1.0426822
C	4.2497918	-3.6284614	1.6528955
H	2.7641492	-2.4165011	0.6606671
H	4.8188097	-3.8590928	0.7283746
H	3.5748034	-4.4813505	1.8574398
H	4.9733799	-3.5616162	2.4922171
H	-0.1720061	5.0827838	-4.7251762

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H	-5.2488564	2.0553366	-2.3339842
C	0.1172585	4.2382352	-5.3883936
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H	1.8561537	5.3645762	-6.0868715
H	-3.7278839	2.9188537	-0.4271701
C	-0.2720218	2.9612543	-4.6533235
C	0.6710509	-1.1123621	-6.0349331
C	1.6199125	4.3622868	-5.6742745
H	1.9591902	3.6169662	-6.4234245
C	0.3994900	1.7441766	-4.8519143
C	-4.3811188	2.0490297	-3.0256942
H	-1.7916931	4.3383264	-6.4820428
C	-1.3832741	2.9618129	-3.7907084
C	-0.7028468	4.3716827	-6.6876997
H	-0.4777484	5.3273584	-7.2058008
H	-1.9004054	3.9167504	-3.6001925
C	2.2094669	-0.6396217	-4.0583672
H	1.1895487	-2.0749823	-6.2247200
H	-0.3819880	-1.2178065	-6.3666494
C	-0.0253287	0.5448310	-4.2491279
C	-2.9271990	3.0025627	-1.1942341
C	-1.8537274	1.7928396	-3.1667542
H	-4.5337342	1.2288029	-3.7544642
H	-4.3864800	3.0044241	-3.5916610
C	0.7515832	-0.7370424	-4.5435850
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C	-3.0668902	1.8829859	-2.2414529
C	2.2507090	-0.3994034	-2.9780485
H	-1.9377014	2.9737072	-0.6987079
H	2.7704232	0.1433290	-4.6106953
H	2.2254825	4.2140501	-4.7575198
H	-3.0314496	4.0131298	-1.6409965
H	-0.4676399	3.5401895	-7.3849256
H	0.2728575	-1.5632665	-3.9806262
H	-3.1330253	0.9237129	-1.6876502
H	1.2813467	1.7159974	-5.5099153
C	-0.7904048	6.5588066	-1.0747700
C	-0.3369051	5.4523730	-0.3514221
C	0.8288773	4.7683844	-0.7717246
C	1.5353578	5.2107991	-1.9115401
C	1.0864724	6.3305951	-2.6234719
C	-0.0781371	6.9992955	-2.2082704
H	-1.7006378	7.0894492	-0.7569675
H	-0.8723611	5.1003849	0.5430493
C	1.3279927	3.6082511	-0.0269169
H	2.4412379	4.6706160	-2.2297903
H	1.6401759	6.6805096	-3.5072635
H	-0.4357580	7.8747750	-2.7720984
O	0.7939369	3.1798227	1.0020246
H	2.2468297	3.1073268	-0.4288656
C	0.1191561	3.5620812	4.4673818
C	-0.3879616	2.5707168	3.6664352
C	-1.4926548	3.2118525	2.9266300
O	-1.6123381	4.5092706	3.2376940
C	-0.6054889	4.8369583	4.2197839
O	-2.3067279	2.7252731	2.1125769
C	0.0560329	1.2039785	3.3922927
H	-1.1246799	5.2620911	5.1068547
H	0.0392623	5.6357101	3.7888741
H	-0.7495839	0.5706329	2.9697976
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H	0.9726026	3.4768890	5.1524331



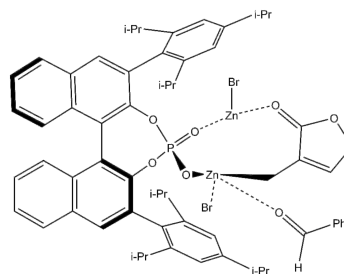
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Br	3.7209288	2.4102063	2.5684619
Zn	-2.4783034	0.9847728	1.1155334
Br	-4.3175109	-0.3591595	1.0554873
C	-0.0521740	-2.6965578	0.8296560
C	-0.6015186	-3.3522726	-0.2770135
C	-0.2787030	-4.7448165	-0.4727258
C	-0.6504472	-5.4694040	-1.6455472
C	0.4727245	-5.4375089	0.5457937
C	0.7605822	-6.8253555	0.3796662
C	0.9509169	-4.7154903	1.6753256
H	1.5247340	-5.2522781	2.4463568
C	0.7511810	-3.3471161	1.8140729
C	-1.7218977	-0.7106257	-2.8262153
C	-2.9477786	-1.2334135	-3.2249527
H	-3.5086876	-0.7257302	-4.0238582
C	-3.5275680	-2.3715082	-2.5986934
C	-4.8360075	-2.8212474	-2.9472089
C	-2.7977092	-3.0607741	-1.5640554
C	-3.4421301	-4.1344354	-0.8806801
C	-1.4684196	-2.6110029	-1.2329985
C	-1.0042666	-1.4322560	-1.8247610
O	-0.3437178	-1.3514567	1.0375591
O	0.2415236	-0.9248638	-1.4264658
P	0.2185368	-0.1688457	0.0270877
O	1.6328002	0.2910546	0.3633779
O	-0.8813398	0.9126450	0.0564570
C	0.3587909	-7.5058038	-0.7591039
C	-0.3391344	-6.8144982	-1.7848222
H	1.3262116	-7.3418935	1.1710392
H	0.5932686	-8.5745584	-0.8780623
H	-1.1843914	-4.9468154	-2.4510561
H	-0.6319498	-7.3481380	-2.7019160
C	-4.7242837	-4.5341444	-1.2289313
C	-5.4240329	-3.8845298	-2.2804216
H	-2.9162325	-4.6358753	-0.0567075
H	-5.2060470	-5.3567325	-0.6788387
H	-6.4384831	-4.2149585	-2.5507155
H	-5.3786889	-2.2904587	-3.7450863
C	2.6573820	-1.9943076	2.7559207
C	1.3635618	-2.5632746	2.9337394
C	3.2092747	-1.2468185	3.8133636
C	0.6632978	-2.4009394	4.1577994
C	1.2746723	-1.6657205	5.1917229
C	2.5438509	-1.0794590	5.0414780
H	4.1980805	-0.7821164	3.6853953
C	-0.7322703	-2.9948559	4.3542820
H	0.7375272	-1.5456174	6.1449676
C	-1.8362119	-1.9542281	4.0818701
H	-1.7565140	-1.0981194	4.7841015
H	-2.8431391	-2.4035344	4.2037203
H	-1.7754064	-1.5555637	3.0512427
C	-0.9175325	-3.6456213	5.7347379
H	-0.8516682	-3.7985154	3.5977106
H	-0.9203123	-2.8944677	6.5519028
H	-0.1128807	-4.3768280	5.9523952

int2

H	-1.8897584	-4.1773256	5.7825910	O	0.7711084	3.1689786	1.0019451
C	3.1867748	-0.2623624	6.1574154	H	2.2996447	3.1222383	-0.3461394
C	2.5713306	1.1471930	6.2411758	C	0.1390024	3.5684137	4.4123714
H	3.0710527	1.7500846	7.0280521	C	-0.3870259	2.5593024	3.6462754
H	1.4901275	1.0945289	6.4918583	C	-1.4953155	3.1888694	2.8993069
H	2.6858415	1.6792179	5.2749285	O	-1.5965938	4.4987147	3.1723427
C	3.1437992	-0.9774028	7.5173581	C	-0.5716817	4.8440864	4.1264716
H	4.2549220	-0.1325723	5.8776373	O	-2.3223558	2.6860717	2.1122552
H	3.7069648	-0.4013879	8.2802053	C	0.0456761	1.1858847	3.4004145
H	3.5850374	-1.9927446	7.4568200	H	-1.0711027	5.3142722	5.0028428
H	2.1041900	-1.0846342	7.8917092	H	0.0815643	5.6134521	3.6550108
C	3.4758335	-2.2680074	1.4918095	H	-0.7594740	0.5498792	2.9826807
C	4.4525799	-1.1478686	1.1069114	H	0.4443827	0.6797501	4.2976295
H	4.8978350	-1.3665956	0.1150591	H	1.0057818	3.4933040	5.0814857
H	5.2923074	-1.0648048	1.8276317				
H	3.9581760	-0.1614892	1.0497934				
C	4.2447120	-3.5983270	1.6369424				
H	2.7574341	-2.3824734	0.6518659				
H	4.8170824	-3.8203580	0.7125507				
H	3.5714191	-4.4546068	1.8317172				
H	4.9652935	-3.5369597	2.4790264				
H	-0.1625543	5.0881720	-4.6745216				
H	1.1313761	-0.3303434	-6.6677956				
H	-5.2707045	2.0409559	-2.3406402				
C	0.1134431	4.2492193	-5.3507971				
H	2.7238653	-1.6010746	-4.2142940				
H	1.8576845	5.3691377	-6.0493146				
H	-3.7602426	2.9065894	-0.4229830				
C	-0.2809172	2.9667477	-4.6277755				
C	0.6542498	-1.1023967	-6.0285067				
C	1.6146584	4.3642493	-5.6468887				
H	1.9417298	3.6261592	-6.4083822				
C	0.3898998	1.7505266	-4.8309665				
C	-4.3993118	2.0409911	-3.0275013				
H	-1.8023846	4.3773741	-6.4283867				
C	-1.3965441	2.9628861	-3.7713280				
C	-0.7151407	4.4056726	-6.6418858				
H	-0.4870405	5.3653219	-7.1513228				
H	-1.9140294	3.9170634	-3.5777652				
C	2.1967810	-0.6381403	-4.0526157				
H	1.1723947	-2.0640247	-6.2238047				
H	-0.3993077	-1.2061679	-6.3584692				
C	-0.0383624	0.5482980	-4.2368748				
C	-2.9573528	2.9946981	-1.1867700				
C	-1.8709283	1.7911858	-3.1561664				
H	-4.5451692	1.2228635	-3.7598076				
H	-4.4054369	2.9974479	-3.5916443				
C	0.7383063	-0.7325461	-4.5361025				
C	-1.1935606	0.5620651	-3.4096207				
C	-3.0888475	1.8769518	-2.2368141				
H	2.2409973	-0.4002964	-2.9720590				
H	-1.9710381	2.9645349	-0.6852382				
H	2.7591894	0.1444536	-4.6039282				
H	2.2261754	4.1979935	-4.7372553				
H	-3.0616372	4.0057977	-1.6327361				
H	-0.4930662	3.5803587	-7.3503240				
H	0.2598010	-1.5602917	-3.9752933				
H	-3.1565962	0.9169624	-1.6844817				
H	1.2746869	1.7246173	-5.4849924				
C	-0.7571136	6.5319996	-1.1345743				
C	-0.3196633	5.4312862	-0.3926320				
C	0.8711989	4.7633690	-0.7633518				
C	1.6174918	5.2153245	-1.8726310				
C	1.1833555	6.3282041	-2.6041953				
C	-0.0053904	6.9818893	-2.2377249				
H	-1.6867472	7.0501186	-0.8542494				
H	-0.8856885	5.0709932	0.4795599				
C	1.3515556	3.6073884	0.0053118				
H	2.5421013	4.6861400	-2.1534995				
H	1.7667303	6.6826794	-3.4668255				
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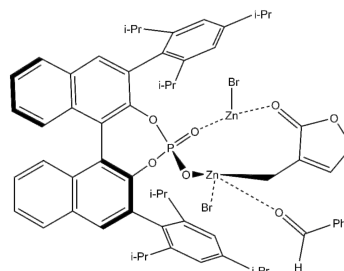


