Supporting Information

Cobalt Pincer Complexes in Catalytic C-H Borylation: The Pincer Ligand Flips Rather Than Dearomatizes

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Cartesian coordinates and energies of the species involved in the text

Cartesian coordinates of the species shown in the following are obtained from the optimizations in gas phase at the level of ωB97XD/BS1, where atoms of the ^{i}PrPNP ligand except N and P use cc-pVDZ and the others (including the Co) use Def2TZVP unless otherwise stated. However, the species of **TS$_{2\text{-}12}$**, **12**, **2^{R}**, **TS$_{9\text{-}10}^{R}$**, **11^{R}**, **TS$_{2\text{-}12}^{R}$**, and **12^{R}** (R= Ir, Ph, Ir_Ph, and Ir_Ph_tBu) are optimized in gas phase at the level of ωB97XD/BS4 (LANL2DZ for Co and 6-31G* for the others). On the basis of gas-phase optimized geometries, single point calculations were conducted in C_6H_6 solvent with the SMD solvent model at the level of ωB97XD/Def2TZVP, where all the atoms use Def2TZVP. Absolute values (in Hartree) of the SCF energy in C_6H_6 solvent and the SCF energy in gas phase together with the thermal correction to Enthalpy and the thermal correction to Gibbs Free Energy in gas phase, are also provided. The free energy in gas phase is obtained by adding the thermal correction to Gibbs Free Energy in gas phase to the SCF energy in gas phase. The free energy in C_6H_6 solvent is obtained by adding the thermal correction to Gibbs Free Energy in gas phase to the SCF energy in C_6H_6 solvent. The enthalpy in C_6H_6 solvent is obtained by adding the thermal correction to Enthalpy in gas phase to the SCF energy in C_6H_6 solvent.

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SCF energy in gas phase: -2076.00426346

Thermal correction to Enthalpy in gas phase: 0.686681

Thermal correction to Gibbs Free Energy in gas phase: 0.582099

SCF energy in solvent: -3314.13141551

Co	0.073950	-0.021061	0.157569
N	0.338115	-1.906709	-0.441020
C	-0.116505	1.890928	0.739962
P	-2.021745	-0.549871	0.359950
P	2.223692	0.037766	0.175692
Si	-0.621729	3.094442	-0.583968
C	-0.808294	2.386803	-2.332144
C	0.631285	4.504019	-0.700896
C	-2.295849	3.894420	-0.225153
H	-0.092926	1.589479	-2.540192
H	-0.680069	3.169637	-3.084917
H	-1.805946	1.965259	-2.470705
H	0.696900	5.032048	0.253920
H	0.356397	5.229693	-1.470884
H	1.629935	4.130154	-0.938010

H	-3.099136	3.153508	-0.229952
H	-2.538179	4.645950	-0.981545
H	-2.303934	4.383833	0.751906
H	-0.848304	1.989350	1.551120
H	0.812016	2.296164	1.165838
C	-0.659392	-2.820656	-0.340279
C	1.520756	-2.320106	-0.964352
C	-3.220253	-0.258820	-1.027634
C	-3.007020	-0.226481	1.896958
C	-1.902792	-2.388990	0.382319
C	2.646761	-1.321499	-0.990136
C	3.292996	1.448630	-0.369154
C	2.997001	-0.498621	1.772084
C	-0.533161	-4.119393	-0.826097
C	1.709152	-3.611319	-1.450457
H	-3.285119	0.840684	-1.095972
C	-4.630394	-0.822727	-0.839657
C	-2.595627	-0.775964	-2.329379
H	-3.819210	-0.974295	1.922757
C	-3.633750	1.171263	1.911612
C	-2.118673	-0.422227	3.130720
H	-1.799517	-2.687460	1.437685
H	-2.790128	-2.906881	-0.009030
H	2.699641	-0.871942	-1.993644
H	3.610809	-1.818153	-0.801191
H	2.953898	2.282077	0.269774
C	2.982641	1.832839	-1.818701
C	4.798669	1.255775	-0.171818
H	4.070342	-0.679202	1.592843
C	2.365023	-1.802732	2.268492
C	2.836988	0.608487	2.819020
H	-1.374353	-4.806757	-0.731899
C	0.664262	-4.524972	-1.401246
H	2.678246	-3.885330	-1.868456
H	-5.250205	-0.590735	-1.720492
H	-5.141609	-0.409284	0.041001
H	-4.617399	-1.919955	-0.735758
H	-2.570284	-1.878311	-2.346231
H	-1.564921	-0.414025	-2.453228
H	-3.186583	-0.446892	-3.198341
H	-4.233548	1.302642	2.826050
H	-4.297286	1.349760	1.053241
H	-2.862543	1.954351	1.902920
H	-1.284528	0.295630	3.122055
H	-1.682844	-1.431624	3.181675
H	-2.705539	-0.268014	4.050261
H	3.425402	2.812544	-2.056438
H	1.902162	1.896779	-2.002449
H	3.409370	1.105924	-2.528537
H	5.164084	0.366601	-0.712038
H	5.077378	1.147661	0.885792
H	5.345603	2.126528	-0.567379
H	2.814495	-2.098084	3.229956
H	2.512016	-2.634892	1.563107
H	1.280677	-1.674074	2.413784
H	1.770842	0.834240	2.978130
H	3.334013	1.544071	2.520295
H	3.272267	0.292259	3.780171
H	0.786223	-5.537850	-1.787708

2

SCF energy in gas phase: -3277.8139751

Thermal correction to Enthalpy in gas phase: 0.748302

Thermal correction to Gibbs Free Energy in gas phase: 0.642266

SCF energy in solvent: -3278.05932703

Co	0.000000	0.000000	0.438563
P	0.515527	2.069819	0.618184
B	0.000000	0.000000	-1.475525
H	-1.451855	0.437685	0.299558
P	-0.515527	-2.069819	0.618184
H	1.451855	-0.437685	0.299558
N	0.000000	0.000000	2.486598
O	-0.328465	-1.082348	-2.305115
O	0.328465	1.082348	-2.305115
C	0.020888	-0.779193	-3.655041
C	-0.020888	0.779193	-3.655041
C	0.973420	1.447729	-4.588311
C	-1.421943	1.333948	-3.903364
C	-0.973420	-1.447729	-4.588311
C	1.421943	-1.333948	-3.903364
H	-0.866725	-2.531716	-4.521930
H	-0.793107	-1.152288	-5.624539
H	-1.998044	-1.192178	-4.323953
H	2.151074	-0.856491	-3.247107
H	1.736094	-1.193562	-4.939071
H	1.420539	-2.402406	-3.683984
H	0.866725	2.531716	-4.521930
H	0.793107	1.152288	-5.624539
H	1.998044	1.192178	-4.323953
H	-2.151074	0.856491	-3.247107
H	-1.736094	1.193562	-4.939071
H	-1.420539	2.402406	-3.683984
C	-0.083036	2.416408	2.330842
C	2.306502	2.528869	0.690768
C	-0.240083	3.438095	-0.372431
C	-2.306502	-2.528869	0.690768
C	0.240083	-3.438095	-0.372431
C	0.083036	-2.416408	2.330842
C	-0.020228	1.163352	3.160625
C	0.020228	-1.163352	3.160625
H	0.431980	3.250678	2.829093
H	-1.143645	2.697750	2.223019
H	2.366208	3.601660	0.937535
C	2.968241	2.287933	-0.669043
C	3.028547	1.743222	1.789474
H	0.269483	3.348661	-1.343711
C	0.000000	4.841021	0.194479
C	-1.731288	3.200203	-0.618337
H	-2.366208	-3.601660	0.937535
C	-2.968241	-2.287933	-0.669043
C	-3.028547	-1.743222	1.789474
H	-0.269483	-3.348661	-1.343711
C	0.000000	-4.841021	0.194479
C	1.731288	-3.200203	-0.618337
H	-0.431980	-3.250678	2.829093
H	1.143645	-2.697750	2.223019
C	-0.013483	1.197092	4.554024
C	0.013483	-1.197092	4.554024
H	4.033816	2.563229	-0.624661
H	2.497908	2.870780	-1.474030
H	2.890403	1.224514	-0.942154
H	2.921261	0.661118	1.617043

H	2.640173	1.971863	2.794039
H	4.101361	1.992697	1.785889
H	-0.432906	5.595388	-0.481535
H	1.066670	5.080561	0.308486
H	-0.484879	4.971119	1.175775
H	-2.312100	3.249066	0.317682
H	-1.908677	2.215674	-1.066175
H	-2.125938	3.977979	-1.291856
H	-4.033816	-2.563229	-0.624661
H	-2.497908	-2.870780	-1.474030
H	-2.890403	-1.224514	-0.942154
H	-2.921261	-0.661118	1.617043
H	-2.640173	-1.971863	2.794039
H	-4.101361	-1.992697	1.785889
H	0.432906	-5.595388	-0.481535
H	-1.066670	-5.080561	0.308486
H	0.484879	-4.971119	1.175775
H	2.312100	-3.249066	0.317682
H	1.908677	-2.215674	-1.066175
H	2.125938	-3.977979	-1.291856
H	-0.027931	2.156862	5.070984
C	0.000000	0.000000	5.260324
H	0.027931	-2.156862	5.070984
H	0.000000	0.000000	6.351622

$TS_{2\text{-}3}$

SCF energy in gas phase: -3277.80827876

Thermal correction to Enthalpy in gas phase: 0.747808

Thermal correction to Gibbs Free Energy in gas phase: 0.643816

SCF energy in solvent: -3278.0540076

Co	0.469674	0.018835	-0.044825
P	0.528491	2.143611	0.131536
B	-1.439790	-0.054768	-0.074696
H	0.111304	-0.040368	-1.521974
P	0.720973	-2.109544	0.017228
H	0.542098	0.033553	1.467699
N	2.501918	0.099319	-0.301347
O	-2.215550	-1.196470	0.174733
O	-2.318639	0.992537	-0.389159
C	-3.594726	-0.842702	0.244525
C	-3.634877	0.479364	-0.583837
C	-4.646712	1.505031	-0.101921
C	-3.813732	0.238681	-2.081489
C	-4.427339	-1.979407	-0.323482
C	-3.935951	-0.634564	1.718601
H	-4.338144	-2.855775	0.320627
H	-5.482818	-1.702323	-0.374614
H	-4.089444	-2.255950	-1.321014
H	-3.348811	0.181479	2.142150
H	-4.995623	-0.418462	1.865353
H	-3.687552	-1.544477	2.266156
H	-4.599933	2.391506	-0.736419
H	-5.661397	1.103560	-0.154083
H	-4.444559	1.812143	0.922733
H	-3.098254	-0.499337	-2.445817
H	-4.822870	-0.101184	-2.321170
H	-3.628289	1.174413	-2.610169
C	2.350276	2.496898	0.132582
C	-0.008179	3.033755	1.668949
C	-0.109441	3.225625	-1.232277
C	-0.302051	-3.333410	-0.926107

C	0.934874	-2.920730	1.665826
C	2.381563	-2.279351	-0.770694
C	3.160798	1.262438	-0.167087
C	3.190390	-1.027974	-0.564078
H	2.648292	2.886443	1.117424
H	2.600071	3.285374	-0.593335
H	0.413574	4.049852	1.577081
C	-1.531579	3.145389	1.775672
C	0.556099	2.400548	2.942796
H	-1.182209	2.976270	-1.251161
C	0.060256	4.732167	-1.020778
C	0.489631	2.789531	-2.572425
H	-1.230216	-3.386888	-0.337488
C	-0.675360	-2.808581	-2.314216
C	0.311084	-4.733982	-1.027059
H	1.172476	-3.981929	1.486204
C	2.097571	-2.297262	2.442939
C	-0.367805	-2.825122	2.465405
H	2.188087	-2.376611	-1.851973
H	2.940339	-3.172803	-0.456182
C	4.549803	1.330458	-0.279915
C	4.579080	-1.027587	-0.673580
H	-1.800068	3.757102	2.651444
H	-1.991509	3.597998	0.886211
H	-1.980000	2.149297	1.897461
H	0.121572	1.403750	3.102644
H	1.649041	2.275204	2.912952
H	0.315552	3.036378	3.809981
H	-0.314898	5.278734	-1.900707
H	-0.491219	5.104777	-0.146018
H	1.119880	5.013045	-0.896260
H	1.563506	3.036261	-2.636745
H	0.378411	1.706447	-2.718882
H	-0.013916	3.314280	-3.399517
H	-1.363791	-3.514450	-2.805926
H	-1.156199	-1.825372	-2.252775
H	0.209243	-2.704649	-2.964149
H	1.250262	-4.726068	-1.603963
H	0.519422	-5.183717	-0.046104
H	-0.384075	-5.407783	-1.552693
H	2.182376	-2.769709	3.434300
H	3.063377	-2.428947	1.930697
H	1.928469	-1.218620	2.583785
H	-0.641553	-1.769043	2.612249
H	-1.208581	-3.314677	1.952682
H	-0.243604	-3.300410	3.451216
H	5.052087	2.291199	-0.162200
C	5.270260	0.169861	-0.528841
H	5.104344	-1.960866	-0.877839
H	6.358015	0.197445	-0.611805

3

SCF energy in gas phase: -3277.81055591

Thermal correction to Enthalpy in gas phase: 0.748313

Thermal correction to Gibbs Free Energy in gas phase: 0.64127

SCF energy in solvent: -3278.05554021

Co	0.440752	0.007581	-0.183906
P	0.586805	2.138448	0.010283
B	-1.464152	-0.013435	-0.061786
H	-0.001324	0.013444	-1.641645
P	0.641716	-2.125002	-0.063464

H	0.565471	-0.013514	1.323123
N	2.476503	0.036839	-0.492208
O	-2.279158	-1.153438	0.013187
O	-2.307354	1.108111	-0.057488
C	-3.624910	-0.767523	0.288781
C	-3.657795	0.693367	-0.253781
C	-4.582574	1.636143	0.495986
C	-3.944626	0.763465	-1.752435
C	-4.570152	-1.731402	-0.406763
C	-3.824602	-0.839568	1.801240
H	-4.479067	-2.722133	0.041565
H	-5.607166	-1.404855	-0.299527
H	-4.337462	-1.816966	-1.466917
H	-3.154064	-0.148258	2.313892
H	-4.852788	-0.609080	2.085528
H	-3.590584	-1.849192	2.140128
H	-4.538114	2.628643	0.044515
H	-5.616727	1.287457	0.446547
H	-4.293154	1.726188	1.541641
H	-3.289362	0.088462	-2.305180
H	-4.982072	0.512627	-1.980234
H	-3.749748	1.779116	-2.099074
C	2.304839	2.448423	-0.593400
C	0.595508	2.870599	1.711759
C	-0.408386	3.364192	-0.960138
C	-0.361486	-3.343213	-1.034466
C	0.743817	-2.915947	1.608240
C	2.343368	-2.365362	-0.739289
C	3.141914	1.204822	-0.473612
C	3.162103	-1.118296	-0.550093
H	2.793685	3.317144	-0.130223
H	2.208018	2.666853	-1.670453
H	0.727016	3.958446	1.592370
C	-0.739410	2.607015	2.414233
C	1.760877	2.341159	2.551656
H	-1.374895	3.370782	-0.433684
C	0.162216	4.785916	-0.980954
C	-0.665909	2.861447	-2.381835
H	-1.300464	-3.402766	-0.462891
C	-0.707355	-2.799115	-2.421947
C	0.253997	-4.742561	-1.137720
H	0.917891	-3.992112	1.444803
C	1.916195	-2.364041	2.423583
C	-0.573657	-2.736271	2.366369
H	2.215231	-2.506783	-1.825898
H	2.859390	-3.255653	-0.352772
C	4.533455	1.249400	-0.404854
C	4.554262	-1.143453	-0.486143
H	-0.743584	3.081959	3.407965
H	-1.596644	2.991118	1.843377
H	-0.887633	1.523633	2.542003
H	1.699840	1.246371	2.644649
H	2.742044	2.592974	2.120669
H	1.722826	2.777578	3.562234
H	-0.529178	5.457512	-1.514366
H	0.311739	5.205802	0.023978
H	1.126432	4.829138	-1.513183
H	0.268446	2.791757	-2.963938
H	-1.124431	1.865595	-2.371647
H	-1.332177	3.561362	-2.911583
H	-1.355689	-3.515074	-2.952140
H	-1.222277	-1.833860	-2.350046

H	0.195050	-2.649720	-3.037981
H	1.185513	-4.733115	-1.726730
H	0.477781	-5.189138	-0.158345
H	-0.444936	-5.420709	-1.652564
H	1.931038	-2.830239	3.421379
H	2.890441	-2.564106	1.951883
H	1.815661	-1.275582	2.551143
H	-0.776488	-1.665660	2.521105
H	-1.429202	-3.158041	1.819958
H	-0.515425	-3.229535	3.349435
H	5.042237	2.212845	-0.366221
C	5.248438	0.057256	-0.390793
H	5.079687	-2.098341	-0.512056
H	6.337668	0.064474	-0.324359

TS_{3-4}

SCF energy in gas phase: -3277.80523291

Thermal correction to Enthalpy in gas phase: 0.747244

Thermal correction to Gibbs Free Energy in gas phase: 0.64068

SCF energy in solvent: -3278.04891911

Co	-0.422058	0.023379	-0.230629
P	-0.460779	2.168403	0.049498
B	1.510899	-0.115164	-0.372552
H	0.611995	-0.056334	-1.459856
P	-0.835077	-2.093578	-0.034679
H	0.181599	-0.054762	1.137068
N	-2.436993	0.197381	-0.573973
O	2.275148	-1.301905	-0.308375
O	2.400018	0.973087	-0.220118
C	3.569238	-0.983800	0.190908
C	3.738047	0.495734	-0.273260
C	4.607741	1.353962	0.629498
C	4.215489	0.608491	-1.720309
C	4.580970	-1.955590	-0.390919
C	3.532805	-1.117510	1.712630
H	4.390087	-2.959028	-0.006822
H	5.597682	-1.672212	-0.108794
H	4.515269	-1.990494	-1.477075
H	2.811741	-0.421689	2.144733
H	4.511233	-0.934957	2.160085
H	3.219154	-2.129982	1.968890
H	4.675631	2.363953	0.221521
H	5.619459	0.947374	0.697614
H	4.187987	1.421447	1.631873
H	3.610875	-0.018895	-2.376862
H	5.263510	0.323065	-1.827778
H	4.103852	1.644088	-2.044684
C	-2.146703	2.609861	-0.547377
C	-0.431094	2.842370	1.771435
C	0.616370	3.356694	-0.881201
C	0.124725	-3.421235	-0.898569
C	-1.102417	-2.793404	1.656425
C	-2.505057	-2.217374	-0.798731
C	-3.043434	1.405555	-0.528863
C	-3.218682	-0.903651	-0.661526
H	-2.597902	3.455439	-0.008522
H	-2.031411	2.922635	-1.598474
H	-0.685820	3.913165	1.704710
C	0.963150	2.693672	2.385603
C	-1.484514	2.151530	2.639016
H	1.607633	3.193995	-0.434031

C	0.227716	4.830072	-0.731087
C	0.722439	2.960756	-2.355896
H	1.103453	-3.381055	-0.397335
C	0.365971	-3.063117	-2.367657
C	-0.459678	-4.830233	-0.766149
H	-1.508792	-3.810279	1.529096
C	-2.128058	-1.959951	2.427526
C	0.223833	-2.872597	2.414731
H	-2.336886	-2.400998	-1.872680
H	-3.113360	-3.048385	-0.413925
C	-4.429012	1.540472	-0.495431
C	-4.608929	-0.832754	-0.637412
H	0.958954	3.048471	3.428190
H	1.725546	3.264035	1.835533
H	1.269701	1.635716	2.378095
H	-1.246990	1.082860	2.737747
H	-2.498542	2.232812	2.217003
H	-1.502923	2.600929	3.644459
H	0.922100	5.460757	-1.308955
H	0.267400	5.175229	0.311915
H	-0.785859	5.029475	-1.116556
H	-0.238219	3.080464	-2.885134
H	1.041253	1.916437	-2.465854
H	1.455261	3.607430	-2.864267
H	1.070581	-3.782601	-2.813483
H	0.787391	-2.055253	-2.470669
H	-0.563774	-3.110352	-2.959354
H	-1.477528	-4.892618	-1.185683
H	-0.500620	-5.176757	0.276298
H	0.164229	-5.547271	-1.323208
H	-2.256876	-2.362118	3.444815
H	-3.116329	-1.958768	1.942532
H	-1.790338	-0.916315	2.503349
H	0.673931	-1.871113	2.497283
H	0.952063	-3.526833	1.912153
H	0.061311	-3.265522	3.430579
H	-4.866724	2.537423	-0.436480
C	-5.230280	0.406167	-0.538472
H	-5.191645	-1.752729	-0.691953
H	-6.317650	0.486499	-0.503361

4

SCF energy in gas phase: -3277.81223238

Thermal correction to Enthalpy in gas phase: 0.750591

Thermal correction to Gibbs Free Energy in gas phase: 0.642644

SCF energy in solvent: -3278.05703093

Co	0.436260	-0.040651	-0.220072
P	0.399372	-2.163803	0.209074
B	-1.610295	0.197349	-0.492538
H	-0.757028	0.111700	-1.481186
P	1.011843	2.034287	0.067991
H	-0.810028	0.165346	0.672983
N	2.342488	-0.308105	-0.748669
O	-2.358949	1.417249	-0.500565
O	-2.557301	-0.872166	-0.356902
C	-3.645468	1.138945	0.025015
C	-3.867143	-0.337034	-0.433415
C	-4.788929	-1.149578	0.461663
C	-4.335839	-0.430606	-1.885657
C	-4.640969	2.138681	-0.538151
C	-3.582366	1.271329	1.548348

H	-4.418056	3.136242	-0.155407
H	-5.660905	1.881438	-0.242595
H	-4.588493	2.173960	-1.625046
H	-2.892213	0.541677	1.975180
H	-4.561492	1.138031	2.011674
H	-3.216055	2.268788	1.797005
H	-4.896173	-2.158548	0.059285
H	-5.782576	-0.698014	0.513265
H	-4.386430	-1.229031	1.470541
H	-3.701008	0.175177	-2.533613
H	-5.371809	-0.107024	-2.003983
H	-4.259128	-1.469679	-2.209393
C	2.051685	-2.714156	-0.388304
C	0.343413	-2.719179	1.972615
C	-0.750530	-3.346834	-0.635459
C	-0.031166	3.470737	-0.454914
C	1.680254	2.551107	1.713653
C	2.467724	2.103935	-1.052970
C	2.925162	-1.530613	-0.700495
C	3.132507	0.758065	-1.037653
H	2.559090	-3.390437	0.315659
H	1.902084	-3.287143	-1.316944
H	0.613966	-3.788153	2.002053
C	-1.071410	-2.538615	2.531485
C	1.357898	-1.935620	2.806047
H	-1.735095	-3.061065	-0.236982
C	-0.486732	-4.825608	-0.342669
C	-0.791997	-3.070996	-2.140632
H	-0.964233	3.309459	0.107332
C	-0.393131	3.367785	-1.940810
C	0.534944	4.854721	-0.128115
H	2.060961	3.581363	1.623487
C	2.838570	1.647711	2.143716
C	0.541488	2.522206	2.737566
H	2.058882	2.281360	-2.059938
H	3.187981	2.906286	-0.836798
C	4.287121	-1.713449	-0.928867
C	4.496192	0.630907	-1.282509
H	-1.088578	-2.764573	3.609181
H	-1.803168	-3.193503	2.037025
H	-1.409645	-1.499118	2.390397
H	1.080219	-0.871411	2.834329
H	2.378954	-2.001815	2.397216
H	1.383870	-2.318776	3.838541
H	-1.207312	-5.452609	-0.891842
H	-0.590387	-5.069717	0.724553
H	0.521768	-5.136339	-0.663729
H	0.161445	-3.324448	-2.635217
H	-1.014944	-2.015070	-2.342988
H	-1.574079	-3.686774	-2.612123
H	-1.236926	4.038044	-2.163969
H	-0.695164	2.348777	-2.216148
H	0.449801	3.677687	-2.581120
H	1.531323	5.004915	-0.576792
H	0.618962	5.035840	0.953083
H	-0.127239	5.633930	-0.538187
H	3.148239	1.890134	3.172684
H	3.719932	1.767764	1.495545
H	2.540659	0.589070	2.111953
H	0.111472	1.509702	2.803284
H	-0.274769	3.210612	2.468890
H	0.909465	2.809537	3.735033

H	4.703070	-2.719444	-0.865632
C	5.091402	-0.622696	-1.227886
H	5.081093	1.523835	-1.504060
H	6.160437	-0.745201	-1.407043

TS_{4-5}

SCF energy in gas phase: -3277.79798424

Thermal correction to Enthalpy in gas phase: 0.749002

Thermal correction to Gibbs Free Energy in gas phase: 0.64364

SCF energy in solvent: -3278.04395796

Co	-0.224844	-0.192831	-0.124826
P	-1.900988	-1.568086	-0.480965
B	1.675064	-0.737163	0.083664
H	0.568041	-1.288776	0.663512
P	0.028558	1.927274	-0.365901
H	0.479945	-0.500350	-1.392738
N	-1.226593	0.316909	1.534077
O	2.579750	-0.024268	0.897744
O	2.412605	-1.684818	-0.650726
C	3.917633	-0.434352	0.599010
C	3.690469	-1.838085	-0.045133
C	4.705793	-2.227370	-1.105870
C	3.578330	-2.953787	0.994938
C	4.727899	-0.445473	1.884272
C	4.527005	0.565455	-0.381366
H	4.840816	0.573840	2.256865
H	5.725327	-0.855319	1.708617
H	4.238161	-1.035514	2.656726
H	3.971535	0.583101	-1.319516
H	5.569000	0.325209	-0.598092
H	4.494114	1.564075	0.057642
H	4.470968	-3.221526	-1.488331
H	5.714323	-2.253127	-0.686471
H	4.690631	-1.532246	-1.943310
H	2.864917	-2.688403	1.776618
H	4.540709	-3.175901	1.459314
H	3.215964	-3.855037	0.499142
C	-2.367541	-1.807010	1.304230
C	-3.560613	-1.184856	-1.230191
C	-1.604779	-3.305010	-1.069017
C	1.641694	2.614251	-0.937103
C	-1.359790	2.960037	-1.051241
C	0.011649	2.383992	1.425990
C	-2.159483	-0.512294	2.040787
C	-1.016053	1.522031	2.101126
H	-3.384359	-2.192722	1.472582
H	-1.657243	-2.552993	1.696506
H	-4.268493	-1.968265	-0.911000
C	-3.477789	-1.187473	-2.758515
C	-4.077330	0.158858	-0.711791
H	-1.481039	-3.179363	-2.158609
C	-2.753322	-4.286987	-0.820360
C	-0.280836	-3.855683	-0.531037
H	2.315396	1.975154	-0.347430
C	1.983832	4.068011	-0.602653
C	1.891219	2.299172	-2.413915
H	-2.189607	2.614349	-0.406949
C	-1.688438	2.535651	-2.485649
C	-1.283683	4.483290	-0.929466
H	1.010973	2.096170	1.793031
H	-0.151014	3.446808	1.655340

