

Cartesian coordinates of all DFT-optimized structures

2n-PhRad

E(PBE0-D3/def2-TZVP) = -1285.872683203 (conv)

Lowest Freq. = 17.45 cm⁻¹

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2n-PhRad (001/c1/pbe0-d3.def2-TZVP)

C	-2.8062755	-1.1065998	0.7114825
C	-3.2617673	0.0268660	-0.1958273
C	-1.3157466	-1.0231886	1.0006801
H	-3.0242119	-2.0652919	0.2237361
H	-3.3714960	-1.1002219	1.6480881
C	-0.4853008	-0.9687417	-0.2798984
H	-1.1064082	-0.1273542	1.5983665
H	-0.9988113	-1.8780778	1.6069215
C	-2.4413188	0.0600054	-1.4766511
H	-3.1400666	0.9819893	0.3303225
H	-4.3266998	-0.0734413	-0.4248151
C	-0.9548112	0.1765389	-1.1737472
H	-0.6862283	-1.8961167	-0.8286014
C	1.0180242	-0.9516696	0.0378011
H	-0.3739945	0.1998029	-2.0988158
H	-0.7709388	1.1300506	-0.6708685
H	-2.6292317	-0.8558757	-2.0512102
H	-2.7568363	0.8944947	-2.1094828
H	1.1673259	-1.1531332	1.1013642
O	1.5610888	0.3746054	-0.2131143
C	1.8831896	-1.9557341	-0.7418075
C	1.4571469	-3.3657560	-0.3353539
C	3.3470999	-1.7650668	-0.3494800
C	1.7334652	-1.7739473	-2.2483008
H	1.5574841	-3.5114884	0.7437572
H	2.0967875	-4.0996293	-0.8307295
H	0.4254408	-3.5893726	-0.6140582
H	0.7105050	-1.9623539	-2.5829313
H	2.3865006	-2.4743150	-2.7747162
H	2.0145328	-0.7627181	-2.5490061
H	3.4777538	-1.8310497	0.7337123
H	3.7280048	-0.7966271	-0.6759256
H	3.9593836	-2.5418036	-0.8136213
S	2.1030296	1.3003443	0.9378453
O	3.1601305	2.0517671	0.3488252
O	2.3030457	0.5338510	2.1252614
C	0.7513537	2.4004065	1.2013081
C	0.6039445	3.5397670	0.4107429
C	-0.4930299	4.3626714	0.6083981
H	1.3542437	3.7629044	-0.3387563
C	-1.4378261	4.0678894	1.5845365
H	-0.6111853	5.2489796	-0.0028760
C	-1.2961268	2.9375652	2.3891586
H	-2.2901915	4.7225941	1.7287557
C	-0.1997557	2.1571513	2.1512490
H	-2.0212221	2.6993297	3.1582819

2n-TS1Aa

E(PBE0-D3/def2-TZVP) = -1285.864402242 (conv)

Lowest Freq. = -890.49 cm⁻¹

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2n-TS1Aa (TS001A/c1/pbe0-d3.def2-TZVP)

C	-2.8535289	-1.3909160	0.6523276
C	-3.3149253	-0.1465925	-0.0913822

C	-1.3697791	-1.3239001	0.9774704
H	-3.0482886	-2.2754865	0.0324453
H	-3.4329285	-1.5210184	1.5704653
C	-0.5243162	-1.1146260	-0.2785603
H	-1.1760360	-0.5043773	1.6785368
H	-1.0493525	-2.2409943	1.4811196
C	-2.4811912	0.0836221	-1.3447201
H	-3.2164669	0.7211356	0.5711194
H	-4.3739876	-0.2257782	-0.3518216
C	-1.0028857	0.1042288	-1.0380167
H	-0.7032903	-1.9793764	-0.9326296
C	0.9752232	-1.0983522	0.0505181
H	-0.3872083	0.3401009	-1.9067810
H	-0.8127452	1.0661033	-0.3020623
H	-2.6839393	-0.7210251	-2.0663218
H	-2.7737094	1.0145789	-1.8396757
H	1.1151147	-1.4686997	1.0682146
O	1.4660472	0.2697288	0.0304378
C	1.8899583	-1.9204868	-0.8695482
C	1.5176232	-3.3949550	-0.7208743
C	3.3357830	-1.7409918	-0.4106826
C	1.7595138	-1.4921517	-2.3271202
H	1.5896627	-3.7171379	0.3216143
H	2.2061407	-4.0080904	-1.3066156
H	0.5070127	-3.6105859	-1.0739157
H	0.7505604	-1.6598802	-2.7120362
H	2.4482557	-2.0697249	-2.9483613
H	2.0053034	-0.4352630	-2.4481304
H	3.4497965	-2.0114503	0.6428747
H	3.6714470	-0.7106562	-0.5299870
H	3.9950244	-2.3857412	-0.9965249
S	1.7615563	1.0703066	1.3533730
O	3.0830093	1.5982119	1.2590145
O	1.3993193	0.2695330	2.4836485
C	0.6268949	2.4098285	1.1943110
C	0.9436889	3.6164416	1.8127850
C	0.0349673	4.6602709	1.7546487
H	1.8949703	3.7275182	2.3198062
C	-1.1701236	4.5087954	1.0805640
H	0.2728794	5.6028446	2.2326090
C	-1.4757987	3.3058692	0.4517386
H	-1.8722467	5.3340342	1.0359024
C	-0.5680245	2.2749507	0.5294389
H	-2.4089801	3.1901546	-0.0892159

2n-TS1Ab

E(PBE0-D3/def2-TZVP) = -1285.861154006 (conv)

Lowest Freq. = -963.80 cm⁻¹

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2n-TS1Ab (TS001A/c2/pbe0-d3.def2-TZVP)

C	-2.8130515	-1.8721880	-1.1013840
C	-3.5321642	-1.2291914	0.0707692
C	-1.3284487	-2.0689881	-0.8248611
H	-2.9299844	-1.2373399	-1.9883681
H	-3.2670282	-2.8362691	-1.3476724
C	-0.6301604	-0.7506987	-0.4694389
H	-1.2018729	-2.7820081	-0.0015596
H	-0.8665946	-2.5145736	-1.7055303
C	-2.8580117	0.0867217	0.4372188
H	-3.5018970	-1.9048351	0.9336542

H	-4.5874172	-1.0644980	-0.1655076
C	-1.3837258	-0.1169860	0.6883350
H	-0.7102777	-0.0878659	-1.3407678
C	0.8605160	-0.8680493	-0.1307518
H	-0.9429085	1.0017676	0.9287981
H	-1.1965897	-0.6569345	1.6226269
H	-2.9903823	0.7980456	-0.3875472
H	-3.3301007	0.5294576	1.3188439
H	0.9730086	-1.2879340	0.8727741
O	1.3272179	0.5135890	-0.0763851
C	1.8127319	-1.6295061	-1.0786394
C	1.6706751	-3.1401316	-0.8749020
C	3.2559285	-1.2807198	-0.7054670
C	1.5778582	-1.2447910	-2.5358373
H	1.8395255	-3.4052041	0.1724419
H	2.4310184	-3.6527992	-1.4687917
H	0.7034610	-3.5381470	-1.1715083
H	0.5896921	-1.5411317	-2.8930064
H	2.3190717	-1.7315553	-3.1742439
H	1.6799034	-0.1655677	-2.6704103
H	3.4477855	-1.4681576	0.3547290
H	3.4952285	-0.2384866	-0.9098731
H	3.9381950	-1.9078728	-1.2837725
S	1.9277272	1.1636237	1.2291857
O	3.2325265	1.6578537	0.9313272
O	1.7417224	0.2627918	2.3263433
C	0.8507277	2.5453707	1.3983951
C	1.3702051	3.8015759	1.6847435
C	0.4916589	4.8617626	1.8547795
H	2.4426864	3.9346256	1.7596947
C	-0.8778360	4.6701950	1.7325829
H	0.8811537	5.8476411	2.0780951
C	-1.3914309	3.4086161	1.4367455
H	-1.5535270	5.5084628	1.8628600
C	-0.5061442	2.3709031	1.2786898
H	-2.4606713	3.2594264	1.3325922

2n-TS1Ba

E(PBE0-D3/def2-TZVP) = -1285.856355867 (conv)

Lowest Freq. = -979.97 cm⁻¹

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2n-TS1Ba (TS001B/c1/pbe0-d3.def2-TZVP)

C	-2.4312743	0.1879947	-1.3213115
C	-3.0691296	-1.1081410	-1.8081286
C	-0.9299968	0.0632200	-1.1854400
H	-2.8544620	0.4416947	-0.3415555
H	-2.6796801	1.0131600	-1.9948838
C	-0.5135649	-1.1115686	-0.3198364
H	-0.4148334	0.1083484	-2.1461876
H	-0.5851770	1.0821560	-0.6006033
C	-2.6722709	-2.2657293	-0.9070843
H	-2.7389116	-1.3171677	-2.8328695
H	-4.1570226	-1.0000484	-1.8437334
C	-1.1589298	-2.4007627	-0.8339312
H	-0.9587771	-0.9257690	0.6669398
C	0.9923333	-1.2192587	-0.0227499
H	-0.8827737	-3.2398285	-0.1889735
H	-0.7861481	-2.6295307	-1.8368298
H	-3.0735086	-2.0994942	0.0997804
H	-3.1098862	-3.2000460	-1.2698924

H	1.0962734	-1.7913258	0.9033841
O	1.4713337	0.1304333	0.2467791
C	2.0084234	-1.8166551	-1.0212570
C	1.8496247	-3.3367184	-1.0975970
C	3.4139169	-1.5489236	-0.4726739
C	1.8978167	-1.2091642	-2.4153808
H	1.8750514	-3.7865810	-0.1013391
H	2.6849351	-3.7520973	-1.6661315
H	0.9326172	-3.6516347	-1.5901698
H	0.9567343	-1.4726057	-2.9025884
H	2.7094721	-1.5819761	-3.0451956
H	1.9779263	-0.1208569	-2.3782410
H	3.5124012	-1.9118419	0.5541937
H	3.6597437	-0.4882613	-0.4749512
H	4.1480155	-2.0756174	-1.0866187
S	1.3777423	0.7753827	1.6771784
O	2.6916665	1.1254240	2.1084143
O	0.5635529	-0.0536686	2.5146581
C	0.5184665	2.2587777	1.2724630
C	0.7424915	3.3958967	2.0425099
C	0.0270504	4.5482493	1.7593594
H	1.4762693	3.3701493	2.8395277
C	-0.8915367	4.5696640	0.7176741
H	0.1933086	5.4396156	2.3520868
C	-1.1035338	3.4325281	-0.0568446
H	-1.4419585	5.4787388	0.5015256
C	-0.3898713	2.2960560	0.2421939
H	-1.8127794	3.4494680	-0.8773410

2n-TS1Bb

E(PBE0-D3/def2-TZVP) = -1285.865358672 (conv)

Lowest Freq. = -1023.10 cm⁻¹

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2n-TS1Bb (TS001B/c2/pbe0-d3.def2-TZVP)