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Zn	1.9922417	0.2441620	2.3805004
Br	4.1161264	-0.1134971	3.3506100
Zn	-2.4137248	0.2174932	0.8431812
Br	-4.2213063	-0.8083476	-0.0977585
C	-0.3885822	-2.8184610	-0.5817413
C	-0.7417912	-2.8843653	-1.9340466
C	-0.4915460	-4.1239553	-2.6321920
C	-0.6351175	-4.2569481	-4.0464912
C	-0.0497981	-5.2747183	-1.8810137
C	0.1598785	-6.5134799	-2.5591473
C	0.2161537	-5.1455139	-0.4883563
H	0.5707945	-6.0253889	0.0701955
C	0.1105321	-3.9244849	0.1674587
C	-1.2364403	0.7166124	-3.1976645
C	-2.3608306	0.5592096	-4.0010937
H	-2.7462473	1.4263784	-4.5575638
C	-3.0748241	-0.6694716	-4.0719901
C	-4.2908107	-0.7704482	-4.8128817
C	-2.6013853	-1.8124076	-3.3313984
C	-3.4166925	-2.9828202	-3.3033081
C	-1.3506285	-1.7096816	-2.6178538
C	-0.7369412	-0.4552677	-2.5502470
O	-0.5717242	-1.6266732	0.1225821
O	0.4579519	-0.3277295	-1.8296413
P	0.3305145	-0.2703926	-0.2038923
O	1.7370585	-0.2641291	0.3686281
O	-0.6593984	0.8332268	0.2652105
C	-0.0197271	-6.6151720	-3.9302659
C	-0.4039736	-5.4706718	-4.6791824
H	0.4858273	-7.3852978	-1.9703774
H	0.1518331	-7.5743532	-4.4421066
H	-0.9229714	-3.3790825	-4.6410463
H	-0.5141444	-5.5440889	-5.7719070
C	-4.6070158	-3.0421550	-4.0142414
C	-5.0415855	-1.9356898	-4.7921707
H	-3.1031318	-3.8408412	-2.6936580
H	-5.2236033	-3.9527411	-3.9673380
H	-5.9831611	-1.9987451	-5.3587157

H	-4.6329610	0.1072329	-5.3835222	H	2.4372486	5.4054808	-0.5887067
C	1.9638774	-3.7183862	1.8510568	H	-3.0125668	4.3174762	-0.1338001
C	0.5687441	-3.7329844	1.5778911	H	1.7774359	6.3552906	-4.2529972
C	2.3828340	-3.5459889	3.1849310	H	0.9722818	0.4106421	-4.2278986
C	-0.3747244	-3.5544856	2.6279955	H	-2.9530261	1.6755998	-1.7309904
C	0.0990240	-3.4054625	3.9431283	H	2.2436192	3.8654356	-3.4705630
C	1.4749393	-3.4066927	4.2465795	C	2.2986972	6.5832571	2.5099919
H	3.4607885	-3.5189499	3.4078723	C	2.3362028	5.1956670	2.3463895
C	-1.8761324	-3.6199297	2.3466623	C	1.2128338	4.5233970	1.8095081
H	-0.6295603	-3.2890137	4.7603395	C	0.0541136	5.2497136	1.4524251
C	-2.7120263	-2.6328503	3.1746786	C	0.0207868	6.6402589	1.6213064
H	-2.7076272	-2.8794519	4.2566592	C	1.1439377	7.3051195	2.1445871
H	-3.7664823	-2.6404732	2.8336047	H	3.1708010	7.1143036	2.9204553
H	-2.3374150	-1.5925795	3.0767452	H	3.2238788	4.6043872	2.6182639
C	-2.3870870	-5.0630707	2.5222799	C	1.2268733	3.0698288	1.6178777
H	-2.0327957	-3.3497315	1.2821035	H	-0.8121067	4.7135434	1.0364741
H	-2.2526490	-5.4031183	3.5706085	H	-0.8778644	7.2097234	1.3403989
H	-1.8335250	-5.7653137	1.8664577	H	1.1212935	8.3985568	2.2711380
H	-3.4657635	-5.1355452	2.2714192	O	2.1887306	2.3503977	1.9249520
C	1.9795260	-3.2665864	5.6791219	H	0.3132006	2.6153876	1.1568401
C	1.7714116	-1.8444156	6.2306165	C	0.0642950	2.3777351	4.5488013
H	2.1792915	-1.7599017	7.2594614	C	-0.3899941	1.3581086	3.7458728
H	0.6916928	-1.5868761	6.2786192	C	-1.7082458	1.8245519	3.2637200
H	2.2871274	-1.0969630	5.5939082	O	-2.0093950	3.0409423	3.7404825
C	1.3657911	-4.3258082	6.6111160	C	-0.9348383	3.4766369	4.6004530
H	3.0765419	-3.4437479	5.6441585	O	-2.5421396	1.2480705	2.5332280
H	1.8121959	-4.2623525	7.6250819	C	0.2051854	0.0773606	3.3728949
H	1.5330992	-5.3516526	6.2245337	H	-1.3627461	3.6642580	5.6101398
H	0.2704020	-4.1829949	6.7232417	H	-0.5608040	4.4486466	4.2057722
C	3.0138094	-3.9293608	0.7590240	H	-0.4987421	-0.5596205	2.8058242
C	4.0724117	-2.8161640	0.7119294	H	0.5294033	-0.4941847	4.2622836
H	4.7846172	-3.0051610	-0.1181135	H	1.0241566	2.4040174	5.0826936
H	4.6578307	-2.7497944	1.6509642				
H	3.6020718	-1.8282351	0.5483844				
C	3.6683593	-5.3170570	0.9033570				
H	2.4900158	-3.9130824	-0.2178886				
H	4.3893224	-5.4989489	0.0793741				
H	2.9142542	-6.1303653	0.8857702				
H	4.2229819	-5.3976244	1.8617455				
H	0.3809552	6.5356969	-1.4991543				
H	2.2735383	2.8006139	-5.6819079				
H	-4.8847122	3.1778845	-2.2040243				
C	1.0731472	6.0187301	-2.2001222				
H	3.4335228	0.2921967	-4.0659254				
H	2.8073358	7.0082459	-1.3004858				
H	-3.9145220	2.8123998	0.1759046				
C	0.4970915	4.6284169	-2.4387774				
C	1.7112078	1.8443632	-5.6374289				
C	2.4587078	5.9814469	-1.5347058				
H	3.2183118	5.5173258	-2.1974897				
C	1.2242137	3.6377063	-3.1210340				
C	-3.8714860	3.4252241	-2.5826986				
H	0.0947735	6.8966513	-3.9661713				
C	-0.8023796	4.3061441	-2.0131054				
C	1.1029363	6.8298342	-3.5095497				
H	1.4706135	7.8615399	-3.3296147				
H	-1.3839694	5.0752251	-1.4791422				
C	2.8830957	1.0780118	-3.5087675				
H	2.2757065	1.0941849	-6.2290886				
H	0.7320257	2.0067658	-6.1323338				
C	0.6908212	2.3635754	-3.3873673				
C	-2.9670258	3.2133624	-0.2395681				
C	-1.3813389	3.0430279	-2.2383472				
H	-3.8094801	3.0870133	-3.6353349				
H	-3.7655139	4.5305518	-2.5814222				
C	1.5306766	1.3672185	-4.1837352				
C	-0.6276465	2.0610442	-2.9471195				
C	-2.7884161	2.7728742	-1.7034284				
H	2.7424946	0.7263871	-2.4681243				
H	-2.1299302	2.8581840	0.3926333				
H	3.5298839	1.9798554	-3.4844731				

int3



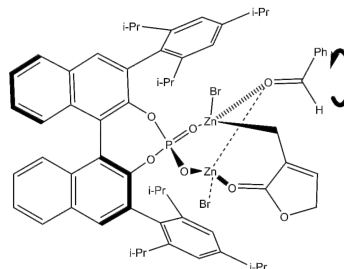
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Zn	-2.4147914	0.2223256	0.8413219
Br	-4.2287432	-0.7912275	-0.0898728
C	-0.3922475	-2.8135058	-0.5834818
C	-0.7476462	-2.8841871	-1.9349058
C	-0.4950700	-4.1246370	-2.6301890
C	-0.6451354	-4.2632478	-4.0430258
C	-0.0440551	-5.2706674	-1.8774834
C	0.1686872	-6.5096755	-2.5532069
C	0.2262322	-5.1359112	-0.4863899
H	0.5881835	-6.0115287	0.0740954
C	0.1150342	-3.9145683	0.1674581
C	-1.2441754	0.7138729	-3.2048242
C	-2.3690886	0.5547555	-4.0067652
H	-2.7542528	1.4215562	-4.5639664
C	-3.0836734	-0.6735217	-4.0747320
C	-4.3002305	-0.7766972	-4.8135210
C	-2.6096417	-1.8147190	-3.3319996
C	-3.4250035	-2.9847519	-3.3001893
C	-1.3580832	-1.7111896	-2.6203522
C	-0.7436024	-0.4568623	-2.5555615