C	-2.906037	-0.159303	3.164027
C	-1.736404	1.931602	3.220211
H	-4.429881	-0.849507	-3.197961
H	-3.264617	-2.189317	-3.160370
H	-2.683813	-0.509663	-3.111101
H	-3.380425	0.967581	-0.973420
H	-4.202210	0.165902	0.381900
H	-5.056269	0.392484	-1.160102
H	-2.496657	-5.279799	-1.223313
H	-3.693375	-3.974333	-1.297809
H	-2.946174	-4.414449	0.257544
H	-0.299966	-3.958512	0.567191
H	0.567781	-3.209906	-0.791211
H	-0.100078	-4.859651	-0.947714
H	3.063734	4.233297	-0.752057
H	1.755822	4.326523	0.442345
H	1.455672	4.781100	-1.250702
H	1.278405	2.934131	-3.073343
H	1.665566	1.246437	-2.640586
H	2.946806	2.488856	-2.668184
H	-2.681107	2.907916	-2.786307
H	-1.680349	1.439969	-2.581193
H	-0.954177	2.941116	-3.198847
H	-0.591974	4.909001	-1.671096
H	-0.957538	4.817490	0.066780
H	-2.274446	4.927480	-1.119772
H	-3.657359	-0.848994	3.549041
C	-2.689483	1.076021	3.763103
H	-1.548779	2.914511	3.652360
H	-3.268104	1.375805	4.638452

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SCF energy in gas phase: -3277.80387118

Thermal correction to Enthalpy in gas phase: 0.750001

Thermal correction to Gibbs Free Energy in gas phase: 0.644437

SCF energy in solvent: -3278.05072196

Co	0.357819	0.192429	-0.435375
P	2.379511	1.048083	-0.491620
B	-1.447558	0.967717	-0.275006
H	-0.222918	1.633930	-0.384296
P	-0.363735	-1.801798	-0.322097
H	0.162280	0.211063	-1.903799
N	0.710018	0.005607	1.532367
O	-2.086040	1.190408	0.959714
O	-2.384284	1.138647	-1.298750
C	-3.486224	1.360509	0.748121
C	-3.550242	1.760941	-0.763435
C	-4.773074	1.250268	-1.506554
C	-3.402634	3.265799	-0.984353
C	-4.006632	2.417859	1.708692
C	-4.178966	0.031052	1.043873
H	-3.924364	2.053190	2.733652
H	-5.057594	2.639720	1.509011
H	-3.433594	3.339778	1.631754
H	-3.851567	-0.750438	0.358415
H	-5.264270	0.117126	0.971686
H	-3.927990	-0.276793	2.060463
H	-4.729930	1.575811	-2.546520
H	-5.690449	1.644166	-1.062914
H	-4.819125	0.162228	-1.496391
H	-2.528916	3.652008	-0.457427

H	-4.284954	3.815371	-0.651656
H	-3.260505	3.447928	-2.049888
C	2.327055	1.772101	1.222331
C	4.023000	0.175460	-0.459507
C	2.735435	2.515034	-1.570553
C	-1.908362	-2.259041	-1.233056
C	0.813077	-3.243939	-0.415285
C	-0.856866	-1.837221	1.462747
C	1.619050	0.799467	2.126195
C	0.097058	-0.966013	2.233451
H	3.307042	2.051455	1.637281
H	1.719811	2.687798	1.138185
H	4.772404	0.880886	-0.062294
C	4.449940	-0.251839	-1.866343
C	3.960307	-1.029434	0.482998
H	2.959629	2.054247	-2.547971
C	3.940121	3.357908	-1.142201
C	1.491105	3.386047	-1.764033
H	-2.445193	-1.297306	-1.221894
C	-2.820816	-3.320028	-0.612069
C	-1.604102	-2.559086	-2.703625
H	1.480000	-3.000218	0.433033
C	1.660448	-3.183844	-1.689675
C	0.258302	-4.650082	-0.182013
H	-1.850579	-1.366901	1.509792
H	-0.931972	-2.837361	1.912885
C	1.913098	0.672749	3.482328
C	0.359747	-1.150741	3.589030
H	5.355794	-0.877023	-1.819221
H	4.677111	0.609924	-2.511214
H	3.661267	-0.841760	-2.359647
H	3.191412	-1.741421	0.150337
H	3.722097	-0.740243	1.517676
H	4.929007	-1.553865	0.498264
H	4.108540	4.173836	-1.863011
H	4.870134	2.773434	-1.086413
H	3.772800	3.823853	-0.157412
H	1.165105	3.844737	-0.815803
H	0.649868	2.799013	-2.154986
H	1.714070	4.204605	-2.466936
H	-3.779670	-3.342632	-1.155839
H	-3.052569	-3.109547	0.443001
H	-2.391007	-4.329570	-0.667083
H	-1.127350	-3.544538	-2.826816
H	-0.943702	-1.792542	-3.135322
H	-2.538351	-2.570601	-3.286592
H	2.559085	-3.814157	-1.590680
H	1.973707	-2.150602	-1.897385
H	1.097670	-3.543774	-2.563922
H	-0.339709	-4.989514	-1.041550
H	-0.373830	-4.714565	0.716565
H	1.084555	-5.369090	-0.058082
H	2.652698	1.330472	3.939185
C	1.269030	-0.311669	4.223804
H	-0.145075	-1.949411	4.132657
H	1.488462	-0.436377	5.285557

$TS_{5\text{-}6}$

SCF energy in gas phase: -3277.79540123

Thermal correction to Enthalpy in gas phase: 0.749033

Thermal correction to Gibbs Free Energy in gas phase: 0.643816

SCF energy in solvent: -3278.04063231

Co	-0.464010	0.097548	-0.620612
P	-2.268547	-1.115234	-0.502782
B	1.380478	-0.838090	-0.781740
H	0.314189	-0.970558	-1.511015
P	0.176777	2.060760	-0.168731
H	-0.759664	0.610661	-1.997654
N	-0.325005	-0.249303	1.339922
O	1.661329	-1.947634	0.017942
O	2.572318	-0.267131	-1.215775
C	3.056727	-1.972267	0.314498
C	3.659065	-1.129590	-0.861353
C	4.860929	-0.280734	-0.485323
C	3.982067	-1.972116	-2.092559
C	3.524546	-3.417435	0.363999
C	3.254443	-1.332135	1.686274
H	3.058892	-3.921901	1.211758
H	4.608231	-3.469359	0.490595
H	3.251698	-3.955402	-0.541804
H	2.977323	-0.279579	1.678762
H	4.288902	-1.413874	2.023733
H	2.609500	-1.839740	2.404904
H	5.207028	0.271597	-1.359785
H	5.681950	-0.908094	-0.131374
H	4.613082	0.439751	0.292726
H	3.127066	-2.585436	-2.379433
H	4.840811	-2.623669	-1.922969
H	4.211707	-1.304183	-2.923064
C	-1.721176	-2.173965	0.921231
C	-3.928313	-0.513694	0.084825
C	-2.737769	-2.366148	-1.791782
C	1.500631	2.870148	-1.179217
C	-1.109227	3.336562	0.263377
C	1.000934	1.781422	1.461875
C	-0.946889	-1.316186	1.879859
C	0.339316	0.611336	2.139149
H	-2.527110	-2.716354	1.437705
H	-1.028300	-2.914019	0.488058
H	-4.500814	-1.385080	0.445510
C	-4.703020	0.148621	-1.057706
C	-3.749472	0.458720	1.253706
H	-3.254155	-1.762670	-2.557577
C	-3.693921	-3.462451	-1.313208
C	-1.496010	-2.967341	-2.456671
H	2.124093	1.993092	-1.416876
C	2.398948	3.910431	-0.502869
C	0.929316	3.396990	-2.498694
H	-1.577481	2.849053	1.139167
C	-2.181253	3.433616	-0.825742
C	-0.633317	4.722951	0.700153
H	2.038720	1.504486	1.213129
H	1.047827	2.651257	2.133080
C	-0.896282	-1.572593	3.248152
C	0.410063	0.414986	3.515880
H	-5.625872	0.614202	-0.676660
H	-4.994287	-0.571822	-1.836385
H	-4.100979	0.937436	-1.536488
H	-3.126201	1.312836	0.949639
H	-3.266213	-0.014373	2.121805
H	-4.727357	0.843318	1.584545
H	-3.969123	-4.120987	-2.152561
H	-4.627182	-3.057934	-0.894706

H	-3.223542	-4.096122	-0.543846
H	-0.860295	-3.501219	-1.731518
H	-0.880171	-2.189347	-2.925918
H	-1.797310	-3.690875	-3.231025
H	3.248858	4.145395	-1.164674
H	2.821152	3.550242	0.447480
H	1.873977	4.854536	-0.301556
H	0.347052	4.320353	-2.346730
H	0.277743	2.650523	-2.976412
H	1.746623	3.636814	-3.197160
H	-3.072986	3.958672	-0.446546
H	-2.474397	2.430972	-1.168140
H	-1.814420	3.990610	-1.701429
H	-0.250339	5.299401	-0.155798
H	0.160287	4.680204	1.461589
H	-1.472682	5.295531	1.127541
H	-1.408786	-2.446509	3.650569
C	-0.206533	-0.696928	4.078808
H	0.949120	1.133987	4.133068
H	-0.160690	-0.872016	5.154902

6

SCF energy in gas phase: -3277.79858129

Thermal correction to Enthalpy in gas phase: 0.749631

Thermal correction to Gibbs Free Energy in gas phase: 0.643148

SCF energy in solvent: -3278.04225397

Co	-0.590095	0.114962	-0.656684
P	-1.857415	-1.587318	-0.404130
B	1.417781	-0.534271	-0.900440
H	0.525108	-0.344460	-1.786543
P	-0.377521	2.216240	-0.332431
H	-1.350028	0.434617	-1.923480
N	-0.185663	-0.074774	1.269936
O	1.806716	-1.819401	-0.543881
O	2.482393	0.344630	-0.720201
C	3.088492	-1.763134	0.092895
C	3.666735	-0.407991	-0.437690
C	4.510049	0.361131	0.564538
C	4.426052	-0.554544	-1.753534
C	3.884857	-2.993822	-0.306650
C	2.865340	-1.769456	1.602124
H	3.412094	-3.884636	0.109124
H	4.903987	-2.937446	0.082110
H	3.927769	-3.107429	-1.388072
H	2.328081	-0.882271	1.933974
H	3.811118	-1.823248	2.143475
H	2.268090	-2.642886	1.866172
H	4.857980	1.290331	0.111155
H	5.385303	-0.220180	0.862085
H	3.938822	0.611066	1.457470
H	3.831074	-1.097692	-2.488611
H	5.375405	-1.074572	-1.616651
H	4.629958	0.439431	-2.152847
C	-1.084332	-2.325152	1.103927
C	-3.626196	-1.358068	0.116841
C	-1.974187	-3.012429	-1.584012
C	0.429723	3.408169	-1.514052
C	-1.862775	3.158300	0.268681
C	0.699728	2.186024	1.167918
C	-0.513166	-1.209516	1.932364
C	0.335969	0.965648	1.965127

H	-1.738429	-2.972002	1.706815
H	-0.244488	-2.932948	0.728218
H	-3.995275	-2.321193	0.508055
C	-4.488307	-0.939903	-1.076993
C	-3.713943	-0.319693	1.238051
H	-2.608791	-2.615358	-2.394639
C	-2.637479	-4.271341	-1.019146
C	-0.607775	-3.332375	-2.194970
H	-0.409775	4.023538	-1.882106
C	1.025743	2.668073	-2.715055
C	1.465030	4.344895	-0.883491
H	-2.175877	2.561273	1.144286
C	-2.982596	3.088486	-0.772108
C	-1.625828	4.597790	0.730103
H	1.720668	2.043613	0.780715
H	0.690605	3.087564	1.795709
C	-0.339199	-1.327536	3.308854
C	0.527225	0.899244	3.342729
H	-5.504940	-0.676413	-0.744348
H	-4.582609	-1.742242	-1.823953
H	-4.052524	-0.061448	-1.579592
H	-3.305624	0.643414	0.896985
H	-3.150840	-0.622317	2.134229
H	-4.763067	-0.168220	1.538169
H	-2.703753	-5.048952	-1.797032
H	-3.658153	-4.085993	-0.653661
H	-2.050164	-4.693615	-0.187339
H	0.105128	-3.693933	-1.438077
H	-0.162060	-2.443340	-2.659939
H	-0.713093	-4.116276	-2.961894
H	1.388788	3.391306	-3.463632
H	0.281754	2.011055	-3.186049
H	1.870865	2.037340	-2.401835
H	2.355884	3.783083	-0.561170
H	1.073416	4.889408	-0.012456
H	1.801044	5.090947	-1.621693
H	-3.919045	3.502466	-0.365220
H	-3.156808	2.050868	-1.089673
H	-2.727224	3.672926	-1.671943
H	-1.335195	5.247757	-0.110637
H	-0.843964	4.672273	1.501158
H	-2.550315	5.017050	1.159070
H	-0.624096	-2.255925	3.804139
C	0.186477	-0.261483	4.028571
H	0.939186	1.762633	3.865558
H	0.324646	-0.331731	5.108484

$TS_{6\text{-}7}$

SCF energy in gas phase: -3277.78793547

Thermal correction to Enthalpy in gas phase: 0.746587

Thermal correction to Gibbs Free Energy in gas phase: 0.638931

SCF energy in solvent: -3278.03236867

Co	-0.473188	0.340110	-0.565513
P	-2.181661	-0.948981	-0.551493
B	1.035745	-0.884478	-0.487965
H	0.194229	-0.214097	-1.797276
P	0.593697	2.186321	-0.311550
H	-1.527521	1.311437	-1.104447
N	-0.608269	0.302133	1.436838
O	0.934786	-2.221876	-0.063917
O	2.401466	-0.566023	-0.556011

C	2.200625	-2.651429	0.434641
C	3.182544	-1.746956	-0.366914
C	4.462596	-1.385804	0.366223
C	3.510755	-2.307182	-1.748633
C	2.359009	-4.141777	0.192433
C	2.215717	-2.359407	1.935356
H	1.632570	-4.691644	0.792939
H	3.358614	-4.477351	0.478363
H	2.192424	-4.392120	-0.853851
H	2.112359	-1.289436	2.126318
H	3.130617	-2.714997	2.412271
H	1.366131	-2.863487	2.398284
H	5.087079	-0.756747	-0.269945
H	5.031649	-2.283628	0.617989
H	4.253158	-0.837918	1.283956
H	2.599981	-2.586999	-2.279832
H	4.165413	-3.178409	-1.688152
H	4.016489	-1.534035	-2.328240
C	-2.051816	-1.628770	1.157725
C	-3.869356	-0.170909	-0.534833
C	-2.492732	-2.433093	-1.623950
C	2.093669	2.750101	-1.262370
C	-0.440427	3.728354	-0.253237
C	1.138183	1.982882	1.439877
C	-1.386776	-0.614713	2.048217
C	0.132987	1.146964	2.184251
H	-2.994998	-1.993358	1.589325
H	-1.356086	-2.479899	1.066439
H	-4.587911	-0.985465	-0.339367
C	-4.208747	0.473667	-1.880782
C	-3.991285	0.861271	0.589385
H	-3.053545	-2.007539	-2.472884
C	-3.370987	-3.503008	-0.966131
C	-1.210290	-3.048353	-2.185414
H	1.956125	3.834407	-1.404168
C	2.097113	2.091313	-2.646492
C	3.432095	2.546103	-0.548487
H	-1.323970	3.399157	0.319514
C	-0.909761	4.103422	-1.661709
C	0.188498	4.929623	0.456526
H	2.057326	1.377965	1.369787
H	1.387364	2.902867	1.984634
C	-1.522633	-0.643374	3.434578
C	0.029142	1.172491	3.572765
H	-5.215678	0.918873	-1.843054
H	-4.197732	-0.246624	-2.712407
H	-3.483822	1.269234	-2.112144
H	-3.226489	1.644385	0.466945
H	-3.869283	0.416051	1.588134
H	-4.983368	1.338716	0.558295
H	-3.637857	-4.278056	-1.702039
H	-4.309846	-3.097433	-0.560263
H	-2.834929	-4.005276	-0.145225
H	-0.594244	-3.486387	-1.387860
H	-0.595107	-2.290913	-2.690144
H	-1.463580	-3.839087	-2.909801
H	2.897513	2.524498	-3.268348
H	1.138639	2.232227	-3.166938
H	2.265232	1.009125	-2.552231
H	3.605867	1.479983	-0.343400
H	3.488556	3.105796	0.397699
H	4.251003	2.905045	-1.192617

H	-1.661540	4.906775	-1.613748
H	-1.357187	3.236855	-2.169655
H	-0.073772	4.474108	-2.277806
H	1.126087	5.250281	-0.026226
H	0.406320	4.728030	1.515338
H	-0.500413	5.788770	0.424815
H	-2.174013	-1.386896	3.894399
C	-0.823611	0.276153	4.207811
H	0.626123	1.884182	4.143445
H	-0.926356	0.281218	5.294067

7

SCF energy in gas phase: -3277.80025365

Thermal correction to Enthalpy in gas phase: 0.749186

Thermal correction to Gibbs Free Energy in gas phase: 0.64272

SCF energy in solvent: -3278.04595371

Co	-0.536453	0.317845	-0.549934
P	-1.975339	-1.250894	-0.641719
B	1.105390	-0.782496	-0.283180
H	-0.248375	0.252379	-1.989563
P	0.493603	2.157653	-0.311918
H	-1.729386	1.216996	-0.847469
N	-0.873626	0.357727	1.434728
O	1.321350	-1.569058	0.863767
O	2.270220	-0.826944	-1.050418
C	2.709937	-1.870710	0.993070
C	3.234653	-1.707639	-0.473495
C	4.609144	-1.064663	-0.589931
C	3.226170	-3.007974	-1.272552
C	2.867646	-3.263976	1.578625
C	3.300397	-0.844036	1.959507
H	2.465621	-3.281202	2.592782
H	3.920581	-3.551241	1.624777
H	2.331181	-4.005459	0.988914
H	3.213258	0.165552	1.555054
H	4.352288	-1.039415	2.174585
H	2.739239	-0.882031	2.894100
H	4.881558	-0.981796	-1.642798
H	5.367851	-1.669420	-0.087789
H	4.622445	-0.063859	-0.160972
H	2.263935	-3.511220	-1.205833
H	4.003143	-3.693919	-0.929998
H	3.409899	-2.772934	-2.321488
C	-2.018873	-1.754244	1.130988
C	-3.736837	-0.807517	-1.020452
C	-1.813327	-2.855739	-1.555925
C	2.249494	2.394617	-0.845338
C	-0.364608	3.747359	-0.732465
C	0.646733	2.246829	1.528602
C	-1.648915	-0.584047	2.000657
C	-0.369720	1.351066	2.187327
H	-2.956091	-2.227263	1.456028
H	-1.205139	-2.491660	1.239503
H	-4.319265	-1.743419	-0.990950
C	-3.836521	-0.206880	-2.425381
C	-4.318354	0.152245	0.019956
H	-2.189961	-2.613128	-2.564122
C	-2.663214	-3.996523	-0.985370
C	-0.353969	-3.283391	-1.691993
H	2.744224	1.569927	-0.305954
C	2.894404	3.715690	-0.422479

C	2.452157	2.113044	-2.336443
H	0.340059	4.563054	-0.499599
C	-1.625315	3.946635	0.113628
C	-0.716805	3.789100	-2.221773
H	1.639987	1.834105	1.772780
H	0.614023	3.266285	1.938077
C	-2.036010	-0.497128	3.336299
C	-0.722043	1.495138	3.527585
H	-4.885048	0.031368	-2.664545
H	-3.465168	-0.892108	-3.202714
H	-3.242198	0.717834	-2.481201
H	-3.705946	1.065066	0.082547
H	-4.370701	-0.296280	1.023655
H	-5.341483	0.443277	-0.265760
H	-2.621902	-4.869840	-1.655305
H	-3.722298	-3.726429	-0.863279
H	-2.281468	-4.322115	-0.004465
H	0.086161	-3.488990	-0.702895
H	0.249836	-2.498647	-2.166751
H	-0.279194	-4.203188	-2.293951
H	3.977561	3.687195	-0.622273
H	2.761320	3.929027	0.649827
H	2.484214	4.565958	-0.989800
H	2.091639	2.946210	-2.959233
H	1.933967	1.192391	-2.635105
H	3.526003	1.986134	-2.547234
H	-2.122645	4.886284	-0.174129
H	-1.411581	4.003781	1.191672
H	-2.330840	3.118324	-0.052023
H	-1.346370	2.923441	-2.480879
H	0.173825	3.762823	-2.864440
H	-1.272793	4.710830	-2.455882
H	-2.682774	-1.264650	3.761636
C	-1.582874	0.568599	4.104856
H	-0.314985	2.324420	4.106478
H	-1.882169	0.665636	5.149748

$TS_{7\text{-}8}$

SCF energy in gas phase: -3277.79804763

Thermal correction to Enthalpy in gas phase: 0.748583

Thermal correction to Gibbs Free Energy in gas phase: 0.645262

SCF energy in solvent: -3278.04405933

Co	0.551080	0.236261	-0.472093
P	1.892818	-1.406372	-0.465112
B	-1.180389	-0.691769	-0.127260
H	0.218481	0.008136	-1.881401
P	-0.407400	2.128865	-0.401875
H	1.782250	0.997405	-0.939053
N	1.033902	0.533510	1.459636
O	-1.995525	-0.440206	0.993187
O	-1.835031	-1.631961	-0.922230
C	-3.111535	-1.329637	1.026357
C	-3.157968	-1.877157	-0.444096
C	-4.117151	-1.105119	-1.346932
C	-3.453108	-3.364834	-0.557230
C	-2.818432	-2.399587	2.076211
C	-4.345991	-0.548618	1.453966
H	-2.637196	-1.908364	3.033045
H	-3.655930	-3.089366	2.194394
H	-1.929961	-2.975806	1.823038
H	-4.517001	0.314931	0.813163

H	-5.236940	-1.179961	1.429566
H	-4.212310	-0.190677	2.475982
H	-3.954310	-1.419375	-2.378246
H	-5.160277	-1.292188	-1.085718
H	-3.931247	-0.033441	-1.294778
H	-2.704991	-3.960032	-0.036811
H	-4.436911	-3.600871	-0.145158
H	-3.445117	-3.656080	-1.608325
C	2.431929	-1.463669	1.305856
C	3.482705	-1.250995	-1.404137
C	1.352294	-3.147546	-0.850711
C	-2.135470	2.385717	-1.010581
C	0.524526	3.651525	-0.902553
C	-0.586520	2.341111	1.422521
C	1.961386	-0.238543	2.052926
C	0.508445	1.581493	2.123149
H	3.517179	-1.597237	1.420236
H	1.960044	-2.336792	1.780763
H	4.051069	-2.177349	-1.222217
C	3.169023	-1.130890	-2.898409
C	4.345705	-0.076329	-0.940834
H	0.736273	-2.997312	-1.752333
C	2.454156	-4.166472	-1.154725
C	0.430648	-3.695922	0.242352
H	-2.694504	1.701393	-0.349528
C	-2.694651	3.797300	-0.825181
C	-2.319637	1.882537	-2.445873
H	-0.129239	4.513870	-0.690359
C	1.805611	3.808746	-0.077928
C	0.850193	3.618786	-2.397661
H	-1.536849	1.846306	1.678806
H	-0.632144	3.385659	1.761768
C	2.440538	0.056219	3.328366
C	0.945048	1.923042	3.401217
H	4.099852	-1.070382	-3.484198
H	2.588259	-1.986737	-3.275901
H	2.576100	-0.221460	-3.081389
H	3.825460	0.877169	-1.110625
H	4.603192	-0.134409	0.128021
H	5.290194	-0.065515	-1.507968
H	2.005337	-5.159656	-1.317052
H	3.032347	-3.919058	-2.055587
H	3.159298	-4.262214	-0.311787
H	1.010730	-4.109350	1.083843
H	-0.244276	-2.922483	0.628286
H	-0.190658	-4.511212	-0.158342
H	-3.775041	3.807884	-1.040524
H	-2.557571	4.171420	0.201409
H	-2.219694	4.513613	-1.514097
H	-1.813278	2.532457	-3.174870
H	-1.921068	0.864724	-2.562402
H	-3.390549	1.872555	-2.706257
H	2.368527	4.688870	-0.426629
H	1.602919	3.950761	0.994359
H	2.446251	2.920484	-0.190533
H	1.401630	2.697385	-2.643368
H	-0.054165	3.651821	-3.021657
H	1.474979	4.483703	-2.671486
H	3.204080	-0.580036	3.776748
C	1.932881	1.156652	4.008249
H	0.509478	2.784962	3.906938
H	2.298191	1.410162	5.004806

8

SCF energy in gas phase: -3277.80317592

Thermal correction to Enthalpy in gas phase: 0.749376

Thermal correction to Gibbs Free Energy in gas phase: 0.64386

SCF energy in solvent: -3278.04855767

Co	-0.000476	-0.629442	-0.567565
P	-2.114579	-0.844693	-0.614656
B	0.006615	1.297302	-0.044450
H	0.060568	-0.031248	-1.903117
P	2.113722	-0.746898	-0.329038
H	-0.045626	-1.996722	-1.267741
N	-0.083614	-1.512375	1.234488
O	0.773123	1.907388	0.967043
O	-0.738149	2.305217	-0.663740
C	0.443404	3.292314	1.099094
C	-0.285329	3.594374	-0.253548
C	0.655932	4.109183	-1.340535
C	-1.483138	4.523416	-0.137910
C	-0.455619	3.440910	2.323039
C	1.725163	4.080407	1.323214
H	0.061474	3.028707	3.190617
H	-0.689516	4.487612	2.525171
H	-1.388181	2.894896	2.196145
H	2.456681	3.888036	0.539974
H	1.522908	5.153369	1.352912
H	2.167127	3.792776	2.278532
H	0.120882	4.115494	-2.290516
H	1.005621	5.121630	-1.130638
H	1.520665	3.455146	-1.450596
H	-2.244697	4.110494	0.521976
H	-1.183789	5.502495	0.243099
H	-1.929204	4.663938	-1.123339
C	-2.302032	-2.243175	0.576773
C	-2.976351	-1.364948	-2.159718
C	-3.259168	0.432469	0.101121
C	3.250251	0.646332	-0.760619
C	3.002314	-2.291529	-0.837819
C	2.216352	-0.801724	1.516005
C	-1.203061	-2.161669	1.605957
C	0.988224	-1.491417	2.048304
H	-2.135845	-3.162116	-0.007100
H	-3.291326	-2.319350	1.050293
H	-4.014085	-1.617642	-1.885960
C	-2.984524	-0.173832	-3.127192
C	-2.342037	-2.585406	-2.827093
H	-2.997262	1.349733	-0.449201
C	-4.756184	0.152887	-0.050461
C	-2.910609	0.665482	1.575386
H	2.893583	1.429380	-0.072530
C	4.732045	0.389681	-0.481567
C	3.018261	1.159636	-2.185420
H	4.040066	-2.204079	-0.474438
C	2.367784	-3.527303	-0.192829
C	3.008607	-2.427262	-2.362530
H	2.184975	0.251196	1.836358
H	3.131669	-1.265282	1.912216
C	-1.304751	-2.767644	2.855981
C	0.948464	-2.087210	3.307454
H	-3.489030	-0.451382	-4.065817
H	-3.502212	0.704274	-2.713762