C	-2.9175727	-0.6121965	0.3842856
C	-3.1931765	0.3460520	-0.7664300
C	-1.4461422	-0.7089342	0.7062250
H	-3.2788446	-1.6139991	0.1102328
H	-3.4808214	-0.3224561	1.2766220
C	-0.5559515	-0.9903916	-0.4904247
H	-1.1000274	0.3926082	1.1538051
H	-1.2397282	-1.3777525	1.5456200
C	-2.3199303	0.0243870	-1.9686385
H	-2.9837835	1.3719427	-0.4440490
H	-4.2518837	0.3114318	-1.0380578
C	-0.8435911	0.0235146	-1.5975201
H	-0.8377534	-1.9846459	-0.8658291
C	0.9056262	-1.0896958	-0.0518585
H	-0.2365837	-0.1802811	-2.4788083
H	-0.5565085	1.0192747	-1.2466482
H	-2.5967311	-0.9591460	-2.3693909
H	-2.4998587	0.7474574	-2.7690209
H	0.9258476	-1.4872688	0.9657922
O	1.4497203	0.2550985	0.0133486
C	1.8718396	-1.9657149	-0.8689995
C	1.3829701	-3.4115678	-0.7968406
C	3.2493224	-1.8906237	-0.2088651
C	1.9973164	-1.5361904	-2.3267164
H	1.2565253	-3.7378455	0.2393794
H	2.1174709	-4.0710587	-1.2644890

H	0.4353276	-3.5564926	-1.3197049
H	1.0848437	-1.7362717	-2.8916381
H	2.8053858	-2.0957246	-2.8045953
H	2.2337736	-0.4733925	-2.4068503
H	3.1965703	-2.1514186	0.8512225
H	3.6787549	-0.8909921	-0.2877510
H	3.9312567	-2.5898802	-0.6980680
S	1.8750326	0.9180009	1.3802883
O	3.0967259	1.6100785	1.1346019
O	1.7931486	-0.0588300	2.4225075
C	0.6059068	2.1176544	1.6228133
C	0.9626566	3.4317050	1.9029901
C	-0.0354905	4.3577297	2.1674161
H	2.0097189	3.7090502	1.9082536
C	-1.3697852	3.9777768	2.1488567
H	0.2324291	5.3839465	2.3878360
C	-1.7225291	2.6627279	1.8539105
H	-2.1435908	4.7082555	2.3578769
C	-0.7218017	1.7558374	1.5999445
H	-2.7660841	2.3682413	1.8273658

2n-INT1A

E(PBE0-D3/def2-TZVP) = -1285.898863725 (conv)

Lowest Freq. = 9.46 cm⁻¹

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2n-INT1A (002A/c1/pbe0-d3.def2-TZVP)

C	-2.8047467	-0.8411262	0.6077526
C	-3.1160794	0.3302562	-0.3097525
C	-1.3211506	-0.9018903	0.9296387
H	-3.1131357	-1.7768531	0.1234230
H	-3.3833517	-0.7636128	1.5327544
C	-0.4659387	-1.0126377	-0.3398678
H	-1.0358326	0.0015682	1.4763283
C	-2.3095411	0.2358855	-1.6041682
H	-2.8607149	1.2637811	0.2032689
H	-4.1852642	0.3688426	-0.5368286
C	-0.8666528	0.0079707	-1.3453204
H	-0.6989598	-2.0040783	-0.7644434
C	1.0334766	-1.0201686	-0.0070726
H	-0.1262109	0.4172817	-2.0187099
H	-2.7187820	-0.5991809	-2.2012016
H	-2.4500026	1.1332876	-2.2128042
H	1.1644401	-1.2227267	1.0592379
O	1.5943061	0.2942639	-0.2601056
C	1.8946849	-2.0383368	-0.7731605
C	1.4599003	-3.4433837	-0.3589180
C	3.3570369	-1.8521621	-0.3723710
C	1.7541250	-1.8693142	-2.2819364
H	1.5391363	-3.5779868	0.7234454
H	2.1085531	-4.1827234	-0.8340267
H	0.4339521	-3.6706138	-0.6558875
H	0.7280944	-2.0369210	-2.6176094
H	2.3950568	-2.5883827	-2.7979940
H	2.0576495	-0.8676412	-2.5927575
H	3.4803076	-1.9108797	0.7121221
H	3.7436666	-0.8873902	-0.7020850
H	3.9681360	-2.6351406	-0.8274583
S	2.0404295	1.2638139	0.8977697
O	3.0192862	2.1076898	0.2987705
O	2.3358257	0.5086555	2.0761410

C	0.5909071	2.2160668	1.1997933
C	0.0433349	2.9604752	0.1630107
C	-1.0990226	3.7040470	0.3997951
H	0.5122572	2.9540174	-0.8127036
C	-1.6806990	3.7051541	1.6618082
H	-1.5384666	4.2850447	-0.4020960
C	-1.1196500	2.9655835	2.6915350
H	-2.5758555	4.2889197	1.8418336
C	0.0233199	2.2129256	2.4635976
H	-1.5712380	2.9719779	3.6762410
H	0.4772354	1.6216007	3.2485433
H	-1.1024040	-1.7524197	1.5832212

2n-INT1B

E(PBE0-D3/def2-TZVP) = -1285.899203295 (conv)

Lowest Freq. = 18.52 cm⁻¹

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2n-INT1B (002B/c1/pbe0-d3.def2-TZVP)

C	-2.7209415	-0.5852996	0.8551333
C	-3.0823950	0.4070512	-0.2464058
C	-1.2631980	-0.8485138	0.9208777
H	-3.2550932	-1.5320298	0.6556340
H	-3.0892011	-0.2390089	1.8254921
C	-0.4665479	-1.0161540	-0.3275212
H	-0.8338925	-1.2011766	1.8534548
C	-2.4013791	0.0356235	-1.5531891
H	-2.7549078	1.4086094	0.0524295
H	-4.1680813	0.4473937	-0.3712096
C	-0.8900664	0.0087716	-1.3870629
H	-0.7135921	-2.0073622	-0.7478674
C	1.0382919	-1.0421562	-0.0212227
H	-0.4020606	-0.2077874	-2.3384711
H	-0.5538336	1.0011886	-1.0798877
H	-2.7581695	-0.9464735	-1.8897055
H	-2.6716156	0.7500262	-2.3360496
H	1.1771894	-1.3025420	1.0307408
O	1.5911232	0.2868026	-0.1985483
C	1.9092206	-2.0194040	-0.8291804
C	1.4921745	-3.4427451	-0.4615611
C	3.3676962	-1.8255647	-0.4156042
C	1.7790150	-1.8137287	-2.3338497
H	1.5774414	-3.6139136	0.6150323
H	2.1459452	-4.1582966	-0.9652238
H	0.4669690	-3.6692692	-0.7617628
H	0.7716033	-2.0418223	-2.6893026
H	2.4702046	-2.4778495	-2.8588027
H	2.0230493	-0.7869585	-2.6135979
H	3.4859697	-1.9121201	0.6677544
H	3.7433442	-0.8472337	-0.7166628
H	3.9907183	-2.5888847	-0.8875339
S	1.9857493	1.2015177	1.0254655
O	3.0378530	2.0273253	0.5351186
O	2.1606962	0.3904887	2.1905570
C	0.5563876	2.2030924	1.2512483
C	0.3111167	3.2358305	0.3559860
C	-0.8269974	4.0079610	0.5146987
H	1.0127936	3.4288744	-0.4459732
C	-1.6994951	3.7533802	1.5652534
H	-1.0300335	4.8158370	-0.1779144
C	-1.4358953	2.7287377	2.4618276

H	-2.5869109	4.3632015	1.6884575
C	-0.3043261	1.9427104	2.3060503
H	-2.1126817	2.5389138	3.2862523
H	-0.0732373	1.1429572	2.9966465

2n-TS2Aa

E(PBE0-D3/def2-TZVP) = -1285.880926802 (conv)

Lowest Freq. = -399.40 cm⁻¹

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2n-TS2Aa (TS002A/c1/pbe0-d3.def2-TZVP)

C	-2.4886598	-1.4129151	-1.1540211
C	-3.2125406	-1.5214591	0.1781524
C	-1.0149108	-1.7429987	-0.9904567
H	-2.5920176	-0.3942655	-1.5503800
H	-2.9465615	-2.0807712	-1.8886679
C	-0.3547418	-0.8041619	0.0155683
H	-0.8915572	-2.7760974	-0.6522411
C	-2.5766565	-0.6354011	1.2423992
H	-3.1866496	-2.5622675	0.5109549
H	-4.2676525	-1.2566803	0.0677027
C	-1.0875908	-0.7413657	1.3206203
H	-0.4619981	0.2118829	-0.3999881
C	1.1526268	-1.0705544	0.1692766
H	-0.6350889	-0.0581886	2.0339012
H	-2.8161999	0.4160281	1.0146471
H	-3.0151749	-0.8292581	2.2253363
H	1.4252905	-1.9220772	-0.4595835
O	1.4806089	-1.4401898	1.5287413
C	2.0796381	0.0979641	-0.1888612
C	1.8762953	0.4374579	-1.6637302
C	3.5280793	-0.3427532	0.0137272
C	1.7936584	1.3204775	0.6779010
H	2.0761042	-0.4294023	-2.2994551
H	2.5669118	1.2314186	-1.9565097
H	0.8641289	0.7886815	-1.8768823
H	0.7778413	1.6973791	0.5339984
H	2.4815630	2.1290388	0.4199786
H	1.9282835	1.0892163	1.7360760
H	3.7511752	-1.2354198	-0.5770524
H	3.7329758	-0.5712031	1.0596427
H	4.2083576	0.4506062	-0.3049152
S	0.9217023	-2.8069185	2.0866664
O	1.7514573	-3.1063420	3.2048134
O	0.7911499	-3.7332463	1.0031238
C	-0.7063256	-2.4086536	2.6825622
C	-0.7679027	-1.6896359	3.9127934
C	-1.8745548	-1.7912445	4.7162755
H	0.0592091	-1.0470441	4.1890759
C	-2.9086214	-2.6790447	4.4004485
H	-1.9280784	-1.2023296	5.6246255
C	-2.7936195	-3.4904771	3.2749718
H	-3.7701633	-2.7649878	5.0507157
C	-1.6954934	-3.3984124	2.4477032
H	-3.5608460	-4.2245955	3.0571938
H	-1.5724395	-4.0658054	1.6050765
H	-0.4935275	-1.6617280	-1.9490666

2n-TS2Ab

E(PBE0-D3/def2-TZVP) = -1285.883272554 (conv)

Lowest Freq. = -333.80 cm⁻¹

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2n-TS2Ab (TS002A/c2/pbe0-d3.def2-TZVP)

C	-1.1969965	2.1848682	-0.1548428
C	-2.5178950	1.4388571	-0.0985026
C	-0.0588578	1.3001095	-0.6443364
H	-0.9522308	2.5583927	0.8471707
H	-1.2786998	3.0624566	-0.8023470
C	0.0893939	0.0340563	0.2177545
H	-0.2348561	1.0125299	-1.6871773
C	-2.3774524	0.1867644	0.7705277
H	-2.8204486	1.1489228	-1.1111649
H	-3.3093927	2.0814582	0.2979326
C	-1.2490994	-0.6451671	0.2722740
H	0.3535595	0.3637038	1.2320144
C	1.1601123	-0.9575851	-0.2355396
H	-1.4720054	-1.2820717	-0.5822507
H	-2.1791799	0.4969584	1.8031697
H	-3.3068811	-0.3849595	0.7769302
H	0.8230982	-1.4714542	-1.1421440
O	1.2410792	-1.9560437	0.8170847
C	2.6099436	-0.4884809	-0.4672115
C	2.7283203	0.2194233	-1.8185759
C	3.5107240	-1.7251847	-0.5405337
C	3.0924041	0.4134367	0.6640860
H	2.3617859	-0.4212288	-2.6252343
H	3.7810164	0.4308022	-2.0201186
H	2.1913614	1.1639308	-1.8676857
H	2.5341933	1.3508886	0.7128910
H	4.1458649	0.6641482	0.5189354
H	3.0002839	-0.0909630	1.6286196
H	3.1430548	-2.4348917	-1.2866110
H	3.5699788	-2.2447255	0.4145060
H	4.5187169	-1.4213531	-0.8321388
S	0.1714852	-3.1077278	0.9059004
O	0.7494141	-4.0690781	1.7835932
O	-0.2433070	-3.4901362	-0.4097999
C	-1.1810903	-2.3222283	1.7335603
C	-0.9029567	-1.6887360	2.9696187
C	-1.9172149	-1.4863925	3.8769242
H	0.1048748	-1.3531813	3.1794946
C	-3.1999151	-1.9785198	3.6336469
H	-1.7064950	-0.9641817	4.8031668
C	-3.4505738	-2.7043290	2.4701983
H	-3.9874863	-1.8270969	4.3612891
C	-2.4542406	-2.9122546	1.5430854
H	-4.4333600	-3.1282821	2.2989352
H	-2.6311988	-3.4973781	0.6490859
H	0.8685983	1.8737490	-0.6225206