O	-0.5792941	-1.6209176	0.1172134	H	1.4823560	7.8531275	-3.3210899
O	0.4509769	-0.3275447	-1.8375224	H	-1.3848374	5.0737184	-1.4891186
P	0.3270912	-0.2673047	-0.2110227	C	2.8783297	1.0677557	-3.5155146
O	1.7336092	-0.2659703	0.3588004	H	2.2650343	1.0867610	-6.2352022
O	-0.6620993	0.8392366	0.2541014	H	0.7217042	1.9992951	-6.1340303
C	-0.0175428	-6.6171400	-3.9224674	C	0.6868079	2.3561957	-3.3907886
C	-0.4117916	-5.4776369	-4.6726646	C	-2.9822163	3.2214024	-0.2588325
H	0.5026768	-7.3776089	-1.9632440	C	-1.3871394	3.0424558	-2.2497686
H	0.1564829	-7.5771453	-4.4318196	H	-3.8077626	3.0940825	-3.6582604
H	-0.9410823	-3.3884394	-4.6379146	H	-3.7642527	4.5382215	-2.6073759
H	-0.5280144	-5.5551733	-5.7644296	C	1.5250771	1.3588408	-4.1875056
C	-4.6156495	-3.0455517	-4.0096781	C	-0.6342715	2.0579969	-2.9557076
C	-5.0509051	-1.9413198	-4.7893395	C	-2.7976403	2.7782648	-1.7210143
H	-3.1098749	-3.8405170	-2.6883607	H	2.7410933	0.7164040	-2.4745729
H	-5.2323823	-3.9557368	-3.9592967	H	-2.1490111	2.8661120	0.3781894
H	-5.9934014	-2.0051214	-5.3541128	H	3.5278246	1.9676759	-3.4933183
H	-4.6433583	0.0999688	-5.3851075	H	2.4425433	5.3844131	-0.5870880
C	1.9651620	-3.6867237	1.8531836	H	-3.0275459	4.3259592	-0.1550890
C	0.5706985	-3.7178707	1.5780327	H	1.7833589	6.3483444	-4.2481078
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C	-0.3764850	-3.5512223	2.6264226	H	-2.9669141	1.6817448	-1.7465521
C	0.0936126	-3.4028130	3.9427101	H	2.2462100	3.8506441	-3.4644382
C	1.4685783	-3.3885892	4.2485324	C	2.2926874	6.5583478	2.5391453
H	3.4565399	-3.4670629	3.4122072	C	2.3285726	5.1730395	2.3563977
C	-1.8769563	-3.6245355	2.3418626	C	1.2058967	4.5097064	1.8088885
H	-0.6377107	-3.2973086	4.7590291	C	0.0490437	5.2412041	1.4599509
C	-2.7187125	-2.6394855	3.1665184	C	0.0175781	6.6296918	1.6478334
H	-2.7209447	-2.8879992	4.2481445	H	1.1398278	7.2865515	2.1818550
H	-3.7708749	-2.6457137	2.8186733	C	3.1649538	7.0827143	2.9579863
H	-2.3436239	-1.5989733	3.0730247	H	3.2130681	4.5730395	2.6201966
C	-2.3826159	-5.0692766	2.5173496	C	1.2228590	3.0554235	1.5998671
H	-2.0332062	-3.3554463	1.2769910	H	-0.8164474	4.7107247	1.0351934
H	-2.2462151	-5.4098000	3.5651660	H	-0.8800295	7.2037732	1.3726126
H	-1.8264033	-5.7691731	1.8615114	H	1.1181646	8.3782673	2.3229755
H	-3.4609532	-5.1463872	2.2666441	O	2.1863715	2.3397663	1.9008762
C	1.9687214	-3.2474848	5.6825182	H	0.3100775	2.6036867	1.1337447
C	1.7417770	-1.8305953	6.2399655	C	0.1049905	2.3406138	4.5590229
H	2.1391017	-1.7480721	7.2730832	C	-0.3654209	1.3386740	3.7418354
H	0.6592504	-1.5833046	6.2797469	C	-1.6740272	1.8355865	3.2590032
H	2.2591595	-1.0757372	5.6133372	O	-1.9531214	3.0543912	3.7494857
C	1.3681568	-4.3199803	6.6076550	C	-0.8734513	3.4592623	4.6156108
H	3.0681052	-3.4087515	5.6483469	O	-2.5143031	1.2844827	2.5206159
H	1.8125025	-4.2575529	7.6225490	C	0.2064501	0.0573238	3.3503506
H	1.5477547	-5.3411708	6.2148185	H	-1.3033591	3.6491968	5.6248946
H	0.2709659	-4.1924973	6.7204680	H	-0.4780297	4.4265749	4.2287989
C	3.0189883	-3.8874426	0.7628968	H	-0.5049712	-0.5635142	2.7755371
C	4.0817100	-2.7777463	0.7289563	H	0.5382351	-0.5300929	4.2260645
H	4.7995415	-2.9660435	-0.0961735	H	1.0665879	2.3398651	5.0903260
H	4.6612005	-2.7148022	1.6716984				
H	3.6186443	-1.7870273	0.5633770				
C	3.6700199	-5.2778027	0.8990989				
H	2.4985198	-3.8621736	-0.2158403				
H	4.3936708	-5.4555782	0.0766828				
H	2.9152387	-6.0901645	0.8742088				
H	4.2207607	-5.3662194	1.8588332				
H	0.3887480	6.5245389	-1.4932492				
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H	3.4261513	0.2808083	-4.0733797				
H	2.8163488	6.9896342	-1.2919070				
H	-3.9310449	2.8209807	0.1536990				
C	0.4988756	4.6199947	-2.4394079				
C	1.7018014	1.8362144	-5.6415359				
C	2.4645222	5.9648646	-1.5301616				
H	3.2236430	5.5016767	-2.1939372				
C	1.2241683	3.6274059	-3.1200279				
C	-3.8739987	3.4332630	-2.6063033				
H	0.1036821	6.8931731	-3.9594775				
C	-0.8037183	4.3025913	-2.0208439				
C	1.1113233	6.8229397	-3.5027195				

7.10.2 Pathway 14d-ma ↔ 14j-mi

TS1; COSMO

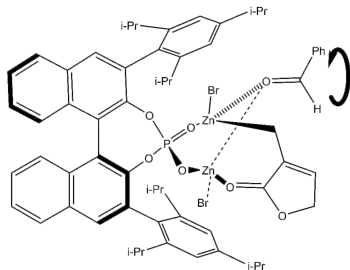


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C	4.7494049	3.5093300	1.1925631

C	2.5910792	4.6167270	1.6180761	C	1.6205479	-5.8347774	-2.8182133
C	3.2733518	5.8709923	1.6170972	H	3.2004585	0.3308573	-3.9789524
C	1.1744998	4.5503488	1.7426705	H	-0.1046681	-6.3200832	-4.0942646
H	0.6090474	5.4868199	1.8676075	H	0.8684934	-4.0710757	3.2783527
C	0.4807119	3.3484274	1.6465285	C	2.1374472	-4.6690026	-1.9847910
C	3.6729116	-1.4288032	0.4554790	C	5.0593093	-1.6335197	-3.2906436
C	4.7715596	-1.6426961	1.2811314	C	0.2989971	-5.4640540	-3.5134541
H	5.3157348	-2.5968735	1.2102885	H	0.4554987	-4.6204074	-4.2202631
C	5.1659880	-0.7002920	2.2722952	C	2.6674019	-3.5122956	-2.5841823
C	6.2356862	-0.9855763	3.1741105	C	3.3531214	-4.8512189	2.3072101
C	4.4318202	0.5346031	2.4132421	H	3.6080387	-6.6324834	-3.3168159
C	4.7592676	1.3893420	3.5093869	C	2.0704358	-4.7090556	-0.5839513
C	3.3828095	0.8343412	1.4663679	C	2.6637366	-6.3492452	-3.8241979
C	3.0277370	-0.1579643	0.5448763	H	2.2824624	-7.2397207	-4.3656440
O	0.5631769	0.9427260	1.5325350	H	1.6221707	-5.5939689	-0.1043712
O	2.0161058	0.1032015	-0.3747106	C	2.7558381	-0.5683113	-3.5047683
P	0.4517479	0.1122025	0.1169536	H	5.7998380	-2.0740481	-2.5922157
O	-0.2913745	0.9542860	-0.9296940	H	5.5245005	-0.7488055	-3.7729191
O	-0.0682843	-1.2845264	0.4520417	C	3.1603256	-2.4348810	-1.8257996
C	4.6424804	5.9377072	1.4073319	C	0.9442843	-4.0599893	2.1709588
C	5.3803441	4.7458136	1.1757099	C	2.5399796	-3.6578900	0.2244198
H	2.6841221	6.7893091	1.7677820	H	3.2722649	-4.9068482	3.4127945
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H	5.3318601	2.5972417	1.0028548	C	3.7655327	-1.2365097	-2.5546398
H	6.4611611	4.8022817	0.9750301	C	3.1200265	-2.5192069	-0.4066821
C	5.7917349	1.0735541	4.3823052	C	2.3963976	-3.7843825	1.7424531
C	6.5513142	-0.1139684	4.2054012	H	1.8429753	-0.2451779	-2.9681503
H	4.1761182	2.3067230	3.6674757	H	0.2663194	-3.2799591	1.7778121
H	6.0186195	1.7476961	5.2223869	H	2.4439197	-1.2509513	-4.3225168
H	7.3736844	-0.3489153	4.8982441	H	-0.4625593	-5.1578017	-2.7675207
H	6.7935387	-1.9263597	3.0446172	H	0.5769176	-5.0389773	1.8008733
C	-1.6927647	3.8708333	0.4705231	H	2.9090995	-5.5795711	-4.5856057
C	-1.0134751	3.3026531	1.5903041	H	4.0488028	-0.4831423	-1.7923806
C	-3.0952202	3.7888489	0.4233344	H	2.6808803	-2.8116136	2.1906863
C	-1.7606447	2.6879108	2.6312734	H	2.7168457	-3.4491596	-3.6832552
C	-3.1660352	2.6588673	2.5424040	Zn	-1.5610066	0.7159319	-2.3744648
C	-3.8581728	3.1977385	1.4465656	Br	-0.9955787	0.9157043	-4.6169624
C	-1.0957473	2.1001400	3.8752267	Zn	-1.9799665	-1.8960821	0.1410183
H	-3.7299923	2.1887424	3.3610701	Br	-2.1018646	-4.1996853	-0.3698800
C	-1.4331727	0.6109562	4.0699838	H	-3.6197165	4.2059280	-0.4520925
H	-2.5200071	0.4558018	4.2357039	C	-5.4974259	-2.9848016	-4.3040696
H	-0.9022932	0.2060152	4.9561935	C	-4.4596343	-2.3965671	-3.5806671
H	-1.1276778	0.0164480	3.1873976	C	-3.1371049	-2.8882976	-3.7146680
C	-1.4450818	2.9282011	5.1265537	C	-2.8716438	-3.9696715	-4.5886709
H	0.0022206	2.1722652	3.7406374	C	-3.9162713	-4.5568414	-5.3107129
H	-2.5331966	2.8941664	5.3447817	C	-5.2266737	-4.0669887	-5.1666402
H	-1.1622513	3.9925291	4.9955196	H	-6.5255320	-2.6048988	-4.2059859
H	-0.9115456	2.5372285	6.0176848	C	-2.0453546	-2.2736170	-2.9782199
C	-5.3818476	3.2001148	1.3424122	H	-1.8425546	-4.3422775	-4.6938434
C	-6.0816821	2.2356138	2.3071940	H	-3.7127310	-5.3980584	-5.9896362
H	-7.1707813	2.2044569	2.0999731	H	-6.0482519	-4.5300069	-5.7346920
H	-5.9601130	2.5568938	3.3627376	O	-2.2107308	-1.2886094	-2.2157070
H	-5.6856035	1.2046684	2.2169862	H	-4.6429894	-1.5490719	-2.9063738
C	-5.9322277	4.6309464	1.5134604	H	-1.0199057	-2.6870672	-3.1331473
H	-5.6263845	2.8781996	0.3033991	C	-5.6705314	-0.5776158	0.0423483
H	-7.0324787	4.6539582	1.3697155	C	-4.3732768	-0.1557048	-0.0703593
H	-5.4772109	5.3340129	0.7876186	C	-4.3468870	0.7036700	-1.2759084
H	-5.7111628	5.0109896	2.5329142	O	-5.5758182	0.8085852	-1.8220054
C	-0.9720981	4.6098653	-0.6600959	C	-6.4963549	0.0177851	-1.0435607
C	-1.2150865	3.9937386	-2.0483441	O	-3.4006498	1.3123812	-1.8029685
H	-0.8030043	4.6450099	-2.8458219	C	-3.1825349	-0.3949401	0.7469885
H	-2.2909552	3.8375193	-2.2666047	H	-6.9691778	-0.7225519	-1.7277405
H	-0.6893249	3.0233450	-2.1349109	H	-7.3019687	0.6903430	-0.6724233
C	-1.3433299	6.1060869	-0.6417626	H	-3.4584045	-0.6364581	1.7925777
H	0.1172221	4.5420559	-0.4739297	H	-2.5424299	0.5100728	0.7587566
H	-0.7536753	6.6653967	-1.3972011	H	-6.0829441	-1.2287411	0.8246965
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H	-2.4183192	6.2604082	-0.8722403				
H	1.3989782	-6.6622766	-2.1091256				
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TS1