H	-1.952227	0.129056	-3.361116
H	-1.308081	-2.368175	-3.128564
H	-2.314606	-3.463215	-2.164308
H	-2.926474	-2.859868	-3.720107
H	-5.337541	0.926462	0.476634
H	-5.085499	0.156242	-1.098931
H	-5.037714	-0.818884	0.389398
H	-3.273868	-0.159021	2.210248
H	-1.826114	0.757795	1.732331
H	-3.388983	1.589005	1.938089
H	5.306482	1.321948	-0.602991
H	4.907891	0.023784	0.542027
H	5.155681	-0.346662	-1.182818
H	3.407992	0.463271	-2.942839
H	1.946784	1.304291	-2.384055
H	3.537333	2.121631	-2.327511
H	2.876871	-4.437159	-0.547935
H	2.442199	-3.514603	0.905153
H	1.303091	-3.594441	-0.466002
H	1.978359	-2.383559	-2.750280
H	3.592246	-1.632253	-2.848395
H	3.451192	-3.391655	-2.658245
H	-2.226358	-3.278823	3.134848
C	-0.217373	-2.721060	3.721634
H	1.828200	-2.048291	3.950026
H	-0.273894	-3.187590	4.706550

TS_{8-9}

SCF energy in gas phase: -3277.78502379

Thermal correction to Enthalpy in gas phase: 0.747798

Thermal correction to Gibbs Free Energy in gas phase: 0.642957

SCF energy in solvent: -3278.03193626

Co	-0.495791	-0.155460	0.498854
P	0.251621	-2.189195	0.397635
P	-1.496518	1.770423	0.333817
H	0.621506	0.356506	1.340185
B	1.261373	0.526140	-0.093018
N	-2.120733	-0.892850	-0.487041
H	-1.203579	-0.544178	1.826763
O	2.439516	-0.250367	-0.214789
O	1.656401	1.867207	-0.289719
C	3.586661	0.593218	-0.232369
C	2.989946	1.920282	-0.783390
C	4.100077	0.730039	1.199852
C	4.655781	-0.045313	-1.102725
C	3.656178	3.187208	-0.274293
C	2.931420	1.946197	-2.310278
H	3.335999	1.164011	1.846652
H	4.350043	-0.259108	1.583725
H	4.995751	1.351561	1.248842
H	5.512888	0.621910	-1.219770
H	5.006429	-0.966924	-0.634926
H	4.267710	-0.292527	-2.089529
H	3.576393	3.268699	0.808325
H	4.712633	3.209880	-0.551944
H	3.171278	4.058984	-0.716766
H	2.341665	2.805964	-2.627700
H	3.926532	2.030574	-2.750302
H	2.451402	1.045476	-2.696013
H	-3.416933	-3.873134	-1.395616

C	-4.299556	-1.956458	-1.883617
H	-4.933754	0.105587	-2.051510
C	-1.328025	-3.088639	0.165436
C	1.007692	-3.019630	1.865274
C	1.250188	-2.823849	-1.035736
C	-3.011224	1.373354	-0.640629
C	-2.153145	2.525137	1.893026
C	-0.868498	3.253941	-0.596660
C	-2.287482	-2.230187	-0.600691
C	-3.097086	-0.091475	-0.956264
H	-1.222280	-4.082846	-0.288630
H	-1.756906	-3.219734	1.171586
H	0.995577	-4.101368	1.647708
C	0.216574	-2.776617	3.152210
C	2.459156	-2.566369	2.048655
H	2.201759	-2.285650	-0.942250
C	0.598835	-2.369152	-2.345759
C	1.527775	-4.328224	-1.039193
H	-3.915960	1.670108	-0.088721
H	-3.019427	1.953157	-1.573555
H	-2.760242	3.396886	1.600095
C	-0.967765	2.996736	2.741210
C	-3.044652	1.569784	2.686459
H	0.101560	3.465117	-0.129023
C	-0.594048	2.884494	-2.059044
C	-1.754318	4.500415	-0.517667
C	-3.345128	-2.788596	-1.311950
C	-4.184883	-0.590215	-1.671862
H	0.188942	-1.704880	3.393305
H	-0.826461	-3.117888	3.081529
H	0.691706	-3.322351	3.983323
H	2.493715	-1.487609	2.258894
H	2.914740	-3.100311	2.897160
H	3.076913	-2.746775	1.157305
H	-0.335065	-2.919105	-2.551741
H	0.363070	-1.294525	-2.310646
H	1.279213	-2.550548	-3.192503
H	0.603595	-4.929118	-1.059672
H	2.102714	-4.597099	-1.939921
H	2.119317	-4.648840	-0.169292
H	-0.348551	3.741034	2.217246
H	-1.322313	3.452902	3.678800
H	-0.323057	2.140569	2.995814
H	-3.428050	2.080223	3.584561
H	-3.914448	1.226788	2.104095
H	-2.478918	0.677837	2.990876
H	-0.124899	1.894894	-2.145606
H	-1.519371	2.888160	-2.658976
H	0.081757	3.625775	-2.512706
H	-1.795849	4.928553	0.493695
H	-1.353593	5.280801	-1.184503
H	-2.788824	4.297593	-0.843392
H	-5.132404	-2.367986	-2.455637

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SCF energy in gas phase: -3277.78906062

Thermal correction to Enthalpy in gas phase: 0.7486

Thermal correction to Gibbs Free Energy in gas phase: 0.641279

SCF energy in solvent: -3278.03518792

Co	0.543841	0.032729	0.698179
P	0.537444	2.182218	0.350363

P	0.678286	-2.125275	0.424183
H	-0.756785	-0.000912	1.456154
B	-1.299058	-0.034424	0.039911
N	2.400113	0.078354	-0.078132
H	1.190876	0.072182	2.118430
O	-2.152409	1.059911	-0.233020
O	-2.071847	-1.200785	-0.173921
C	-3.494625	0.607293	-0.379359
C	-3.279582	-0.862471	-0.843377
C	-4.174431	0.699968	0.985177
C	-4.211183	1.499566	-1.378035
C	-4.367979	-1.836199	-0.426911
C	-3.026806	-0.973057	-2.347268
H	-3.667757	0.066667	1.715095
H	-4.121703	1.731178	1.335721
H	-5.224569	0.407292	0.935308
H	-5.212773	1.119007	-1.590961
H	-4.311761	2.504907	-0.965605
H	-3.658122	1.570496	-2.313370
H	-4.455175	-1.891369	0.656782
H	-5.333806	-1.541007	-0.843443
H	-4.129788	-2.834374	-0.798206
H	-2.675021	-1.980833	-2.572885
H	-3.932977	-0.787728	-2.926426
H	-2.256041	-0.268715	-2.663891
H	4.656951	2.282994	-1.266318
C	4.871486	0.130760	-1.377974
H	4.802693	-2.023374	-1.163335
C	2.340893	2.481261	0.176774
C	0.035772	3.368511	1.678414
C	-0.107538	2.965673	-1.208400
C	2.499663	-2.308565	0.287547
C	0.232995	-3.295487	1.786616
C	0.106473	-3.005763	-1.110792
C	3.006789	1.251180	-0.358785
C	3.084936	-1.063298	-0.303952
H	2.596397	3.371866	-0.412498
H	2.731958	2.632444	1.195600
H	0.436492	4.354835	1.387876
C	0.622637	2.986029	3.039101
C	-1.490705	3.462422	1.771832
H	-1.188668	2.784878	-1.158023
C	0.428460	2.193452	-2.417274
C	0.137640	4.469086	-1.349363
H	2.881820	-2.378143	1.318653
H	2.826582	-3.207997	-0.250546
H	0.731503	-4.252329	1.553223
C	-1.281061	-3.528620	1.837045
C	0.737223	-2.803961	3.145448
H	-0.986508	-2.926894	-1.053994
C	0.560329	-2.220464	-2.343773
C	0.489303	-4.483363	-1.212674
C	4.224819	1.310243	-1.031071
C	4.305354	-1.071978	-0.974093
H	0.276475	1.988363	3.343671
H	1.722146	2.956168	3.034864
H	0.312236	3.724979	3.795284
H	-1.916518	2.487750	2.051951
H	-1.773375	4.198609	2.540555
H	-1.956579	3.761830	0.822123
H	1.505061	2.374040	-2.576526
H	0.282171	1.111471	-2.281011

H	-0.095277	2.504484	-3.334716
H	1.209654	4.726259	-1.333040
H	-0.259900	4.821525	-2.314776
H	-0.360506	5.051707	-0.560989
H	-1.677796	-3.940597	0.898262
H	-1.521604	-4.234204	2.647659
H	-1.812792	-2.584742	2.027197
H	0.488306	-3.545566	3.921525
H	1.826194	-2.651101	3.164881
H	0.276608	-1.840336	3.404166
H	0.302252	-1.156232	-2.240422
H	1.650189	-2.293600	-2.498064
H	0.072847	-2.611509	-3.250645
H	0.071243	-5.083881	-0.391797
H	0.101443	-4.903804	-2.154547
H	1.580847	-4.636840	-1.221527
H	5.816537	0.149660	-1.922675

$TS_{9\text{-}10}$

SCF energy in gas phase: -3277.78184317

Thermal correction to Enthalpy in gas phase: 0.746252

Thermal correction to Gibbs Free Energy in gas phase: 0.638159

SCF energy in solvent: -3278.02569421

Co	0.520555	0.120501	0.709803
P	0.111174	2.196054	0.263294
P	1.048123	-1.953773	0.377278
H	-0.397302	-0.072626	1.849396
B	-1.277171	-0.263531	0.060531
N	2.411831	0.512280	0.100108
H	0.778556	0.178894	2.224977
O	-2.365166	0.632742	0.062196
O	-1.780036	-1.496786	-0.395888
C	-3.585471	-0.071118	-0.148431
C	-3.093314	-1.327607	-0.923192
C	-4.165685	-0.410955	1.223014
C	-4.548246	0.821162	-0.912521
C	-3.896917	-2.592552	-0.677980
C	-2.952634	-1.079927	-2.424455
H	-3.485419	-1.053954	1.783475
H	-4.297914	0.513110	1.787021
H	-5.134128	-0.907734	1.142828
H	-5.461572	0.279141	-1.168292
H	-4.822889	1.676913	-0.293831
H	-4.098009	1.196905	-1.830157
H	-3.878452	-2.877187	0.372532
H	-4.936041	-2.457989	-0.987119
H	-3.474493	-3.414497	-1.258286
H	-2.406046	-1.913589	-2.867631
H	-3.923272	-1.002312	-2.917364
H	-2.386468	-0.166861	-2.615431
H	4.275190	3.052467	-1.101328
C	4.925247	0.988801	-1.022887
H	5.245121	-1.129997	-0.709905
C	1.825489	2.861602	0.092714
C	-0.593238	3.359832	1.530410
C	-0.677291	2.776554	-1.319988
C	2.882973	-1.824949	0.492554
C	0.670734	-3.278914	1.618232
C	0.828028	-2.818295	-1.253313
C	2.788942	1.762630	-0.239428
C	3.309243	-0.488833	-0.035004

H	1.908277	3.693462	-0.620125
H	2.111321	3.258855	1.079684
H	-0.288411	4.372360	1.211962
C	-0.004889	3.094471	2.918501
C	-2.122567	3.309925	1.597568
H	-1.713950	2.421844	-1.229666
C	-0.037293	2.042758	-2.500548
C	-0.691530	4.289476	-1.548805
H	3.124268	-1.846874	1.567102
H	3.432579	-2.645355	0.010909
H	1.367116	-4.108245	1.403905
C	-0.764648	-3.796885	1.477760
C	0.914226	-2.806095	3.053818
H	-0.264186	-2.883673	-1.353027
C	1.341069	-1.913727	-2.377171
C	1.425967	-4.222618	-1.356438
C	4.026972	2.028936	-0.819510
C	4.564368	-0.285359	-0.602026
H	-0.303463	2.100655	3.280884
H	1.094773	3.122891	2.932009
H	-0.368391	3.854546	3.628608
H	-2.461186	2.315591	1.919947
H	-2.486069	4.057611	2.320438
H	-2.597836	3.514645	0.627787
H	1.014910	2.341039	-2.647380
H	-0.057215	0.955947	-2.336510
H	-0.576681	2.267517	-3.434278
H	0.324595	4.712905	-1.607448
H	-1.186727	4.517828	-2.506346
H	-1.236307	4.831500	-0.762775
H	-0.986138	-4.169156	0.467735
H	-0.935366	-4.618564	2.191137
H	-1.486692	-2.995392	1.690975
H	0.739706	-3.639751	3.752876
H	1.939557	-2.443833	3.217763
H	0.234696	-1.981995	3.312983
H	0.952003	-0.891813	-2.263086
H	2.442617	-1.857951	-2.385178
H	1.024800	-2.300911	-3.358480
H	0.976290	-4.927510	-0.642454
H	1.255366	-4.628324	-2.366760
H	2.516115	-4.224718	-1.191588
H	5.895794	1.170585	-1.486869

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SCF energy in gas phase: -3277.79713991

Thermal correction to Enthalpy in gas phase: 0.749483

Thermal correction to Gibbs Free Energy in gas phase: 0.644255

SCF energy in solvent: -3278.03956448

Co	-0.438892	0.051151	-0.641984
P	-0.386555	2.046953	0.076716
P	-0.850917	-1.954790	-0.017327
N	-2.450633	0.249548	-0.695013
B	1.472580	-0.133706	-0.328012
H	-0.247800	-0.383757	-2.163218
H	-0.190532	0.496231	-2.148387
O	2.107045	-0.576959	0.842259
O	2.471619	0.147773	-1.272422
C	3.495904	-0.793883	0.593805
C	3.754485	0.118055	-0.646216
C	3.684684	-2.278897	0.289941

C	4.286536	-0.425889	1.838423
C	4.779421	-0.415533	-1.632352
C	4.111340	1.551758	-0.258915
H	4.737268	-2.535256	0.158149
H	3.291546	-2.859383	1.126067
H	3.141687	-2.566889	-0.610340
H	4.037082	-1.115550	2.646195
H	5.360753	-0.494511	1.651417
H	4.054277	0.583248	2.174342
H	4.896049	0.289877	-2.456242
H	5.752308	-0.541863	-1.151396
H	4.468007	-1.371760	-2.049301
H	5.124570	1.624734	0.140050
H	4.039969	2.182168	-1.146268
H	3.417020	1.935573	0.489371
H	-6.295776	0.583038	-0.490667
C	-0.349838	2.555485	1.864847
C	-2.070712	2.632217	-0.458796
C	0.733282	3.327761	-0.680195
C	-1.216490	-2.496950	1.726252
C	0.121607	-3.408307	-0.648134
C	-2.498358	-2.161272	-0.854933
C	-3.228854	-0.849534	-0.763299
C	-3.014655	1.463827	-0.546764
H	-0.647865	3.615798	1.920032
C	-1.358405	1.734132	2.665741
C	1.055713	2.395407	2.452622
H	-2.494704	3.435182	0.162877
H	-1.937861	3.043175	-1.473385
H	1.707208	3.125331	-0.206420
C	0.351244	4.781434	-0.384365
C	0.919360	3.101102	-2.182037
H	-1.389176	-3.585424	1.718680
C	-0.012219	-2.203672	2.624768
C	-2.487197	-1.827586	2.259800
H	0.956735	-3.477742	0.070190
C	0.717900	-3.132074	-2.030686
C	-0.628137	-4.744744	-0.653706
H	-2.262434	-2.364321	-1.912463
H	-3.119426	-2.990316	-0.484735
C	-4.617576	-0.760160	-0.702545
C	-4.398257	1.614314	-0.468023
H	-1.403190	2.088510	3.707871
H	-2.376675	1.791789	2.248532
H	-1.059766	0.676926	2.674778
H	1.431058	1.371903	2.288947
H	1.775248	3.099458	2.007046
H	1.040440	2.586932	3.537478
H	1.089391	5.465489	-0.832600
H	-0.630465	5.037570	-0.815418
H	0.314755	5.001928	0.691983
H	-0.034633	3.177367	-2.730601
H	1.595394	3.867627	-2.594390
H	1.352071	2.112516	-2.381934
H	0.894549	-2.723878	2.282723
H	0.228834	-1.130773	2.623199
H	-0.220377	-2.523454	3.658503
H	-3.395298	-2.215981	1.775080
H	-2.588232	-2.008751	3.341772
H	-2.464828	-0.739376	2.102527
H	-0.072585	-3.010695	-2.789831
H	1.323937	-2.216360	-2.044048

H 1.349817 -3.978186 -2.345842
H 0.055095 -5.562135 -0.934344
H -1.060818 -5.002391 0.323237
H -1.445129 -4.737734 -1.393347
C -5.210337 0.488797 -0.552810
H -5.219798 -1.667385 -0.754926
H -4.825967 2.608448 -0.336301

11

SCF energy in gas phase: -3276.60284223

Thermal correction to Enthalpy in gas phase: 0.731735

Thermal correction to Gibbs Free Energy in gas phase: 0.624484

SCF energy in solvent: -3276.84634414

Co 0.539781 0.027189 -0.171158
P 0.777398 -2.069946 -0.086655
P 0.513925 2.129909 0.012756
B -1.406324 -0.085461 -0.029980
N 2.506238 0.145616 -0.361713
O -2.255537 -0.064082 -1.152307
O -2.222334 -0.188151 1.112559
C -3.611374 0.092721 -0.734594
C -3.572365 -0.452995 0.726575
C -3.946076 1.582065 -0.799110
C -4.516716 -0.674734 -1.683259
C -4.513832 0.242848 1.695937
C -3.791770 -1.962859 0.800170
H -3.345235 2.146245 -0.084808
H -3.718339 1.948023 -1.801247
H -5.000377 1.772035 -0.589848
H -5.552097 -0.657292 -1.334494
H -4.482970 -0.215113 -2.672115
H -4.198084 -1.711020 -1.782841
H -4.284644 1.303570 1.782989
H -5.552443 0.134619 1.374321
H -4.415938 -0.205363 2.685735
H -3.559107 -2.305708 1.808635
H -4.824248 -2.233070 0.571933
H -3.133404 -2.485834 0.105509
H 5.211844 -1.877578 -0.362190
C 5.289683 0.275013 -0.150192
H 4.986184 2.414540 -0.036302
C 2.523800 -2.273184 -0.670489
C -0.181012 -3.246470 -1.141104
C 0.838196 -2.890299 1.572444
C 2.279745 2.578663 -0.334942
C -0.441600 3.206211 -1.146036
C 0.242711 2.902107 1.674179
C 3.259626 -0.980902 -0.434540
C 3.137106 1.341731 -0.262145
H 3.061724 -3.125454 -0.229186
H 2.479082 -2.444320 -1.758712
H -1.181618 -3.239809 -0.676097
C 0.339235 -4.684359 -1.163783
C -0.335189 -2.666282 -2.550521
H 1.286917 -3.889353 1.435001
C -0.563582 -3.046429 2.165980
C 1.740170 -2.079308 2.507925
H 2.332381 2.960813 -1.367971
H 2.674607 3.372981 0.315930
H -1.483638 3.067902 -0.815831
C -0.346577 2.638320 -2.565055

C	-0.104414	4.696711	-1.091034
H	0.666754	3.920796	1.639548
C	-1.243815	2.993240	2.029655
C	1.003136	2.088643	2.725606
C	4.647013	-0.946010	-0.318596
C	4.521808	1.433183	-0.137591
H	1.355877	-4.737067	-1.586874
H	0.367469	-5.135555	-0.160962
H	-0.307976	-5.316708	-1.792463
H	0.632856	-2.618285	-3.076691
H	-1.002054	-3.303032	-3.153669
H	-0.759393	-1.652552	-2.513013
H	-1.068072	-2.070397	2.234230
H	-1.198528	-3.710463	1.559674
H	-0.500770	-3.481869	3.176119
H	1.339350	-1.062738	2.639917
H	1.799555	-2.563204	3.495832
H	2.766419	-1.982203	2.120959
H	-0.664429	1.585559	-2.582254
H	-0.990569	3.212407	-3.250629
H	0.682336	2.693869	-2.958577
H	-0.749778	5.262060	-1.782394
H	-0.246683	5.120360	-0.085637
H	0.938913	4.887352	-1.391616
H	-1.791752	3.665313	1.351199
H	-1.715232	1.998789	1.990466
H	-1.362700	3.390659	3.050332
H	2.072527	1.985309	2.482321
H	0.926209	2.567805	3.714681
H	0.577910	1.075350	2.793486
H	6.374701	0.324192	-0.045661

2 (at ωB97XD/BS4)

SCF energy in gas phase: -2039.75589001

Thermal correction to Enthalpy in gas phase: 0.756123

Thermal correction to Gibbs Free Energy in gas phase: 0.650965

SCF energy in solvent: -3278.059742

Co	0.000000	0.000000	0.428515
P	0.511093	2.082707	0.612209
B	0.000000	0.000000	-1.478097
H	-1.475326	0.434384	0.282254
P	-0.511093	-2.082707	0.612209
H	1.475326	-0.434384	0.282254
N	0.000000	0.000000	2.486905
O	-0.318213	-1.091124	-2.301003
O	0.318213	1.091124	-2.301003
C	0.031555	-0.780298	-3.652793
C	-0.031555	0.780298	-3.652793
C	0.955942	1.465462	-4.589183
C	-1.444650	1.318210	-3.896873
C	-0.955942	-1.465462	-4.589183
C	1.444650	-1.318210	-3.896873
H	-0.837956	-2.551843	-4.518299
H	-0.777287	-1.171346	-5.630025
H	-1.987713	-1.220724	-4.326347
H	2.166183	-0.829356	-3.234246
H	1.763818	-1.173193	-4.934606
H	1.457627	-2.390339	-3.676483
H	0.837956	2.551843	-4.518299
H	0.777287	1.171346	-5.630025
H	1.987713	1.220724	-4.326347

H	-2.166183	0.829356	-3.234246
H	-1.763818	1.173193	-4.934606
H	-1.457627	2.390339	-3.676483
C	-0.108797	2.420176	2.333785
C	2.315164	2.528872	0.702538
C	-0.242723	3.456551	-0.392087
C	-2.315164	-2.528872	0.702538
C	0.242723	-3.456551	-0.392087
C	0.108797	-2.420176	2.333785
C	-0.035149	1.163903	3.161279
C	0.035149	-1.163903	3.161279
H	0.399854	3.252400	2.833319
H	-1.165816	2.696539	2.224677
H	2.394381	3.598694	0.934766
C	2.981917	2.252368	-0.648901
C	3.004516	1.736650	1.818417
H	0.260066	3.366154	-1.360665
C	0.000000	4.857952	0.178984
C	-1.734994	3.215184	-0.631921
H	-2.394381	-3.598694	0.934766
C	-2.981917	-2.252368	-0.648901
C	-3.004516	-1.736650	1.818417
H	-0.260066	-3.366154	-1.360665
C	0.000000	-4.857952	0.178984
C	1.734994	-3.215184	-0.631921
H	-0.399854	-3.252400	2.833319
H	1.165816	-2.696539	2.224677
C	-0.029206	1.196380	4.553206
C	0.029206	-1.196380	4.553206
H	4.048435	2.502854	-0.598771
H	2.532901	2.832033	-1.461432
H	2.880004	1.191937	-0.901762
H	2.843950	0.663095	1.670273
H	2.629703	2.008148	2.811863
H	4.082910	1.934536	1.805698
H	-0.442303	5.609713	-0.485347
H	1.062971	5.096883	0.279329
H	-0.470610	4.977582	1.162467
H	-2.309966	3.263487	0.301028
H	-1.904544	2.233421	-1.075336
H	-2.130067	3.986792	-1.304267
H	-4.048435	-2.502854	-0.598771
H	-2.532901	-2.832033	-1.461432
H	-2.880004	-1.191937	-0.901762
H	-2.843950	-0.663095	1.670273
H	-2.629703	-2.008148	2.811863
H	-4.082910	-1.934536	1.805698
H	0.442303	-5.609713	-0.485347
H	-1.062971	-5.096883	0.279329
H	0.470610	-4.977582	1.162467
H	2.309966	-3.263487	0.301028
H	1.904544	-2.233421	-1.075336
H	2.130067	-3.986792	-1.304267
H	-0.055989	2.150369	5.069458
C	0.000000	0.000000	5.257677
H	0.055989	-2.150369	5.069458
H	0.000000	0.000000	6.343483

9 (at ωB97XD/BS4)