2n-TS2Ba

E(PBE0-D3/def2-TZVP) = -1285.881516641 (conv)

Lowest Freq. = -399.07 cm⁻¹

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2n-TS2Ba (TS002B/c1/pbe0-d3.def2-TZVP)

C	-2.3757768	0.0868560	0.9926646
C	-2.9188684	0.4546354	-0.3819659
C	-0.9067020	-0.1867725	1.0216074
H	-2.8799734	-0.8316158	1.3354532
H	-2.6287621	0.8523843	1.7307414
C	-0.3395131	-0.9890112	-0.1202523

H	-0.5315287	-0.4991533	1.9941500
C	-2.4162982	-0.5009722	-1.4481061
H	-2.6086869	1.4703266	-0.6349285
H	-4.0118671	0.4584719	-0.3527825
C	-0.8958005	-0.5569065	-1.4727053
H	-0.6993859	-2.0182909	0.0556170
C	1.1766620	-1.0814581	0.0164797
H	-0.5760716	-1.2597735	-2.2422830
H	-0.4885959	0.4200672	-1.7484590
H	-2.8073439	-1.5085328	-1.2550352
H	-2.7924403	-0.2058300	-2.4315277
H	1.3710682	-1.4651137	1.0230901
O	1.7452006	0.2475238	-0.0386993
C	2.0007547	-1.9554593	-0.9459850
C	1.3237856	-3.3155170	-1.0860153
C	3.3753375	-2.1528172	-0.3022778
C	2.2117266	-1.3217859	-2.3203203
H	1.1515114	-3.7779973	-0.1097279
H	1.9650586	-3.9880243	-1.6604220
H	0.3658005	-3.2481684	-1.6060643
H	1.2921085	-1.2413928	-2.8980492
H	2.9076672	-1.9381672	-2.8947462
H	2.6451907	-0.3254194	-2.2279151
H	3.2894511	-2.6408747	0.6720550
H	3.8826282	-1.1973382	-0.1583095
H	4.0040722	-2.7777962	-0.9406024
S	1.6998693	1.1398733	1.2624429
O	2.6066712	2.2054668	0.9979423
O	1.8712920	0.3145233	2.4197629
C	0.0445673	1.7786510	1.2610957
C	-0.2997126	2.6031181	0.1536123
C	-1.2492418	3.5873589	0.2935721
H	0.1938372	2.4434976	-0.7966456
C	-1.8292051	3.8494683	1.5348216
H	-1.5284055	4.1825010	-0.5684517
C	-1.4077152	3.1305929	2.6548923
H	-2.5680366	4.6343933	1.6367227
C	-0.4573242	2.1441943	2.5411744
H	-1.8122137	3.3677416	3.6322281
H	-0.0947908	1.6125428	3.4121513

2n-TS2Bb

E(PBE0-D3/def2-TZVP) = -1285.873720036 (conv)

Lowest Freq. = -383.25 cm⁻¹

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2n-TS2Bb (TS002B/c2/pbe0-d3.def2-TZVP)

C	-2.2731686	0.3009741	0.1817790
C	-2.6485935	1.4155881	-0.7951654
C	-0.7937734	0.1291220	0.2630347
H	-2.7269128	-0.6273683	-0.1832981
H	-2.6902181	0.4861006	1.1739538
C	-0.0871531	-0.0530418	-1.0476325
H	-0.2904759	0.7698610	0.9812732
C	-2.0233372	1.1403697	-2.1514868
H	-2.2956414	2.3822635	-0.4173832
H	-3.7373992	1.4837998	-0.8729817
C	-0.5106729	1.0458571	-2.0368151
H	-0.4651322	-0.9885866	-1.4790277
C	1.4351108	-0.2603683	-0.8931196
H	-0.0662765	0.8446634	-3.0152941

H	-0.1345813	2.0160613	-1.7042783
H	-2.4243518	0.2022763	-2.5536907
H	-2.2866440	1.9267437	-2.8644389
H	1.7616554	-0.9372679	-1.6885340
O	1.6826164	-0.9474456	0.3624828
C	2.4349293	0.9174705	-0.8744697
C	2.0712736	1.9780262	0.1601052
C	2.5641390	1.5448188	-2.2644035
C	3.8153365	0.3469918	-0.5261354
H	1.1188554	2.4639541	-0.0583454
H	2.8408958	2.7536901	0.1794503
H	2.0139740	1.5432620	1.1600973
H	3.8469244	-0.0648286	0.4810028
H	4.5622980	1.1407281	-0.5988133
H	4.0988974	-0.4459706	-1.2237514
H	1.7059204	2.1468190	-2.5523890
H	2.7172540	0.7789808	-3.0298973
H	3.4392459	2.1984846	-2.2774833
S	0.9046203	-2.2682540	0.7189506
O	1.6968944	-2.8960696	1.7226220
O	0.5732689	-2.9637893	-0.4877964
C	-0.5917471	-1.6748551	1.4684891
C	-0.4664625	-1.0758999	2.7566800
C	-1.5336167	-1.0713645	3.6175850
H	0.4687679	-0.6015571	3.0283852
C	-2.7155270	-1.7473388	3.2933950
H	-1.4451572	-0.5683150	4.5735488
C	-2.7952517	-2.4590268	2.0995637
H	-3.5457021	-1.7537183	3.9887113
C	-1.7414655	-2.4659256	1.2117243
H	-3.6851261	-3.0346393	1.8719472
H	-1.7784899	-3.0512755	0.3018492

2n-INT2Aa

E(PBE0-D3/def2-TZVP) = -1285.906985522 (conv)

Lowest Freq. = 23.68 cm⁻¹

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2n-INT2Aa (002_spiroA/c1/pbe0-d3.def2-TZVP)

C	-2.4214748	-1.7230014	-0.2046301
C	-2.8964248	-0.5516724	0.6421574
C	-0.9054181	-1.8436180	-0.1935055
H	-2.7544057	-1.5817344	-1.2410405
H	-2.8807386	-2.6518826	0.1442651
C	-0.2661432	-0.5396942	-0.6543264
H	-0.5890692	-2.6520760	-0.8598165
C	-2.2077434	0.7537831	0.2607619
H	-2.7148389	-0.7696059	1.6970191
H	-3.9782627	-0.4269065	0.5386950
C	-0.6810530	0.6710802	0.1896765
H	-0.7045279	-0.3223128	-1.6355444
C	1.2534007	-0.6585676	-0.8551771
H	-2.5604448	1.0578357	-0.7317856
H	-2.4976504	1.5517795	0.9498363
H	1.5940619	-1.6245874	-0.4725389
O	1.9499109	0.3567845	-0.0905372
C	1.7473635	-0.5184851	-2.3000845
C	1.1175384	-1.6309475	-3.1347239
C	3.2648736	-0.6913687	-2.3178981
C	1.3855967	0.8449561	-2.8816401
H	1.3650691	-2.6165866	-2.7312461

H	1.4998125	-1.5845236	-4.1568500
H	0.0296461	-1.5479623	-3.1873632
H	0.3044880	1.0001011	-2.9258987
H	1.7676854	0.9268739	-3.9018246
H	1.8251354	1.6509954	-2.2915966
H	3.5533799	-1.6556665	-1.8908281
H	3.7613860	0.0931162	-1.7464682
H	3.6344213	-0.6536804	-3.3453849
S	1.7286391	0.2877803	1.4734892
O	2.6162993	1.2522316	2.0289224
O	1.7926513	-1.0823363	1.8871092
C	-0.0260030	0.8647936	1.6095608
C	0.0031123	2.3308654	1.8909776
C	-0.5404491	2.8791515	3.0058473
H	0.4786147	2.9581901	1.1462504
C	-1.1403350	2.0800477	3.9966763
H	-0.5034630	3.9548297	3.1359634
C	-1.1514943	0.6838603	3.8332858
H	-1.5639696	2.5317631	4.8840208
C	-0.6301741	0.0868161	2.7294501
H	-1.5794214	0.0611413	4.6111395
H	-0.6041168	-0.9906991	2.6571491
H	-0.5390402	-2.1105386	0.8020039
H	-0.3364242	1.5496777	-0.3635475

2n-INT2Ab

E(PBE0-D3/def2-TZVP) = -1285.914165913 (conv)

Lowest Freq. = 39.87 cm⁻¹

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2n-INT2Ab (002_spiroA/c2/pbe0-d3.def2-TZVP)

C	-2.5369677	-1.5561380	-0.9896035
C	-3.1825783	-0.8541737	0.1879598
C	-1.0606684	-1.8165390	-0.7383767
H	-2.6449854	-0.9309744	-1.8843944
H	-3.0418568	-2.5015426	-1.2068688
C	-0.2717429	-0.5527807	-0.3952934
H	-0.6355567	-2.2801213	-1.6274063
C	-2.4331021	0.4257220	0.5001868
H	-3.1662315	-1.5139535	1.0639692
H	-4.2332372	-0.6340312	-0.0200514
C	-0.9549258	0.1720582	0.7827617
H	-0.3012233	0.1097637	-1.2686610
C	1.1998669	-0.8414690	-0.0838523
H	-0.8801812	-0.4845138	1.6593183
H	-2.5180368	1.1161325	-0.3471013
H	-2.8767731	0.9366506	1.3583375
H	1.2689238	-1.4277048	0.8392122
O	1.8268926	0.4433103	0.1825358
C	2.0935069	-1.5235965	-1.1445644
C	1.8990483	-3.0416566	-1.1175113
C	3.5596797	-1.2722153	-0.7760552
C	1.8319620	-0.9675162	-2.5403408
H	2.0803726	-3.4368094	-0.1143960
H	2.6247607	-3.5059268	-1.7893765
H	0.9104797	-3.3668137	-1.4331945
H	0.8272312	-1.2020262	-2.8989525
H	2.5430408	-1.3947961	-3.2513277
H	1.9579341	0.1177269	-2.5569291
H	3.7632727	-1.5707664	0.2556379
H	3.8345763	-0.2240687	-0.8808106

H	4.2008736	-1.8651985	-1.4322366
S	1.4498514	1.1434107	1.5449854
O	2.2384320	2.3258848	1.6019131
O	1.5014066	0.1826047	2.6069339
C	-0.3037284	1.5279323	1.2042150
C	-0.3386905	2.5592011	0.1291570
C	-0.8047074	3.8154858	0.3479380
H	0.0502180	2.2824085	-0.8423517
C	-1.2927944	4.2138020	1.6058834
H	-0.7987618	4.5286470	-0.4688427
C	-1.3169993	3.2834170	2.6620167
H	-1.6479135	5.2243355	1.7593526
C	-0.8723312	2.0120456	2.4960263
H	-1.7073715	3.5843306	3.6278504
H	-0.8900316	1.3013531	3.3139738
H	-0.9509328	-2.5408904	0.0783342