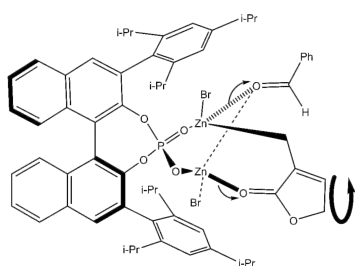
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H	0.6054406	5.4853224	1.8654760
C	0.4783058	3.3475319	1.6478038
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C	4.7665230	-1.6435353	1.2745754
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C	5.1621900	-0.7054551	2.2689768
C	6.2320876	-0.9934151	3.1688993
C	4.4284961	0.5288935	2.4149576
C	4.7573680	1.3797212	3.5133709
C	3.3792058	0.8325171	1.4699146
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O	0.5598338	0.9421162	1.5365425
O	2.0120378	0.1085007	-0.3735741
P	0.4484582	0.1149755	0.1180089
O	-0.3018960	0.9566836	-0.9225436
O	-0.0667666	-1.2844855	0.4509961
C	4.6412388	5.9349080	1.4223557
C	5.3789586	4.7431047	1.1934729
H	2.6821870	6.7870130	1.7748152
H	5.1545627	6.9084854	1.4180302
H	5.3293130	2.5944898	1.0197861
H	6.4605273	4.7988158	0.9970132
C	5.7905105	1.0609745	4.3836962
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H	4.1743541	2.2966866	3.6738095
H	6.0185462	1.7325734	5.2254367
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C	-1.6895119	3.8647642	0.4599854
C	-1.0156073	3.3023082	1.5855894
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C	-5.3826948	3.2153887	1.3266935
C	-6.0906948	2.2567309	2.2914693
H	-7.1805402	2.2347503	2.0860744

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C	2.1266644	-4.6579273	-1.9962953
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H	0.4826584	-4.6115719	-4.2658578
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H	3.6035385	-6.6332879	-3.2924345
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C	2.6691258	-6.3505803	-3.8175676
H	2.2936784	-7.2435436	-4.3590954
H	1.5958160	-5.5799238	-0.1190400
C	2.7617574	-0.5535836	-3.5027948
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H	5.5302336	-0.7479600	-3.7753347
C	3.1590549	-2.4289566	-1.8324113
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C	2.5238177	-3.6500255	0.2144163
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H	3.1112250	-5.8437352	1.8896801
C	3.7696281	-1.2312116	-2.5576163
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C	2.3776196	-3.7773321	1.7322044
H	1.8527602	-0.2245476	-2.9637883
H	0.2426523	-3.2937106	1.7640159
H	2.4422251	-1.2309038	-4.3219814
H	-0.4626363	-5.1235962	-2.8198048
H	0.5685181	-5.0489435	1.7958802
H	2.9318212	-5.5880253	-4.5802402
H	4.0578857	-0.4826684	-1.7923257
H	2.6542737	-2.8023623	2.1807808
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Br	-0.9931671	0.8617939	-4.6258245
Zn	-1.9676358	-1.9125963	0.1235843
Br	-2.0851155	-4.2047656	-0.4144302
H	-3.6122034	4.1990967	-0.4706456
C	-5.5012996	-3.0583779	-4.2329431
C	-4.4665621	-2.4602544	-3.5131678
C	-3.1331675	-2.9011107	-3.6951147
C	-2.8536460	-3.9420892	-4.6108943
C	-3.8949095	-4.5378046	-5.3307927
C	-5.2165611	-4.0984303	-5.1404249
H	-6.5390655	-2.7183788	-4.0962258
C	-2.0435029	-2.2678640	-2.9666712
H	-1.8157110	-4.2773261	-4.7491315
H	-3.6795002	-5.3476473	-6.0434890
H	-6.0356643	-4.5688047	-5.7061263

O	-2.2221595	-1.2903366	-2.1985507
H	-4.6589253	-1.6461211	-2.8011755
H	-1.0102657	-2.6509231	-3.1453044
C	-5.6595474	-0.5914633	0.0685350
C	-4.3614058	-0.1728954	-0.0451558
C	-4.3352584	0.6963725	-1.2480276
O	-5.5699949	0.8104717	-1.7851516
C	-6.4875125	0.0196410	-1.0088043
O	-3.3907807	1.3000740	-1.7758539
C	-3.1703108	-0.4202844	0.7652584
H	-6.9699514	-0.7115800	-1.6972175
H	-7.2866469	0.6942205	-0.6254822
H	-3.4404962	-0.6739655	1.8093240
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H	-6.0691689	-1.2472062	0.8483832

TS2; COSMO



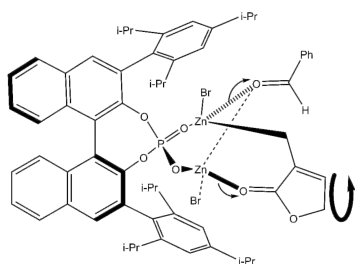
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C	2.4487335	4.6817085	1.3877500
C	3.1716707	5.9022474	1.2296062
C	1.0691064	4.6902510	1.7531189
H	0.5821427	5.6552487	1.9588254
C	0.3284716	3.5180987	1.8293213
C	3.1449248	-1.4059487	0.1822684
C	4.3120809	-1.6799486	0.8835644
H	4.8368466	-2.6314728	0.7077633
C	4.8388131	-0.7676801	1.8432446
C	5.9899593	-1.1007104	2.6187920
C	4.1879176	0.5042722	2.0547647
C	4.6914314	1.3548356	3.0851864
C	3.0399362	0.8499970	1.2482883
C	2.5266348	-0.1393276	0.4002836
O	0.2851294	1.1267085	1.7050673
O	1.3949122	0.1170302	-0.3635516
P	-0.0818092	0.3387128	0.3218668
O	-0.7715572	1.3023527	-0.6850849
O	-0.8103283	-0.9254710	0.7583531
C	4.4978846	5.9012527	0.8228933
C	5.1521948	4.6711303	0.5478111
H	2.6473484	6.8510265	1.4243612
H	5.0396964	6.8512764	0.6990867
H	4.9992626	2.5199747	0.4863722
H	6.1962132	4.6729438	0.1990213
C	5.8021060	0.9928150	3.8352733
C	6.4691852	-0.2375174	3.5926407
H	4.1803152	2.3048298	3.2933490
H	6.1638506	1.6635329	4.6295449
H	7.3534115	-0.5101371	4.1886161
H	6.4820406	-2.0692052	2.4375114
C	-2.1051132	3.8342598	1.1755269
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C	-3.4667526	3.6180659	1.4625994
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C	-2.9239064	2.6191429	3.5832532
C	-3.9000544	2.9914534	2.6434171
C	-0.5600878	2.4218295	4.4472639
H	-3.2360068	2.1322184	4.5199403
C	-0.6962288	0.9418334	4.8437463
H	-1.6762493	0.7260439	5.3168756
H	0.0924418	0.6633099	5.5728939
H	-0.6033073	0.2779139	3.9628823
C	-0.6874233	3.3512914	5.6696619
H	0.4641462	2.5625303	4.0456851
H	-1.6915260	3.2653750	6.1354175
H	-0.5380654	4.4133191	5.3866649
H	0.0658547	3.0906125	6.4419339
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C	-5.6600559	1.3039847	3.3891547
H	-6.7516671	1.1088031	3.4262113
H	-5.2638647	1.1423797	4.4128486
H	-5.1899563	0.5369375	2.7413890
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H	-5.8910680	2.8494017	1.9045743
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H	-5.8190413	4.8120876	3.4582690
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H	-3.5932143	4.3662118	-1.3132977
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H	-0.6608537	4.1692527	-0.3614735
H	-1.4387457	6.4631671	-1.0340023
H	-1.1141555	6.4009208	0.7293359
H	-2.7980637	6.3494966	0.1326816
H	0.1520568	-5.6339058	-3.4121786
H	4.6280058	-1.9665006	-4.4102444
H	3.3727026	-4.1778776	1.7939036
C	1.2200076	-5.4114143	-3.6390958
H	3.1856175	0.8183061	-3.9213680
H	0.8896080	-5.8616084	-5.7475301
H	-0.3972477	-3.9619138	2.3491636
C	1.6411953	-4.2941000	-2.6886029
C	4.8647017	-1.3772252	-3.4998376
C	1.3116140	-5.0471797	-5.1250957
H	2.3655499	-4.9035113	-5.4432929
C	2.3793237	-3.1745795	-3.1043965
C	2.3273165	-4.5417257	1.8403275
H	1.9314279	-7.0047108	-2.2852943
C	1.3144575	-4.3892415	-1.3196646
C	2.0273610	-6.6926930	-3.3444735
H	1.6830252	-7.5328235	-3.9824739
H	0.6946987	-5.2359303	-0.9829761
C	2.6643311	-0.1006357	-3.5837517
H	5.5418433	-1.9886206	-2.8695506
H	5.4197382	-0.4731282	-3.8246257
C	2.8410992	-2.2030759	-2.1937760
C	-0.0965984	-4.0597856	1.2869486
C	1.7529031	-3.4494385	-0.3703382
H	2.0442950	-4.6305827	2.9095055
H	2.3039706	-5.5587668	1.3949705
C	3.5921030	-0.9854529	-2.7288521
C	2.5683136	-2.3696885	-0.8115343
C	1.3584634	-3.6009795	1.0984606
H	1.7733248	0.2082812	-3.0021435
H	-0.7924889	-3.4305910	0.6998177
H	2.3051054	-0.6378105	-4.4863922
H	0.7541892	-4.1197329	-5.3610105
H	-0.2407286	-5.1214980	0.9961776
H	3.1059158	-6.5266951	-3.5488922
H	3.9147692	-0.3779828	-1.8585366

H	1.4412100	-2.5953616	1.5618022
H	2.6096855	-3.0448901	-4.1719012
Zn	-0.8630094	0.8629762	-2.5440437
Br	-1.0692004	1.9450886	-4.5328166
Zn	-2.7740057	-0.7338099	1.3972092
Br	-3.0459390	-1.9768581	3.3425612
H	-4.2235959	3.9125030	0.7183984
C	-1.3485190	-2.2949219	-6.3590431
C	-1.0045302	-1.8563352	-5.0772388
C	-1.3337088	-2.6497417	-3.9528685
C	-2.0118113	-3.8786811	-4.1249729
C	-2.3587694	-4.3097255	-5.4096497
C	-2.0246269	-3.5196181	-6.5248445
H	-1.0918192	-1.6820983	-7.2359417
C	-1.0003763	-2.2191932	-2.6023718
H	-2.2814300	-4.4747701	-3.2399226
H	-2.8929127	-5.2614597	-5.5476194
H	-2.2943261	-3.8612393	-7.5361065
O	-0.5480132	-1.0973112	-2.2982792
H	-0.4807419	-0.8996355	-4.9339735
H	-1.1318111	-2.9597700	-1.7801956
C	-6.2249627	-0.8518033	-0.0784251
C	-4.9329008	-0.6406436	-0.4558507
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O	-5.7637546	-2.3691189	-1.7909629
C	-6.8099580	-1.9588051	-0.8963852
O	-3.6176157	-1.7681159	-2.1884864
C	-3.8688622	0.2458980	0.0322425
H	-7.1194538	-2.8397249	-0.2885838
H	-7.6914078	-1.6493935	-1.5027259
H	-4.2459035	1.1769533	0.4938364
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TS2



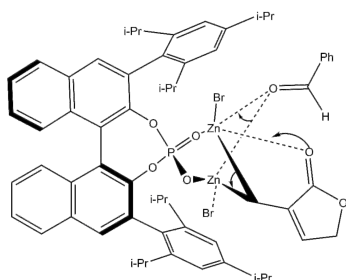
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C	2.4496982	4.6850800	1.3794758
C	3.1740946	5.9039846	1.2198680
C	1.0707117	4.6944901	1.7465371
H	0.5837712	5.6595518	1.9519499
C	0.3289399	3.5234840	1.8252981
C	3.1329626	-1.4064731	0.1829753
C	4.2975491	-1.6834260	0.8869158
H	4.8169510	-2.6384826	0.7141289
C	4.8277711	-0.7709882	1.8440302
C	5.9766120	-1.1055781	2.6213900
C	4.1822452	0.5042724	2.0506175
C	4.6891707	1.3562379	3.0778461
C	3.0360096	0.8523779	1.2428529
C	2.5192883	-0.1367193	0.3964542
O	0.2843268	1.1331451	1.7024524
O	1.3885165	0.1207762	-0.3674049