SCF energy in gas phase: -2039.7317659

Thermal correction to Enthalpy in gas phase: 0.756629

Thermal correction to Gibbs Free Energy in gas phase: 0.650204

SCF energy in solvent: -3278.03566609

Co	0.550079	0.069813	0.722030
P	0.359867	2.221148	0.336055
P	0.820346	-2.088349	0.412615
H	-0.775078	-0.069014	1.478788
B	-1.303571	-0.128310	0.112130
N	2.398096	0.250601	-0.029594
H	1.198787	0.158305	2.174069
O	-2.220957	0.911413	-0.166184
O	-1.973652	-1.349172	-0.140760
C	-3.522499	0.359366	-0.364008
C	-3.180828	-1.082149	-0.851099
C	-4.248888	0.371200	0.984407
C	-4.274537	1.221689	-1.370211
C	-4.208417	-2.148432	-0.494173
C	-2.865290	-1.135768	-2.350606
H	-3.716054	-0.242069	1.718374
H	-4.283166	1.398317	1.360348
H	-5.276424	0.002060	0.897243
H	-5.243582	0.775472	-1.621929
H	-4.457672	2.212614	-0.941588
H	-3.698969	1.352113	-2.290075
H	-4.334486	-2.231532	0.587834
H	-5.180766	-1.922330	-0.946943
H	-3.876130	-3.121749	-0.870260
H	-2.437364	-2.114019	-2.592176
H	-3.762964	-0.993860	-2.961839
H	-2.130203	-0.370230	-2.619558
H	4.501230	2.606786	-1.195257
C	4.881118	0.483128	-1.287351
H	4.964339	-1.663870	-1.071337
C	2.152867	2.650954	0.188928
C	-0.248022	3.394550	1.648574
C	-0.322138	2.929431	-1.255497
C	2.666321	-2.131256	0.321329
C	0.431475	-3.313955	1.760340
C	0.337622	-2.981383	-1.156860
C	2.919296	1.465083	-0.312724
C	3.168903	-0.838929	-0.246551
H	2.350706	3.542392	-0.414348
H	2.510282	2.854528	1.206105
H	0.093472	4.398372	1.361173
C	0.335160	3.049486	3.022011
C	-1.779668	3.392649	1.715145
H	-1.379256	2.655391	-1.228730
C	0.316621	2.192835	-2.436608
C	-0.201658	4.447420	-1.407902
H	3.024659	-2.187173	1.357181
H	3.072156	-2.993072	-0.217087
H	1.019791	-4.217578	1.548580
C	-1.057178	-3.683216	1.756269
C	0.836903	-2.773283	3.134638
H	-0.754421	-2.975088	-1.125747
C	0.773275	-2.141799	-2.360399
C	0.825017	-4.427444	-1.271940
C	4.140850	1.610532	-0.961573
C	4.397449	-0.756280	-0.892795
H	0.069609	2.027079	3.304439
H	1.427545	3.113999	3.045347
H	-0.056684	3.748134	3.771538

H	-2.145658	2.402410	2.000726
H	-2.116059	4.117894	2.465556
H	-2.244382	3.649865	0.758365
H	1.373800	2.460830	-2.560309
H	0.257074	1.109539	-2.289557
H	-0.198979	2.447914	-3.369963
H	0.840163	4.788604	-1.368411
H	-0.602589	4.754638	-2.381503
H	-0.762352	4.987636	-0.638726
H	-1.374910	-4.136222	0.812041
H	-1.258997	-4.400119	2.560918
H	-1.676498	-2.795936	1.915265
H	0.606353	-3.520289	3.904285
H	1.904760	-2.542502	3.198931
H	0.300043	-1.846677	3.354866
H	0.435783	-1.107201	-2.244498
H	1.864857	-2.133157	-2.474760
H	0.346663	-2.546980	-3.285671
H	0.441685	-5.061753	-0.466500
H	0.482186	-4.858934	-2.220281
H	1.919396	-4.498288	-1.265975
H	5.828518	0.570664	-1.809813

$TS_{9\text{-}10}$ (at ωB97XD/BS4)

SCF energy in gas phase: -2039.72394303

Thermal correction to Enthalpy in gas phase: 0.75373

Thermal correction to Gibbs Free Energy in gas phase: 0.646464

SCF energy in solvent: -3278.02620711

Co	0.520246	0.124953	0.718886
P	0.089692	2.201382	0.254251
P	1.048549	-1.957578	0.371513
H	-0.410850	-0.070219	1.872734
B	-1.277504	-0.269601	0.086231
N	2.416815	0.525789	0.129396
H	0.788674	0.190491	2.265942
O	-2.366576	0.626394	0.078442
O	-1.764120	-1.508841	-0.374815
C	-3.583003	-0.088607	-0.143042
C	-3.075358	-1.342280	-0.917595
C	-4.170979	-0.434738	1.228393
C	-4.547717	0.803581	-0.914245
C	-3.875482	-2.617487	-0.685017
C	-2.916313	-1.088089	-2.420347
H	-3.486005	-1.074012	1.794723
H	-4.315070	0.490089	1.795495
H	-5.138044	-0.941940	1.142752
H	-5.463180	0.259045	-1.173103
H	-4.825715	1.663886	-0.296680
H	-4.093911	1.180636	-1.834285
H	-3.873348	-2.903391	0.369399
H	-4.913700	-2.492504	-1.013816
H	-3.434017	-3.439815	-1.257762
H	-2.354530	-1.917200	-2.862346
H	-3.884022	-1.015925	-2.928475
H	-2.353748	-0.166214	-2.600544
H	4.280408	3.064078	-1.060545
C	4.940470	1.011251	-0.960418
H	5.264807	-1.099400	-0.640463
C	1.816104	2.877284	0.086798
C	-0.628481	3.376253	1.519557
C	-0.698089	2.767184	-1.347245

C	2.894523	-1.815369	0.519884
C	0.658143	-3.311733	1.593569
C	0.857904	-2.789777	-1.290678
C	2.789822	1.776795	-0.215441
C	3.320223	-0.472645	0.005233
H	1.898388	3.686054	-0.646518
H	2.089443	3.305724	1.059276
H	-0.326359	4.386595	1.209375
C	-0.051843	3.100733	2.911426
C	-2.158849	3.316519	1.572121
H	-1.726920	2.402886	-1.268216
C	-0.031048	2.035792	-2.514633
C	-0.723069	4.279816	-1.581115
H	3.121674	-1.849327	1.592679
H	3.452504	-2.624995	0.037875
H	1.357351	-4.133709	1.386471
C	-0.774510	-3.830633	1.422254
C	0.870305	-2.842772	3.036426
H	-0.226536	-2.832667	-1.425062
C	1.429606	-1.868521	-2.372998
C	1.439369	-4.200947	-1.402383
C	4.034172	2.045996	-0.777283
C	4.580872	-0.262796	-0.543335
H	-0.342952	2.103863	3.253763
H	1.042098	3.139566	2.935743
H	-0.430516	3.845718	3.621945
H	-2.491190	2.319361	1.870761
H	-2.529175	4.046324	2.302298
H	-2.623074	3.537626	0.606096
H	1.016851	2.339397	-2.638672
H	-0.049090	0.954821	-2.348747
H	-0.551825	2.255438	-3.454443
H	0.285959	4.706257	-1.635636
H	-1.213972	4.498815	-2.537197
H	-1.272494	4.815439	-0.801131
H	-0.973487	-4.196388	0.410563
H	-0.954295	-4.653054	2.125044
H	-1.496322	-3.034508	1.623904
H	0.662290	-3.670012	3.726059
H	1.892312	-2.500301	3.226233
H	0.201297	-2.010416	3.272019
H	1.082710	-0.840927	-2.228215
H	2.526899	-1.860219	-2.354868
H	1.118690	-2.206792	-3.368356
H	0.959400	-4.907228	-0.718067
H	1.296557	-4.582455	-2.420882
H	2.517874	-4.217353	-1.202153
H	5.912639	1.196276	-1.406614

11 (at ωB97XD/BS4)

SCF energy in gas phase: -2038.55652806

Thermal correction to Enthalpy in gas phase: 0.739764

Thermal correction to Gibbs Free Energy in gas phase: 0.632453

SCF energy in solvent: -3276.84706231

Co	0.537587	0.031602	-0.162269
P	0.790687	-2.066391	-0.078670
P	0.486059	2.133743	0.020797
B	-1.395795	-0.090714	-0.019558
N	2.504432	0.169522	-0.366285
O	-2.234563	-0.052051	-1.151990
O	-2.217838	-0.220216	1.119889

C	-3.597607	0.076503	-0.739776
C	-3.562484	-0.498131	0.713611
C	-3.955367	1.565866	-0.779830
C	-4.484837	-0.688736	-1.715291
C	-4.525521	0.164910	1.692307
C	-3.757562	-2.017087	0.755187
H	-3.366006	2.127368	-0.048094
H	-3.724427	1.956430	-1.776128
H	-5.017480	1.738866	-0.574365
H	-5.528264	-0.692781	-1.378500
H	-4.445889	-0.210771	-2.699450
H	-4.148816	-1.721921	-1.831054
H	-4.317609	1.232305	1.798672
H	-5.564268	0.040965	1.363975
H	-4.422414	-0.297214	2.679341
H	-3.526031	-2.379587	1.761204
H	-4.786356	-2.303089	0.510996
H	-3.081827	-2.514489	0.052383
H	5.227878	-1.821936	-0.399786
C	5.288390	0.324627	-0.183955
H	4.966084	2.454479	-0.060743
C	2.548261	-2.251865	-0.681111
C	-0.160982	-3.275590	-1.124292
C	0.877383	-2.883491	1.593620
C	2.261847	2.605426	-0.326091
C	-0.485398	3.202276	-1.150847
C	0.201433	2.917160	1.687271
C	3.270062	-0.949862	-0.449809
C	3.127192	1.371843	-0.268704
H	3.093573	-3.092053	-0.235594
H	2.503562	-2.433325	-1.763268
H	-1.144910	-3.321513	-0.639835
C	0.422443	-4.689270	-1.175849
C	-0.370934	-2.686293	-2.523489
H	1.329063	-3.876965	1.466352
C	-0.521286	-3.039410	2.197119
C	1.780345	-2.053903	2.512579
H	2.317136	3.010691	-1.345342
H	2.645105	3.385016	0.342619
H	-1.523270	3.067052	-0.824878
C	-0.385746	2.620657	-2.564597
C	-0.149296	4.694041	-1.105753
H	0.611468	3.936243	1.656386
C	-1.289574	2.988383	2.031565
C	0.961238	2.108775	2.743629
C	4.656551	-0.900881	-0.347889
C	4.510932	1.474262	-0.159306
H	1.421497	-4.691171	-1.628530
H	0.500446	-5.142156	-0.181968
H	-0.213867	-5.340386	-1.787142
H	0.581157	-2.565071	-3.055553
H	-0.997872	-3.356211	-3.124780
H	-0.859621	-1.709522	-2.462806
H	-1.037725	-2.074198	2.231993
H	-1.141556	-3.732259	1.617451
H	-0.449167	-3.436589	3.217072
H	1.376344	-1.043251	2.630792
H	1.846085	-2.521462	3.502505
H	2.798621	-1.959754	2.118205
H	-0.722440	1.579707	-2.569833
H	-1.011910	3.197466	-3.256574
H	0.642764	2.654306	-2.946095

H	-0.794783	5.249789	-1.796525
H	-0.290746	5.119029	-0.106206
H	0.888229	4.881849	-1.407879
H	-1.835013	3.658535	1.357408
H	-1.745466	1.993438	1.978756
H	-1.420084	3.371614	3.050971
H	2.027156	2.012270	2.505382
H	0.876093	2.587289	3.726956
H	0.541219	1.099646	2.809767
H	6.368559	0.383600	-0.092092

$TS_{2\text{-}12}$ (at ωB97XD/BS4)

SCF energy in gas phase: -2039.69758865

Thermal correction to Enthalpy in gas phase: 0.750364

Thermal correction to Gibbs Free Energy in gas phase: 0.643656

SCF energy in solvent: -3278.00231411

Co	-0.415349	0.045729	-0.028426
P	-0.495641	2.248742	0.040196
B	1.499994	-0.081837	-0.060245
H	-0.673043	0.341944	-1.728196
P	-0.803091	-2.106836	0.042376
H	0.058627	-0.075143	1.372920
N	-2.436556	0.157316	0.094495
O	2.226488	-1.251568	-0.309790
O	2.398263	0.957906	0.197576
C	3.603390	-1.027286	0.022313
C	3.724393	0.523153	-0.126303
C	4.709207	1.187676	0.827365
C	4.012719	0.963164	-1.564446
C	4.479511	-1.837066	-0.924667
C	3.809863	-1.504575	1.462623
H	4.321628	-2.906328	-0.749776
H	5.540403	-1.618056	-0.757330
H	4.237745	-1.627123	-1.968993
H	3.196094	-0.924223	2.158627
H	4.857974	-1.427765	1.770620
H	3.504393	-2.553267	1.536779
H	4.720261	2.268062	0.650908
H	5.724401	0.806205	0.668025
H	4.430069	1.019970	1.870078
H	3.324193	0.482405	-2.266383
H	5.040015	0.729533	-1.863600
H	3.867538	2.045485	-1.638986
C	-2.035898	2.252671	-0.909553
C	-0.678099	3.082278	1.687319
C	0.684223	3.315836	-0.911623
C	-1.134067	-2.967832	-1.570437
C	0.245761	-3.304486	1.001485
C	-2.447425	-2.105295	0.913678
C	-2.985029	1.290960	-0.424538
C	-3.208632	-0.882735	0.464553
H	-2.438468	3.174931	-1.327904
H	-1.235751	1.145708	-1.668643
H	-1.016673	4.111162	1.510388
C	0.678913	3.106842	2.401645
C	-1.733118	2.364859	2.535418
H	1.636700	3.185653	-0.387437
C	0.294238	4.797817	-0.908692
C	0.871193	2.797849	-2.340050
H	-1.460413	-3.990463	-1.342630
C	0.162812	-3.016573	-2.386098

C	-2.251470	-2.275691	-2.358092
H	1.200407	-3.280276	0.465221
C	-0.294033	-4.738120	1.023669
C	0.509539	-2.797769	2.422694
H	-3.029551	-3.019472	0.754040
H	-2.231187	-2.025894	1.986282
C	-4.391238	1.387423	-0.541174
C	-4.587417	-0.830707	0.383362
H	0.565674	3.523477	3.409603
H	1.416630	3.715536	1.868486
H	1.084889	2.092920	2.487452
H	-1.458784	1.315064	2.683323
H	-2.720692	2.393828	2.065126
H	-1.810871	2.847046	3.517409
H	1.011603	5.371983	-1.507163
H	0.290779	5.226005	0.098670
H	-0.698229	4.952038	-1.348067
H	-0.053863	2.887360	-2.920299
H	1.172405	1.748092	-2.342328
H	1.647803	3.383708	-2.846174
H	-0.017585	-3.511037	-3.347801
H	0.960000	-3.560137	-1.868850
H	0.526740	-2.001598	-2.577606
H	-2.008325	-1.223606	-2.536094
H	-3.212798	-2.317073	-1.836321
H	-2.375780	-2.769796	-3.328838
H	0.360064	-5.370625	1.635244
H	-0.337571	-5.183805	0.025557
H	-1.297730	-4.785120	1.463497
H	-0.398354	-2.821896	3.037352
H	0.888869	-1.773963	2.416343
H	1.251779	-3.439749	2.911386
H	-4.828864	2.291166	-0.951913
C	-5.177816	0.336522	-0.126684
H	-5.189367	-1.677657	0.693986
H	-6.259592	0.405278	-0.202194

12 (at ωB97XD/BS4)

SCF energy in gas phase: -2038.55357575

Thermal correction to Enthalpy in gas phase: 0.737675

Thermal correction to Gibbs Free Energy in gas phase: 0.629887

SCF energy in solvent: -3276.85178263

Co	-0.538122	0.007292	0.452916
P	-0.901012	2.213740	0.246197
B	1.451886	0.111742	0.293718
P	-0.476687	-2.186463	0.161543
H	0.679703	0.189431	1.377246
N	-2.438779	-0.181487	0.010222
O	2.287170	-1.002472	0.182307
O	2.166738	1.266586	0.003774
C	3.639387	-0.538377	0.040550
C	3.432070	0.891882	-0.557179
C	4.473779	1.920406	-0.136551
C	3.282388	0.892995	-2.080115
C	4.413131	-1.501824	-0.848809
C	4.249631	-0.516640	1.444694
H	4.477838	-2.480989	-0.363513
H	5.432776	-1.136174	-1.014048
H	3.930333	-1.636613	-1.818850
H	3.711322	0.180184	2.095195
H	5.306389	-0.231231	1.424439

H	4.168889	-1.517422	1.879916
H	4.242905	2.886590	-0.595890
H	5.473931	1.616357	-0.465361
H	4.485371	2.056584	0.947090
H	2.542951	0.155292	-2.407608
H	4.233587	0.681931	-2.579388
H	2.932270	1.878741	-2.400557
C	-2.602319	2.206220	-0.196396
C	-0.689266	3.268671	1.762080
C	-0.000172	3.118134	-1.108762
C	-0.309020	-2.825441	-1.581734
C	0.503970	-3.355910	1.213747
C	-2.242381	-2.555989	0.530194
C	-3.187232	0.960852	-0.289892
C	-3.071972	-1.390687	0.050296
H	-3.179920	3.098256	-0.415971
H	-1.212758	4.216138	1.576069
C	0.783361	3.559305	2.064239
C	-1.371947	2.560143	2.936129
H	1.050622	3.141535	-0.806927
C	-0.512952	4.545797	-1.310483
C	-0.112234	2.298775	-2.396843
H	-0.737800	-3.837064	-1.573404
C	1.144717	-2.918399	-2.048937
C	-1.130639	-1.961711	-2.547659
H	1.528883	-3.246987	0.844633
C	0.068563	-4.818221	1.092481
C	0.488989	-2.872978	2.668019
H	-2.593338	-3.498448	0.096117
H	-2.334712	-2.637730	1.620786
C	-4.562967	0.788132	-0.687309
C	-4.386760	-1.576371	-0.294109
H	0.873061	4.113818	3.006357
H	1.255845	4.156481	1.277580
H	1.355436	2.629805	2.158034
H	-0.857726	1.619110	3.167474
H	-2.415071	2.324788	2.701552
H	-1.350156	3.191078	3.833042
H	0.037336	5.034508	-2.124119
H	-0.389194	5.160623	-0.412208
H	-1.574918	4.546972	-1.581550
H	-1.161461	2.179194	-2.690227
H	0.317185	1.300832	-2.261096
H	0.421290	2.794330	-3.217656
H	1.177940	-3.347322	-3.057267
H	1.760124	-3.544239	-1.395176
H	1.601377	-1.926436	-2.080350
H	-0.795622	-0.919149	-2.519838
H	-2.197979	-1.971329	-2.309702
H	-1.007882	-2.336946	-3.570613
H	0.712708	-5.454698	1.710473
H	0.133421	-5.184670	0.062637
H	-0.961854	-4.959294	1.439255
H	-0.521166	-2.893989	3.094333
H	0.868404	-1.849868	2.744184
H	1.120106	-3.521828	3.286520
H	-5.121270	1.673441	-0.973819
C	-5.138932	-0.442011	-0.692272
H	-4.833057	-2.562817	-0.243101
H	-6.177719	-0.558560	-0.990601

2^{Ir} (at ωB97XD/BS4)

SCF energy in gas phase: -1999.48832027

Thermal correction to Enthalpy in gas phase: 0.756808

Thermal correction to Gibbs Free Energy in gas phase: 0.649613

SCF energy in solvent: -1999.75647353

Ir	0.000000	0.000000	0.309237
P	1.490649	1.684646	0.615897
B	0.000000	0.000000	-1.703558
H	-1.219060	1.156558	0.272747
P	-1.490649	-1.684646	0.615897
H	1.219060	-1.156558	0.272747
N	0.000000	0.000000	2.530772
O	-0.727117	-0.879477	-2.526175
O	0.727117	0.879477	-2.526175
C	-0.275495	-0.731028	-3.873299
C	0.275495	0.731028	-3.873299
C	1.442695	0.978291	-4.820980
C	-0.819787	1.777023	-4.105529
C	-1.442695	-0.978291	-4.820980
C	0.819787	-1.777023	-4.105529
H	-1.758468	-2.024539	-4.752124
H	-1.154011	-0.777567	-5.859416
H	-2.299679	-0.350094	-4.566543
H	1.667548	-1.603827	-3.434571
H	1.180528	-1.772610	-5.139880
H	0.411861	-2.768511	-3.884547
H	1.758468	2.024539	-4.752124
H	1.154011	0.777567	-5.859416
H	2.299679	0.350094	-4.566543
H	-1.667548	1.603827	-3.434571
H	-1.180528	1.772610	-5.139880
H	-0.411861	2.768511	-3.884547
C	1.079028	2.186659	2.369293
C	3.299728	1.262276	0.668430
C	1.437506	3.281099	-0.334611
C	-3.299728	-1.262276	0.668430
C	-1.437506	-3.281099	-0.334611
C	-1.079028	-2.186659	2.369293
C	0.547953	1.035135	3.192440
C	-0.547953	-1.035135	3.192440
H	1.909381	2.682425	2.884091
H	0.270022	2.923245	2.270850
H	3.855921	2.184552	0.880054
C	3.732221	0.708754	-0.693906
C	3.589361	0.249956	1.780786
H	1.927986	3.022130	-1.280683
C	2.198054	4.431244	0.334577
C	0.000000	3.686858	-0.666507
H	-3.855921	-2.184552	0.880054
C	-3.732221	-0.708754	-0.693906
C	-3.589361	-0.249956	1.780786
H	-1.927986	-3.022130	-1.280683
C	-2.198054	-4.431244	0.334577
C	0.000000	-3.686858	-0.666507
H	-1.909381	-2.682425	2.884091
H	-0.270022	-2.923245	2.270850
C	0.572634	1.053995	4.584515
C	-0.572634	-1.053995	4.584515
H	4.801617	0.466938	-0.677222
H	3.556205	1.418249	-1.508400
H	3.166933	-0.201133	-0.920059
H	2.986637	-0.652977	1.635337

H	3.373928	0.652897	2.776940
H	4.648148	-0.033532	1.759882
H	2.199638	5.307800	-0.323497
H	3.241600	4.183781	0.552586
H	1.716907	4.731584	1.273216
H	-0.585092	3.887439	0.239051
H	-0.504306	2.893758	-1.219610
H	0.006891	4.602147	-1.271134
H	-4.801617	-0.466938	-0.677222
H	-3.556205	-1.418249	-1.508400
H	-3.166933	0.201133	-0.920059
H	-2.986637	0.652977	1.635337
H	-3.373928	-0.652897	2.776940
H	-4.648148	0.033532	1.759882
H	-2.199638	-5.307800	-0.323497
H	-3.241600	-4.183781	0.552586
H	-1.716907	-4.731584	1.273216
H	0.585092	-3.887439	0.239051
H	0.504306	-2.893758	-1.219610
H	-0.006891	-4.602147	-1.271134
H	1.022279	1.892693	5.105584
C	0.000000	0.000000	5.285639
H	-1.022279	-1.892693	5.105584
H	0.000000	0.000000	6.371384

$TS_{9\text{-}10}^{Ir}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1999.43198195

Thermal correction to Enthalpy in gas phase: 0.754066

Thermal correction to Gibbs Free Energy in gas phase: 0.643945

SCF energy in solvent: -1999.69896265

Ir	0.379959	-0.008441	-0.639681
P	0.567778	-2.231613	-0.192399
P	0.620808	2.217762	-0.248188
H	-0.053790	-0.047452	-2.538591
B	-1.579543	0.022005	-0.159843
N	2.560471	-0.035405	-0.075078
H	0.673215	-0.065498	-2.865652
O	-2.380342	-1.103498	0.148668
O	-2.373403	1.171334	0.077335
C	-3.726702	-0.691993	0.372391
C	-3.539884	0.795277	0.807127
C	-4.480349	-0.831535	-0.954408
C	-4.354359	-1.599652	1.423744
C	-4.684551	1.728636	0.433625
C	-3.216068	0.933336	2.299555
H	-4.044159	-0.177942	-1.716411
H	-4.391743	-1.865352	-1.303108
H	-5.544219	-0.591653	-0.850012
H	-5.362011	-1.258032	1.688167
H	-4.432755	-2.618457	1.029798
H	-3.746908	-1.634950	2.331634
H	-4.836100	1.756602	-0.648052
H	-5.619492	1.414978	0.912675
H	-4.454540	2.745823	0.767848
H	-2.898434	1.961318	2.502543
H	-4.083680	0.711157	2.930401
H	-2.395015	0.265407	2.579750
H	4.751889	-2.208391	1.262729
C	4.937218	-0.060920	1.360669
H	4.795572	2.090184	1.266115
C	2.424326	-2.468311	-0.151787

C	0.035916	-3.586121	-1.362734
C	0.023601	-2.856390	1.479203
C	2.482176	2.401465	-0.157243
C	0.185241	3.541972	-1.494017
C	0.016264	2.948083	1.357653
C	3.132473	-1.208463	0.271091
C	3.157025	1.125444	0.271190
H	2.733974	-3.313778	0.471816
H	2.728991	-2.700664	-1.179452
H	0.496575	-4.520608	-1.014699
C	0.506943	-3.312406	-2.793675
C	-1.490354	-3.735918	-1.346483
H	-1.042649	-2.602712	1.497135
C	0.726023	-2.048413	2.574697
C	0.203121	-4.358245	1.714687
H	2.815520	2.638037	-1.175782
H	2.797839	3.235082	0.478203
H	0.752418	4.444705	-1.227937
C	-1.315639	3.855808	-1.451585
C	0.584123	3.114677	-2.908990
H	-1.072493	2.884415	1.252292
C	0.422795	2.049489	2.526594
C	0.421441	4.402237	1.612460
C	4.322965	-1.249623	0.991076
C	4.346637	1.140965	0.993276
H	0.059647	-2.389577	-3.174409
H	1.594351	-3.214944	-2.877745
H	0.199723	-4.136961	-3.447745
H	-1.791489	-4.536752	-2.032585
H	-1.881209	-3.972640	-0.352593
H	-1.965816	-2.802196	-1.658990
H	1.788064	-2.315926	2.649908
H	0.660400	-0.977387	2.366156
H	0.266165	-2.249195	3.549371
H	1.252335	-4.662655	1.610247
H	-0.105363	-4.612648	2.735816
H	-0.393823	-4.968198	1.030671
H	-1.619027	4.317218	-0.506806
H	-1.572828	4.550571	-2.260107
H	-1.905158	2.941606	-1.569908
H	0.418445	3.942603	-3.608380
H	1.635455	2.817171	-2.987829
H	-0.021765	2.263880	-3.233532
H	0.057353	1.033708	2.363277
H	1.514008	2.002863	2.640450
H	0.004498	2.433156	3.465077
H	0.092527	5.080966	0.819963
H	-0.026640	4.751647	2.550323
H	1.507879	4.508530	1.718907
H	5.860723	-0.070581	1.931320

11^{Ir} (at ωB97XD/BS4)

SCF energy in gas phase: -1998.26866106

Thermal correction to Enthalpy in gas phase: 0.73969

Thermal correction to Gibbs Free Energy in gas phase: 0.629114

SCF energy in solvent: -1998.53114366

Ir	0.355808	-0.004596	-0.146760
P	0.555462	-2.243356	0.010255
P	0.696393	2.218761	-0.050103
B	-1.660169	0.052310	0.004268
N	2.534445	-0.074927	-0.384107