2n-INT2Ba

E(PBE0-D3/def2-TZVP) = -1285.909118767 (conv)

Lowest Freq. = 41.41 cm⁻¹

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2n-INT2Ba (002_spiroB/c1/pbe0-d3.def2-TZVP)

C	-2.4169087	0.0205353	0.9619434
C	-2.9608214	0.4163309	-0.4018711
C	-0.8899576	-0.0461611	1.0246607
H	-2.7986475	-0.9754269	1.2156983
H	-2.7838416	0.7009664	1.7344786
C	-0.3378153	-0.9117613	-0.1294079
H	-0.6244965	-0.5696123	1.9497758
C	-2.4163442	-0.4930525	-1.4887838
H	-2.6961443	1.4541889	-0.6201449
H	-4.0535244	0.3714629	-0.3836147
C	-0.8938035	-0.5334475	-1.4990165
H	-0.7275769	-1.9156131	0.0878711
C	1.1760289	-1.0470169	0.0066176
H	-0.5729286	-1.2733167	-2.2329806
H	-0.4895748	0.4226796	-1.8375573
H	-2.7922824	-1.5113678	-1.3252834
H	-2.7846088	-0.1818596	-2.4702396
H	1.3564796	-1.4757929	0.9982021
O	1.7771925	0.2738375	0.0151003
C	1.9906929	-1.9002303	-0.9797704
C	1.3012569	-3.2506572	-1.1521560
C	3.3637685	-2.1297641	-0.3430968
C	2.2083681	-1.2283720	-2.3346911
H	1.1355974	-3.7376151	-0.1867530
H	1.9322289	-3.9118185	-1.7504921
H	0.3384401	-3.1644054	-1.6595420
H	1.2886259	-1.1064161	-2.9044279
H	2.8870447	-1.8414902	-2.9328146
H	2.6658453	-0.2458948	-2.2119216
H	3.2734644	-2.6466630	0.6158485
H	3.8798485	-1.1840619	-0.1701693
H	3.9858025	-2.7412493	-1.0007713
S	1.5464822	1.1139821	1.3368723
O	2.2563388	2.3316940	1.1441098
O	1.8140023	0.2902596	2.4786242
C	-0.2702802	1.3834229	1.2301842
C	-0.4815021	2.3812747	0.1436539
C	-0.9817417	3.6221755	0.3819696

H	-0.1623235	2.1136260	-0.8532871
C	-1.3474538	4.0383817	1.6730156
H	-1.0948647	4.3088397	-0.4495396
C	-1.1785012	3.1501532	2.7519740
H	-1.7401756	5.0329973	1.8379901
C	-0.6796895	1.9017197	2.5699299
H	-1.4565729	3.4657268	3.7514264
H	-0.5451267	1.2288117	3.4083865

2n-INT2Bb

E(PBE0-D3/def2-TZVP) = -1285.904893825 (conv)

Lowest Freq. = 40.27 cm⁻¹

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2n-INT2Bb (002_spiroB/c2/pbe0-d3.def2-TZVP)

C	-2.1275122	0.8579397	-0.3575888
C	-2.8986556	0.0618715	-1.3985779
C	-0.6279207	0.6772675	-0.5547732
H	-2.3998608	0.5312575	0.6527299
H	-2.3852344	1.9180111	-0.4218800
C	-0.2534963	-0.8106099	-0.4091585
C	-2.4804694	-1.3990984	-1.4030772
H	-2.7083295	0.4953498	-2.3876656
H	-3.9741577	0.1499499	-1.2215681
C	-0.9708621	-1.5658557	-1.5264747
H	-0.6765557	-1.1710472	0.5377205
C	1.2706928	-0.9610757	-0.2716275
H	-0.7322803	-2.6282933	-1.4937723
H	-0.6293343	-1.1943021	-2.4988500
H	-2.8096111	-1.8713358	-0.4690531
H	-2.9808523	-1.9354534	-2.2141172
H	1.5152405	-0.7620657	0.7770292
O	1.8955513	0.0895047	-1.0462736
C	1.9982656	-2.2754465	-0.5895855
C	1.3555969	-3.3978804	0.2221762
C	3.4455214	-2.1134624	-0.1163668
C	2.0248029	-2.6101651	-2.0794190
H	1.3714448	-3.1654524	1.2910611
H	1.9180608	-4.3232761	0.0792244
H	0.3216563	-3.5916341	-0.0655452
H	1.0481920	-2.8833592	-2.4744869
H	2.6962962	-3.4560788	-2.2458269
H	2.4045995	-1.7656862	-2.6571287
H	3.4907669	-1.8570247	0.9451391
H	3.9585852	-1.3274084	-0.6711464
H	3.9904423	-3.0485724	-0.2645377
S	1.9598280	1.4786445	-0.2769604
O	2.2173809	2.4443207	-1.2951718
O	2.8350661	1.3608002	0.8472689
C	0.1839017	1.6492163	0.3390528
C	-0.1742729	3.0670432	0.0542340
C	-0.4367559	3.9664605	1.0362509
H	-0.1813292	3.3653317	-0.9867902
C	-0.4220642	3.5945310	2.3931104
H	-0.6713566	4.9896373	0.7651909
C	-0.1551507	2.2573899	2.7342451
H	-0.6275687	4.3256884	3.1639657
C	0.1229068	1.3232497	1.7876274
H	-0.1764686	1.9597448	3.7765620
H	0.3145802	0.3019864	2.0897340
H	-0.3942064	0.9649390	-1.5876369

2n-TS3Aa

E(PBE0-D3/def2-TZVP) = -1285.899083150 (conv)

Lowest Freq. = -273.98 cm⁻¹

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2n-TS3Aa (TS003A/c1/pbe0-d3.def2-TZVP)

C	-2.5086599	-1.5835349	-0.3720377
C	-3.0303181	-0.4301318	0.4705111
C	-0.9893985	-1.6669573	-0.3437304
H	-2.8343536	-1.4418342	-1.4103974
H	-2.9420197	-2.5303943	-0.0384238
C	-0.3428864	-0.3334384	-0.7164689
H	-0.6541171	-2.4385800	-1.0391350
C	-2.3849035	0.8821031	0.0560726
H	-2.8296714	-0.6211616	1.5296462
H	-4.1166350	-0.3516359	0.3724909
C	-0.8505957	0.8506288	0.1288722
H	-0.7085129	-0.0915103	-1.7222911
C	1.1889381	-0.4461650	-0.8068266
H	-2.6647092	1.1037696	-0.9807815
H	-2.7610163	1.7059682	0.6680319
H	1.5305750	-1.2690439	-0.1697792
O	1.8173207	0.7599753	-0.3236177
C	1.7706110	-0.6613800	-2.2168869
C	1.1544128	-1.9009963	-2.8574798
C	3.2771801	-0.8786968	-2.0834017
C	1.5129152	0.5523061	-3.1065491
H	1.3070963	-2.7909931	-2.2412870
H	1.6315450	-2.0824189	-3.8233957
H	0.0837921	-1.7843666	-3.0392512
H	0.4455780	0.7302504	-3.2603086
H	1.9602089	0.3881271	-4.0897178
H	1.9527021	1.4544606	-2.6800611
H	3.4932293	-1.7451766	-1.4525727
H	3.7660405	-0.0096720	-1.6425330
H	3.7190389	-1.0580769	-3.0664498
S	1.8217554	0.9532033	1.2650317
O	2.4332179	2.2327741	1.4712955
O	2.3748188	-0.2263653	1.8772560
C	-0.4078202	1.0190001	1.5888937
C	-0.5492696	2.3626890	2.0828758
C	-0.6308415	2.6386591	3.4215790
H	-0.5333484	3.1724392	1.3621729
C	-0.6512416	1.6016485	4.3571960
H	-0.6866958	3.6686150	3.7536173
C	-0.6193762	0.2796716	3.9140797
H	-0.7079664	1.8215173	5.4160189
C	-0.5430365	-0.0156699	2.5754073
H	-0.6613546	-0.5301951	4.6328985
H	-0.4987043	-1.0497793	2.2711120
H	-0.6440899	-1.9935466	0.6399846
H	-0.4894337	1.7539147	-0.3716600

2n-TS3Ab

E(PBE0-D3/def2-TZVP) = -1285.901521818 (conv)

Lowest Freq. = -277.16 cm⁻¹

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2n-TS3Ab (TS003A/c2/pbe0-d3.def2-TZVP)

C	-2.5289138	-1.7039610	-1.0332850
C	-3.2246079	-1.0973076	0.1655295

C	-1.0374836	-1.8345579	-0.7827914
H	-2.6983889	-1.0672951	-1.9102582
H	-2.9432324	-2.6866665	-1.2752265
C	-0.3357330	-0.5237198	-0.4179315
H	-0.5740434	-2.2470112	-1.6765976
C	-2.5981191	0.2432679	0.4828198
H	-3.1271133	-1.7676667	1.0279818
H	-4.2952665	-0.9751400	-0.0206294
C	-1.0856625	0.1645653	0.7494233
H	-0.3771016	0.1343671	-1.2938591
C	1.1450142	-0.7723333	-0.0871428
H	-0.9354039	-0.4555990	1.6429489
H	-2.7649319	0.9303602	-0.3555892
H	-3.0777930	0.7026660	1.3508919
H	1.2090037	-1.3436411	0.8458644
O	1.7694950	0.5115981	0.1502902
C	2.0618991	-1.4744974	-1.1231170
C	1.8948708	-2.9962443	-1.0761981
C	3.5194327	-1.2017139	-0.7309446
C	1.8260688	-0.9412880	-2.5324806
H	2.0318436	-3.3687505	-0.0574219
H	2.6658340	-3.4562134	-1.6988322
H	0.9337481	-3.3524692	-1.4379783
H	0.8301381	-1.1840100	-2.9096045
H	2.5533994	-1.3758063	-3.2224905
H	1.9482545	0.1440642	-2.5613079
H	3.7050981	-1.4779323	0.3103815
H	3.7881149	-0.1538875	-0.8517231
H	4.1779673	-1.8023871	-1.3624984
S	1.5167513	1.1814316	1.5784545
O	2.3388773	2.3554020	1.5859116
O	1.6637619	0.1799320	2.6080817
C	-0.6834431	1.5920407	1.1170535
C	-0.5301915	2.5751127	0.0980967
C	-0.5766099	3.9165237	0.3982827
H	-0.3163226	2.2572445	-0.9143452
C	-0.8513735	4.3467885	1.6943513
H	-0.4045652	4.6450497	-0.3853762
C	-1.1212075	3.4059068	2.6899037
H	-0.8746314	5.4047793	1.9238284
C	-1.0839832	2.0639611	2.4057663
H	-1.3711842	3.7357733	3.6914593
H	-1.2903308	1.3320797	3.1792120
H	-0.8719351	-2.5628150	0.0210962

2n-TS3Ba

E(PBE0-D3/def2-TZVP) = -1285.899233573 (conv)

Lowest Freq. = -284.40 cm⁻¹

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2n-TS3Ba (TS003B/c1/pbe0-d3.def2-TZVP)

C	-2.5121141	-0.2289415	0.9089419
C	-3.0678017	0.1983107	-0.4391393
C	-0.9850847	-0.0804423	0.9925992
H	-2.7564611	-1.2841641	1.0789818
H	-2.9798972	0.3397633	1.7167716
C	-0.3412734	-0.8797505	-0.1644018
H	-0.6606096	-0.5739657	1.9158023
C	-2.4158991	-0.5845585	-1.5673191
H	-2.9060080	1.2712420	-0.5814081
H	-4.1507145	0.0464948	-0.4552114