P	-0.0882132	0.3436715	0.3216622
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O	-0.8140414	-0.9192808	0.7623512
C	4.4998186	5.9017172	0.8132758
C	5.1527439	4.6712396	0.5395711
H	2.6505454	6.8534206	1.4134466
H	5.0422268	6.8512144	0.6885139
H	4.9972792	2.5199958	0.4808224
H	6.1968676	4.6716605	0.1912312
C	5.7977386	0.9923080	3.8292875
C	6.4592668	-0.2413360	3.5918198
H	4.1817189	2.3090625	3.2813660
H	6.1620809	1.6645587	4.6209889
H	7.3418743	-0.5158499	4.1892197
H	6.4642233	-2.0771033	2.4442957
C	-2.1062342	3.8375404	1.1773788
C	-1.1340298	3.4413732	2.1388023
C	-3.4664800	3.6197936	1.4682509
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C	-2.9172181	2.6227005	3.5873914
C	-3.8960304	2.9936834	2.6503351
C	-0.5517271	2.4291647	4.4465108
H	-3.2259554	2.1339606	4.5241087
C	-0.6843181	0.9494677	4.8453606
H	-1.6623316	0.7309502	5.3209854
H	0.1063351	0.6732086	5.5730492
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H	-0.5315609	4.4224540	5.3828021
H	0.0765062	3.1024175	6.4391692
C	-5.3769846	2.7338409	2.8996529
C	-5.6551759	1.3074703	3.4040001
H	-6.7469084	1.1135594	3.4458503
H	-5.2563945	1.1458034	4.4264644
H	-5.1878688	0.5375492	2.7578933
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H	-5.8893584	2.8513531	1.9181527
H	-7.0535110	3.6337592	4.0030668
H	-5.8096323	4.8161106	3.4691809
H	-5.4762630	3.7292253	4.8519454
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H	-2.1189692	4.2983576	-2.3026047
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H	0.1430807	-5.6320987	-3.4173686
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H	3.3355466	-4.1722906	1.8085447
C	1.2130018	-5.4126163	-3.6389830
H	3.2070948	0.8103354	-3.9211724
H	0.8913977	-5.8657923	-5.7487373
H	-0.4392385	-3.9411064	2.3336812
C	1.6323114	-4.2945512	-2.6884056
C	4.8721438	-1.3948703	-3.4866522
C	1.3118517	-5.0513982	-5.1252558
H	2.3675426	-4.9112574	-5.4388840
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C	2.2887378	-4.5325954	1.8477174
H	1.9153437	-7.0044135	-2.2789539
C	1.2988218	-4.3858775	-1.3211248
C	2.0157895	-6.6951803	-3.3383418
H	1.6733854	-7.5364125	-3.9759233
H	0.6750961	-5.2300012	-0.9851215
C	2.6792615	-0.1052773	-3.5848160

H	5.5416060	-2.0094188	-2.8515755
H	5.4348961	-0.4950164	-3.8098701
C	2.8365630	-2.2073396	-2.1915496
C	-0.1293059	-4.0446514	1.2748883
C	1.7345963	-3.4458536	-0.3710054
H	1.9970621	-4.6162478	2.9147599
H	2.2660548	-5.5513403	1.4063954
C	3.5970952	-0.9946450	-2.7243138
C	2.5560936	-2.3701922	-0.8105854
C	1.3286512	-3.5915219	1.0952434
H	1.7870876	0.2097183	-3.0088423
H	-0.8190150	-3.4151712	0.6810088
H	2.3215718	-0.6407190	-4.4891062
H	0.7578324	-4.1231255	-5.3659125
H	-0.2754325	-5.1071460	0.9875519
H	3.0954797	-6.5316518	-3.5374052
H	3.9180452	-0.3882050	-1.8526760
H	1.4108728	-2.5848350	1.5561069
H	2.6122460	-3.0517179	-4.1691451
Zn	-0.8717516	0.8672309	-2.5442305
Br	-1.0527203	1.9534392	-4.5300669
Zn	-2.7783721	-0.7337779	1.4138624
Br	-3.0396940	-1.9560228	3.3644058
H	-4.2253805	3.9126998	0.7255635
C	-1.3357420	-2.2689822	-6.3693578
C	-0.9966070	-1.8379583	-5.0835527
C	-1.3311956	-2.6372323	-3.9659647
C	-2.0112615	-3.8626978	-4.1482867
C	-2.3530450	-4.2862154	-5.4365893
C	-2.0122706	-3.4910679	-6.5457386
H	-1.0758596	-1.6496678	-7.2407456
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H	-2.2885864	-4.4606932	-3.2669517
H	-2.8895406	-5.2355331	-5.5820828
H	-2.2780716	-3.8265936	-7.5601163
O	-0.5475596	-1.0950581	-2.3020233
H	-0.4757294	-0.8808665	-4.9319290
H	-1.1336517	-2.9587627	-1.7923347
C	-6.2057705	-0.9075464	-0.0749540
C	-4.9182432	-0.6639705	-0.4484383
C	-4.6079578	-1.6303851	-1.5432085
O	-5.7014795	-2.4156303	-1.7848679
C	-6.7581995	-2.0309896	-0.8946655
O	-3.5705477	-1.7579392	-2.1758882
C	-3.8751865	0.2419043	0.0445634
H	-7.0470656	-2.9195395	-0.2868075
H	-7.6461684	-1.7464493	-1.5047674
H	-4.2709694	1.1633079	0.5094686
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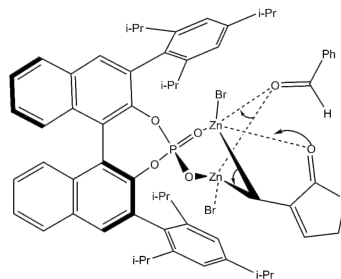


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C	1.9973602	4.7518067	2.1163250
C	2.7057562	5.9882983	2.1977144

C	0.5709334	4.7199398	2.1577032
H	0.0252705	5.6634818	2.3081872
C	-0.1368441	3.5363679	1.9957010
C	3.1040686	-1.2524170	0.7921686
C	4.0678951	-1.5572555	1.7458676
H	4.6241583	-2.5039652	1.6657204
C	4.3327580	-0.6923261	2.8460881
C	5.2656516	-1.0600440	3.8621750
C	3.6292783	0.5646946	2.9532546
C	3.8539067	1.3642750	4.1148545
C	2.7038024	0.9433944	1.9108179
C	2.4293320	-0.0003815	0.9128931
O	-0.0872915	1.1573877	1.7116605
O	1.5111338	0.2916885	-0.0842941
P	-0.0931000	0.4670927	0.2306916
O	-0.5303987	1.5137825	-0.8383545
O	-0.8623093	-0.8353251	0.3618498
C	4.0897917	6.0278362	2.1105885
C	4.8215213	4.8242823	1.9282962
H	2.1265369	6.9173540	2.3181520
H	4.6209022	6.9901312	2.1687426
H	4.7417040	2.6785387	1.7153302
H	5.9175827	4.8595880	1.8329900
C	4.7547176	0.9692249	5.0945490
C	5.4801172	-0.2450890	4.9634593
H	3.2921672	2.3003266	4.2381895
H	4.9018264	1.6005732	5.9841269
H	6.1970935	-0.5438968	5.7432527
H	5.8023708	-2.0163456	3.7600072
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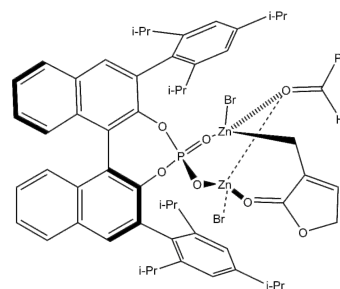
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C	1.9920527	4.7565942	2.1081143
C	2.6975839	5.9943604	2.1860604
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H	0.0172455	5.6620939	2.3044140
C	-0.1396154	3.5352187	1.9965163
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TS3

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H	-2.4080151	3.0338179	-1.7727553	H	-4.5894450	-2.0875183	-5.0021909
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H	3.1382364	-4.1748914	-5.2424828				
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H	3.3910906	-6.6227365	-2.3201643				
C	1.9305373	-4.3346630	-1.1111660				
C	3.3707117	-6.1904932	-3.3405246				
H	3.2543617	-7.0218068	-4.0664954				
H	1.4245531	-5.2915648	-0.8987785				
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C	2.1015140	-3.4115184	-0.0621391				
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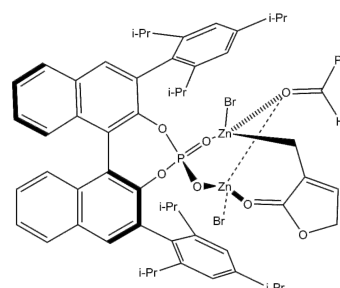


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C	5.2117914	-0.6046297	2.6648298
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O	0.2102618	-1.5240174	0.6787280
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C	5.2265579	4.8248290	1.5802077
H	2.3984852	6.7544945	1.8439306
H	4.8864102	6.9830395	1.7140406
H	5.2912290	2.6740620	1.4696752
H	6.3182241	4.9258706	1.4816380
C	5.5749713	1.1688682	4.8388205
C	6.4139055	0.0308591	4.7030541
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H	5.7010652	1.8417560	5.7008123
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H	6.8519630	-1.7418411	3.5390426
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C	-6.0586674	4.1644942	0.8306116	H	-2.9701328	-3.7127719	-1.6022354
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H	-0.5826502	6.1834770	-1.7337706	H	-5.7867518	-1.7606939	0.6523148
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H	-2.2774817	5.8512703	-1.2495717				
H	1.3945433	-6.1208445	-2.5428788				
H	5.3843999	-2.0785330	-3.7316527				
H	4.8582547	-4.7802454	1.7168647				
C	1.4197512	-5.1092848	-3.0061320				
H	3.9378600	0.7861445	-3.5026672				
H	-0.6663880	-5.2492733	-3.7029853				
H	1.4269736	-4.5296390	3.3206242				
C	2.2250600	-4.2146859	-2.0714611				
C	5.5744773	-1.4036164	-2.8706446				
C	-0.0332156	-4.5939760	-3.0678861				
H	-0.0617643	-3.5679338	-3.4927682				
C	2.8922912	-3.0656439	-2.5292034				
C	3.8346610	-5.0747311	2.0270145				
H	3.0773446	-5.5774804	-4.3753817				
C	2.2363207	-4.4755266	-0.6904989				
C	2.0182812	-5.2507428	-4.4122267				
H	1.4480255	-5.9960667	-5.0034192				
H	1.7235009	-5.3783722	-0.3210872				
C	3.3945467	-0.1291048	-3.1887921				
H	6.2154470	-1.9515237	-2.1500414				
H	6.1458747	-0.5289711	-3.2457912				
C	3.5110193	-2.1633113	-1.6465435				
C	1.4062557	-4.3589172	2.2242124				
C	2.8386237	-3.6071060	0.2377390				
H	3.8567530	-5.3065166	3.1124030				
H	3.5813307	-6.0103937	1.4853247				
C	4.2524084	-0.9556691	-2.2170938				
C	3.4627530	-2.4218552	-0.2490441				
C	2.8049218	-3.9690374	1.7226262				
H	2.4395648	0.1787299	-2.7220642				
H	0.6720524	-3.5615406	2.0060452				
H	3.1466327	-0.6958276	-4.1099037				
H	-0.4780230	-4.5525429	-2.0531315				
H	1.0309457	-5.2902978	1.7533256				
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H	4.5231219	-0.2933670	-1.3691100				