O	-2.520779	-1.070955	0.060960
O	-2.477556	1.207022	-0.014562
C	-3.859184	-0.654986	-0.200788
C	-3.830269	0.839684	0.251509
C	-4.098102	-0.814498	-1.706662
C	-4.822304	-1.545244	0.575558
C	-4.762851	1.763584	-0.523074
C	-4.063355	1.007339	1.757119
H	-3.421262	-0.168119	-2.274668
H	-3.887645	-1.851615	-1.987268
H	-5.130691	-0.580647	-1.988513
H	-5.855369	-1.193708	0.468936
H	-4.769965	-2.569118	0.190512
H	-4.568444	-1.572347	1.638038
H	-4.510501	1.780743	-1.586053
H	-5.807453	1.448723	-0.414057
H	-4.673600	2.785001	-0.138316
H	-3.822463	2.037534	2.038072
H	-5.102639	0.804851	2.038513
H	-3.407588	0.339672	2.325603
H	5.045428	-2.299903	-0.150079
C	5.291403	-0.156272	-0.135221
H	5.178560	1.996850	-0.219762
C	2.338600	-2.519054	-0.495423
C	-0.423499	-3.400683	-1.059633
C	0.505361	-3.014767	1.701847
C	2.489429	2.371745	-0.570975
C	-0.215183	3.413704	-1.138221
C	0.705205	3.020850	1.627595
C	3.172589	-1.266810	-0.340239
C	3.245169	1.076051	-0.377533
H	2.806227	-3.360906	0.027588
H	2.326128	-2.776345	-1.563204
H	-1.433266	-3.303934	-0.642775
C	0.021259	-4.863297	-1.012442
C	-0.479928	-2.856675	-2.490277
H	0.921316	-4.028436	1.619431
C	-0.933970	-3.099615	2.218433
C	1.382408	-2.200325	2.658019
H	2.486151	2.594690	-1.646398
H	3.010267	3.199887	-0.077191
H	-1.231502	3.375862	-0.727398
C	-0.291341	2.856423	-2.563130
C	0.305251	4.851733	-1.108080
H	1.139270	4.024213	1.518986
C	-0.721005	3.140290	2.172060
C	1.585244	2.206575	2.581368
C	4.556216	-1.332864	-0.201650
C	4.630360	1.060794	-0.240478
H	1.049911	-4.981345	-1.375752
H	-0.030248	-5.279398	-0.000887
H	-0.622952	-5.476322	-1.654067
H	0.503305	-2.883628	-2.977209
H	-1.163599	-3.462226	-3.097349
H	-0.829455	-1.819739	-2.489302
H	-1.412663	-2.116009	2.186092
H	-1.546052	-3.781772	1.619593
H	-0.939579	-3.463669	3.252962
H	0.987995	-1.182890	2.749664
H	1.394668	-2.666097	3.650773
H	2.418965	-2.123774	2.309198
H	-0.684694	1.835390	-2.552813

H	-0.947220	3.484011	-3.178082
H	0.693274	2.837322	-3.047649
H	-0.297197	5.486281	-1.769019
H	0.261458	5.287597	-0.104632
H	1.343620	4.909545	-1.458202
H	-1.345647	3.793054	1.553702
H	-1.199686	2.156676	2.198970
H	-0.702488	3.553624	3.187743
H	2.617871	2.119606	2.223847
H	1.611225	2.680724	3.569848
H	1.184259	1.193005	2.686763
H	6.370296	-0.187811	-0.017841

$TS_{2\text{-}12}^{Ir}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1999.42058399

Thermal correction to Enthalpy in gas phase: 0.751189

Thermal correction to Gibbs Free Energy in gas phase: 0.643952

SCF energy in solvent: -1999.69214218

Ir	-0.301946	0.023457	0.075561
P	-0.651265	2.317510	0.099861
B	1.725389	-0.021476	-0.008303
H	-0.602118	0.379817	-1.764193
P	-0.663126	-2.234833	0.052382
H	-0.014789	-0.111446	1.641437
N	-2.490110	0.025082	0.013347
O	2.588320	1.081515	-0.044930
O	2.497046	-1.195491	-0.036546
C	3.905887	0.627791	-0.368921
C	3.875118	-0.851784	0.132746
C	4.731891	-1.821408	-0.671663
C	4.197157	-0.981542	1.624608
C	4.926486	1.521176	0.324439
C	4.061919	0.736730	-1.889069
H	4.870698	2.533611	-0.088386
H	5.944374	1.145199	0.168580
H	4.735790	1.583891	1.398333
H	3.339126	0.092435	-2.400577
H	5.070661	0.465669	-2.218581
H	3.864138	1.770241	-2.189972
H	4.643619	-2.828347	-0.250558
H	5.788293	-1.530576	-0.639069
H	4.411269	-1.862742	-1.715355
H	3.590861	-0.285989	2.214009
H	5.255291	-0.791720	1.834141
H	3.957214	-1.998887	1.949874
C	-2.159607	2.197465	-0.899644
C	-0.974870	3.134762	1.732836
C	0.500615	3.460342	-0.795387
C	-0.735647	-3.071837	-1.604652
C	0.289346	-3.424919	1.111501
C	-2.405259	-2.289897	0.725978
C	-3.058189	1.144601	-0.520650
C	-3.200957	-1.099931	0.237603
H	-2.618958	3.097920	-1.306364
H	-1.202747	1.120813	-1.680528
H	-1.362166	4.140311	1.525115
C	0.332250	3.243433	2.526135
C	-2.037549	2.363343	2.520981
H	1.433557	3.384234	-0.225227
C	0.017406	4.914360	-0.809701
C	0.798137	2.959093	-2.211014

H	-0.888139	-4.144275	-1.427617
C	0.598382	-2.866825	-2.333749
C	-1.900841	-2.546624	-2.449245
H	1.202596	-3.607880	0.532426
C	-0.441179	-4.752164	1.345073
C	0.707584	-2.783207	2.436574
H	-2.923769	-3.228313	0.503488
H	-2.291688	-2.222847	1.816425
C	-4.453133	1.137715	-0.771923
C	-4.560029	-1.147833	-0.000994
H	0.138770	3.676114	3.514787
H	1.071698	3.875796	2.023745
H	0.776236	2.251078	2.664312
H	-1.703326	1.340459	2.722597
H	-2.985293	2.309183	1.976925
H	-2.223307	2.862641	3.479392
H	0.725869	5.535723	-1.369993
H	-0.065198	5.337701	0.196330
H	-0.959148	5.005796	-1.299666
H	-0.104885	2.952024	-2.831612
H	1.213941	1.949987	-2.185722
H	1.530795	3.622512	-2.685835
H	0.595854	-3.424454	-3.277607
H	1.457958	-3.193904	-1.741306
H	0.744831	-1.804532	-2.555713
H	-1.827338	-1.461774	-2.582436
H	-2.874464	-2.767018	-2.000694
H	-1.875708	-3.011178	-3.441641
H	0.218383	-5.452089	1.870480
H	-0.757961	-5.234630	0.414932
H	-1.329325	-4.608209	1.971361
H	-0.161461	-2.469630	3.027455
H	1.331276	-1.906299	2.257602
H	1.274779	-3.506372	3.034802
H	-4.921965	2.026557	-1.180615
C	-5.186407	0.005359	-0.504765
H	-5.122232	-2.055200	0.190044
H	-6.256343	-0.003345	-0.693855

12^{Ir} (at ωB97XD/BS4)

SCF energy in gas phase: -1998.26507384

Thermal correction to Enthalpy in gas phase: 0.736895

Thermal correction to Gibbs Free Energy in gas phase: 0.628488

SCF energy in solvent: -1998.5355464

Ir	-0.413793	0.010594	0.400442
P	-0.839679	2.295585	0.215101
B	1.593652	0.097925	0.095895
P	-0.489443	-2.278045	0.146330
H	0.765086	0.152918	1.497772
N	-2.405340	-0.132879	-0.242307
O	2.334700	1.251831	-0.155397
O	2.443550	-1.015775	0.044371
C	3.620059	0.865847	-0.654603
C	3.798095	-0.550000	-0.019767
C	4.630037	-1.524825	-0.842187
C	4.323319	-0.495328	1.417650
C	4.648746	1.900740	-0.219687
C	3.525040	0.826384	-2.182266
H	4.440955	2.856393	-0.711344
H	5.660148	1.585580	-0.500505
H	4.617594	2.062901	0.860136

H	2.800465	0.073638	-2.511162
H	4.493196	0.608329	-2.645018
H	3.179806	1.801286	-2.539295
H	4.666302	-2.495841	-0.337993
H	5.657094	-1.158318	-0.950864
H	4.208884	-1.677428	-1.838506
H	3.744714	0.214569	2.017370
H	5.379157	-0.207676	1.455276
H	4.217591	-1.486191	1.869874
C	-2.505644	2.273488	-0.374712
C	-0.756203	3.306558	1.768150
C	0.162906	3.238359	-1.035659
C	-0.147522	-2.995081	-1.540725
C	0.296269	-3.439854	1.351903
C	-2.316957	-2.530697	0.282363
C	-3.094119	1.042374	-0.568012
C	-3.051834	-1.340857	-0.293968
H	-3.056549	3.175264	-0.620792
H	-1.224320	4.276006	1.551633
C	0.696435	3.528363	2.199775
C	-1.567277	2.608113	2.863076
H	1.192270	3.211736	-0.667352
C	-0.303271	4.688592	-1.186747
C	0.119786	2.498197	-2.374873
H	-0.696950	-3.946459	-1.563876
C	1.332012	-3.281505	-1.802966
C	-0.723478	-2.078859	-2.627868
H	1.367457	-3.328126	1.142100
C	-0.116059	-4.902568	1.166755
C	0.049643	-2.957947	2.785404
H	-2.656984	-3.461656	-0.182976
H	-2.547571	-2.592628	1.353707
C	-4.426255	0.902184	-1.105740
C	-4.321331	-1.483471	-0.784230
H	0.729592	4.049134	3.164174
H	1.255968	4.128600	1.475062
H	1.217229	2.570268	2.309429
H	-1.107081	1.648457	3.126545
H	-2.591896	2.411364	2.531426
H	-1.606541	3.230802	3.764914
H	0.296613	5.197139	-1.951209
H	-0.202037	5.258091	-0.256710
H	-1.351246	4.735982	-1.504977
H	-0.907826	2.424284	-2.748143
H	0.518788	1.484992	-2.271131
H	0.720659	3.031574	-3.121890
H	1.443554	-3.735381	-2.794682
H	1.762972	-3.970588	-1.069203
H	1.913586	-2.358907	-1.767809
H	-0.236568	-1.097860	-2.602482
H	-1.799206	-1.917446	-2.511265
H	-0.552655	-2.525799	-3.614251
H	0.409820	-5.535869	1.890506
H	0.119191	-5.278440	0.165985
H	-1.191380	-5.034941	1.335585
H	-1.009951	-3.029785	3.058404
H	0.360561	-1.916692	2.910652
H	0.613304	-3.579152	3.490831
H	-4.944697	1.803890	-1.414244
C	-5.008955	-0.318239	-1.219399
H	-4.795714	-2.457568	-0.805908
H	-6.012022	-0.407027	-1.628376

2^{Ph} (at ωB97XD/BS4)

SCF energy in gas phase: -1860.14543413

Thermal correction to Enthalpy in gas phase: 0.659545

Thermal correction to Gibbs Free Energy in gas phase: 0.564933

SCF energy in solvent: -3098.38013273

Co	0.000004	0.011035	0.000006
P	2.148842	-0.166258	0.024241
H	0.075906	-0.021187	1.551237
P	-2.148826	-0.166316	-0.024184
H	-0.075929	-0.021206	-1.551246
N	0.000018	-2.020795	-0.000036
C	2.310069	-1.869479	0.748163
C	3.073481	-0.289518	-1.581392
C	3.186977	0.946734	1.092815
C	-3.073467	-0.289754	1.581441
C	-3.186979	0.946793	-1.092604
C	-2.310030	-1.869472	-0.748254
C	1.115225	-2.694125	0.340302
C	-1.115162	-2.694123	-0.340466
H	3.246676	-2.380216	0.498097
H	2.274957	-1.744570	1.837071
H	4.121500	-0.520095	-1.349754
C	2.991695	1.052457	-2.315385
C	2.508105	-1.418058	-2.448826
H	2.855500	1.947665	0.788126
C	4.699374	0.826969	0.879764
C	2.839265	0.780082	2.576582
H	-4.121490	-0.520271	1.349745
C	-2.991690	1.052140	2.315587
C	-2.508169	-1.418410	2.448770
H	-2.855605	1.947688	-0.787690
C	-4.699376	0.826848	-0.879682
C	-2.839113	0.780452	-2.576377
H	-3.246625	-2.380248	-0.498220
H	-2.274925	-1.744479	-1.837151
C	1.146886	-4.085764	0.341609
C	-1.146774	-4.085763	-0.341947
H	3.552753	1.004575	-3.256062
H	3.396000	1.880546	-1.722808
H	1.947799	1.289006	-2.542477
H	1.434293	-1.270399	-2.608266
H	2.658169	-2.404366	-1.995376
H	3.008415	-1.422828	-3.424426
H	5.223077	1.483248	1.584501
H	5.007064	1.117186	-0.128871
H	5.049449	-0.196874	1.062655
H	3.314625	-0.116586	2.993935
H	1.759998	0.702788	2.730000
H	3.213266	1.640792	3.141634
H	-3.552767	1.004155	3.256249
H	-3.395990	1.880295	1.723096
H	-1.947802	1.288667	2.542730
H	-1.434363	-1.270798	2.608282
H	-2.658236	-2.404665	1.995205
H	-3.008533	-1.423274	3.424342
H	-5.223093	1.483252	-1.584293
H	-5.007144	1.116793	0.129009
H	-5.049352	-0.196981	-1.062839
H	-3.314443	-0.116136	-2.993948
H	-1.759824	0.703170	-2.729700

H	-3.213041	1.641273	-3.141301
H	2.060476	-4.601884	0.617119
C	0.000068	-4.789783	-0.000211
H	-2.060344	-4.601880	-0.617531
H	0.000088	-5.875491	-0.000282
C	-0.000038	1.950488	-0.000001
C	-0.100916	2.702962	-1.184806
C	0.100775	2.703001	1.184784
C	-0.104120	4.098032	-1.192413
H	-0.177950	2.180811	-2.134465
C	0.103933	4.098072	1.192351
H	0.177783	2.180888	2.134466
C	-0.000098	4.809218	-0.000042
H	-0.184552	4.630852	-2.137919
H	0.184329	4.630920	2.137844
H	-0.000115	5.896090	-0.000060

$TS_{9\text{-}10}^{Ph}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1860.11067741

Thermal correction to Enthalpy in gas phase: 0.655625

Thermal correction to Gibbs Free Energy in gas phase: 0.558876

SCF energy in solvent: -3098.34361072

Co	0.000010	-0.001403	0.635916
P	-2.156279	0.136933	0.379218
P	2.156290	0.136959	0.379163
H	0.000018	-0.773755	1.915886
N	-0.000014	2.000731	0.047749
H	0.000001	0.460589	2.120583
H	-2.149726	4.454808	-0.776937
C	-0.000077	4.608191	-0.916136
H	2.149589	4.454822	-0.777183
C	-2.409552	1.976384	0.370258
C	-3.342272	-0.507121	1.653489
C	-2.918018	-0.349999	-1.251506
C	2.409556	1.976414	0.370024
C	3.342316	-0.506943	1.653487
C	2.918014	-0.350136	-1.251522
C	-1.162379	2.666690	-0.118905
C	1.162328	2.666699	-0.119032
H	-3.296940	2.302046	-0.182961
H	-2.549199	2.282071	1.415027
H	-4.349160	-0.158396	1.389924
C	-3.001128	-0.006741	3.059518
C	-3.310522	-2.041134	1.614000
H	-2.577494	-1.377803	-1.416668
C	-2.318476	0.527456	-2.360052
C	-4.447239	-0.306558	-1.306486
H	2.549343	2.282189	1.414748
H	3.296876	2.302023	-0.183336
H	4.349201	-0.158275	1.389836
C	3.310533	-2.040961	1.614205
C	3.001241	-0.006365	3.059461
H	2.577436	-1.377933	-1.416608
C	2.318525	0.527266	-2.360140
C	4.447237	-0.306774	-1.306512
C	-1.194752	3.962478	-0.625549
C	1.194635	3.962485	-0.625687
H	-1.983062	-0.296518	3.335776
H	-3.075709	1.082174	3.148599
H	-3.698007	-0.444530	3.784119
H	-2.311570	-2.406878	1.871299

H	-4.026148	-2.450114	2.336722
H	-3.560117	-2.443759	0.626937
H	-2.793900	1.515703	-2.382811
H	-1.243675	0.675663	-2.223252
H	-2.476114	0.061029	-3.338540
H	-4.835284	0.684752	-1.038723
H	-4.786940	-0.523869	-2.326168
H	-4.912018	-1.041488	-0.642805
H	3.560004	-2.443723	0.627168
H	4.026228	-2.449861	2.336903
H	2.311600	-2.406646	1.871663
H	3.698102	-0.444120	3.784100
H	3.075916	1.082554	3.148407
H	1.983160	-0.296028	3.335783
H	1.243737	0.675572	-2.223356
H	2.794027	1.515473	-2.382997
H	2.476119	0.060738	-3.338587
H	4.911985	-1.041681	-0.642784
H	4.786922	-0.524171	-2.326180
H	4.835333	0.684535	-1.038819
H	-0.000104	5.612265	-1.328910
C	0.000003	-1.715090	-0.426632
C	0.000063	-2.935916	0.281079
C	-0.000066	-1.865264	-1.827438
C	0.000043	-4.185108	-0.338990
H	0.000128	-2.910471	1.369345
C	-0.000089	-3.105306	-2.469977
H	-0.000096	-0.985926	-2.464675
C	-0.000038	-4.281699	-1.727961
H	0.000091	-5.087646	0.269142
H	-0.000147	-3.147729	-3.557696
H	-0.000056	-5.251019	-2.219627

11^{Ph} (at ωB97XD/BS4)

SCF energy in gas phase: -1858.96181576

Thermal correction to Enthalpy in gas phase: 0.641482

Thermal correction to Gibbs Free Energy in gas phase: 0.542175

SCF energy in solvent: -3097.18133001

Co	-0.000021	0.032206	0.265487
P	-2.150771	0.170944	0.143959
P	2.150746	0.170911	0.144015
N	0.000006	2.019163	0.501465
H	-2.148017	4.614267	0.308264
C	0.000068	4.809021	0.261083
H	2.148142	4.614192	0.308524
C	-2.446037	1.940571	0.630592
C	-3.333836	-0.767318	1.233890
C	-2.910101	0.057238	-1.554028
C	2.446021	1.940476	0.630868
C	3.333788	-0.767500	1.233842
C	2.910086	0.057406	-1.553994
C	-1.164020	2.718292	0.477611
C	1.164058	2.718254	0.477755
H	-3.261280	2.425571	0.082573
H	-2.731723	1.951076	1.690299
H	-4.296035	-0.236201	1.230191
C	-2.788783	-0.795909	2.666422
C	-3.549533	-2.196849	0.719377
H	-2.720378	-0.982264	-1.852330
C	-2.133160	0.966303	-2.511640
C	-4.413050	0.337920	-1.629613

H	2.731528	1.950858	1.690624
H	3.261372	2.425503	0.083034
H	4.296010	-0.236425	1.230160
C	3.549419	-2.196997	0.719198
C	2.788793	-0.796181	2.666393
H	2.720287	-0.982035	-1.852456
C	2.133211	0.966654	-2.511491
C	4.413065	0.337957	-1.629551
C	-1.191482	4.103117	0.343910
C	1.191585	4.103076	0.344056
H	-1.827268	-1.317966	2.694980
H	-2.635164	0.207522	3.078800
H	-3.488200	-1.323097	3.326268
H	-2.601049	-2.739448	0.660557
H	-4.211502	-2.739288	1.405049
H	-4.012036	-2.219472	-0.272207
H	-2.253658	2.024703	-2.246641
H	-1.064621	0.736495	-2.485237
H	-2.493731	0.838638	-3.539049
H	-4.644484	1.366670	-1.327555
H	-4.766133	0.217135	-2.660785
H	-4.999726	-0.336361	-0.998862
H	4.011850	-2.219559	-0.272421
H	4.211426	-2.739502	1.404782
H	2.600920	-2.739569	0.660405
H	3.488203	-1.323470	3.326166
H	2.635256	0.207225	3.078865
H	1.827249	-1.318181	2.694944
H	1.064633	0.737022	-2.485023
H	2.253902	2.025012	-2.246425
H	2.493683	0.839008	-3.538937
H	4.999690	-0.336533	-0.998976
H	4.766112	0.217382	-2.660761
H	4.644609	1.366611	-1.327257
H	0.000094	5.888550	0.146629
C	-0.000011	-1.849603	-0.131699
C	-0.000147	-2.858548	0.854736
C	0.000139	-2.320280	-1.461483
C	-0.000133	-4.219730	0.548272
H	-0.000294	-2.573130	1.907314
C	0.000170	-3.677200	-1.786552
H	0.000266	-1.597537	-2.279544
C	0.000034	-4.640853	-0.780433
H	-0.000249	-4.956260	1.349835
H	0.000302	-3.985081	-2.830756
H	0.000053	-5.699473	-1.026173

$TS_{2\text{-}12}^{Ph}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1860.09306108

Thermal correction to Enthalpy in gas phase: 0.653438

Thermal correction to Gibbs Free Energy in gas phase: 0.558229

SCF energy in solvent: -3098.32734131

Co	-0.020692	0.043977	-0.041352
P	-2.212830	-0.257388	0.016718
H	-0.296716	-0.136101	-1.790368
P	2.159283	-0.123147	0.169468
H	0.055323	0.093569	1.434577
N	0.045574	-1.948808	-0.108206
C	-2.073099	-1.669783	-1.109805
C	-3.041937	-0.745382	1.604173
C	-3.352015	0.971084	-0.775964

C	3.262454	-0.247074	-1.326213
C	3.101279	0.961493	1.343303
C	2.243242	-1.837567	0.881695
C	-1.024015	-2.558815	-0.691761
C	1.130638	-2.653986	0.272013
H	-2.954596	-2.125559	-1.560186
H	-1.074702	-0.736113	-1.796157
H	-4.052677	-1.089741	1.351258
C	-3.137497	0.465826	2.538907
C	-2.299263	-1.897172	2.288395
H	-3.195703	1.893072	-0.200992
C	-4.829696	0.569192	-0.699894
C	-2.939039	1.253927	-2.223909
H	4.197119	-0.715638	-0.989198
C	3.584868	1.136659	-1.900615
C	2.627897	-1.152537	-2.387276
H	3.079803	1.945534	0.857297
C	4.558030	0.528198	1.543828
C	2.380620	1.104543	2.686759
H	3.215590	-2.321612	0.741324
H	2.066813	-1.739437	1.960179
C	-0.982444	-3.953114	-0.919947
C	1.208044	-4.020342	0.083965
H	-3.665170	0.190527	3.459544
H	-3.671132	1.308379	2.086346
H	-2.134167	0.809871	2.812586
H	-1.259793	-1.619782	2.493560
H	-2.295986	-2.803329	1.675824
H	-2.787009	-2.135450	3.241247
H	-5.440357	1.308129	-1.231361
H	-5.199872	0.516684	0.328490
H	-5.001491	-0.404070	-1.175210
H	-3.050414	0.360999	-2.848766
H	-1.903344	1.592413	-2.281981
H	-3.580128	2.041201	-2.636693
H	4.186534	1.028782	-2.810412
H	4.153380	1.756166	-1.199406
H	2.672082	1.680643	-2.160025
H	1.660795	-0.754344	-2.709722
H	2.461856	-2.169408	-2.016532
H	3.287762	-1.217468	-3.260276
H	5.060120	1.220367	2.229228
H	5.129098	0.518466	0.610636
H	4.615707	-0.472582	1.988811
H	2.310880	0.146690	3.215848
H	1.371768	1.496063	2.549791
H	2.939398	1.795624	3.328334
H	-1.830532	-4.437441	-1.391906
C	0.124458	-4.670628	-0.527804
H	2.090117	-4.567940	0.396810
H	0.161305	-5.744238	-0.689888
C	-0.065533	1.970102	-0.115286
C	0.246115	2.641680	-1.311066
C	-0.404315	2.789244	0.974044
C	0.235357	4.032273	-1.413971
H	0.488566	2.057065	-2.196965
C	-0.421199	4.181673	0.885778
H	-0.670357	2.328531	1.922888
C	-0.096615	4.814772	-0.310849
H	0.483318	4.505354	-2.361784
H	-0.690811	4.773983	1.757724
H	-0.107523	5.898855	-0.384317

12^{Ph} (at ωB97XD/BS4)

SCF energy in gas phase: -1858.93527062

Thermal correction to Enthalpy in gas phase: 0.637681

Thermal correction to Gibbs Free Energy in gas phase: 0.539953

SCF energy in solvent: -3097.16799293

Co	-0.021550	-0.080352	0.086141
P	-2.221778	-0.253803	0.241026
P	2.176404	-0.222486	0.011813
H	0.006458	-0.027434	1.512303
N	-0.004422	-2.068425	0.084278
C	-2.396755	-1.996816	0.306713
C	-3.158871	0.535259	1.631160
C	-3.062726	0.334794	-1.313946
C	2.918943	0.124634	-1.653032
C	3.263286	0.619984	1.248963
C	2.443441	-2.034123	0.235252
C	-1.229852	-2.728236	0.142631
C	1.145838	-2.793623	0.051265
H	-3.354511	-2.505273	0.356048
H	-4.155387	0.071968	1.611588
C	-3.306430	2.051176	1.462817
C	-2.495446	0.185582	2.965942
H	-2.869697	1.412177	-1.381678
C	-4.572636	0.083240	-1.311863
C	-2.403089	-0.364771	-2.507757
H	3.884250	-0.397784	-1.695688
C	3.148738	1.620347	-1.892416
C	1.989585	-0.473055	-2.717819
H	3.101942	1.688380	1.055786
C	4.748833	0.286149	1.075384
C	2.796360	0.325701	2.679002
H	3.225616	-2.418879	-0.428527
H	2.792932	-2.200900	1.261679
C	-1.230646	-4.162070	0.023693
C	1.173217	-4.162904	-0.063471
H	-3.850285	2.467243	2.319365
H	-3.860837	2.318992	0.557720
H	-2.327402	2.537782	1.412526
H	-1.530457	0.696383	3.058001
H	-2.320690	-0.891557	3.053783
H	-3.131656	0.505650	3.799584
H	-5.012515	0.401600	-2.264813
H	-5.084022	0.628846	-0.512351
H	-4.786120	-0.984949	-1.187144
H	-2.589925	-1.443096	-2.469898
H	-1.314739	-0.227441	-2.518460
H	-2.799270	0.026017	-3.452254
H	3.533429	1.774668	-2.907275
H	3.878780	2.042867	-1.194686
H	2.217964	2.186797	-1.791674
H	1.034790	0.066075	-2.735977
H	1.776444	-1.533158	-2.541105
H	2.439851	-0.378442	-3.712302
H	5.343255	0.828463	1.819389
H	5.127479	0.559665	0.085869
H	4.933079	-0.784501	1.224850
H	2.953383	-0.725727	2.946369
H	1.734624	0.547935	2.813177
H	3.370663	0.933204	3.387206
H	-2.187803	-4.673259	0.026982