C	-0.8923940	-0.5170888	-1.5401658
H	-0.6805444	-1.9065749	0.0294441
C	1.1753838	-0.9603128	-0.0061540
H	-0.5091091	-1.2241400	-2.2763126
H	-0.5371466	0.4638588	-1.8609463
H	-2.7152747	-1.6369273	-1.4811110
H	-2.7844490	-0.2388294	-2.5370405
H	1.3514221	-1.3537214	1.0012431
O	1.7625419	0.3600750	-0.0475505
C	2.0119841	-1.8436066	-0.9524059
C	1.3350432	-3.2024061	-1.1056631
C	3.3723147	-2.0486820	-0.2808388
C	2.2563341	-1.2088647	-2.3208489
H	1.1383690	-3.6609623	-0.1321321
H	1.9895036	-3.8780854	-1.6611681
H	0.3902470	-3.1375838	-1.6492733
H	1.3481698	-1.1049995	-2.9127553
H	2.9481955	-1.8366902	-2.8879177
H	2.7080352	-0.2218319	-2.2160927
H	3.2644875	-2.5455612	0.6867980
H	3.8765915	-1.0951600	-0.1159962
H	4.0141606	-2.6683754	-0.9113090
S	1.6027784	1.2156547	1.2990893
O	2.2741760	2.4517655	1.0299546
O	1.9935290	0.4063155	2.4274267
C	-0.6510837	1.4020984	1.2086617
C	-0.7436090	2.3863794	0.1741307
C	-0.8782805	3.7214801	0.4718622
H	-0.6236483	2.0876122	-0.8558327
C	-1.0101157	4.1532978	1.7895184
H	-0.8853453	4.4451412	-0.3347374
C	-1.0333896	3.2102945	2.8194035
H	-1.1074942	5.2084842	2.0119564
C	-0.9008905	1.8747074	2.5414339
H	-1.1677949	3.5329426	3.8452662
H	-0.9168344	1.1463080	3.3444461

2n-TS3Bb

E(PBE0-D3/def2-TZVP) = -1285.900149534 (conv)

Lowest Freq. = -276.65 cm⁻¹

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2n-TS3Bb (TS003B/c2/pbe0-d3.def2-TZVP)

C	-2.5258548	0.9113013	-0.1909890
C	-3.2103512	0.1145298	-1.2884803
C	-1.0049151	0.8387570	-0.3331938
H	-2.8120481	0.5266484	0.7951898
H	-2.8455740	1.9562951	-0.2211797
C	-0.5373237	-0.6283072	-0.2429729
C	-2.7063161	-1.3176477	-1.3210334
H	-3.0067461	0.5930715	-2.2538613
H	-4.2951202	0.1359444	-1.1515579
C	-1.1869998	-1.3897731	-1.3967015
H	-0.9380296	-1.0535877	0.6871632
C	0.9909148	-0.7072733	-0.1136169
H	-0.8878908	-2.4368415	-1.3801275
H	-0.8356025	-0.9758097	-2.3484354
H	-3.0380038	-1.8366305	-0.4129373
H	-3.1456816	-1.8579752	-2.1641615
H	1.2331464	-0.4210181	0.9151386
O	1.5789973	0.2941835	-0.9746378

C	1.7521990	-2.0260135	-0.3308067
C	1.0981059	-3.1181030	0.5118982
C	3.1767262	-1.8091749	0.1871104
C	1.8470329	-2.4410142	-1.7981578
H	1.0555714	-2.8275693	1.5658551
H	1.6885180	-4.0350181	0.4484451
H	0.0844702	-3.3541848	0.1849372
H	0.8951347	-2.7616897	-2.2173153
H	2.5452727	-3.2767004	-1.8897918
H	2.2289067	-1.6197362	-2.4066643
H	3.1768626	-1.5151942	1.2397365
H	3.6880956	-1.0274887	-0.3757445
H	3.7519488	-2.7329162	0.0908609
S	1.6896985	1.7226719	-0.2459408
O	1.8292663	2.6703066	-1.3128168
O	2.6816469	1.6522638	0.7911929
C	-0.3453223	1.8193911	0.6284240
C	-0.5911332	3.2198528	0.3796843
C	-0.4476280	4.1548374	1.3683029
H	-0.8101037	3.5248019	-0.6370111
C	-0.1512687	3.7650461	2.6790285
H	-0.5767570	5.2050464	1.1344746
C	-0.0568502	2.4067046	2.9876060
H	-0.0307785	4.5101646	3.4553612
C	-0.1935777	1.4549297	2.0100381
H	0.1069642	2.0990013	4.0137811
H	-0.1586468	0.4065356	2.2784627
H	-0.7609557	1.1873824	-1.3445563

2o-PhRad

E(PBE0-D3/def2-TZVP) = -1287.067723955 (conv)

Lowest Freq. = 12.63 cm⁻¹

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2o-PhRad (011/c2/pbe0-d3.def2-TZVP)

C	-0.9902818	-0.5142136	-0.9502745
C	-3.3064139	0.2689905	-0.3149725
C	-1.8733885	0.0612428	0.1442288
H	-0.9757265	0.1663869	-1.8068940
C	0.4332354	-0.7884493	-0.5101243
H	-1.4661976	1.0182820	0.4842611
H	-1.8582540	-0.6034096	1.0155136
H	-3.3139355	0.9277580	-1.1924712
H	0.4251848	-1.3877503	0.4045639
O	1.0328180	0.4988095	-0.1745312
C	1.3421048	-1.4797437	-1.5373723
C	0.7706093	-2.8650218	-1.8371207
C	2.7338749	-1.6528207	-0.9335800
C	1.4503431	-0.6712038	-2.8264835
H	0.6234466	-3.4422107	-0.9197060
H	1.4664844	-3.4200718	-2.4703792
H	-0.1830651	-2.8130743	-2.3646844
H	0.4916396	-0.6014748	-3.3442745
H	2.1589345	-1.1494931	-3.5071598
H	1.8063322	0.3410056	-2.6250821
H	2.6876579	-2.1759271	0.0259396
H	3.2241277	-0.6922801	-0.7736904
H	3.3624509	-2.2409620	-1.6062865
S	1.3065831	0.9447082	1.3100653
O	0.8855508	-0.0845257	2.2103094
O	0.8116019	2.2734202	1.4337410

C	3.0667197	1.0089781	1.3452826
C	3.7920741	0.1112666	2.1242860
C	5.1772192	0.1848814	2.1288473
H	3.2582495	-0.6250678	2.7131516
C	5.8413743	1.1353561	1.3652952
H	5.7451487	-0.5086578	2.7368210
C	5.1248748	2.0424311	0.5815780
H	6.9248113	1.1796700	1.3768145
C	3.7650721	1.9318448	0.6166456
H	5.6304844	2.7915996	-0.0160476
H	-1.4238739	-1.4552685	-1.3005566
H	-3.7275230	-0.6870353	-0.6513067
C	-4.1984422	0.8603078	0.7626990
H	-4.1924186	0.2021165	1.6404248
H	-3.7739452	1.8135788	1.1000644
C	-5.6318140	1.0795377	0.3085782
H	-5.6343882	1.7371012	-0.5685116
H	-6.0531725	0.1252654	-0.0285764
C	-6.5140299	1.6724340	1.3932903
H	-6.1308858	2.6414552	1.7247858
H	-6.5530707	1.0187016	2.2691166
H	-7.5381811	1.8215317	1.0437824

2o-TS1(1,8)a

E(PBE0-D3/def2-TZVP) = -1287.054539856 (conv)

Lowest Freq. = -931.44 cm⁻¹

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2o-TS1(1,8)a (TS005A/c2/pbe0-d3.def2-TZVP)

C	0.3421544	0.1371297	2.1678095
C	0.9509391	1.5270097	0.0914720
C	-0.0651814	1.2326172	1.1745973
H	0.0310919	0.4226582	3.1743301
C	-0.1857457	-1.2707319	1.9069943
H	-0.2108102	2.1617386	1.7401381
H	-1.0338932	1.0135083	0.7193892
H	1.9762917	1.3585472	0.4336761
H	0.5325442	-1.9925645	2.3074166
O	-0.2743550	-1.4822493	0.4714783
C	-1.5549268	-1.6387977	2.5017663
C	-1.4509304	-1.5908900	4.0252987
C	-1.8941986	-3.0698774	2.0879567
C	-2.6599211	-0.6982009	2.0332389
H	-0.6382216	-2.2261943	4.3884874
H	-2.3806333	-1.9565006	4.4670208
H	-1.2871752	-0.5792457	4.4014002
H	-2.4938601	0.3256494	2.3756695
H	-3.6207989	-1.0285443	2.4355052
H	-2.7382202	-0.6918764	0.9440777
H	-1.1088927	-3.7661165	2.3940827
H	-2.0111323	-3.1581539	1.0080227
H	-2.8276281	-3.3822358	2.5620332
S	0.9351972	-2.1889237	-0.2565533
O	0.7230050	-3.6016592	-0.2885409
O	2.1590055	-1.6838966	0.2881592
C	0.6474908	-1.5232156	-1.8558768
C	0.4526620	-2.3756667	-2.9348481
C	0.2297158	-1.8246362	-4.1881702
H	0.4700007	-3.4474384	-2.7777332
C	0.1896692	-0.4473071	-4.3515365
H	0.0785759	-2.4757981	-5.0405314

C	0.3821089	0.4014395	-3.2624805
H	0.0057498	-0.0254745	-5.3336268
C	0.6165895	-0.1585350	-2.0300946
H	0.3451952	1.4769170	-3.3956880
H	1.4328130	0.0853358	2.1924232
H	0.8324942	0.7066947	-0.8123004
C	0.7961778	2.8669215	-0.5871199
H	-0.1442715	2.8879570	-1.1532406
H	0.6922419	3.6474042	0.1798810
C	1.9596210	3.2231682	-1.4991851
H	2.8719870	3.2914581	-0.8968008
H	2.1343564	2.4066248	-2.2070647
C	1.7435626	4.5228120	-2.2534772
H	1.6039530	5.3605339	-1.5645768
H	0.8523735	4.4686237	-2.8857065
H	2.5932294	4.7599815	-2.8971726

2o-TS1(1,8)b

E(PBE0-D3/def2-TZVP) = -1287.055189953 (conv)

Lowest Freq. = -887.89 cm⁻¹

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2o-TS1(1,8)b (TS005B/c1/pbe0-d3.def2-TZVP)