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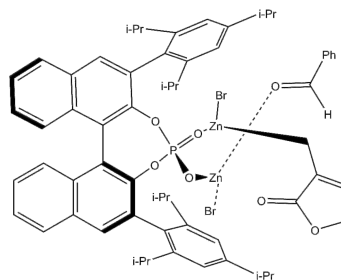


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C	4.6579384	3.5608156	1.5937327
C	2.4253328	4.5818981	1.7723527
C	3.0522182	5.8637801	1.8006884
C	1.0074805	4.4584359	1.7548175
H	0.3942013	5.3720652	1.7874126
C	0.3779381	3.2251601	1.6349935
C	3.9052489	-1.3789249	0.7198966
C	4.9496405	-1.5511938	1.6195592
H	5.5656229	-2.4615946	1.5607972
C	5.2056580	-0.6139577	2.6623489
C	6.2216733	-0.8564811	3.6347150
C	4.3939927	0.5753913	2.7742132
C	4.5974697	1.4268971	3.9011908
C	3.3932406	0.8351258	1.7656281
C	3.1634384	-0.1598372	0.8112835
O	0.5555725	0.8288296	1.6249948
O	2.1807757	0.0466357	-0.1533076
P	0.6080128	-0.0964713	0.2672064

O	-0.1780408	0.5623613	-0.8765309	H	6.1234055	-0.5155901	-3.2526936
O	0.2091363	-1.5134727	0.6891792	C	3.4900319	-2.1497231	-1.6515806
C	4.4308284	5.9860756	1.7260314	C	1.3892653	-4.3594887	2.2145406
C	5.2355899	4.8226316	1.6030881	C	2.8196406	-3.6000026	0.2284528
H	2.4128912	6.7584409	1.8640762	H	3.8410811	-5.3129302	3.0934546
H	4.9011292	6.9810395	1.7415887	H	3.5607581	-6.0092751	1.4643599
H	5.2939729	2.6717959	1.4868532	C	4.2316292	-0.9411122	-2.2199624
H	6.3277273	4.9207421	1.5074754	C	3.4443893	-2.4137823	-0.2551761
C	5.5819418	1.1513417	4.8401516	C	2.7871163	-3.9680649	1.7119211
C	6.4145119	0.0099723	4.6997326	H	2.4221463	0.2039393	-2.7142627
H	3.9549662	2.3092811	4.0270859	H	0.6555783	-3.5591088	2.0069996
H	5.7131364	1.8214531	5.7034792	H	3.1174115	-0.6710218	-4.1075562
H	7.1979727	-0.1941805	5.4453687	H	-0.4930125	-4.5804246	-2.0541586
H	6.8404739	-1.7616412	3.5304999	H	1.0090204	-5.2861544	1.7386837
C	-1.6883575	3.5231989	0.2125483	H	1.9401876	-4.6099997	-4.9835911
C	-1.1023341	3.1056339	1.4442686	H	4.5065598	-0.2825554	-1.3703722
C	-3.0758911	3.3735979	0.0454625	H	3.0906118	-3.0708423	2.2874013
C	-1.9209844	2.5640874	2.4704280	H	2.8946478	-2.8721699	-3.6135177
C	-3.3099922	2.4671393	2.2594576	Zn	-1.2229449	-0.0321263	-2.3999730
C	-3.9109593	2.8569153	1.0525933	Br	-0.3465920	0.0357860	-4.5438489
C	-1.3462926	2.1082693	3.8104204	Zn	-1.6805198	-2.1550653	0.4648666
H	-3.9326150	2.0540742	3.0664992	Br	-2.1419611	-4.4422917	0.7726298
C	-1.6175785	0.6171597	4.0809346	H	-3.5286527	3.6719959	-0.9143520
H	-2.7048093	0.4079712	4.1645875	C	-4.4830567	-1.7505476	-5.4734392
H	-1.1464998	0.3025692	5.0348399	C	-3.5587081	-1.7678667	-4.4259434
H	-1.2025353	-0.0154559	3.2725826	C	-3.6691104	-2.7498699	-3.4098960
C	-1.8547786	2.9951692	4.9620504	C	-4.7105493	-3.7141045	-3.4744409
H	-0.2458757	2.2376755	3.7668634	C	-5.6376467	-3.6815239	-4.5203923
H	-2.9550677	2.9117475	5.0843157	C	-5.5226025	-2.6979660	-5.5205506
H	-1.6183330	4.0632473	4.7809410	H	-4.3894795	-0.9914623	-6.2641417
H	-1.3880942	2.6972918	5.9237831	C	-2.7863636	-2.8378871	-2.2580867
C	-5.4152690	2.7689761	0.8047754	H	-4.7810845	-4.4807497	-2.6862464
C	-6.1593593	1.8333080	1.7651019	H	-6.4465616	-4.4259576	-4.5658518
H	-7.2203799	1.7278881	1.4591612	H	-6.2476062	-2.6741151	-6.3489008
H	-6.1598554	2.2298055	2.8017962	O	-1.9091974	-2.0151356	-1.8910732
H	-5.7054676	0.8226522	1.7871687	H	-2.7339562	-1.0393709	-4.4113094
C	-6.0471882	4.1756998	0.8184207	H	-2.9246171	-3.7305068	-1.5981444
H	-5.5401832	2.3620150	-0.2259207	C	-5.3579601	-1.2078372	-0.1720986
H	-7.1278173	4.1321660	0.5687434	C	-4.1172596	-0.6226201	-0.2271628
H	-5.5536789	4.8515180	0.0920045	C	-4.0759653	0.0601338	-1.5444923
H	-5.9452992	4.6348992	1.8237717	O	-5.2670863	-0.0192802	-2.1700588
C	-0.8775237	4.1780794	-0.9078512	C	-6.1456225	-0.8441631	-1.3827719
C	-1.0633386	3.5118474	-2.2804577	O	-3.1310729	0.6343901	-2.1097374
H	-0.5014608	4.0656823	-3.0596953	C	-2.9921534	-0.6053950	0.6957039
H	-2.1245263	3.4719544	-2.6000667	H	-6.4358713	-1.7103261	-2.0220485
H	-0.6647306	2.4811360	-2.2689052	H	-7.0680774	-0.2622000	-1.1591337
C	-1.1987527	5.6844892	-0.9790845	H	-3.3276621	-0.7103138	1.7457442
H	0.1958721	4.0795247	-0.6509932	H	-2.4124167	0.3312647	0.5916174
H	-0.5618642	6.1884529	-1.7351856	H	-5.7536743	-1.8199233	0.6494014
H	-1.0345329	6.1845967	-0.0030642				
H	-2.2589507	5.8540369	-1.2618824				
H	1.4013631	-6.1146640	-2.5643974				
H	5.3572935	-2.0615591	-3.7411515				
H	4.8393245	-4.7831132	1.6966496				
C	1.4085959	-5.0992099	-3.0198751				
H	3.9179765	0.8049548	-3.5005433				
H	-0.6779632	-5.2675327	-3.7083573				
H	1.4121651	-4.5386122	3.3093780				
C	2.2064321	-4.2008865	-2.0822092				
C	5.5507812	-1.3898286	-2.8786176				
C	-0.0524973	-4.6065000	-3.0713413				
H	-0.0977917	-3.5787626	-3.4904668				
C	2.8705458	-3.0491410	-2.5363844				
C	3.8161599	-5.0762550	2.0092528				
H	3.0667494	-5.5281879	-4.4007742				
C	2.2171388	-4.4651212	-0.7021879				
C	2.0018242	-5.2209468	-4.4298769				
H	1.4424728	-5.9724481	-5.0236345				
H	1.7055762	-5.3695931	-0.3351395				
C	3.3729157	-0.1087986	-3.1859087				
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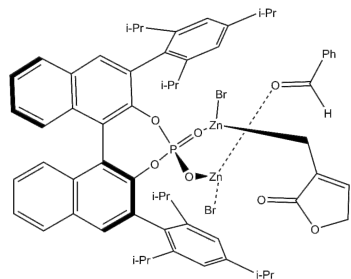


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C	4.2574520	3.5999744	1.7310016
C	2.0822923	4.7142679	2.0654732
C	2.7719743	5.9634003	2.1070574
C	0.6581451	4.6629200	2.1493239