C	-0.062410	-4.851594	-0.091497
H	2.118205	-4.693630	-0.092353
H	-0.075797	-5.934283	-0.187471
C	-0.018992	1.837803	-0.043554
C	-0.330282	2.442786	-1.274292
C	0.330745	2.712437	0.998976
C	-0.293345	3.825417	-1.458937
H	-0.608459	1.826649	-2.129236
C	0.367548	4.095964	0.829863
H	0.570554	2.305715	1.979198
C	0.056371	4.663075	-0.403809
H	-0.541246	4.247644	-2.430131
H	0.638570	4.734969	1.667315
H	0.083407	5.740506	-0.539660

2$^{\mathbf{Ir\_Ph}}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1819.87051288

Thermal correction to Enthalpy in gas phase: 0.659429

Thermal correction to Gibbs Free Energy in gas phase: 0.56212

SCF energy in solvent: -1820.07002944

Ir	0.000011	0.064772	-0.000016
P	-2.255074	-0.218931	0.004777
H	-0.060591	0.088514	-1.678670
P	2.255028	-0.219422	-0.004793
H	0.060638	0.088591	1.678637
N	-0.000231	-2.100100	0.000048
C	0.000258	2.117599	-0.000030
C	0.251628	2.873573	1.163094
C	-0.250920	2.873640	-1.163154
C	0.256449	4.267807	1.168419
H	0.442196	2.349684	2.096143
C	-0.255375	4.267875	-1.168476
H	-0.441617	2.349808	-2.096207
C	0.000631	4.979843	-0.000028
H	0.456844	4.800033	2.096241
H	-0.455628	4.800156	-2.096297
H	0.000777	6.066657	-0.000028
C	-2.364262	-1.965064	-0.637296
C	-3.147087	-0.271040	1.629530
C	-3.336830	0.807656	-1.106283
C	3.147007	-0.271844	-1.629551
C	3.336971	0.807053	1.106200
C	2.363821	-1.965534	0.637407
C	-1.139487	-2.771296	-0.271364
C	1.138887	-2.771525	0.271481
H	-3.277399	-2.487985	-0.332621
H	-2.382964	-1.877978	-1.730667
H	-4.192708	-0.537496	1.428792
C	-3.079829	1.118311	2.273052
C	-2.543327	-1.334462	2.550959
H	-3.049242	1.830048	-0.827021
C	-4.842755	0.626438	-0.892771
C	-2.971850	0.617846	-2.582613
H	4.192546	-0.538630	-1.428825
C	3.080179	1.117518	-2.273093
C	2.542879	-1.335077	-2.550954
H	3.049679	1.829474	0.826737
C	4.842875	0.625417	0.892884
C	2.971780	0.617614	2.582523
H	3.276858	-2.488675	0.332815
H	2.382483	-1.878374	1.730773

C	-1.167674	-4.162565	-0.263366
C	1.166789	-4.162799	0.263513
H	-3.582508	1.109543	3.247123
H	-3.558342	1.886225	1.655112
H	-2.035463	1.414113	2.419685
H	-1.479883	-1.133579	2.716504
H	-2.643640	-2.345118	2.138435
H	-3.056597	-1.319321	3.519507
H	-5.394102	1.232023	-1.621257
H	-5.166690	0.938060	0.104341
H	-5.144543	-0.418389	-1.039531
H	-3.386666	-0.318916	-2.975772
H	-1.888929	0.607386	-2.730636
H	-3.398866	1.435126	-3.173953
H	3.582858	1.108582	-3.247164
H	3.558927	1.885292	-1.655161
H	2.035906	1.413642	-2.419730
H	1.479491	-1.133858	-2.716459
H	2.642887	-2.345764	-2.138434
H	3.056115	-1.320099	-3.519523
H	5.394291	1.230989	1.621327
H	5.167005	0.936784	-0.104243
H	5.144378	-0.419461	1.039861
H	3.386281	-0.319194	2.975902
H	1.888837	0.607511	2.730428
H	3.398970	1.434880	3.173759
H	-2.096187	-4.680621	-0.478489
C	-0.000515	-4.866632	0.000080
H	2.095194	-4.681043	0.478651
H	-0.000626	-5.952170	0.000091

$TS_{9\text{-}10}^{Ir\_Ph}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1819.81040153

Thermal correction to Enthalpy in gas phase: 0.655409

Thermal correction to Gibbs Free Energy in gas phase: 0.558951

SCF energy in solvent: -1820.01108106

Ir	-0.000051	-0.052345	-0.602468
P	2.222440	0.187283	-0.148883
P	-2.222395	0.188021	-0.148680
H	-0.000056	0.130841	-2.318530
N	0.000357	2.100546	-0.234910
H	-0.000123	-0.937168	-2.052031
H	2.149550	4.580008	0.511656
C	0.001054	4.759722	0.594652
H	-2.147545	4.580780	0.512761
C	2.439787	2.021406	-0.371828
C	3.533439	-0.564385	-1.234259
C	2.859273	-0.117672	1.580138
C	-2.439229	2.022349	-0.370529
C	-3.533689	-0.562633	-1.234409
C	-2.859205	-0.117563	1.580230
C	1.169022	2.764486	-0.059094
C	-1.167973	2.764892	-0.058474
H	3.283719	2.434201	0.190959
H	2.656083	2.171043	-1.437105
H	4.503376	-0.139727	-0.944375
C	3.288665	-0.267230	-2.715330
C	3.547469	-2.081035	-0.996808
H	2.560164	-1.151559	1.792880
C	2.111783	0.795849	2.556860
C	4.373160	0.022378	1.760642

H	-2.656591	2.172794	-1.435471
H	-3.282469	2.435058	0.193361
H	-4.503482	-0.137842	-0.944230
C	-3.548189	-2.079411	-0.997803
C	-3.288864	-0.264772	-2.715328
H	-2.560010	-1.151497	1.792619
C	-2.111684	0.795718	2.557164
C	-4.373082	0.022417	1.760847
C	1.193934	4.088101	0.364263
C	-1.192181	4.088529	0.364874
H	4.054663	-0.764555	-3.321841
H	2.306304	-0.636789	-3.025097
H	3.331779	0.802656	-2.945258
H	2.573543	-2.516483	-1.243430
H	4.307730	-2.553094	-1.629845
H	3.767628	-2.344035	0.042788
H	2.463770	1.832403	2.481707
H	1.037283	0.788644	2.353018
H	2.273471	0.464864	3.588719
H	4.725687	1.015136	1.452579
H	4.635094	-0.100622	2.818241
H	4.935695	-0.725431	1.194555
H	-3.768395	-2.342923	0.041653
H	-4.308609	-2.550882	-1.631088
H	-2.574405	-2.515017	-1.244693
H	-4.055269	-0.761201	-3.322059
H	-3.331217	0.805275	-2.944646
H	-2.306788	-0.634844	-3.025390
H	-1.037220	0.788772	2.353101
H	-2.463852	1.832243	2.482454
H	-2.273122	0.464335	3.588934
H	-4.935633	-0.725347	1.194718
H	-4.634950	-0.100676	2.818452
H	-4.725661	1.015191	1.452886
H	0.001326	5.789184	0.938251
C	-0.000350	-1.955585	0.279088
C	-0.000978	-3.149931	-0.468784
C	0.000093	-2.132764	1.677548
C	-0.001149	-4.412744	0.120450
H	-0.001306	-3.087349	-1.555493
C	-0.000061	-3.391109	2.281641
H	0.000539	-1.258863	2.323443
C	-0.000685	-4.545679	1.506187
H	-0.001637	-5.298548	-0.510987
H	0.000305	-3.463856	3.367323
H	-0.000807	-5.527963	1.970765

11$^{\mathbf{Ir\_Ph}}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1818.66342759

Thermal correction to Enthalpy in gas phase: 0.641564

Thermal correction to Gibbs Free Energy in gas phase: 0.541491

SCF energy in solvent: -1818.85787644

Ir	0.000000	0.022737	-0.000116
P	2.243311	-0.226265	-0.059446
P	-2.243317	-0.226137	0.059571
N	-0.000077	-2.116402	-0.000253
C	0.000060	2.062220	-0.000091
C	-0.314553	2.822444	-1.147904
C	0.314797	2.822401	1.147717
C	-0.311600	4.216662	-1.155548
H	-0.563008	2.304809	-2.073352

C	0.311974	4.216619	1.155378
H	0.563220	2.304735	2.073156
C	0.000216	4.928747	-0.000079
H	-0.557165	4.750573	-2.071655
H	0.557605	4.750496	2.071487
H	0.000272	6.015487	-0.000073
C	2.454317	-2.044636	0.283457
C	3.125169	0.021763	-1.673362
C	3.306856	0.617174	1.208094
C	-3.124837	0.021389	1.673758
C	-3.307085	0.617740	-1.207483
C	-2.454460	-2.044383	-0.283894
C	1.163710	-2.810742	0.104029
C	-1.163923	-2.810634	-0.104596
H	3.247590	-2.494503	-0.324757
H	2.766778	-2.149710	1.329708
H	4.139424	-0.390292	-1.580878
C	3.206547	1.517501	-1.996586
C	2.378746	-0.739025	-2.774421
H	3.124562	1.681257	1.007639
C	4.804740	0.324804	1.096759
C	2.781278	0.322341	2.618144
H	-4.139071	-0.390742	1.581403
C	-3.206305	1.517037	1.997390
C	-2.378103	-0.739617	2.774455
H	-3.124567	1.681751	-1.006849
C	-4.804983	0.325584	-1.095792
C	-2.781946	0.323119	-2.617741
H	-3.247822	-2.494369	0.324114
H	-2.766828	-2.149105	-1.330210
C	1.187127	-4.201213	0.091548
C	-1.187461	-4.201104	-0.092256
H	3.653465	1.665217	-2.986780
H	3.818302	2.064008	-1.270851
H	2.208300	1.969227	-1.996347
H	1.355609	-0.358632	-2.867525
H	2.314134	-1.813259	-2.564502
H	2.892146	-0.614338	-3.735224
H	5.351308	0.842821	1.893659
H	5.223168	0.655394	0.141103
H	5.009051	-0.748247	1.203282
H	3.046847	-0.691566	2.942287
H	1.691452	0.415968	2.662524
H	3.224508	1.019546	3.337901
H	-3.652996	1.664452	2.987731
H	-3.818308	2.063651	1.271944
H	-2.208116	1.968888	1.997008
H	-1.354972	-0.359168	2.867409
H	-2.313457	-1.813795	2.564257
H	-2.891285	-0.615207	3.735411
H	-5.351682	0.843831	-1.892452
H	-5.223094	0.656079	-0.139965
H	-5.009497	-0.747415	-1.202447
H	-3.047784	-0.690675	-2.942019
H	-1.692115	0.416564	-2.662400
H	-3.225249	1.020553	-3.337229
H	2.140100	-4.714291	0.170746
C	-0.000197	-4.912512	-0.000394
H	-2.140478	-4.714093	-0.171484
H	-0.000243	-5.997845	-0.000440

$TS_{2\text{-}12}^{Ir\text{-}Ph}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1819.80702749

Thermal correction to Enthalpy in gas phase: 0.653519

Thermal correction to Gibbs Free Energy in gas phase: 0.556316

SCF energy in solvent: -1820.00967112

Ir	-0.019968	0.101763	0.033725
P	-2.275674	-0.443932	0.026653
H	-0.347802	-0.173194	-1.831550
P	2.271308	-0.062227	0.128145
H	0.062146	0.291780	1.610692
N	0.159054	-2.032079	-0.039679
C	-2.002969	-1.892878	-1.026527
C	-3.067924	-0.911245	1.637735
C	-3.511608	0.641192	-0.827238
C	3.279294	-0.146762	-1.431222
C	3.267985	1.020824	1.258464
C	2.408911	-1.783716	0.832898
C	-0.888024	-2.697294	-0.612089
C	1.314122	-2.660965	0.272843
H	-2.849219	-2.430237	-1.453296
H	-1.033860	-0.848125	-1.775047
H	-4.035568	-1.371166	1.400646
C	-3.293946	0.341445	2.491505
C	-2.219006	-1.941291	2.388909
H	-3.509118	1.564180	-0.233506
C	-4.925544	0.048836	-0.835738
C	-3.056289	1.003690	-2.244164
H	4.259054	-0.557626	-1.154103
C	3.470285	1.254972	-2.021047
C	2.636214	-1.092847	-2.450195
H	3.275417	1.989730	0.743261
C	4.712038	0.543679	1.447120
C	2.566034	1.232104	2.603309
H	3.393127	-2.234662	0.669325
H	2.263561	-1.676323	1.915603
C	-0.759614	-4.087414	-0.846599
C	1.473876	-4.015373	0.058656
H	-3.743686	0.066305	3.452604
H	-3.959127	1.064077	2.007325
H	-2.339900	0.841862	2.691018
H	-1.222284	-1.541407	2.601817
H	-2.099716	-2.865605	1.816093
H	-2.701358	-2.192597	3.340903
H	-5.602247	0.715360	-1.382599
H	-5.333971	-0.078421	0.171509
H	-4.944782	-0.925343	-1.338462
H	-2.969515	0.111654	-2.874232
H	-2.094040	1.519461	-2.231274
H	-3.794676	1.671978	-2.701756
H	3.970068	1.186054	-2.993882
H	4.084429	1.894420	-1.378727
H	2.506377	1.753566	-2.168181
H	1.647576	-0.730739	-2.748040
H	2.516459	-2.107717	-2.057115
H	3.266562	-1.151353	-3.344937
H	5.254007	1.245467	2.090923
H	5.259768	0.475971	0.502066
H	4.745825	-0.438801	1.932928
H	2.413483	0.287959	3.139455
H	1.593202	1.707549	2.464904
H	3.182556	1.878080	3.238882
H	-1.588951	-4.624542	-1.293981

C	0.406703	-4.732038	-0.507719
H	2.405325	-4.505525	0.318650
H	0.507012	-5.799589	-0.682084
C	-0.191274	2.143174	-0.078082
C	-0.513250	2.964874	1.018949
C	0.006034	2.819725	-1.298715
C	-0.624206	4.350774	0.912168
H	-0.685850	2.506086	1.990343
C	-0.101707	4.203905	-1.419259
H	0.242841	2.239070	-2.189430
C	-0.417066	4.983826	-0.309983
H	-0.875585	4.938842	1.792321
H	0.060031	4.674000	-2.386892
H	-0.502354	6.063535	-0.397128

12$^{\mathbf{Ir\_Ph}}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1818.64623068

Thermal correction to Enthalpy in gas phase: 0.637986

Thermal correction to Gibbs Free Energy in gas phase: 0.538577

SCF energy in solvent: -1818.85012033

Ir	-0.010189	0.019218	0.109502
P	-2.286580	-0.445414	0.171597
P	2.282423	-0.122443	-0.004185
H	0.029267	0.118927	1.645998
N	0.134622	-2.125460	0.136366
C	-2.276431	-2.202471	0.160686
C	-3.310855	0.182694	1.581874
C	-3.155224	0.153629	-1.362534
C	2.972091	0.085752	-1.711833
C	3.387882	0.850442	1.115726
C	2.570199	-1.907058	0.392821
C	-1.048719	-2.853637	0.099589
C	1.337245	-2.757769	0.150621
H	-3.189389	-2.789625	0.152141
H	-4.282194	-0.324492	1.500601
C	-3.516975	1.698614	1.503117
C	-2.668071	-0.224242	2.910348
H	-3.060411	1.246666	-1.354337
C	-4.634575	-0.235386	-1.404976
C	-2.413559	-0.393437	-2.586417
H	3.981001	-0.347543	-1.720667
C	3.047729	1.567477	-2.094840
C	2.094970	-0.697658	-2.697208
H	3.195948	1.890980	0.823289
C	4.874886	0.532156	0.933111
C	2.958166	0.696239	2.578587
H	3.435013	-2.311187	-0.144200
H	2.809109	-1.958596	1.462667
C	-0.940778	-4.282637	-0.008540
C	1.462174	-4.122053	0.031299
H	-4.074793	2.046449	2.380676
H	-4.081044	1.996340	0.613286
H	-2.554778	2.221614	1.480076
H	-1.738809	0.333381	3.072832
H	-2.432832	-1.293159	2.929328
H	-3.346261	-0.000286	3.741992
H	-5.089786	0.099048	-2.344936
H	-5.203954	0.212641	-0.584193
H	-4.750935	-1.324216	-1.347864
H	-2.439161	-1.488280	-2.595908
H	-1.358738	-0.088992	-2.595993

H	-2.870758	-0.023588	-3.511434
H	3.368775	1.666583	-3.138015
H	3.763019	2.117650	-1.474828
H	2.070447	2.052352	-1.990686
H	1.092198	-0.255556	-2.759861
H	1.980075	-1.749314	-2.414128
H	2.531374	-0.660250	-3.701503
H	5.475982	1.146200	1.613164
H	5.221545	0.731900	-0.085561
H	5.086287	-0.518633	1.164990
H	3.131433	-0.321009	2.948185
H	1.898733	0.929453	2.712996
H	3.541614	1.377022	3.207986
H	-1.857185	-4.861238	-0.060655
C	0.278273	-4.890162	-0.056345
H	2.440141	-4.589444	0.043606
H	0.342822	-5.971187	-0.149138
C	-0.150777	2.054019	-0.031621
C	0.137034	2.951038	1.014885
C	-0.515909	2.649829	-1.255520
C	0.066264	4.333631	0.855863
H	0.415011	2.557885	1.990869
C	-0.580610	4.031506	-1.430407
H	-0.756638	2.017853	-2.111305
C	-0.291082	4.886577	-0.371303
H	0.292468	4.983932	1.697935
H	-0.864642	4.439434	-2.397808
H	-0.345449	5.963985	-0.498858

2$^{\text{Ir\_Ph\_tBu}}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1977.07438532

Thermal correction to Enthalpy in gas phase: 0.780013

Thermal correction to Gibbs Free Energy in gas phase: 0.678685

SCF energy in solvent: -1977.32486497

Ir	0.000003	-0.059584	-0.000035
P	-2.275601	0.255920	0.122027
H	0.016972	-0.071589	1.676966
P	2.275572	0.256135	-0.122078
H	-0.016949	-0.071498	-1.677037
N	-0.000100	2.105907	0.000107
C	0.000132	-2.117327	0.000005
C	-0.312481	-2.878740	-1.145056
C	0.312892	-2.878612	1.145110
C	-0.317309	-4.273025	-1.151709
H	-0.558262	-2.360216	-2.066553
C	0.317922	-4.272895	1.151867
H	0.558643	-2.359977	2.066558
C	0.000351	-4.986552	0.000106
H	-0.569208	-4.803034	-2.067986
H	0.569918	-4.802801	2.068176
H	0.000434	-6.073208	0.000145
C	-2.272972	1.962614	0.876487
C	-3.191789	0.503965	-1.522402
C	-3.333314	-0.744904	1.329933
C	3.191701	0.503863	1.522431
C	3.333344	-0.744347	-1.330218
C	2.272815	1.962971	-0.876222
C	-1.097041	2.777731	0.405240
C	1.096785	2.777898	-0.404899
H	-3.208636	2.512726	0.732133

H	-2.151336	1.793375	1.953744
C	-2.953483	-0.718693	-2.422465
C	-2.554169	1.719210	-2.221952
C	-4.595117	-0.011256	1.816080
C	-2.474172	-1.060280	2.566920
C	2.953313	-0.718966	2.422248
C	2.554061	1.718979	2.222186
C	4.595137	-0.010534	-1.816143
C	2.474235	-1.059387	-2.567311
H	3.208422	2.513144	-0.731738
H	2.151237	1.793906	-1.953514
C	-1.124070	4.168720	0.410400
C	1.123681	4.168891	-0.409843
H	-3.495862	-0.578886	-3.366561
H	-3.294141	-1.655136	-1.974036
H	-1.888649	-0.816105	-2.643808
H	-1.466891	1.613508	-2.283438
H	-2.796838	2.663189	-1.721537
H	-2.948353	1.781797	-3.243889
H	-5.115000	-0.653048	2.538336
H	-5.302149	0.217268	1.018464
H	-4.349098	0.921847	2.335040
H	-2.094212	-0.158282	3.056910
H	-1.617197	-1.681018	2.306051
H	-3.098073	-1.601577	3.290080
H	3.495526	-0.579295	3.366460
H	3.294097	-1.655313	1.973718
H	1.888446	-0.816486	2.643393
H	1.466775	1.613295	2.283558
H	2.796798	2.663056	1.721990
H	2.948166	1.781339	3.244168
H	5.115049	-0.652117	-2.538565
H	5.302150	0.217794	-1.018454
H	4.349102	0.922702	-2.334855
H	2.094265	-0.157252	-3.057039
H	1.617270	-1.680223	-2.306641
H	3.098162	-1.600458	-3.290618
H	-2.018803	4.685757	0.740289
C	-0.000229	4.872973	0.000329
H	2.018370	4.686064	-0.739637
H	-0.000280	5.958508	0.000416
C	3.710537	-2.081788	-0.671254
H	4.440456	-1.957612	0.134568
H	2.827452	-2.594009	-0.273863
H	4.165364	-2.734981	-1.426264
C	4.697589	0.766712	1.393606
H	5.095121	1.034627	2.380765
H	5.246687	-0.115613	1.053951
H	4.920332	1.599353	0.716703
C	-3.710493	-2.082163	0.670589
H	-4.440354	-1.957752	-0.135251
H	-2.827395	-2.594298	0.273119
H	-4.165385	-2.735548	1.425394
C	-4.697666	0.766809	-1.393444
H	-5.095270	1.034816	-2.380549
H	-5.246741	-0.115545	-1.053826
H	-4.920354	1.599390	-0.716450

$TS_{9\text{-}10}^{Ir\_Ph\_tBu}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1976.99429973

Thermal correction to Enthalpy in gas phase: 0.774901

Thermal correction to Gibbs Free Energy in gas phase: 0.666481

SCF energy in solvent: -1977.24658219

Ir	0.000028	-0.036850	-0.519416
P	2.288322	0.227438	-0.117591
P	-2.288276	0.227444	-0.117614
H	-0.000012	0.360696	-2.164533
N	0.000010	2.113574	-0.195742
H	-0.000018	-0.862267	-1.955467
H	2.148810	4.643950	0.345413
C	-0.000060	4.819866	0.457979
H	-2.148907	4.643937	0.345008
C	2.410311	2.051425	-0.472060
C	3.531267	-0.487231	-1.369615
C	3.052422	0.128384	1.638213
C	-2.410249	2.051367	-0.472394
C	-3.531258	-0.487442	-1.369483
C	-3.052371	0.128755	1.638201
C	1.164685	2.795160	-0.098457
C	-1.164690	2.795149	-0.098658
H	3.298520	2.532093	-0.053844
H	2.491579	2.117766	-1.565460
C	2.833434	-0.580805	-2.736694
C	3.915682	-1.914375	-0.947759
C	2.098287	0.953456	2.520872
C	4.467728	0.708285	1.783112
H	-2.491311	2.117521	-1.565823
H	-3.298540	2.532085	-0.054403
C	-3.915830	-1.914437	-0.947267
C	-2.833413	-0.581430	-2.736527
C	-2.098530	0.954405	2.520637
C	-4.467860	0.708261	1.782856
C	1.192780	4.140583	0.248921
C	-1.192856	4.140576	0.248694
H	3.569066	-0.904785	-3.484385
H	2.013907	-1.301322	-2.713856
H	2.414152	0.376237	-3.064426
H	3.037966	-2.502946	-0.657028
H	4.395236	-2.422360	-1.793943
H	4.631005	-1.917282	-0.121051
H	2.127327	2.021260	2.275726
H	1.066361	0.609840	2.406840
H	2.391922	0.849230	3.572621
H	4.570648	1.719045	1.374650
H	4.715524	0.765648	2.851164
H	5.220693	0.067340	1.316534
H	-4.631118	-1.917063	-0.120526
H	-4.395488	-2.422563	-1.793307
H	-3.038171	-2.503046	-0.656439
H	-3.569048	-0.905612	-3.484128
H	-2.414125	0.375515	-3.064528
H	-2.013900	-1.301957	-2.713485
H	-1.066406	0.611449	2.406347
H	-2.128335	2.022195	2.275530
H	-2.391827	0.849971	3.572458
H	-5.220618	0.066920	1.316483
H	-4.715701	0.765942	2.850882
H	-4.571065	1.718842	1.374018
H	-0.000091	5.865426	0.748817
C	-0.000001	-2.025722	0.141295
C	-0.000202	-3.127908	-0.737432
C	0.000143	-2.367532	1.507935

C	-0.000310	-4.451227	-0.296987
H	-0.000292	-2.945987	-1.810214
C	0.000041	-3.685508	1.965530
H	0.000382	-1.571898	2.248418
C	-0.000200	-4.743820	1.063330
H	-0.000479	-5.257318	-1.027312
H	0.000159	-3.879424	3.035968
H	-0.000286	-5.772826	1.411953
C	3.083272	-1.314117	2.171568
H	3.210132	-1.288299	3.261828
H	2.167776	-1.861158	1.952093
H	3.920499	-1.884761	1.764907
C	4.800697	0.361749	-1.554467
H	5.357929	0.515003	-0.629720
H	5.468746	-0.150289	-2.258799
H	4.576333	1.344593	-1.982715
C	-4.800595	0.361625	-1.554583
H	-5.468657	-0.150500	-2.258838
H	-5.357860	0.515137	-0.629898
H	-4.576101	1.344350	-1.983035
C	-3.082770	-1.313590	2.171984
H	-2.166894	-1.860222	1.953100
H	-3.210169	-1.287498	3.262174
H	-3.919490	-1.884801	1.765084

11$^{\text{Ir\_Ph\_tBu}}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1975.86673538