C	-0.1008291	0.3673116	1.8027325
C	0.3829993	1.7602032	-0.3453186
C	-0.5406575	1.4587945	0.8195564
H	-0.4120451	0.6486890	2.8103572
C	-0.6111744	-1.0482312	1.5480310
H	-0.6377106	2.3927010	1.3885306
H	-1.5385072	1.2488416	0.4306255
H	0.2966498	0.8878141	-1.2011694
H	0.1175350	-1.7567405	1.9530187
O	-0.6912536	-1.2686822	0.1117260
C	-1.9737557	-1.4362463	2.1460533
C	-1.8678390	-1.3785649	3.6692552
C	-2.2881666	-2.8754986	1.7408736
C	-3.0986430	-0.5203507	1.6759477
H	-1.0427026	-1.9966117	4.0342015
H	-2.7896862	-1.7593568	4.1145772
H	-1.7225498	-0.3620387	4.0397789
H	-2.9594393	0.5056656	2.0235877
H	-4.0528648	-0.8755696	2.0728912
H	-3.1727989	-0.5120721	0.5864784
H	-1.4886673	-3.5559667	2.0454306
H	-2.4095451	-2.9717702	0.6621243
H	-3.2131104	-3.2022872	2.2217602
S	0.5035145	-2.0244439	-0.5890352
O	0.2537767	-3.4312592	-0.5996977
O	1.7357829	-1.5474628	-0.0349393
C	0.2699911	-1.3809386	-2.2052135
C	0.1664263	-2.2464049	-3.2867803
C	0.0263714	-1.7091557	-4.5580523
H	0.1913777	-3.3165886	-3.1198340
C	-0.0168584	-0.3336064	-4.7392075
H	-0.0539985	-2.3702143	-5.4124176
C	0.0803028	0.5271442	-3.6473113
H	-0.1296803	0.0752880	-5.7374081
C	0.2258898	-0.0196320	-2.3960609
H	0.0439668	1.6022250	-3.7880447
H	0.9887256	0.3295663	1.8310055
H	-0.0041487	2.6224196	-0.9001663
C	1.8533749	1.9253365	-0.0525625
H	1.9769560	2.6523649	0.7642058
H	2.2700845	0.9806646	0.3089203
C	2.6558349	2.3834663	-1.2594641
H	2.5234808	1.6576519	-2.0689144
H	2.2494158	3.3328212	-1.6280328
C	4.1348100	2.5398314	-0.9546902
H	4.5650622	1.5927721	-0.6187831
H	4.2992255	3.2765355	-0.1631869
H	4.6939335	2.8663374	-1.8342824

2o-TS1(1,7)a

E(PBE0-D3/def2-TZVP) = -1287.061856220 (conv)

Lowest Freq. = -949.17 cm⁻¹

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2o-TS1(1,7)a (TS004B/c3/pbe0-d3.def2-TZVP)

C	-0.0265505	-0.9614871	-1.0550254
C	-2.2755384	-0.0907761	-0.2313620
C	-0.8653041	-0.4995797	0.1111363
H	0.0331274	-0.1753759	-1.8141199
C	1.3739022	-1.3925265	-0.6670744
H	-0.3376155	0.5048664	0.5839557
H	-0.8269637	-1.2048919	0.9467222
H	-2.2507733	0.7786828	-0.9006841
H	1.3326856	-1.9921500	0.2458858
O	2.1366799	-0.1930354	-0.3634502
C	2.1656776	-2.1802272	-1.7211613
C	1.4462314	-3.5017409	-1.9872172
C	3.5516629	-2.4865539	-1.1566772
C	2.3029657	-1.3900267	-3.0184511
H	1.2449772	-4.0403510	-1.0567081
H	2.0737023	-4.1423891	-2.6107738
H	0.4998061	-3.3611554	-2.5131204
H	1.3330445	-1.2102182	-3.4881802
H	2.9161706	-1.9464255	-3.7313688
H	2.7840425	-0.4265342	-2.8403003
H	3.4794132	-3.0385316	-0.2152021
H	4.1200943	-1.5750953	-0.9690757
H	4.1149680	-3.0996332	-1.8639307
S	2.5323445	0.2065971	1.1108647
O	3.9280338	0.4986767	1.1131817
O	1.9980178	-0.7626223	2.0177291
C	1.6557031	1.7253586	1.2794985
C	2.3356612	2.8786565	1.6497391
C	1.6212387	4.0595262	1.7923477
H	3.4058163	2.8380150	1.8122030
C	0.2540730	4.0877503	1.5576469
H	2.1391259	4.9657783	2.0821764
C	-0.4216418	2.9287526	1.1788901
H	-0.2936114	5.0176110	1.6651368
C	0.2995681	1.7666194	1.0549636
H	-1.4888615	2.9542129	0.9877194
H	-0.5328126	-1.8114598	-1.5265543
H	-2.7541541	-0.8939055	-0.8096929
C	-3.1263289	0.2196246	0.9890010
H	-3.2112448	-0.6828440	1.6060527
H	-2.6134000	0.9579537	1.6162180
C	-4.5152370	0.7284523	0.6433231
H	-4.4247175	1.6339237	0.0316948
H	-5.0240404	-0.0099620	0.0130117
C	-5.3596953	1.0229368	1.8705626
H	-4.8841959	1.7775771	2.5033159
H	-5.4956960	0.1246031	2.4787865
H	-6.3503509	1.3933236	1.5983668

2o-TS1(1,7)b

E(PBE0-D3/def2-TZVP) = -1287.062709652 (conv)

Lowest Freq. = -949.51 cm⁻¹

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2o-TS1(1,7)b (TS004A/c3/pbe0-d3.def2-TZVP)

C	-0.4637553	-0.4707349	-1.7017679
C	-1.6316213	-0.9272039	0.5499908
C	-1.3381379	0.0332531	-0.5756154
H	-0.3959526	0.2871388	-2.4862402
C	0.9404738	-0.8651724	-1.2859074
H	-2.2556608	0.4807029	-0.9702125
H	-0.7845812	1.0077626	-0.0658810
H	-2.1025485	-1.8299744	0.1338522
H	0.9133055	-1.4591951	-0.3707945
O	1.6505478	0.3670283	-0.9802849
C	1.7672704	-1.6389916	-2.3235630
C	1.0954255	-2.9885023	-2.5727045
C	3.1589861	-1.8897158	-1.7457959
C	1.8887843	-0.8651366	-3.6320653
H	0.9291080	-3.5289571	-1.6364220
H	1.7379122	-3.6076478	-3.2026844
H	0.1363189	-2.8875998	-3.0844557
H	0.9189723	-0.7299592	-4.1164969
H	2.5314527	-1.4091681	-4.3283468
H	2.3312811	0.1186923	-3.4644782
H	3.0995135	-2.4200240	-0.7912067
H	3.7004775	-0.9578033	-1.5794214
H	3.7434610	-2.5023997	-2.4360226
S	2.1436770	0.7199761	0.4746715
O	3.5184663	1.0885480	0.3886252
O	1.7372323	-0.3192002	1.3724129
C	1.2052734	2.1751434	0.7964647
C	1.8373625	3.2986051	1.3156335
C	1.0743319	4.4187926	1.6112138
H	2.9091169	3.2842377	1.4725993
C	-0.2950415	4.4184623	1.3851141
H	1.5552778	5.3007613	2.0165727
C	-0.9215639	3.2924132	0.8549071
H	-0.8811280	5.3009379	1.6172174
C	-0.1514966	2.1903799	0.5746828
H	-1.9904778	3.2911825	0.6700728
H	-0.9492070	-1.3450803	-2.1500370
H	-0.6979334	-1.2543929	1.0175471
C	-2.5332721	-0.3335942	1.6190875
H	-2.0582075	0.5664109	2.0266624
H	-3.4757832	-0.0035755	1.1636122
C	-2.8308667	-1.2977899	2.7545429
H	-3.3025386	-2.2002792	2.3486830
H	-1.8852572	-1.6239778	3.2014665
C	-3.7208302	-0.6921701	3.8254420
H	-4.6838083	-0.3828007	3.4092653
H	-3.2542997	0.1920476	4.2683454
H	-3.9200591	-1.4014299	4.6317189

2o-TS1(1,6)a

E(TPSS-D3/def2-TZVP) = -1287.056547430 (conv)

Lowest Freq. = -1022.71 cm⁻¹

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2o-TS1(1,6)a (TS006A/c1/pbe0-d3.def2-TZVP)

C	0.1829566	-0.8384313	0.6258183
C	-1.9072824	-0.4453148	-0.7318140
C	-0.4117443	-0.7193417	-0.7538980
H	-0.2497618	-1.6579133	1.2045541
C	1.6803031	-0.7762763	0.8131444
H	-0.2371244	-1.6486263	-1.3094945
H	0.1008779	0.0727475	-1.3082480
H	-2.4111953	-1.2145243	-0.1329512
H	1.8827208	-0.8434782	1.8855096
O	2.1238267	0.5412143	0.3765061
C	2.5787241	-1.8224807	0.1293266
C	2.0154767	-3.2066974	0.4386510
C	3.9765254	-1.7027960	0.7367097
C	2.6871327	-1.6225881	-1.3799731
H	1.9072522	-3.3621854	1.5159782
H	2.6934148	-3.9748661	0.0599827
H	1.0406883	-3.3632795	-0.0288635
H	1.7437279	-1.7991442	-1.8953804
H	3.4194585	-2.3264183	-1.7832281
H	3.0256563	-0.6134362	-1.6183388
H	3.9542760	-1.8509007	1.8190272
H	4.4106889	-0.7206770	0.5424976
H	4.6378284	-2.4559057	0.3017656
S	2.4167172	1.6708709	1.4346712
O	3.1824602	2.6553617	0.7480225
O	2.9141342	1.0741749	2.6354378
C	0.8166786	2.3374133	1.7740106
C	0.7139059	3.6841616	2.1083114
C	-0.5245376	4.1971684	2.4601018
H	1.5961735	4.3127239	2.0805524
C	-1.6479119	3.3811530	2.4763398
H	-0.6140883	5.2452814	2.7188388
C	-1.5454505	2.0371584	2.1282967
H	-2.6123058	3.7930391	2.7522892
C	-0.3071335	1.5455902	1.7896129
H	-2.4231019	1.4001311	2.1249248
H	-0.1696470	0.1672749	1.2407400
H	-2.0908118	0.5080118	-0.2248573
C	-2.5237083	-0.3998868	-2.1187089
H	-2.0050288	0.3569966	-2.7198892
H	-2.3525347	-1.3573294	-2.6264486
C	-4.0125697	-0.0965496	-2.1061838
H	-4.5288995	-0.8517192	-1.5021803
H	-4.1788727	0.8612680	-1.5998278
C	-4.6206882	-0.0510751	-3.4969144
H	-4.4952743	-1.0072116	-4.0125056
H	-4.1421934	0.7176547	-4.1099289
H	-5.6897395	0.1696575	-3.4619868

2o-TS1(1,6)b

E(TPSS-D3/def2-TZVP) = -1287.057616079 (conv)

Lowest Freq. = -889.21 cm⁻¹

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2o-TS1(1,6)b (TS006B/c1/pbe0-d3.def2-TZVP)

C	0.2514167	-0.5724118	0.0364775
C	-2.2516105	-1.0159324	0.1171158
C	-0.8521694	-1.5193075	0.4467087
H	-0.0791587	0.5209741	0.4675299
C	1.6185482	-0.8654220	0.6205819
H	-0.7782081	-1.6924934	1.5249918
H	-0.6971815	-2.4944621	-0.0326586
H	-2.9801030	-1.7527179	0.4721127
H	1.4997688	-1.4914835	1.5079403
O	2.2611925	0.3674311	1.0651459
C	2.6293421	-1.5400234	-0.3193215
C	2.0099730	-2.8291504	-0.8522927
C	3.8832563	-1.8830342	0.4819873
C	3.0039501	-0.6281017	-1.4837496
H	1.6972551	-3.4894821	-0.0387905
H	2.7458183	-3.3674708	-1.4538782
H	1.1434095	-2.6332941	-1.4876065
H	2.1379188	-0.3686851	-2.0971349
H	3.7226946	-1.1355759	-2.1315244
H	3.4606307	0.2964842	-1.1285825
H	3.6460235	-2.5519563	1.3138338
H	4.3507920	-0.9862796	0.8899508
H	4.6115909	-2.3869950	-0.1578874
S	1.8825044	1.0115302	2.4534565
O	3.0400644	1.7062288	2.9070503
O	1.2617239	0.0167570	3.2732538
C	0.6694420	2.2025721	1.9861719
C	0.6601398	3.4647429	2.5667362
C	-0.3368109	4.3579511	2.2019341
H	1.4301823	3.7346331	3.2795314
C	-1.3009620	4.0011529	1.2684549
H	-0.3560367	5.3461268	2.6453867
C	-1.2827146	2.7374452	0.6808142
H	-2.0705061	4.7121076	0.9885259
C	-0.2931821	1.8684312	1.0665376
H	-2.0273044	2.4586426	-0.0569869
H	0.2874563	-0.3896731	-1.0384199
H	-2.4442969	-0.1016085	0.6903074
C	-2.4995778	-0.7471532	-1.3579493
H	-1.8165565	0.0305113	-1.7192989
H	-2.2648686	-1.6484121	-1.9390018
C	-3.9274905	-0.3172061	-1.6510366
H	-4.6161919	-1.0966447	-1.3060683
H	-4.1626232	0.5740433	-1.0570408
C	-4.1719165	-0.0309137	-3.1220188
H	-3.9753364	-0.9164613	-3.7326470
H	-3.5169581	0.7675135	-3.4820899
H	-5.2033297	0.2770728	-3.3065525