H	0.1038092	5.6031336	2.2876867	H	-0.5443968	-4.0437941	2.2416295
C	-0.0369246	3.4665391	2.0285145	C	2.1544821	-4.0513631	-2.4764103
C	3.1843241	-1.2887700	0.7147766	C	5.4211093	-1.0839068	-2.6822496
C	4.2172708	-1.5780498	1.5971852	C	2.0515858	-4.6314109	-4.9797463
H	4.7842540	-2.5138607	1.4777586	H	3.1155381	-4.4120835	-5.2083967
C	4.5473781	-0.7043226	2.6738267	C	2.9213816	-2.9032724	-2.7304011
C	5.5537336	-1.0573532	3.6226874	C	2.2360065	-4.5300856	2.0942444
C	3.8359370	0.5433535	2.8298526	H	2.5734256	-6.7601476	-2.2440353
C	4.1269324	1.3455900	3.9746683	C	1.6609020	-4.2308232	-1.1676441
C	2.8398654	0.9121891	1.8506415	C	2.7321244	-6.3671825	-3.2682508
C	2.5158617	-0.0384908	0.8739906	H	2.4881284	-7.1752984	-3.9886792
O	0.0471150	1.0820931	1.8269852	H	1.0207432	-5.1038428	-0.9620302
O	1.5338277	0.2430132	-0.0684855	C	3.2417384	0.1861449	-3.0155907
P	-0.0473852	0.3719277	0.3616406	H	6.0088456	-1.7222753	-1.9918766
O	-0.5935613	1.3760078	-0.6940257	H	6.0067037	-0.1630747	-2.8823097
O	-0.7730569	-0.9450567	0.5973953	C	3.2435595	-1.9799315	-1.7155175
C	4.1501990	6.0258216	1.9621662	C	-0.0976004	-4.0768815	1.2281116
C	4.8943842	4.8336063	1.7576623	C	1.9469870	-3.3365735	-0.1209559
H	2.1820618	6.8836657	2.2420744	H	1.8085241	-4.6784425	3.1073367
H	4.6663371	6.9975301	1.9901466	H	2.3012781	-5.5236570	1.6025708
H	4.8437870	2.6854377	1.5649790	C	4.0484198	-0.7343568	-2.0808234
H	5.9844814	4.8869781	1.6145945	C	2.7883612	-2.2200635	-0.3931017
C	5.0982895	0.9637792	4.8901166	C	1.3547171	-3.5728614	1.2684356
C	5.8312692	-0.2392000	4.7075222	H	2.2770708	0.4625047	-2.5452788
H	3.5612740	2.2733746	4.1365996	H	-0.7311191	-3.4420235	0.5802075
H	5.2965507	1.5968938	5.7684071	H	3.0121042	-0.3057084	-3.9835286
H	6.6045062	-0.5274940	5.4357870	H	1.4622584	-3.7162222	-5.1864446
H	6.0957212	-2.0059319	3.4835373	H	-0.1644834	-5.1258994	0.8711319
C	-2.2725792	3.7565136	0.8603515	H	3.8112467	-6.1281605	-3.3730509
C	-1.5293239	3.3235510	1.9958293	H	4.2388798	-0.1683043	-1.1461483
C	-3.6515729	3.4726226	0.8082967	H	1.3424152	-2.5905559	1.7862002
C	-2.1871707	2.6200287	3.0464721	H	3.2872760	-2.7119430	-3.7499943
C	-3.5616465	2.3490338	2.9327913	Zn	-0.2838003	1.0760160	-2.5558392
C	-4.3143358	2.7545866	1.8169274	Br	-0.0607735	2.1659477	-4.5395154
C	-1.4543797	2.1700119	4.3094307	Zn	-2.8346515	-0.9526113	0.6247787
H	-4.0576282	1.7891592	3.7409321	Br	-3.5511270	-2.1996078	2.4572664
C	-1.6360646	0.6698026	4.5972554	H	4.2324538	3.7971970	-0.0694522
H	-2.6884030	0.4178994	4.8415315	C	-0.9255493	-2.1976448	-6.3915099
H	-1.0131929	0.3655255	5.4636579	C	-0.6227853	-1.7166219	-5.1151323
H	-1.3444275	0.0528612	3.7257326	C	-0.8779742	-2.5274369	-3.9815773
C	-1.8803762	3.0340932	5.5123077	C	-1.4452399	-3.8148488	-4.1400669
H	-0.3703074	2.3485119	4.1573624	C	-1.7497500	-4.2870328	-5.4214947
H	-2.9616721	2.9091275	5.7310814	C	-1.4863232	-3.4816213	-6.5442289
H	-1.6985589	4.1113348	5.3204013	H	-0.7227424	-1.5750986	-7.2757236
H	-1.3158737	2.7457605	6.4233858	C	-0.5494249	-2.0687308	-2.6391265
C	-5.7982064	2.4277292	1.7027204	H	-1.6710463	-4.4158909	-3.2471969
C	-6.0696317	0.9165343	1.8076395	H	-2.1958318	-5.2843887	-5.5496805
H	-7.1455469	0.6988111	1.6451143	H	-1.7210214	-3.8571299	-7.5522858
H	-5.7946499	0.5174348	2.8053682	O	-0.1622424	-0.9161805	-2.3564535
H	-5.4852998	0.3405794	1.0629690	H	-0.1774090	-0.7180452	-4.9837879
C	-6.6229957	3.2162799	2.7371523	H	-0.6313389	-2.8009977	-1.8064268
H	-6.1218977	2.7604903	0.6911787	C	-5.9360480	-0.7170912	-1.7864471
H	-7.7078492	3.0158631	2.6155858	C	-4.6026214	-0.8642918	-1.5548929
H	-6.4595473	4.3084567	2.6370504	C	-4.2724579	-2.2804261	-1.8844984
H	-6.3418583	2.9268640	3.7714721	O	-5.3841521	-2.9177747	-2.3490934
C	-1.6208582	4.5002535	-0.3049024	C	-6.4984803	-2.0095585	-2.2903489
C	-2.1624732	4.0746831	-1.6805339	O	-3.1968740	-2.8533691	-1.7533069
H	-1.5235718	4.4792897	-2.4911860	C	-3.5543875	-0.0018042	-0.9945238
H	-3.1922706	4.4477741	-1.8593791	H	-7.2676236	-2.4514398	-1.6170823
H	-2.1863688	2.9719357	-1.7804608	H	-6.9490692	-1.9317537	-3.3053517
C	-1.7611126	6.0260360	-0.1344606	H	-3.8785660	1.0347099	-0.7878097
H	-0.5397597	4.2505323	-0.2877892	H	-2.6619863	0.0174466	-1.6546293
H	-1.2512964	6.5646856	-0.9602017	H	-6.5421095	0.1867003	-1.6348728
H	-1.3290228	6.3788916	0.8224164				
H	-2.8312500	6.3221155	-0.1434305				
H	0.8078109	-5.4104994	-3.4088008				
H	5.3206872	-1.6298876	-3.6433939				
H	3.2678814	-4.1452477	2.2130308				
C	1.8738337	-5.1133941	-3.5352498				
H	3.7918128	1.1244339	-3.2321825				
H	1.7191719	-5.4148210	-5.6901448				

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C	2.8368073	3.4970409	1.8647993
C	4.2481111	3.5957178	1.6814575
C	2.0776729	4.7174146	2.0194335
C	2.7704379	5.9647084	2.0431927
C	0.6544265	4.6688622	2.1157086
H	0.1017641	5.6107775	2.2490395
C	-0.0441271	3.4730043	2.0144159
C	3.1491029	-1.2985458	0.7086588
C	4.1846639	-1.5875939	1.5878451
H	4.7444951	-2.5279763	1.4699683
C	4.5271227	-0.7086963	2.6559178
C	5.5365156	-1.0599010	3.6014416
C	3.8250240	0.5446971	2.8058589
C	4.1291086	1.3547981	3.9414022
C	2.8245304	0.9116246	1.8308719
C	2.4884717	-0.0434340	0.8623386
O	0.0359270	1.0863317	1.8352852
O	1.5011953	0.2378247	-0.0745085
P	-0.0776737	0.3674923	0.3748791
O	-0.6333797	1.3687709	-0.6787873
O	-0.7987231	-0.9477642	0.6215457
C	4.1473056	6.0231070	1.8888827
C	4.8875337	4.8278128	1.6923158
H	2.1831526	6.8874971	2.1722118
H	4.6652364	6.9940882	1.9035321
H	4.8304442	2.6775612	1.5218631
H	5.9769061	4.8772933	1.5428502
C	5.1038707	0.9746262	4.8531760
C	5.8268643	-0.2346264	4.6767819
H	3.5702599	2.2875527	4.0976360
H	5.3122027	1.6141544	5.7243880
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H	6.0706781	-2.0136449	3.4674559
C	-2.2922503	3.7426476	0.8652818
C	-1.5365358	3.3290273	1.9993955
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C	-2.1800383	2.6367134	3.0658781
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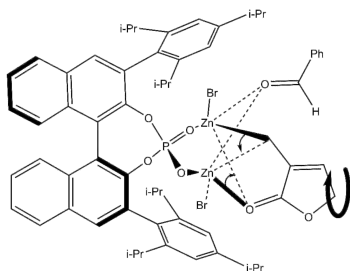
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C	-1.6555042	4.4761805	-0.3146182
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H	-0.5741045	4.2269330	-0.3084765
H	-1.2956422	6.5356481	-0.9920193
H	-1.3505934	6.3644949	0.7927596
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H	0.7704058	-5.3943540	-3.4412107
H	5.3788646	-1.7196761	-3.5720180
H	3.1504115	-4.0750045	2.2599289
C	1.8500140	-5.1345459	-3.5332607
H	3.8625131	1.0694608	-3.2472401
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H	-0.6689459	-3.9851704	2.1754309
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C	5.4542332	-1.1545858	-2.6196633
C	2.0928550	-4.6768052	-4.9760357
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C	2.9201122	-2.9364339	-2.7252464
C	2.1277769	-4.4749610	2.1156350
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C	3.3010281	0.1352933	-3.0424731
H	6.0127901	-1.7851136	-1.8987934
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C	-0.1859080	-4.0627732	1.1814731
C	1.8858927	-3.3312195	-0.1321174
H	1.6708251	-4.6096435	3.1174892
H	2.2201138	-5.4764875	1.6451501
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C	1.2603311	-3.5441608	1.2462577
H	2.3182285	0.4205661	-2.6182298
H	-0.8032664	-3.4666063	0.4828570
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H	1.5411537	-3.7462421	-5.2150161
H	-0.2331194	-5.1279651	0.8720387
H	3.7455040	-6.2100489	-3.2939840
H	4.2333605	-0.2018336	-1.1376596
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Zn	-0.2730313	1.0872456	-2.5341154
Br	0.0370460	2.2314983	-4.4716955
Zn	-2.8681905	-0.9573853	0.7274778
Br	-3.5240200	-2.1529230	2.5984631
H	-4.2600392	3.7575290	-0.0470307
C	-0.6629206	-2.0454886	-6.4688779
C	-0.4346390	-1.6171327	-5.1584116
C	-0.7938000	-2.4550550	-4.0747270
C	-1.3919566	-3.7146732	-4.3164037
C	-1.6229889	-4.1323372	-5.6317497
C	-1.2542886	-3.3019478	-6.7050849
H	-0.3786127	-1.4003259	-7.3135804
C	-0.5405608	-2.0491483	-2.6965866
H	-1.7062677	-4.3302560	-3.4610970
H	-2.0952664	-5.1069990	-5.8248696
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H	-0.6648309	-2.8121298	-1.8984408
C	-5.9822505	-0.8417431	-1.5881524
C	-4.6293030	-0.9435638	-1.4724127
C	-4.2697421	-2.3162313	-1.9380302
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C	-6.5323297	-2.1239012	-2.1315459
O	-3.1659008	-2.8433900	-1.9618057
C	-3.5843591	-0.0692376	-0.9293394
H	-7.2232620	-2.6425238	-1.4275954
H	-7.0735546	-2.0029801	-3.0977318
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C	-3.4526757	2.3849697	2.3621352
C	-4.0584767	2.9215220	1.2146930
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H	-4.0677063	1.8566271	3.1052488
C	-1.7811518	0.3229945	3.9026058
H	-2.8677203	0.1228106	4.0110395
H	-1.2714834	-0.1447814	4.7697916
H	-1.4268706	-0.1907460	2.9877735
C	-1.9680924	2.5539665	5.1176459
H	-0.3814830	1.9511275	3.8072516
H	-3.0694808	2.4750956	5.2333340
H	-1.7098014	3.6320866	5.0916010
H	-1.5036778	2.1099495	6.0223322
C	-5.5538431	2.8168162	0.9259310
C	-6.3095576	1.8484062	1.8441608
H	-7.3611785	1.7385841	1.5095993
H	-6.3385649	2.2195763	2.8899785
H	-5.8528042	0.8380770	1.8626289
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H	-5.6286268	2.4341463	-0.1192801
H	-7.2876660	4.1436122	0.6723286
H	-5.7232675	4.9134236	0.2564727
H	-6.1559555	4.6465952	1.9730792
C	-1.0595332	4.5879209	-0.5219216
C	-1.2460037	4.1331822	-1.9775992
H	-0.6273619	4.7635770	-2.6494162
H	-2.2973497	4.2132213	-2.3198340
H	-0.9346940	3.0796525	-2.1044984
C	-1.4035225	6.0832684	-0.3678652
H	0.0166537	4.4688433	-0.2912431
H	-0.7790900	6.7018849	-1.0453962
H	-1.2427224	6.4415344	0.6693006
H	-2.4679263	6.2730592	-0.6205909
H	0.2871944	-6.3584053	-0.7135684
H	4.0780868	-3.1542170	-3.9425339
H	3.4648474	-4.1689638	3.9677518
C	0.6351561	-5.8083192	-1.6145671
H	2.8654585	-0.2304977	-4.1571996
H	-1.1802926	-6.3033769	-2.7419970
H	1.2491428	-2.9139621	4.1015371
C	1.4051289	-4.5929469	-1.1128608
C	4.4930291	-2.3277403	-3.3280469
C	-0.6118843	-5.4073665	-2.4158634
C	-0.3336216	-4.8394714	-3.3268577
H	1.9797701	-3.6601053	-1.9981877
C	3.3260196	-4.2983497	2.8742136
H	2.4283856	-7.0645551	-1.8354692
C	1.5837623	-4.3905568	0.2649216
C	1.5424468	-6.7519821	-2.4244189
H	0.9911747	-7.6655455	-2.7300138
H	1.1151457	-5.1004781	0.9640776
C	2.3639298	-0.9443513	-3.4711035
H	5.0089468	-1.6238572	-4.0139046
H	5.2523208	-2.7655350	-2.6487734
C	2.7272643	-2.5609823	-1.5369161
C	1.0952172	-3.0824389	3.0152534
C	2.3177489	-3.3074472	0.7801966
H	4.3292409	-4.3192977	2.4009187
H	2.8584507	-5.2916899	2.7095297
C	3.3847097	-1.6107989	-2.5349562
C	2.9015957	-2.3886189	-0.1398262
C	2.4527806	-3.1678172	2.2986190
H	1.6108149	-0.3810741	-2.8865747
H	0.4889274	-2.2483761	2.6130941
H	1.8350949	-1.6919422	-4.0979735
H	-1.2946850	-4.7809828	-1.8076544