Thermal correction to Enthalpy in gas phase: 0.761425

Thermal correction to Gibbs Free Energy in gas phase: 0.657345

SCF energy in solvent: -1976.11210258

Ir	0.000013	-0.064917	-0.226526
P	-2.252979	0.264312	-0.043813
P	2.253062	0.263851	-0.043833
N	0.000222	2.041281	-0.668633
C	-0.000286	-2.099308	0.019982
C	-0.000541	-2.926406	-1.128340
C	-0.000330	-2.807041	1.240413
C	-0.000830	-4.318502	-1.070877
H	-0.000515	-2.464412	-2.114069
C	-0.000606	-4.199672	1.314773
H	-0.000180	-2.258004	2.177055
C	-0.000865	-4.973024	0.157635
H	-0.001033	-4.893823	-1.994526
H	-0.000622	-4.682868	2.289931
H	-0.001082	-6.058270	0.211780
C	-2.441332	1.935409	-0.842241
C	-3.504421	-0.787795	-0.993097
C	-2.843179	0.576039	1.732008
C	2.843348	0.575587	1.731956
C	3.504337	-0.788500	-0.993056
C	2.441725	1.934859	-0.842359
C	-1.166236	2.730662	-0.763911
C	1.166820	2.730409	-0.763978
H	-2.637493	1.741804	-1.904141
H	-3.290544	2.514285	-0.464138
C	-3.683041	-2.127077	-0.259773
C	-2.859451	-1.075071	-2.361546
C	-4.355826	0.761548	1.895536
C	-2.145586	1.857512	2.223237
C	2.357623	-0.581807	2.617200
C	2.145984	1.857191	2.223174

C	4.870636	-0.130191	-1.241920
C	2.859155	-1.076042	-2.361346
H	3.291103	2.513572	-0.464367
H	2.637761	1.741141	-1.904264
C	-1.191230	4.118679	-0.841493
C	1.192112	4.118420	-0.841580
H	-4.257094	-2.813214	-0.895380
H	-4.236089	-2.011655	0.677984
H	-2.718110	-2.597245	-0.042953
H	-1.916330	-1.610240	-2.247001
H	-2.664719	-0.161259	-2.934501
H	-3.542484	-1.696955	-2.954491
H	-4.567684	1.073517	2.926402
H	-4.908032	-0.165378	1.718338
H	-4.754074	1.536605	1.230921
H	-2.530397	2.759541	1.735277
H	-1.066032	1.804633	2.055112
H	-2.319396	1.967523	3.301004
H	2.721646	-0.435494	3.642710
H	2.699420	-1.560385	2.269901
H	1.265239	-0.602168	2.633447
H	1.066414	1.804461	2.055130
H	2.530914	2.759123	1.735143
H	2.319894	1.967213	3.300924
H	5.465471	-0.786349	-1.890254
H	5.444261	0.027353	-0.327804
H	4.777322	0.832397	-1.757356
H	2.663877	-0.162321	-2.934260
H	1.916294	-1.611616	-2.246538
H	3.542295	-1.697655	-2.954461
H	-2.147047	4.629530	-0.892289
C	0.000519	4.829117	-0.859498
H	2.148041	4.629056	-0.892440
H	0.000633	5.913371	-0.908442
C	-2.357519	-0.581485	2.617146
H	-2.699283	-1.560026	2.269698
H	-1.265132	-0.601855	2.633452
H	-2.721592	-0.435300	3.642655
C	-4.870746	-0.129418	-1.241646
H	-5.465591	-0.785323	-1.890227
H	-5.444340	0.027740	-0.327443
H	-4.777477	0.833387	-1.756691
C	4.356048	0.760894	1.895358
H	4.568038	1.072907	2.926187
H	4.908103	-0.166123	1.718181
H	4.754360	1.535845	1.230656
C	3.683067	-2.127666	-0.259537
H	4.236361	-2.012140	0.678059
H	2.718155	-2.597736	-0.042421
H	4.256905	-2.813935	-0.895198

$TS_{2\text{-}12}^{Ir\_Ph\_tBu}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1977.01048063

Thermal correction to Enthalpy in gas phase: 0.773626

Thermal correction to Gibbs Free Energy in gas phase: 0.671301

SCF energy in solvent: -1977.26406849

Ir	0.009734	0.096869	0.031787
P	-2.323192	-0.248394	-0.085001
H	-0.222565	-0.156245	-1.845055
P	2.283582	-0.302630	0.178629
H	0.065431	0.275619	1.602385

N	-0.012143	-2.044760	-0.014651
C	-2.080011	-1.711332	-1.135372
C	-3.224957	-0.806271	1.489859
C	-3.398287	0.929948	-1.101759
C	3.191590	-0.561976	-1.465823
C	3.338539	0.693012	1.388146
C	2.211602	-2.003040	0.946538
C	-1.088978	-2.616343	-0.633076
C	1.046839	-2.780943	0.385116
H	-2.940096	-2.173292	-1.619625
H	-0.959239	-0.765842	-1.807800
C	-3.804360	0.391118	2.255338
C	-2.201008	-1.500623	2.407860
C	-4.834559	0.414955	-1.279081
C	-2.761535	1.073373	-2.496254
C	2.941527	0.660181	-2.364507
C	2.573539	-1.786242	-2.167466
C	4.582924	-0.060964	1.887642
C	2.471977	1.023023	2.617303
H	3.144578	-2.566110	0.841611
H	2.046069	-1.831635	2.017346
C	-1.100936	-4.020611	-0.811635
C	1.064203	-4.153848	0.238957
H	-4.142662	0.056348	3.244198
H	-4.668021	0.830650	1.748531
H	-3.052187	1.173662	2.405578
H	-1.412212	-0.815128	2.724771
H	-1.728581	-2.359864	1.924248
H	-2.726153	-1.865737	3.300087
H	-5.357870	1.063545	-1.992876
H	-5.401978	0.441505	-0.344462
H	-4.864073	-0.605343	-1.677093
H	-2.710626	0.119401	-3.029272
H	-1.757066	1.497290	-2.432312
H	-3.379296	1.761346	-3.086702
H	3.505102	0.539190	-3.298327
H	3.245454	1.604172	-1.905740
H	1.880715	0.736282	-2.614425
H	1.487221	-1.701830	-2.259385
H	2.807368	-2.723320	-1.653036
H	2.991050	-1.851937	-3.179715
H	5.112035	0.575757	2.607453
H	5.288823	-0.309936	1.095256
H	4.313934	-0.985010	2.411083
H	2.049240	0.129946	3.089712
H	1.651494	1.691313	2.354659
H	3.103830	1.525578	3.360448
H	-1.955927	-4.482262	-1.293788
C	-0.039712	-4.774290	-0.367536
H	1.920542	-4.729462	0.572103
H	-0.050639	-5.853419	-0.492183
C	0.047398	2.148722	-0.036087
C	-0.206897	2.958019	1.090485
C	0.312293	2.852422	-1.226996
C	-0.189221	4.350355	1.038873
H	-0.449026	2.481070	2.038064
C	0.331664	4.244998	-1.293835
H	0.499010	2.293768	-2.140761
C	0.084092	5.008661	-0.157070
H	-0.397193	4.923850	1.939561
H	0.538874	4.734016	-2.243212
H	0.097823	6.094052	-0.203323

C	-3.425190	2.331932	-0.467862
H	-3.905779	2.349186	0.512001
H	-2.419445	2.743421	-0.364492
H	-3.999213	2.998091	-1.124711
C	-4.327243	-1.832965	1.181010
H	-4.789235	-2.154714	2.123149
H	-5.120593	-1.436166	0.545311
H	-3.909811	-2.719659	0.693079
C	4.699524	-0.812277	-1.332392
H	5.102168	-1.070084	-2.319920
H	5.241631	0.070403	-0.983243
H	4.922539	-1.649385	-0.661652
C	3.736635	2.024990	0.730786
H	4.196662	2.672152	1.487697
H	4.467749	1.892473	-0.072338
H	2.861080	2.548167	0.330655

12$^{\text{Ir\_Ph\_tBu}}$ (at ωB97XD/BS4)

SCF energy in gas phase: -1975.85108729

Thermal correction to Enthalpy in gas phase: 0.757898

Thermal correction to Gibbs Free Energy in gas phase: 0.653418

SCF energy in solvent: -1976.10520172

Ir	-0.043065	0.030210	0.136980
P	-2.346981	-0.384829	0.012788
P	2.270677	-0.254001	0.113288
H	-0.011360	0.134314	1.674464
N	0.018819	-2.117640	0.382851
C	-2.375138	-2.139480	0.159791
C	-3.558355	0.326128	1.260349
C	-2.821091	-0.014860	-1.782486
C	2.969205	-0.540376	-1.621785
C	3.392249	0.847228	1.151716
C	2.395940	-1.912780	0.921078
C	-1.175370	-2.819514	0.309172
C	1.179214	-2.768306	0.651757
H	-3.296732	-2.708609	0.099304
C	-3.629249	1.858642	1.207542
C	-3.004908	-0.091477	2.634589
C	-3.977557	-0.883741	-2.290608
C	-1.546846	-0.418203	-2.552447
C	2.592357	0.639155	-2.532144
C	2.290405	-1.803436	-2.187455
C	4.731198	0.191829	1.528257
C	2.627853	1.151799	2.453648
H	3.317338	-2.443281	0.660201
H	2.436245	-1.717459	1.999796
C	-1.109382	-4.253975	0.385030
C	1.267166	-4.137638	0.741960
H	-4.158069	2.220723	2.098869
H	-4.180099	2.218878	0.336088
H	-2.636025	2.314068	1.193295
H	-2.037161	0.382957	2.829054
H	-2.873661	-1.175854	2.703079
H	-3.704170	0.227704	3.417698
H	-4.123792	-0.705197	-3.364252
H	-4.920507	-0.649458	-1.788117
H	-3.765795	-1.947624	-2.147907
H	-1.296730	-1.471138	-2.384320
H	-0.684643	0.208072	-2.263669
H	-1.686107	-0.265343	-3.630468
H	3.066382	0.502980	-3.512229

H	2.901862	1.609305	-2.136753
H	1.511787	0.676223	-2.692274
H	1.198651	-1.743598	-2.138919
H	2.595756	-2.714658	-1.664820
H	2.574752	-1.910782	-3.241435
H	5.284386	0.877071	2.182457
H	5.365683	-0.017038	0.665932
H	4.588547	-0.741326	2.083526
H	2.335482	0.244634	2.994195
H	1.730479	1.738716	2.254296
H	3.279614	1.735102	3.115779
H	-2.033432	-4.813306	0.281782
C	0.079463	-4.888457	0.585427
H	2.216644	-4.615993	0.953284
H	0.114735	-5.973423	0.639964
C	-0.068869	2.083686	0.016839
C	-0.213937	2.895540	1.161498
C	0.103743	2.792753	-1.188529
C	-0.162224	4.286948	1.116711
H	-0.382082	2.424006	2.128141
C	0.153035	4.185107	-1.250830
H	0.201706	2.249297	-2.125851
C	0.028117	4.947143	-0.093725
H	-0.276633	4.857407	2.035545
H	0.290557	4.673850	-2.212690
H	0.070444	6.031734	-0.135281
C	-3.126865	1.464674	-2.039608
H	-4.124935	1.731285	-1.679408
H	-2.396594	2.128934	-1.568589
H	-3.112016	1.657294	-3.120602
C	-4.963000	-0.265649	1.080858
H	-5.607148	0.070955	1.903390
H	-5.426516	0.067605	0.146916
H	-4.950680	-1.360446	1.094283
C	4.487945	-0.752175	-1.658641
H	4.778826	-1.060611	-2.670626
H	5.038203	0.164161	-1.427732
H	4.814690	-1.539204	-0.970624
C	3.633562	2.176384	0.418786
H	4.132565	2.875122	1.101438
H	4.283593	2.053456	-0.453438
H	2.692821	2.636562	0.098167

$TS_{11\text{-}13}$

SCF energy in gas phase: -3508.83879528

Thermal correction to Enthalpy in gas phase: 0.836931

Thermal correction to Gibbs Free Energy in gas phase: 0.72217

SCF energy in solvent: -3509.08636608

Co	0.363801	0.141543	0.395876
P	0.019925	2.259072	0.182206
P	1.001004	-1.377276	-1.082900
B	-1.551921	-0.137412	0.156834
C	0.626675	-1.071750	1.965001
H	0.083815	0.429306	1.811330
N	2.353640	0.708190	0.274103
O	-2.506172	-0.184136	1.174060
O	-2.224818	-0.294920	-1.065719
C	-3.753959	-0.647421	0.657630
C	-3.640757	-0.285311	-0.857594
C	-4.882678	0.045420	1.401696
C	-3.824464	-2.153233	0.904714

C	-4.154758	1.115488	-1.176742
C	-4.291504	-1.280030	-1.805496
H	-5.851951	-0.218818	0.972725
H	-4.875287	-0.267544	2.446365
H	-4.770931	1.128111	1.373977
H	-3.696252	-2.340149	1.971388
H	-4.784242	-2.568395	0.592985
H	-3.029240	-2.677505	0.372101
H	-3.883470	1.369983	-2.201462
H	-5.240088	1.174234	-1.082320
H	-3.709415	1.858539	-0.515929
H	-5.368391	-1.330868	-1.629694
H	-4.129891	-0.959845	-2.835875
H	-3.876400	-2.279480	-1.693353
C	-0.272670	-2.080403	2.344162
C	1.824185	-1.042642	2.702388
C	0.026030	-3.026794	3.313724
H	-1.241358	-2.127405	1.868975
C	2.132726	-1.981584	3.675389
H	2.547977	-0.257734	2.515238
C	1.238790	-2.995267	3.984030
H	-0.703064	-3.794762	3.548458
H	3.078237	-1.912448	4.202113
H	1.474226	-3.731413	4.742503
C	0.017161	3.239620	-1.398716
C	1.580870	2.873062	0.979947
C	-1.306816	3.107200	1.170897
C	1.244194	-1.008726	-2.888989
C	0.365779	-3.109986	-0.919491
C	2.753180	-1.531800	-0.507067
C	3.269256	-0.160820	-0.188949
C	2.706316	1.971802	0.561586
H	0.154681	4.301676	-1.136899
C	-1.317168	3.073861	-2.129116
C	1.186173	2.820601	-2.292328
H	1.814723	3.926159	0.766654
H	1.427387	2.770380	2.065570
H	-2.236462	2.808655	0.657692
C	-1.398268	2.572870	2.603934
C	-1.225445	4.637561	1.169374
H	1.930450	-0.143975	-2.821741
C	-0.046683	-0.515959	-3.550453
C	1.932455	-2.072755	-3.747102
H	0.073834	-3.124382	0.142777
C	-0.902316	-3.328999	-1.751396
C	1.368367	-4.249354	-1.126751
H	2.698596	-2.101230	0.435027
H	3.424969	-2.066108	-1.191703
C	4.599922	0.214956	-0.362092
C	4.023956	2.405651	0.427867
H	-2.153859	3.518570	-1.569921
H	-1.279924	3.562867	-3.115287
H	-1.550699	2.009097	-2.280822
H	2.163142	3.027582	-1.830502
H	1.139797	1.745263	-2.511665
H	1.148917	3.365860	-3.248647
H	-0.478638	2.776526	3.176020
H	-2.225302	3.076842	3.128768
H	-1.587697	1.493360	2.622820
H	-1.314675	5.071590	0.163850
H	-2.042218	5.055440	1.778447
H	-0.279370	4.991672	1.610179

H	-0.588900	0.181698	-2.899399
H	0.180700	-0.014417	-4.504996
H	-0.729619	-1.350708	-3.765500
H	1.276878	-2.941110	-3.910868
H	2.174061	-1.656740	-4.738632
H	2.871800	-2.436607	-3.304964
H	-1.590660	-2.477001	-1.669950
H	-0.665644	-3.474239	-2.817161
H	-1.424552	-4.236413	-1.407727
H	1.747280	-4.294551	-2.157882
H	2.229308	-4.178369	-0.447438
H	0.872446	-5.210994	-0.917043
C	4.982741	1.512138	-0.038015
H	5.320083	-0.506646	-0.747762
H	4.283038	3.436264	0.670568
H	6.019609	1.829376	-0.161529

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SCF energy in gas phase: -3508.8418747

Thermal correction to Enthalpy in gas phase: 0.839219

Thermal correction to Gibbs Free Energy in gas phase: 0.724446

SCF energy in solvent: -3509.09058983

Co	-0.336796	0.113861	-0.471111
P	-0.028591	2.256183	-0.241550
P	-1.063295	-1.321154	1.104368
B	1.565621	-0.157761	-0.185102
C	-0.530221	-1.305154	-1.844045
H	0.024324	0.687614	-1.762132
N	-2.351023	0.680741	-0.442732
O	2.565085	-0.182382	-1.150674
O	2.170840	-0.320195	1.070925
C	3.799078	-0.611919	-0.573001
C	3.595830	-0.276778	0.940180
C	4.939520	0.130884	-1.248076
C	3.936495	-2.109818	-0.835441
C	4.057004	1.129599	1.311456
C	4.217134	-1.271904	1.907303
H	5.894073	-0.104249	-0.771905
H	4.997724	-0.168287	-2.295150
H	4.786969	1.208507	-1.213999
H	3.842168	-2.288105	-1.906855
H	4.903773	-2.488546	-0.501039
H	3.151076	-2.673870	-0.330131
H	3.723378	1.357679	2.324080
H	5.144064	1.216146	1.278338
H	3.630717	1.874836	0.640952
H	5.302837	-1.295367	1.790247
H	3.992172	-0.972113	2.931991
H	3.832314	-2.278492	1.758036
C	0.384322	-2.335800	-2.098225
C	-1.646744	-1.297566	-2.697126
C	0.190625	-3.301533	-3.077345
H	1.295160	-2.392500	-1.517808
C	-1.857278	-2.253757	-3.681649
H	-2.387310	-0.510307	-2.604028
C	-0.940433	-3.274944	-3.876840
H	0.935840	-4.077491	-3.216703
H	-2.742289	-2.192789	-4.306050
H	-1.097595	-4.023841	-4.643385
C	-0.123092	3.299851	1.298329
C	-1.539422	2.830078	-1.156069

C	1.357538	3.090306	-1.167259
C	-1.390691	-0.806728	2.858900
C	-0.434575	-3.062696	1.122770
C	-2.782675	-1.513239	0.449966
C	-3.284393	-0.166335	0.022153
C	-2.686067	1.934538	-0.784793
H	-0.242763	4.349356	0.984453
C	1.167442	3.167091	2.110709
C	-1.344998	2.925641	2.138005
H	-1.790785	3.886093	-0.982466
H	-1.314434	2.701776	-2.225702
H	2.256336	2.794036	-0.601139
C	1.538392	2.566941	-2.596389
C	1.277798	4.622099	-1.174874
H	-2.059251	0.057220	2.690601
C	-0.121726	-0.283009	3.539759
C	-2.137153	-1.787983	3.765542
H	-0.096261	-3.176009	0.082405
C	0.792227	-3.216692	2.027792
C	-1.460586	-4.171017	1.380301
H	-2.684512	-2.147217	-0.445282
H	-3.483706	-1.999593	1.140838
C	-4.622127	0.213610	0.116863
C	-4.008365	2.371894	-0.731746
H	2.032266	3.603982	1.589527
H	1.069184	3.681007	3.079867
H	1.402613	2.109975	2.306110
H	-2.290772	3.091072	1.600609
H	-1.306850	1.869444	2.433054
H	-1.375098	3.531987	3.057188
H	0.654041	2.772986	-3.220811
H	2.392630	3.083348	-3.062581
H	1.735496	1.489558	-2.617244
H	1.332768	5.064975	-0.171229
H	2.117398	5.032546	-1.756945
H	0.349975	4.975824	-1.653188
H	0.481494	0.321046	2.849835
H	-0.381642	0.327967	4.419190
H	0.515566	-1.110049	3.884485
H	-1.506408	-2.649800	4.029726
H	-2.415623	-1.288299	4.707479
H	-3.062235	-2.171604	3.310445
H	1.496997	-2.384513	1.896510
H	0.507687	-3.261719	3.090876
H	1.313517	-4.158101	1.791081
H	-1.889844	-4.124935	2.391252
H	-2.286091	-4.153818	0.655068
H	-0.965294	-5.150177	1.278808
C	-4.989218	1.494333	-0.281758
H	-5.358980	-0.490622	0.503092
H	-4.254319	3.393837	-1.020475
H	-6.030910	1.814171	-0.221909

$TS_{11\text{-}15}$

SCF energy in gas phase: -3508.81309779

Thermal correction to Enthalpy in gas phase: 0.837259

Thermal correction to Gibbs Free Energy in gas phase: 0.72242

SCF energy in solvent: -3509.06062831

Co	0.372669	-0.239361	-0.207849
P	-0.645513	-2.121939	-0.048869
P	1.215080	1.740219	0.281782

B	-1.411995	0.610170	-0.307569
N	0.935780	-0.695384	1.726480
H	0.477810	-0.408733	-1.676377
C	1.851367	-0.722314	-1.622458
O	-2.304757	0.482626	-1.381000
O	-2.014409	1.475110	0.628514
C	-3.344688	1.455492	-1.294694
C	-3.339801	1.831363	0.225607
C	-2.955242	2.617093	-2.207771
C	-4.641080	0.838160	-1.795036
C	-3.560972	3.307867	0.518869
C	-4.318472	1.006880	1.056807
H	-2.809858	2.232111	-3.217365
H	-3.727068	3.388195	-2.237064
H	-2.017786	3.073035	-1.890073
H	-5.475712	1.533238	-1.678440
H	-4.543242	0.598900	-2.854632
H	-4.877365	-0.081993	-1.263162
H	-4.538901	3.634211	0.158111
H	-3.523962	3.474053	1.596542
H	-2.797378	3.930672	0.055330
H	-4.108765	1.172153	2.114226
H	-5.352731	1.293138	0.858620
H	-4.210817	-0.057714	0.856961
C	2.540768	-1.945894	-1.573313
C	2.374427	0.199397	-2.547130
C	3.692509	-2.193523	-2.308017
H	2.200825	-2.735495	-0.919120
C	3.519773	-0.031585	-3.289546
H	1.848591	1.136899	-2.692041
C	4.200963	-1.233589	-3.167119
H	4.197069	-3.147452	-2.201645
H	3.875779	0.727255	-3.977282
H	5.098093	-1.424206	-3.742603
H	2.008809	-1.556335	5.344331
C	-2.304031	-2.274389	0.775920
C	0.456689	-2.999535	1.154777
C	-0.710399	-3.177081	-1.566376
C	0.429771	3.352443	-0.192203
C	3.055188	1.978108	0.091928
C	1.004473	1.688009	2.106970
C	1.212928	0.286439	2.603946
C	0.948954	-1.976148	2.145317
H	-2.959911	-1.682145	0.115862
H	-0.021102	-3.843846	1.672239
H	1.309675	-3.408711	0.596647
H	0.186161	-2.833060	-2.104884
H	-0.630452	3.069779	-0.153968
H	3.217432	1.929371	-0.994761
H	1.626173	2.407725	2.656866
H	-0.055241	1.945127	2.273528
C	1.606749	0.009907	3.911975
C	1.342429	-2.320295	3.435442
C	1.694187	-1.312925	4.328299
H	1.831592	0.831676	4.592234
H	1.359187	-3.368970	3.733372
C	-2.274298	-1.598864	2.153542
H	-3.295541	-1.536262	2.560434
H	-1.674885	-2.182073	2.870682
H	-1.866428	-0.580625	2.102630
C	-2.886370	-3.684813	0.897335
H	-3.832779	-3.647155	1.460210

H	-3.103711	-4.138121	-0.078120
H	-2.212733	-4.363499	1.445168
C	-0.577017	-4.692306	-1.393806
H	-1.429509	-5.140465	-0.865285
H	-0.517369	-5.168742	-2.385593
H	0.338765	-4.966652	-0.848821
C	-1.917450	-2.778537	-2.425274
H	-1.819407	-3.215643	-3.431036
H	-2.864848	-3.144524	-1.998857
H	-1.992373	-1.685577	-2.525325
C	0.762284	3.698331	-1.645960
H	0.179552	4.574889	-1.971106
H	1.827843	3.940996	-1.784915
H	0.510856	2.863874	-2.318449
C	0.577590	4.555285	0.744953
H	1.588075	4.983582	0.749572
H	-0.112100	5.351351	0.418556
H	0.309376	4.304730	1.781704
C	3.810388	0.794501	0.710490
H	3.775163	0.828135	1.811881
H	3.402423	-0.168908	0.378654
H	4.869702	0.835685	0.413601
C	3.640725	3.298413	0.598641
H	4.739867	3.262015	0.530291
H	3.307953	4.161030	0.006504
H	3.388435	3.491226	1.654088

$TS_{11\text{-}15\_iso}$

SCF energy in gas phase: -3508.81148977

Thermal correction to Enthalpy in gas phase: 0.837446

Thermal correction to Gibbs Free Energy in gas phase: 0.723291

SCF energy in solvent: -3509.05900165

Co	0.041672	-0.478400	0.480894
P	2.253546	-0.322757	0.533484
P	-1.964630	-1.019387	-0.140285
B	-0.157099	1.158083	-0.671794
C	-0.443496	0.190230	2.345403
N	0.527157	-2.029330	-0.875597
H	0.183180	-0.888373	1.992947
O	0.014058	2.471052	-0.227642
O	-0.474379	1.220639	-2.043058
C	-0.422742	3.407674	-1.213974
C	-0.386038	2.561694	-2.532180
C	0.507738	4.610473	-1.204452
C	-1.826227	3.862032	-0.820118
C	0.926976	2.684962	-3.300005
C	-1.545785	2.813331	-3.483673
H	0.230183	5.321619	-1.985875
H	0.432754	5.117157	-0.241479
H	1.545689	4.319501	-1.353247
H	-1.790544	4.259976	0.194298
H	-2.202754	4.638570	-1.488356
H	-2.528672	3.030449	-0.822197
H	0.946954	1.927489	-4.084633
H	1.033265	3.667225	-3.763600
H	1.781173	2.517521	-2.646622
H	-1.555509	3.852401	-3.820223
H	-1.442421	2.173640	-4.361535
H	-2.503969	2.593124	-3.015577
C	0.165755	1.404032	2.725469