2o-TS1(1,5)

E(TPSS-D3/def2-TZVP+COSMO) = -1287.054479377 (conv)

Lowest Freq. = -1060.34 cm⁻¹

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2o-TS1(1,5) (TS009/c1c/pbe0-d3.def2-TZVP)

C	-0.4700040	-0.5989635	-0.0325199
C	-2.2366890	-0.3038144	-1.8000311
C	-0.7505249	-0.2463768	-1.4894664
H	-0.6351903	-1.6654005	0.1401828
C	0.9003121	-0.2517552	0.5012053
H	-0.2166107	-0.9256028	-2.1603807
H	-0.3758907	0.7599361	-1.6979748
H	-2.6251374	-1.3000442	-1.5525152
H	0.7932725	-0.3598974	1.7291709
O	1.2333255	1.1342535	0.3398478
C	2.1391125	-1.0606826	0.1110789
C	1.8278543	-2.5482452	0.2416030
C	3.2862280	-0.7070618	1.0596100
C	2.5820994	-0.7463900	-1.3206599
H	1.4484754	-2.7921266	1.2381330
H	2.7400317	-3.1273683	0.0825458
H	1.0933955	-2.8784545	-0.4953370
H	1.8444002	-1.0648203	-2.0565784
H	3.5153988	-1.2742177	-1.5323298
H	2.7599881	0.3218310	-1.4505224
H	3.0446334	-0.9666418	2.0926520
H	3.5182062	0.3580673	1.0215157
H	4.1836945	-1.2598363	0.7734821
S	0.5390389	2.2552125	1.2228073
O	-0.8669439	2.2629360	0.9708552
O	1.3077824	3.4332845	1.0077763
C	0.8258969	1.6373633	2.8461075
C	1.0839409	2.5106682	3.8964716
C	1.2507442	1.9801939	5.1661536
H	1.1574184	3.5757932	3.7122256
C	1.1739463	0.6087198	5.3775822
H	1.4508019	2.6429453	5.9993267
C	0.9342429	-0.2612785	4.3168956
H	1.3118977	0.2100199	6.3766607
C	0.7537317	0.2839349	3.0671837
H	0.8948601	-1.3323276	4.4807849
H	-1.2014803	-0.0745186	0.5870026
H	-2.7626667	0.4008648	-1.1456069
C	-2.5573746	0.0153183	-3.2496602
H	-2.1664652	1.0103457	-3.4953844
H	-2.0274801	-0.6876379	-3.9049657
C	-4.0438080	-0.0313781	-3.5624666
H	-4.4328699	-1.0255534	-3.3134952
H	-4.5702128	0.6717388	-2.9071193
C	-4.3557517	0.2906948	-5.0133889
H	-3.8653282	-0.4169035	-5.6878531
H	-4.0054310	1.2923441	-5.2774127
H	-5.4288707	0.2508318	-5.2131921

2o-INT1

E(PBE0-D3/def2-TZVP) = -1287.096925690 (conv)

Lowest Freq. = 11.12 cm⁻¹

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2o-INT1 (012/c1/pbe0-d3.def2-TZVP)

C	-1.8606216	-0.1792937	0.3981845
C	-2.5837608	0.0890771	1.7083204
C	-0.6689398	-1.0472083	0.5356613
H	-1.5681510	0.7872280	-0.0467975
H	-2.5590811	-0.6200597	-0.3273980
C	-0.0465764	-1.7440434	-0.6171476
H	-0.1922823	-1.1362706	1.5079072
H	-2.9446857	-0.8574707	2.1274111
H	-0.1429386	-2.8313356	-0.4972734
C	1.4339635	-1.4349708	-0.7853450
H	1.9422241	-1.5145397	0.1790516
O	1.5192216	-0.0472359	-1.2091598
C	2.1973328	-2.2975385	-1.8039313
C	2.2157517	-3.7409702	-1.3032789
C	3.6387158	-1.7994153	-1.8937478
C	1.5503591	-2.2299547	-3.1834864
H	2.6199606	-3.8044590	-0.2889608
H	2.8536147	-4.3458431	-1.9517480
H	1.2232780	-4.1955702	-1.3056582
H	0.5466765	-2.6610986	-3.1847679
H	2.1506612	-2.7908485	-3.9038145
H	1.4842390	-1.1977446	-3.5330521
H	4.1176653	-1.7919554	-0.9114323
H	3.6922731	-0.7891447	-2.3019307
H	4.2160737	-2.4562930	-2.5486026
S	2.3322199	1.0406666	-0.4057954
O	3.0355538	1.7986607	-1.3871761
O	3.0253685	0.4178550	0.6797591
C	1.0540302	2.0565262	0.2501401
C	0.3680627	2.9110368	-0.6027596
C	-0.6350764	3.7133195	-0.0867386
H	0.6306359	2.9479937	-1.6525927
C	-0.9358176	3.6669477	1.2686481
H	-1.1789850	4.3828513	-0.7421378
C	-0.2344318	2.8186259	2.1119620
H	-1.7178105	4.3010505	1.6698238
C	0.7654984	2.0030847	1.6042929
H	-0.4645594	2.7914639	3.1703323
H	1.3303012	1.3367168	2.2432348
H	-0.5699651	-1.4856875	-1.5417139
H	-1.8659099	0.4894403	2.4331859
C	-3.7419415	1.0603569	1.5644654
H	-4.4766351	0.6475392	0.8636631
H	-3.3736190	1.9853134	1.1064908
C	-4.4160650	1.3777162	2.8872706
H	-5.2479676	2.0740841	2.7602672
H	-3.7083013	1.8290392	3.5887744
H	-4.8095586	0.4723578	3.3576002

2o-TS2a

E(PBE0-D3/def2-TZVP) = -1287.082526187 (conv)

Lowest Freq. = -368.58 cm⁻¹

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2o-TS2a (TS007A/c1/pbe0-d3.def2-TZVP)

C	-1.6721638	0.4181099	0.7194970
C	-2.5865876	-0.7763451	0.9985248
C	-0.2283561	0.0580325	0.7386864
H	-1.8700945	1.1888825	1.4700610
H	-1.9331340	0.8498962	-0.2531356
C	0.3047330	-0.6920164	-0.4343474

H	0.1717908	-0.2414871	1.7053276
H	-2.4249093	-1.5556912	0.2447706
H	-0.1786793	-1.6775659	-0.4695435
C	1.8028480	-0.8995773	-0.3907872
H	2.0840092	-1.3362137	0.5731873
O	2.4439894	0.3964708	-0.4750270
C	2.4120830	-1.7615729	-1.5034678
C	1.8275936	-3.1691805	-1.4069532
C	3.9212614	-1.8403217	-1.2797731
C	2.1306620	-1.1748268	-2.8834494
H	1.9468430	-3.5824269	-0.4013226
H	2.3494180	-3.8316864	-2.1011025
H	0.7669772	-3.1953734	-1.6649817
H	1.0620197	-1.1600929	-3.1097397
H	2.6195202	-1.7799865	-3.6504914
H	2.5155365	-0.1565311	-2.9631241
H	4.1501108	-2.2535449	-0.2935277
H	4.3857129	-0.8565412	-1.3491211
H	4.3772008	-2.4888129	-2.0314157
S	2.4207962	1.3475361	0.7832451
O	3.3588151	2.3732019	0.4742519
O	2.5657781	0.5724811	1.9779173
C	0.7876148	2.0342614	0.7384190
C	0.3652874	2.6295414	-0.4773783
C	-0.6190057	3.5905696	-0.4622138
H	0.8089487	2.3047434	-1.4101520
C	-1.1393229	4.0602095	0.7439969
H	-0.9687738	4.0084585	-1.3992678
C	-0.6410279	3.5645117	1.9486759
H	-1.9012590	4.8296168	0.7450237
C	0.3328770	2.5922136	1.9597088
H	-1.0080107	3.9599808	2.8888418
H	0.7449935	2.2210373	2.8899568
H	0.0219723	-0.1799595	-1.3605817
H	-2.3165701	-1.2227084	1.9628898
C	-4.0573303	-0.3931433	1.0123293
H	-4.3190982	0.0601186	0.0494796
H	-4.2169682	0.3857245	1.7663978
C	-4.9724325	-1.5725981	1.2903229
H	-6.0227706	-1.2732911	1.2957679
H	-4.7500294	-2.0227910	2.2616674
H	-4.8528689	-2.3513120	0.5319577

2o-TS2b

E(PBE0-D3/def2-TZVP) = -1287.079617640 (conv)

Lowest Freq. = -416.64 cm⁻¹

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2o-TS2b (TS007B/c1/pbe0-d3.def2-TZVP)

C	-0.7862781	-0.5918123	1.2258266
C	-2.0365337	-0.3299486	2.0512160
C	-0.7751895	0.1297604	-0.0886541
H	-0.6979735	-1.6717405	1.0358208
H	0.1034178	-0.3388203	1.8125837
C	-0.1810108	-0.5595860	-1.2740355
H	-1.6844647	0.6834408	-0.3076791
H	-2.1517268	0.7497878	2.1945761
H	-0.7036072	-1.5150509	-1.4130437
C	1.3038602	-0.8317830	-1.1228222
H	1.5113201	-1.2659660	-0.1397081
O	1.9835203	0.4459708	-1.1809233

C	1.9520841	-1.7288084	-2.1841185
C	1.3438013	-3.1254855	-2.0774509
C	3.4478918	-1.8226778	-1.8882212
C	1.7413360	-1.1731221	-3.5890365
H	1.4304854	-3.5207478	-1.0613229
H	1.8739313	-3.8085297	-2.7448557
H	0.2901065	-3.1422599	-2.3628936
H	0.6849727	-1.1609337	-3.8673636
H	2.2655161	-1.7960824	-4.3175006
H	2.1329214	-0.1575164	-3.6721397
H	3.6247692	-2.1954148	-0.8754997
H	3.9334814	-0.8509567	-1.9785907
H	3.9246102	-2.5112082	-2.5896919
S	1.9623324	1.3860581	0.0845740
O	2.8602794	2.4413396	-0.2416498
O	2.1659820	0.6063617	1.2678374
C	0.3051346	2.0123573	0.0933787
C	-0.1250224	2.6856125	-1.0850012
C	-1.1753842	3.5671596	-1.0172441
H	0.3557241	2.4632780	-2.0292256
C	-1.7498581	3.8990182	0.2128733
H	-1.5409216	4.0325340	-1.9253487
C	-1.2113745	3.3783471	1.3885525
H	-2.5725275	4.6018627	0.2559461
C	-0.1643039	2.4861989	1.3481310
H	-1.6056296	3.6927637	2.3481016
H	0.2782578	2.0965437	2.2558429
H	-0.3448397	0.0263053	-2.1810623
H	-2.9201081	-0.6556502	1.4885083
C	-2.0112128	-1.0213187	3.4031280
H	-1.1263700	-0.6888313	3.9577658
H	-1.8859099	-2.1004282	3.2561998
C	-3.2607444	-0.7584260	4.2248452
H	-3.2188188	-1.2613051	5.1933906
H	-4.1556807	-1.1116750	3.7050578
H	-3.3902458	0.3113853	4.4109270