7.10.3 Pathway 14d-ma ↔ 14d-mi

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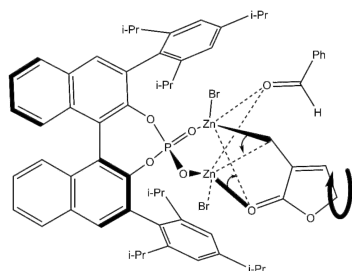


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C	4.4285641	3.8576990	1.2081915
C	2.2268022	4.7473247	1.8555212
C	2.8077456	6.0501940	1.9152740
C	0.8253041	4.5600252	2.0163557
H	0.1915429	5.4409013	2.1995396
C	0.2223917	3.3192663	1.8390294
C	3.6102497	-1.2084171	0.4434964
C	4.8055230	-1.3436050	1.1383556
H	5.3604061	-2.2920504	1.0657336
C	5.2560945	-0.3510895	2.0543453
C	6.4286525	-0.5577728	2.8417559
C	4.4476868	0.8238314	2.2780071
C	4.8056397	1.6821930	3.3616658
C	3.3012941	1.0594630	1.4252449
C	2.9371064	0.0499220	0.5255709
O	0.4833748	0.9306261	1.6406756
O	1.8746834	0.2562245	-0.3566098
P	0.3209939	0.2167546	0.1658473
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O	-0.1773592	-1.2121257	0.4176341
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C	4.9587235	5.1399818	1.2499211
H	2.1591591	6.9027669	2.1712361
H	4.5845392	7.2558029	1.6677991
H	5.0647045	3.0139066	0.9075541
H	6.0142724	5.3009173	0.9825143
C	5.9396645	1.4419141	4.1262110
C	6.7749950	0.3267887	3.8518574
H	4.1665508	2.5426977	3.5994121
H	6.1869500	2.1195339	4.9576199
H	7.6773979	0.1524394	4.4574066

H	0.4937869	-4.0056140	2.8957508
H	1.9114644	-6.2591965	-3.3487086
H	3.8705187	-0.8024331	-1.9490473
H	2.9775628	-2.2164763	2.5088299
H	1.8541448	-3.8004245	-3.0845032
Zn	-2.3798571	0.4848790	-1.0905526
Br	-3.6700516	1.4367437	-2.8360280
Zn	-1.7437024	-2.3085814	-0.0816704
Br	-2.0541764	-4.1785614	1.2973831
H	-3.6824850	3.9895244	-0.6299025
C	-1.8248500	-3.7398001	-5.7239431
C	-1.7776028	-2.9283604	-4.5861979
C	-1.1457071	-1.6638326	-4.6578852
C	-0.5819358	-1.2159605	-5.8758671
C	-0.6190086	-2.0405641	-7.0056406
C	-1.2395787	-3.3013049	-6.9275323
H	-2.3192317	-4.7217268	-5.6767565
C	-1.0937476	-0.7926390	-3.4876641
H	-0.1065824	-0.2231389	-5.9209080
H	-0.1707570	-1.7032492	-7.9520636
H	-1.2749581	-3.9470981	-7.8186541
O	-1.3766236	-1.1538121	-2.3321280
H	-2.2409377	-3.2391908	-3.6380682
H	-0.7987660	0.2719072	-3.6708504
C	-5.8766958	-0.7699755	-0.8751211
C	-4.6166641	-1.1626784	-0.5422780
C	-4.3154404	-2.3194282	-1.4076192
O	-5.3580624	-2.6304830	-2.1914638
C	-6.4021026	-1.6610508	-1.9519500
O	-3.2405286	-2.9374021	-1.4761026
C	-3.5282602	-0.5930755	0.2726372
H	-7.3343678	-2.2052866	-1.6863911
H	-6.5768627	-1.1147223	-2.9056105
H	-3.1992004	-1.3131195	1.0637817
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TS1



Energy (Hartree) = -11970.0101431
number of imaginary frequencies: 1

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C	4.4269290	3.8580133	1.1960959
C	2.2257805	4.7476643	1.8442098
C	2.8062161	6.0505974	1.8992329
C	0.8251312	4.5589980	2.0087386
H	0.1904736	5.4394530	2.1907717
C	0.2228627	3.3174474	1.8362441
C	3.6063879	-1.2106480	0.4438158
C	4.8015056	-1.3462273	1.1385110
H	5.3534336	-2.2965829	1.0684219
C	5.2555314	-0.3520816	2.0507699
C	6.4286329	-0.5577443	2.8369733
C	4.4497131	0.8249392	2.2720017
C	4.8112179	1.6861052	3.3519604
C	3.3024675	1.0599285	1.4205781

C	2.9361188	0.0493554	0.5231005
O	0.4857058	0.9289256	1.6412400
O	1.8736655	0.2552213	-0.3585593
P	0.3211058	0.2146632	0.1666847
O	-0.4948845	1.0935038	-0.7966007
O	-0.1722942	-1.2160247	0.4175373
C	4.1473604	6.2460279	1.6086184
C	4.9561194	5.1404391	1.2334881
H	2.1574393	6.9034545	2.1537441
H	4.5811740	7.2568906	1.6456223
H	5.0628064	3.0134077	0.8974377
H	6.0111833	5.3012717	0.9642918
C	5.9459770	1.4464755	4.1149708
C	6.7784988	0.3292659	3.8430937
H	4.1740223	2.5485097	3.5875834
H	6.1960250	2.1266182	4.9434330
H	7.6816701	0.1552555	4.4475322
H	7.0371440	-1.4551779	2.6439011
C	-1.8527266	3.7551578	0.4941746
C	-1.2576556	3.1857859	1.6639955
C	-3.2312255	3.5777753	0.2903887
C	-2.0611435	2.4754819	2.5923022
C	-3.4496809	2.3787286	2.3648182
C	-4.0572288	2.9119409	1.2170142
C	-1.4777546	1.8324718	3.8481344
H	-4.0630296	1.8508978	3.1096589
C	-1.7729594	0.3222105	3.9079517
H	-2.8588736	0.1200017	4.0192949
H	-1.2608126	-0.1433211	4.7746957
H	-1.4195992	-0.1931135	2.9938641
C	-1.9616401	2.5557811	5.1185307
H	-0.3764258	1.9522590	3.8069414
H	-3.0626666	2.4759208	5.2363485
H	-1.7051843	3.6341339	5.0896763
H	-1.4953857	2.1145724	6.0235915
C	-5.5526888	2.8054109	0.9296599
C	-6.3063389	1.8363829	1.8490727
H	-7.3586121	1.7253869	1.5165662
H	-6.3346960	2.2077874	2.8947682
H	-5.8485024	0.8265837	1.8673504
C	-6.2169652	4.1964927	0.9598140
H	-5.6278737	2.4227288	-0.1155839
H	-7.2885956	4.1309863	0.6792233
H	-5.7253620	4.9016572	0.2611959
H	-6.1548396	4.6344849	1.9779031
C	-1.0640057	4.5813499	-0.5251935
C	-1.2505673	4.1239602	-1.9800836
H	-0.6335113	4.7543468	-2.6532346
H	-2.3019497	4.2006678	-2.3227398
H	-0.9367272	3.0711844	-2.1056047
C	-1.4119563	6.0759411	-0.3729903
H	0.0126645	4.4655140	-0.2952377
H	-0.7897807	6.6954678	-1.0516857
H	-1.2519905	6.4362642	0.6635514
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H	0.2664009	-6.3513073	-0.7018517
H	4.0714353	-3.1675536	-3.9352050
H	3.4485549	-4.1756800	3.9726987
C	0.6181766	-5.8061044	-1.6042091
H	2.8681631	-0.2387127	-4.1568357
H	-1.1956003	-6.3039958	-2.7322313
H	1.2449427	-2.9001464	4.1070361
C	1.3901156	-4.5908044	-1.1051561
C	4.4879727	-2.3406689	-3.3224969
C	-0.6265197	-5.4070678	-2.4098505
H	-0.3450737	-4.8446005	-3.3234409
C	1.9679375	-3.6616999	-1.9920886
C	3.3082586	-4.3041595	2.8793184
H	2.4096605	-7.0664296	-1.8148234
C	1.5701224	-4.3867646	0.2719536
C	1.5260578	-6.7547891	-2.4074769

H	0.9742584	-7.6686442	-2.7112809
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C	2.3636666	-0.9502000	-3.4703052
H	5.0071591	-1.6403100	-4.0095549
H	5.2447754	-2.7794077	-2.6413750
C	2.7195004	-2.5647912	-1.5328528
C	1.0888091	-3.0674036	3.0209851
C	2.3084435	-3.3059579	0.7854460
H	4.3110594	-4.3347982	2.4057164
H	2.8319510	-5.2932940	2.7154179
C	3.3810585	-1.6187141	-2.5321255
C	2.8946370	-2.3905055	-0.1362968
C	2.4452886	-3.1658748	2.3036545
H	1.6121826	-0.3835289	-2.8868578
H	0.4906766	-2.2273311	2.6196831
H	1.8330161	-1.6969329	-4.0967396
H	-1.3101077	-4.7777841	-1.8057868
H	0.4776386	-3.9841268	2.9020382
H	1.8992010	-6.2665343	-3.3324600
H	3.8687750	-0.8108960	-1.9470830
H	2.9793134	-2.2194939	2.5129568
H	1.8420608	-3.8038597	-3.0782106
Zn	-2.3847066	0.4811013	-1.0803078
Br	-3.6879292	1.4302750	-2.8148285
Zn	-1.7359585	-2.3183076	-0.0787258
Br	-2.0492152	-4.1913255	1.2902292
H	-3.6848138	3.9755783	-0.6305877
C	-1.7875960	-3.7176409	-5.7365872
C	-1.7544711	-2.9081917	-4.5968599
C	-1.1362861	-1.6372646	-4.6634019
C	-0.5726318	-1.1810495	-5.8775503
C	-0.5953566	-2.0034196	-7.0091398
C	-1.2020344	-3.2708230	-6.9363658
H	-2.2709673	-4.7051895	-5.6929460
C	-1.0971157	-0.7704015	-3.4879223
H	-0.1072744	-0.1832922	-5.9177828
H	-0.1465825	-1.6592634	-7.9528794
H	-1.2262605	-3.9152284	-7.8289096
O	-1.3767946	-1.1440015	-2.3373549
H	-2.2179232	-3.2257793	-3.6508352
H	-0.8161901	0.2995426	-3.6634522
C	-5.8694382	-0.7775002	-0.8640453
C	-4.6099774	-1.1736745	-0.5350168
C	-4.3053083	-2.3177467	-1.4183734
O	-5.3480024	-2.6175521	-2.2088930
C	-6.3911095	-1.6530114	-1.9563381
O	-3.2300156	-2.9296947	-1.4972002
C	-3.5228792	-0.6110891	0.2851856
H	-7.3246017	-2.2016765	-1.7025099
H	-6.5623998	-1.0911371	-2.9019470
H	-3.1944719	-1.3369164	1.0711812
H	-3.8366501	0.2665196	0.8847941
H	-6.4249223	0.0768720	-0.4575879