2o-INT2a

E(PBE0-D3/def2-TZVP) = -1287.113142432 (conv)

Lowest Freq. = 34.34 cm⁻¹

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2o-INT2a (013A/c1/pbe0-d3.def2-TZVP)

C	-1.7293783	0.3507040	0.7762013
C	-2.4026031	-0.9545915	1.1658282
C	-0.2059075	0.2818185	0.7284476
H	-2.0201651	1.1250784	1.4934171
H	-2.1040025	0.6868994	-0.1975726
C	0.2768059	-0.6115824	-0.4109593
H	0.1527236	-0.1413108	1.6742448
H	-2.1873608	-1.7351795	0.4274898
H	-0.1540638	-1.6036058	-0.2693495
C	1.7817600	-0.7583182	-0.4810929
H	2.1534884	-1.1821220	0.4581822
O	2.3693051	0.5631559	-0.6111930
C	2.3346772	-1.6007336	-1.6368653
C	1.7751018	-3.0165929	-1.5195247
C	3.8555454	-1.6567137	-1.5050818
C	1.9641929	-1.0058636	-2.9923983
H	1.9666706	-3.4405048	-0.5295389
H	2.2560976	-3.6643526	-2.2557752
H	0.6997052	-3.0507791	-1.7052857
H	0.8849778	-1.0135592	-3.1611867
H	2.4232305	-1.5928480	-3.7913180
H	2.3213706	0.0215254	-3.0817891
H	4.1500529	-2.0797678	-0.5407737
H	4.2977319	-0.6634880	-1.5871079
H	4.2770393	-2.2856616	-2.2926334
S	2.2039961	1.5197714	0.6379279
O	2.8523315	2.7333328	0.2772588
O	2.5834146	0.8151174	1.8266500
C	0.3777039	1.7290634	0.6636999
C	-0.0141606	2.4710711	-0.5660234
C	-0.5482722	3.7185951	-0.5172892
H	0.1635278	1.9915415	-1.5201363
C	-0.7677305	4.3810182	0.7042078
H	-0.8106631	4.2153987	-1.4446981
C	-0.4427910	3.7301539	1.9092044
H	-1.1838147	5.3797946	0.7172180
C	0.0843150	2.4794891	1.9184901
H	-0.6257273	4.2330948	2.8522481
H	0.3342476	1.9840963	2.8493084
H	-0.1070548	-0.2339557	-1.3628620
H	-1.9836057	-1.3099164	2.1156158
C	-3.9103538	-0.8172228	1.3031953
H	-4.3252343	-0.4521483	0.3568149
H	-4.1336907	-0.0453074	2.0481871
C	-4.5901233	-2.1177855	1.6927884
H	-5.6710675	-1.9937479	1.7865666
H	-4.2135297	-2.4867602	2.6507592
H	-4.4087128	-2.8963009	0.9465034

2o-INT2B

E(PBE0-D3/def2-TZVP) = -1287.106251729 (conv)

Lowest Freq. = 35.40 cm⁻¹

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2o-INT2B (013B/c1/pbe0-d3.def2-TZVP)

C	-0.9543751	-0.5659383	1.1266587
C	-2.3147200	-0.3237694	1.7620968
C	-0.7084784	0.2821401	-0.1295464
H	-0.8895012	-1.6235970	0.8473082
H	-0.1610849	-0.4120762	1.8606678
C	-0.0442348	-0.5246377	-1.2476065
H	-1.6879199	0.5950661	-0.5071134
H	-2.4446948	0.7448347	1.9661336
H	-0.6176125	-1.4444925	-1.3770396
C	1.4007307	-0.8636836	-0.9539700
H	1.4861966	-1.3492859	0.0242565
O	2.1249636	0.3935008	-0.8742971
C	2.1320080	-1.7372214	-1.9787586
C	1.4421103	-3.0982910	-2.0344662
C	3.5708376	-1.9316697	-1.5041321
C	2.1333648	-1.0954870	-3.3629255
H	1.3725128	-3.5501871	-1.0408161
H	2.0179201	-3.7770012	-2.6674780
H	0.4358304	-3.0340913	-2.4532847
H	1.1249355	-1.0114428	-3.7743484
H	2.7186808	-1.7066196	-4.0538788
H	2.5796833	-0.0997635	-3.3338860
H	3.5977379	-2.3805765	-0.5074388
H	4.1063129	-0.9829861	-1.4607000
H	4.1042031	-2.5955675	-2.1883948
S	1.8143692	1.2978610	0.3852427
O	2.5833874	2.4803320	0.2008933
O	1.9685262	0.5162201	1.5764381
C	0.0259338	1.6495082	0.1333431
C	-0.0811810	2.5366071	-1.0625391
C	-0.5965835	3.7901580	-0.9954522
H	0.2769889	2.1478834	-2.0069085
C	-1.0374534	4.3438093	0.2203399
H	-0.6635844	4.3793054	-1.9032661
C	-0.9281712	3.5818586	1.3974443
H	-1.4382894	5.3482963	0.2522956
C	-0.4305619	2.3184368	1.3859986
H	-1.2461237	4.0114957	2.3409610
H	-0.3253351	1.7620995	2.3077676
H	-0.0950638	0.0168442	-2.1942221
H	-3.1002059	-0.5872618	1.0423932
C	-2.5185598	-1.1112394	3.0447353
H	-1.7382239	-0.8339416	3.7625825
H	-2.3731879	-2.1785100	2.8407545
C	-3.8870651	-0.8896194	3.6643795
H	-4.0084627	-1.4618207	4.5865935
H	-4.6835693	-1.1911782	2.9784693
H	-4.0429903	0.1656988	3.9047157

2o-TS3a

E(PBE0-D3/def2-TZVP) = -1287.103378560 (conv)

Lowest Freq. = -280.60 cm⁻¹

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2o-TS3a (TS008A/c1/pbe0-d3.def2-TZVP)

C	-1.8636904	0.2067701	0.8048965
C	-2.3319195	-1.1784292	1.2183896
C	-0.3421810	0.3589938	0.6797913
H	-2.2224782	0.9328562	1.5418310
H	-2.3286574	0.4922420	-0.1466143
C	0.1925691	-0.4520673	-0.5004056
H	0.1098491	-0.0359695	1.5980155
H	-2.0470363	-1.9242392	0.4682038
H	-0.2402720	-1.4508382	-0.4359718
C	1.6989661	-0.6155695	-0.5412862
H	2.0445776	-1.0307924	0.4123106
O	2.3254263	0.6801421	-0.6972879
C	2.2505215	-1.5030388	-1.6669376
C	1.6866936	-2.9133122	-1.5078303
C	3.7706837	-1.5644663	-1.5263136
C	1.8890398	-0.9504128	-3.0425810
H	1.8684982	-3.3044408	-0.5026126
H	2.1739087	-3.5856098	-2.2176157
H	0.6133330	-2.9547708	-1.7033278
H	0.8106238	-0.9637064	-3.2166737
H	2.3531312	-1.5607277	-3.8209248
H	4.0579632	-1.9494016	-0.5439836
H	4.2209211	-0.5790159	-1.6467894
H	4.1900409	-2.2287368	-2.2855692
S	2.2287183	1.6483647	0.5747990
O	2.8890589	2.8537452	0.1730407
O	2.6675530	0.9311742	1.7470205
C	-0.0209236	1.8517913	0.6394031
C	-0.2586222	2.6010313	-0.5534472
C	-0.3885878	3.9683287	-0.5151909
H	-0.2783770	2.0870085	-1.5059401
C	-0.3701988	4.6529336	0.6991629
H	-0.5163689	4.5182531	-1.4402860
C	-0.2588680	3.9355974	1.8928985
H	-0.4621841	5.7316326	0.7181228
C	-0.1327274	2.5705141	1.8747302
H	-0.2837368	4.4594648	2.8412856
H	-0.0440427	2.0130235	2.8006129
H	-0.1611937	-0.0234024	-1.4418122
H	-1.8232223	-1.4703794	2.1456557
C	-3.8363219	-1.2499695	1.4268828
H	-4.3419628	-0.9447214	0.5036835
H	-4.1288377	-0.5175226	2.1875566
C	-4.3108942	-2.6326686	1.8374540
H	-5.3926527	-2.6585035	1.9847266
H	-3.8404303	-2.9485391	2.7726381
H	-4.0613669	-3.3770136	1.0761802
H	2.2456776	0.0743979	-3.1598926

2o-TS3b

E(PBE0-D3/def2-TZVP) = -1287.097572518 (conv)

Lowest Freq. = -316.92 cm⁻¹

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2o-TS3b (TS008B/c1/pbe0-d3.def2-TZVP)

C	-0.9813968	-0.5809595	1.0766488
C	-2.3527009	-0.4939592	1.7301598
C	-0.8654305	0.2393077	-0.2131003
H	-0.7847379	-1.6321690	0.8390189
H	-0.2001315	-0.2947331	1.7858068
C	-0.0626329	-0.5023332	-1.2902301
H	-1.8812973	0.3249300	-0.6213381
H	-2.6405071	0.5542527	1.8685514
H	-0.5674976	-1.4562495	-1.4560240
C	1.3881880	-0.7697211	-0.9443551
H	1.4673668	-1.1922921	0.0631632
O	2.0927527	0.4961011	-0.9413438
C	2.1528388	-1.7001093	-1.8962910
C	1.5137268	-3.0862730	-1.8488624
C	3.5946172	-1.8098799	-1.4029164
C	2.1411915	-1.1681975	-3.3262073
H	1.4484573	-3.4593344	-0.8226478
H	2.1228763	-3.7912443	-2.4189775
H	0.5116168	-3.0969948	-2.2820425
H	1.1326993	-1.1517458	-3.7459761
H	2.7518846	-1.8094814	-3.9661503
H	2.5511431	-0.1575820	-3.3719497
H	3.6296054	-2.1733448	-0.3721786
H	4.1008226	-0.8450676	-1.4363621
H	4.1511239	-2.5117786	-2.0283975
S	1.7655978	1.4493480	0.3021006
O	2.4697573	2.6653677	0.0297409
O	2.0173503	0.7297936	1.5266897
C	-0.4478140	1.7050963	-0.0004196
C	-0.4577983	2.5582844	-1.1538385
C	-0.5317607	3.9221278	-1.0353647
H	-0.3566204	2.1127039	-2.1352379
C	-0.6792340	4.5221040	0.2160437
H	-0.4882666	4.5380252	-1.9260194
C	-0.7927253	3.7171479	1.3502904
H	-0.7266416	5.6002104	0.3035527
C	-0.7288484	2.3498896	1.2520470
H	-0.9438063	4.1732276	2.3217536
H	-0.7990979	1.7462916	2.1463497
H	-0.0995325	0.0369914	-2.2389209
H	-3.1003683	-0.9171679	1.0475625
C	-2.4220518	-1.2155483	3.0649593
H	-1.6835114	-0.7791250	3.7470342
H	-2.1209084	-2.2604003	2.9261174
C	-3.8011819	-1.1591125	3.6977580
H	-3.8248565	-1.6794656	4.6575775
H	-4.5509427	-1.6217966	3.0499802
H	-4.1113169	-0.1251346	3.8722454