C	-1.531828	-0.205889	3.144414
H	-1.817829	2.401260	5.293319
C	-1.435065	1.785750	4.489275
C	-0.325854	2.185727	3.752541
H	0.995661	1.782670	2.147352
C	-2.027094	0.574320	4.177192
H	-2.007893	-1.158249	2.955821
H	0.156068	3.131810	3.972080
H	-2.881024	0.223761	4.745858
H	1.475881	-4.738474	-3.475724
C	3.088261	0.567730	-0.875474
C	2.652803	-2.097872	0.226756
C	3.284368	0.039934	2.040937
C	-3.289260	0.244232	-0.405358
C	-2.795300	-2.474426	0.705037
C	-1.649681	-1.644610	-1.836053
C	-0.351096	-2.393863	-1.829189
C	1.747019	-2.595636	-0.856492
H	2.275874	0.575757	-1.620437
C	3.363848	2.025154	-0.487619
C	4.294036	-0.097721	-1.545506
H	3.707907	-2.302001	0.002870
H	2.390110	-2.616131	1.163228
H	3.113854	1.112405	2.229498
C	2.791070	-0.729059	3.273231
C	4.792699	-0.179504	1.872047
H	-2.806711	0.883265	-1.162970
C	-3.508634	1.092354	0.850219
C	-4.622202	-0.232839	-0.984096
H	-3.425135	-2.008007	1.483035
C	-1.759016	-3.374439	1.391847
C	-3.690084	-3.353170	-0.179040
H	-2.461380	-2.239839	-2.271958
H	-1.507208	-0.737480	-2.444915
C	-0.043896	-3.373278	-2.771621
C	2.125239	-3.568719	-1.778222
H	3.644014	2.609330	-1.379302
H	2.472241	2.492798	-0.043537
H	4.196790	2.111300	0.225931
H	4.640033	0.531125	-2.381992
H	5.146082	-0.235208	-0.864956
H	4.034160	-1.079820	-1.967665
H	3.376381	-0.418971	4.152959
H	1.734070	-0.541879	3.493012
H	2.935371	-1.814883	3.155224
H	5.235615	0.462636	1.100747
H	5.305146	0.046446	2.820546
H	5.026058	-1.226135	1.619879
H	-3.944085	0.499289	1.669222
H	-2.568773	1.527865	1.215901
H	-4.210108	1.912595	0.627091
H	-5.195261	-0.822749	-0.252235
H	-5.239872	0.640602	-1.248084
H	-4.498404	-0.835464	-1.896415
H	-1.132113	-3.883971	0.642560
H	-1.080040	-2.815172	2.048045
H	-2.267683	-4.150602	1.985460
H	-4.231881	-4.079918	0.447323
H	-4.435533	-2.791256	-0.753477
H	-3.082305	-3.935997	-0.889827
C	1.210656	-3.972166	-2.745619
H	-0.784320	-3.646058	-3.524033

H 3.122989 -4.005260 -1.725782

$TS_{13\text{-}14}$

SCF energy in gas phase: -3508.8335483

Thermal correction to Enthalpy in gas phase: 0.838847

Thermal correction to Gibbs Free Energy in gas phase: 0.725442

SCF energy in solvent: -3509.08223301

Co 0.404079 0.109147 0.324763
P 0.108826 2.241491 -0.075112
P 0.584476 -1.760664 -0.853516
B -1.580826 -0.108132 0.250920
C 1.127233 -0.628094 2.052878
H -0.744874 0.119585 1.296399
N 2.256595 0.437381 -0.336009
O -2.468274 0.943079 -0.033713
O -2.327443 -1.284204 0.400953
C -3.788617 0.425284 -0.198432
C -3.702134 -0.931747 0.569086
C -4.039168 0.248494 -1.693121
C -4.779009 1.422295 0.378015
C -4.581260 -2.037225 0.012090
C -3.949368 -0.781579 2.069107
H -5.066317 -0.059070 -1.895374
H -3.860350 1.200849 -2.194420
H -3.362328 -0.491403 -2.119436
H -4.775409 2.332351 -0.223914
H -5.791590 1.013062 0.367888
H -4.520042 1.690934 1.400700
H -4.431631 -2.949912 0.590174
H -5.635102 -1.758853 0.080689
H -4.347836 -2.254208 -1.028679
H -4.995524 -0.561859 2.287443
H -3.680271 -1.715503 2.562991
H -3.330135 0.010452 2.492818
C 2.364927 -0.246613 2.590788
C 0.421359 -1.573742 2.815384
C 2.870530 -0.772568 3.774275
H 2.977006 0.488430 2.075186
C 0.912564 -2.112605 3.997123
H -0.558134 -1.900612 2.477624
C 2.148858 -1.717416 4.486401
H 3.835101 -0.438568 4.142171
H 0.323329 -2.843078 4.541468
H 2.538321 -2.132279 5.408179
C -0.411655 2.855048 -1.751510
C 1.863223 2.782348 0.085036
C -0.791278 3.351114 1.119781
C 0.559196 -1.658661 -2.714561
C -0.098490 -3.415189 -0.345608
C 2.397792 -1.954691 -0.569797
C 3.022224 -0.604707 -0.721040
C 2.756031 1.687185 -0.413437
H -1.398008 2.374716 -1.862775
C 0.524327 2.274973 -2.815783
C -0.578981 4.361408 -1.953777
H 2.106308 3.747467 -0.381301
H 2.034839 2.881433 1.169728
H -1.772596 3.506270 0.642983
C -0.129462 4.715533 1.356930
C -1.024103 2.652751 2.463798
H 1.278043 -0.833068 -2.872454

C	1.080344	-2.863468	-3.502929
C	-0.791464	-1.172008	-3.244477
H	-0.379279	-3.225993	0.701812
C	-1.376723	-3.800222	-1.099048
C	0.901260	-4.576656	-0.362782
H	2.495774	-2.257840	0.484872
H	2.900207	-2.701074	-1.198410
C	4.304636	-0.419909	-1.230307
C	4.032426	1.934159	-0.911704
H	0.097246	2.409228	-3.821755
H	1.505274	2.778855	-2.804879
H	0.693291	1.201717	-2.655070
H	-0.911526	4.565585	-2.984632
H	-1.325909	4.798404	-1.276341
H	0.372530	4.900075	-1.810661
H	0.142291	5.238595	0.431235
H	-0.813867	5.368967	1.920938
H	0.783335	4.610121	1.964103
H	-1.691508	1.789056	2.357906
H	-0.082245	2.286603	2.900925
H	-1.483829	3.356872	3.175651
H	2.073275	-3.190963	-3.161325
H	0.400650	-3.724854	-3.432390
H	1.170654	-2.605668	-4.570675
H	-1.142138	-0.299925	-2.672737
H	-0.707063	-0.878342	-4.302987
H	-1.560390	-1.955952	-3.177099
H	-2.089390	-2.969062	-1.135337
H	-1.160397	-4.134307	-2.124805
H	-1.868493	-4.638514	-0.580594
H	0.396766	-5.496935	-0.026798
H	1.295033	-4.768983	-1.372747
H	1.751275	-4.409111	0.312485
C	4.817913	0.867324	-1.331932
H	4.886173	-1.287379	-1.541854
H	4.396482	2.960068	-0.966290
H	5.818246	1.037345	-1.732958

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SCF energy in gas phase: -3508.84304989

Thermal correction to Enthalpy in gas phase: 0.838798

Thermal correction to Gibbs Free Energy in gas phase: 0.719398

SCF energy in solvent: -3509.090535

Co	-0.366168	-0.000621	0.135815
P	-0.358377	-2.178189	-0.212392
P	-0.306515	2.191267	-0.101133
B	1.598176	-0.031405	0.181764
C	-1.868022	-0.015773	1.540934
H	0.624863	-0.032581	1.270337
N	-1.710228	0.055980	-1.370343
O	2.455517	1.088968	0.283228
O	2.432391	-1.171836	0.210999
C	3.805183	0.683265	0.090101
C	3.759180	-0.797127	0.567459
C	4.716426	1.592068	0.896166
C	4.123344	0.812294	-1.399324
C	3.891726	-0.933025	2.082903
C	4.739555	-1.727191	-0.125692
H	5.750649	1.243231	0.851386
H	4.682024	2.603372	0.487672
H	4.407053	1.638455	1.938849

H	3.930046	1.838989	-1.713150
H	5.167445	0.577971	-1.612968
H	3.486696	0.153284	-1.991586
H	3.652239	-1.958558	2.366068
H	4.904080	-0.709243	2.423241
H	3.194807	-0.267980	2.595507
H	5.768780	-1.402610	0.043237
H	4.633422	-2.737002	0.274054
H	4.556745	-1.765958	-1.198474
C	-1.562607	-0.041810	2.915870
C	-3.243752	-0.012108	1.265175
C	-2.527051	-0.063163	3.914851
H	-0.521968	-0.046522	3.226277
C	-4.227837	-0.033057	2.248917
H	-3.589760	0.007280	0.233640
C	-3.875515	-0.059317	3.587917
H	-2.223129	-0.083356	4.956230
H	-5.275143	-0.029089	1.964553
H	-4.634075	-0.076223	4.361102
C	0.832216	-3.028585	-1.354923
C	-1.938351	-2.334403	-1.125217
C	-0.596672	-3.224413	1.289032
C	0.881272	3.063597	-1.229447
C	-0.462134	3.179852	1.451052
C	-1.902595	2.426830	-0.966068
C	-2.189426	1.232949	-1.823239
C	-2.204023	-1.081239	-1.901202
H	1.795398	-2.932944	-0.839861
C	0.926108	-2.217614	-2.652521
C	0.574431	-4.508346	-1.644619
H	-2.017693	-3.231023	-1.752877
H	-2.725544	-2.389611	-0.354267
H	-1.258494	-2.567182	1.877173
C	-1.304348	-4.573668	1.136116
C	0.722326	-3.350553	2.055844
H	1.848381	2.929399	-0.729701
C	0.647427	4.558677	-1.452445
C	0.941371	2.306725	-2.560553
H	-1.049310	2.483704	2.072217
C	0.908580	3.348268	2.113813
C	-1.234765	4.500468	1.387256
H	-2.671305	2.426108	-0.174865
H	-1.990610	3.367427	-1.524240
C	-2.995543	1.311891	-2.955989
C	-3.009307	-1.073380	-3.037376
H	1.068917	-1.148234	-2.438067
H	1.774833	-2.569428	-3.259409
H	0.016431	-2.323437	-3.267665
H	0.751642	-5.137132	-0.762305
H	-0.449340	-4.706193	-2.001605
H	1.262374	-4.853791	-2.433117
H	-0.663556	-5.337914	0.676154
H	-1.591247	-4.945257	2.132762
H	-2.226656	-4.502217	0.540658
H	1.168389	-2.364177	2.243744
H	0.549224	-3.845211	3.023920
H	1.460677	-3.949334	1.497602
H	0.824785	5.144895	-0.541036
H	1.346057	4.930421	-2.219348
H	-0.370632	4.784905	-1.808790
H	0.023850	2.453382	-3.154815
H	1.786227	2.668416	-3.167146

H	1.070047	1.227497	-2.392857
H	1.437080	2.388409	2.197451
H	1.555485	4.031716	1.539834
H	0.787124	3.771723	3.122677
H	-0.697475	5.281582	0.832199
H	-2.228744	4.382986	0.931407
H	-1.392990	4.875801	2.410939
C	-3.376955	0.142038	-3.601446
H	-3.327932	2.288034	-3.308904
H	-3.353042	-2.019262	-3.455811
H	-3.991210	0.176304	-4.502467

$TS_{14\text{-}15}$

SCF energy in gas phase: -3508.8340116

Thermal correction to Enthalpy in gas phase: 0.838529

Thermal correction to Gibbs Free Energy in gas phase: 0.725189

SCF energy in solvent: -3509.08155186

Co	0.245598	-0.053476	-0.147478
P	-0.515021	-2.094877	0.204048
P	1.173265	1.972656	0.085466
B	-1.604563	0.622546	-0.202048
C	1.672483	-0.841436	-1.416258
H	-0.630523	0.305647	-1.311153
N	1.276784	-0.455794	1.557863
O	-2.083857	1.944028	-0.275602
O	-2.740155	-0.218513	-0.267378
C	-3.502053	1.959622	-0.139915
C	-3.887201	0.536838	-0.641161
C	-4.063997	3.107756	-0.960201
C	-3.834146	2.169500	1.337466
C	-4.025239	0.463769	-2.160782
C	-5.114026	-0.069266	0.018615
H	-5.156320	3.092706	-0.952463
H	-3.734706	4.056864	-0.534143
H	-3.720576	3.062775	-1.992146
H	-3.383328	3.103452	1.674595
H	-4.910777	2.233199	1.503360
H	-3.434320	1.356629	1.945512
H	-4.106368	-0.581823	-2.458421
H	-4.913788	0.991315	-2.511680
H	-3.148497	0.888381	-2.652015
H	-5.998086	0.547011	-0.160098
H	-5.302597	-1.059558	-0.399393
H	-4.973117	-0.176298	1.093105
C	1.396804	-0.963803	-2.790201
C	2.963926	-1.254038	-1.058363
C	2.317554	-1.432265	-3.718353
H	0.418062	-0.672330	-3.158941
C	3.905184	-1.724774	-1.967405
H	3.275751	-1.203359	-0.015781
C	3.587790	-1.815527	-3.312979
H	2.042331	-1.495053	-4.765918
H	4.890175	-2.021067	-1.621527
H	4.313376	-2.179007	-4.030517
C	-1.865247	-2.419918	1.447168
C	0.964505	-2.800403	1.023717
C	-0.769740	-3.181247	-1.262099
C	0.349992	3.615057	-0.260603
C	2.941888	2.025005	-0.477428
C	1.362006	1.925459	1.914888
C	1.788938	0.544957	2.303455

C	1.561629	-1.731881	1.892049
H	-2.784291	-2.223421	0.878055
C	-1.795608	-1.399125	2.590818
C	-1.931369	-3.831814	2.038742
H	0.781974	-3.717318	1.597683
H	1.676731	-3.035857	0.218201
H	0.168961	-2.986567	-1.805856
C	-0.875261	-4.691636	-1.038301
C	-1.915035	-2.666308	-2.136364
H	-0.362701	3.357311	-1.056367
C	1.242097	4.755756	-0.757706
C	-0.467787	4.118477	0.934813
H	3.241856	1.006664	-0.184615
C	3.074666	2.077072	-2.004696
C	3.915381	2.987296	0.208191
H	2.021415	2.692863	2.340640
H	0.350468	2.080615	2.318269
C	2.629959	0.301139	3.385536
C	2.380895	-2.040031	2.975971
H	-1.686112	-0.374238	2.213426
H	-2.709637	-1.458637	3.202608
H	-0.940531	-1.606200	3.256162
H	-2.025576	-4.619703	1.283596
H	-1.048254	-4.057836	2.657771
H	-2.807479	-3.905050	2.702985
H	-1.875992	-4.983570	-0.686851
H	-0.705824	-5.212618	-1.993894
H	-0.132728	-5.071436	-0.320621
H	-1.776903	-1.607443	-2.390789
H	-1.960954	-3.248867	-3.069673
H	-2.886844	-2.760979	-1.626340
H	1.842017	4.486692	-1.634769
H	0.602466	5.605584	-1.045390
H	1.920254	5.115961	0.030415
H	0.188686	4.494524	1.736311
H	-1.104806	4.956721	0.610418
H	-1.128475	3.343772	1.338129
H	2.290712	1.491979	-2.502760
H	3.042715	3.108748	-2.384439
H	4.039473	1.642290	-2.307672
H	3.735658	4.036651	-0.060671
H	3.892611	2.905700	1.304961
H	4.941939	2.742534	-0.109690
C	2.931976	-1.011568	3.729123
H	3.028496	1.140569	3.955158
H	2.585658	-3.084811	3.209568
H	3.585165	-1.229197	4.575492

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SCF energy in gas phase: -3508.8506709

Thermal correction to Enthalpy in gas phase: 0.839525

Thermal correction to Gibbs Free Energy in gas phase: 0.724641

SCF energy in solvent: -3509.09887304

Co	0.410659	-0.048514	-0.282814
P	0.435265	-2.219586	-0.182673
P	0.326479	2.101734	-0.013118
B	-1.593241	0.001634	-0.328428
C	2.422250	-0.041228	-0.561248
H	0.233869	0.000896	-1.727300
N	0.513126	-0.133961	1.747365
O	-2.416111	0.183992	0.790899

O	-2.414861	-0.114402	-1.447156
C	-3.800323	0.079533	0.449897
C	-3.788241	0.117730	-1.126185
C	-4.538801	1.236395	1.108961
C	-4.320030	-1.232240	1.031971
C	-4.187806	1.465463	-1.724323
C	-4.637215	-0.957112	-1.792939
H	-5.597019	1.234305	0.840373
H	-4.462809	1.140978	2.193048
H	-4.112407	2.197532	0.824546
H	-4.134676	-1.236430	2.106766
H	-5.392018	-1.348838	0.864795
H	-3.810734	-2.091684	0.599290
H	-3.984005	1.443656	-2.795016
H	-5.250463	1.665817	-1.577900
H	-3.623056	2.291094	-1.298027
H	-5.693885	-0.821336	-1.553202
H	-4.521927	-0.882822	-2.874879
H	-4.339475	-1.958061	-1.492780
C	2.978006	0.061956	-1.846856
C	3.372961	-0.067438	0.471673
C	4.344317	0.101622	-2.088999
H	2.310422	0.122937	-2.699062
C	4.745759	-0.032835	0.253955
H	3.043917	-0.097005	1.507307
C	5.245593	0.043172	-1.036091
H	4.707607	0.179299	-3.108229
H	5.426354	-0.062068	1.098371
H	6.313286	0.067116	-1.216972
C	-1.144779	-3.163081	0.081683
C	1.282099	-2.407230	1.441316
C	1.359510	-3.323759	-1.354451
C	-0.978090	3.099974	-0.859450
C	1.914083	3.064666	-0.049723
C	-0.228917	2.175250	1.746186
C	0.223181	0.949101	2.488149
C	0.872370	-1.282995	2.349415
H	-1.733166	-2.468834	0.702628
C	-1.018262	-4.485853	0.843114
C	-1.886766	-3.377381	-1.241668
H	1.162667	-3.385277	1.922362
H	2.352146	-2.273054	1.224888
H	0.886167	-4.314769	-1.252179
C	1.152579	-2.845341	-2.797030
C	2.850716	-3.491024	-1.044126
H	-1.881926	2.610050	-0.462226
C	-0.986151	2.889624	-2.376369
C	-1.062228	4.581055	-0.485723
H	2.637182	2.301301	0.272760
C	2.287076	3.444209	-1.486865
C	2.055667	4.256555	0.901048
H	0.050290	3.091386	2.280916
H	-1.328329	2.128999	1.704190
C	0.289775	0.914061	3.880115
C	0.925577	-1.390454	3.737064
H	-0.701833	-4.344368	1.886080
H	-1.995769	-4.993469	0.869064
H	-0.307619	-5.177153	0.361231
H	-1.968912	-2.447942	-1.821410
H	-1.383160	-4.137548	-1.859270
H	-2.905352	-3.750008	-1.044350
H	1.688846	-1.903160	-2.965951

H	1.543246	-3.599045	-3.499189
H	0.095004	-2.669809	-3.035908
H	3.020237	-3.997130	-0.082098
H	3.314172	-4.113535	-1.825759
H	3.376475	-2.525177	-1.029955
H	-0.982667	1.819432	-2.623410
H	-1.894303	3.340836	-2.807530
H	-0.120246	3.364318	-2.858721
H	-0.223089	5.154594	-0.906144
H	-1.989176	5.014708	-0.894684
H	-1.073662	4.740731	0.603192
H	2.144817	2.601686	-2.177862
H	1.693322	4.298764	-1.847809
H	3.348452	3.731964	-1.532701
H	1.322954	5.052796	0.708385
H	1.969410	3.959673	1.956595
H	3.058102	4.696884	0.776488
C	0.634776	-0.273732	4.512679
H	0.054593	1.810847	4.453440
H	1.213212	-2.337060	4.194617
H	0.680971	-0.328497	5.601590

$TS_{15\text{-}16}$

SCF energy in gas phase: -3508.83433279

Thermal correction to Enthalpy in gas phase: 0.838177

Thermal correction to Gibbs Free Energy in gas phase: 0.724345

SCF energy in solvent: -3509.08116893

Co	-0.433253	0.089964	-0.056836
P	-0.265166	2.285854	0.244309
P	-0.897912	-2.008136	0.264320
B	1.414228	-0.280016	-1.068566
C	-2.175106	0.282787	-1.056611
H	0.232210	-0.135033	-1.541205
N	0.180554	-0.029030	1.830753
O	2.024551	-1.540627	-1.020907
O	2.376735	0.672567	-1.391059
C	3.443620	-1.362502	-1.012368
C	3.599556	0.014017	-1.731440
C	4.093518	-2.534465	-1.725921
C	3.898267	-1.327835	0.446331
C	3.635444	-0.111883	-3.252605
C	4.773037	0.850959	-1.254373
H	5.171387	-2.381986	-1.814910
H	3.926425	-3.450005	-1.156546
H	3.676535	-2.674252	-2.721336
H	3.617677	-2.264561	0.930151
H	4.980267	-1.216965	0.527705
H	3.420209	-0.512296	0.990854
H	3.541025	0.883274	-3.687837
H	4.570814	-0.554180	-3.599278
H	2.804231	-0.718743	-3.613554
H	5.716301	0.335359	-1.448049
H	4.787765	1.799650	-1.792576
H	4.704790	1.066054	-0.190203
C	-2.234674	0.264862	-2.459912
C	-3.422269	0.449050	-0.430701
C	-3.416291	0.404375	-3.176956
H	-1.315487	0.135494	-3.024916
C	-4.616655	0.587112	-1.128185
H	-3.475303	0.481519	0.652911
C	-4.623328	0.566388	-2.514223

H	-3.392530	0.385352	-4.261379
H	-5.546582	0.713008	-0.583562
H	-5.549198	0.673881	-3.066003
C	1.358997	3.178744	0.067803
C	-0.517245	2.279619	2.064077
C	-1.590256	3.396717	-0.403518
C	-0.720725	-3.201847	-1.136487
C	-2.466100	-2.447156	1.148253
C	0.424460	-2.418071	1.476900
C	0.584605	-1.211771	2.359246
C	0.130696	1.053391	2.642564
H	1.671651	2.946664	-0.961191
C	2.400854	2.566141	1.013077
C	1.345625	4.697037	0.260494
H	-0.194259	3.193484	2.582401
H	-1.607001	2.179362	2.208497
H	-2.458042	2.720558	-0.363746
C	-1.958967	4.652154	0.391773
C	-1.336803	3.688352	-1.886622
H	0.003923	-2.677657	-1.777267
C	-2.029618	-3.324275	-1.926867
C	-0.113635	-4.565085	-0.793988
H	-3.249474	-2.155407	0.429526
C	-2.647134	-3.923558	1.511722
C	-2.637407	-1.577771	2.400801
H	0.259418	-3.325062	2.074744
H	1.328707	-2.554624	0.868337
C	1.067187	-1.307584	3.660065
C	0.592582	1.013106	3.954934
H	2.394931	1.470128	0.981934
H	3.407419	2.906376	0.724971
H	2.231241	2.886952	2.053477
H	0.754234	5.218745	-0.502585
H	0.953731	4.981402	1.250746
H	2.376019	5.083198	0.197026
H	-1.197466	5.440399	0.331055
H	-2.895378	5.070985	-0.011175
H	-2.135446	4.434204	1.456017
H	-1.144006	2.759462	-2.442655
H	-2.223053	4.164536	-2.333408
H	-0.481605	4.365866	-2.036607
H	-2.457359	-2.338723	-2.161034
H	-1.839216	-3.845379	-2.878069
H	-2.789336	-3.905804	-1.382730
H	-0.736786	-5.145156	-0.097848
H	-0.005734	-5.161194	-1.714575
H	0.888526	-4.463539	-0.352733
H	-2.698145	-4.575395	0.630262
H	-1.830435	-4.287891	2.156092
H	-3.585883	-4.056698	2.072962
H	-1.946088	-1.887634	3.201375
H	-2.449620	-0.516743	2.189407
H	-3.661813	-1.679311	2.791066
C	1.095089	-0.176043	4.468690
H	1.404570	-2.275252	4.032238
H	0.543146	1.915178	4.565264
H	1.472857	-0.228425	5.490682

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SCF energy in gas phase: -3096.92966761

Thermal correction to Enthalpy in gas phase: 0.635286

Thermal correction to Gibbs Free Energy in gas phase: 0.5374

SCF energy in solvent: -3097.17604288

Co	-0.035284	0.016684	-0.012627
P	-2.093627	0.598410	-0.193618
P	2.103507	-0.249115	0.079577
C	-0.482776	-1.860165	0.092069
N	0.372264	1.961414	-0.053013
C	-0.384023	-2.745968	-0.994361
C	-1.000046	-2.432879	1.267618
C	-0.775064	-4.077243	-0.927092
H	-0.002900	-2.377642	-1.943337
C	-1.392850	-3.761999	1.355132
H	-1.119672	-1.810352	2.151834
C	-1.286758	-4.598295	0.252699
H	-0.683214	-4.711927	-1.802422
H	-1.791445	-4.147039	2.287994
H	-1.596214	-5.634592	0.312054
C	-3.304353	-0.129981	-1.386797
C	-1.930815	2.338931	-0.784465
C	-3.046972	0.751219	1.387108
C	2.936439	-0.361733	-1.585716
C	2.957485	-1.457955	1.183849
C	2.599412	1.392515	0.753736
C	1.606248	2.417481	0.281185
C	-0.571697	2.867324	-0.408096
H	-4.125104	0.599548	-1.506044
C	-3.886714	-1.452120	-0.871132
C	-2.633327	-0.340726	-2.748069
H	-2.002290	2.311476	-1.883075
H	-2.721842	3.018326	-0.433601
H	-3.158223	-0.296380	1.714900
C	-2.181703	1.472476	2.426330
C	-4.435185	1.383591	1.276759
H	2.160583	0.055976	-2.248553
C	3.134108	-1.827136	-1.991767
C	4.208172	0.465362	-1.790228
H	2.727194	-2.430657	0.717405
C	4.475391	-1.305984	1.307647
C	2.288995	-1.449702	2.563083
H	2.497934	1.299493	1.847219
H	3.630987	1.710165	0.550041
C	1.934910	3.769400	0.231488
C	-0.304562	4.234203	-0.449073
H	-4.444319	-1.328552	0.068596
H	-4.584527	-1.864004	-1.617177
H	-3.094481	-2.196005	-0.699239
H	-2.205920	0.586242	-3.160213
H	-1.821363	-1.077168	-2.662697
H	-3.367860	-0.719035	-3.476598
H	-2.004472	2.523822	2.142557
H	-2.680174	1.475444	3.408420
H	-1.199615	0.986046	2.528561
H	-5.094228	0.835468	0.588196
H	-4.926337	1.398119	2.262869
H	-4.378675	2.428304	0.929504
H	2.231282	-2.427316	-1.806793
H	3.372456	-1.893691	-3.064813
H	3.966809	-2.292263	-1.441381
H	5.011404	0.182801	-1.093041
H	4.590372	0.313448	-2.812700
H	4.020153	1.543205	-1.672278

H	4.992736	-1.436768	0.347437
H	4.749224	-0.315829	1.707571
H	4.876200	-2.060546	2.003417
H	2.497022	-0.514441	3.109114
H	1.200795	-1.567988	2.478460
H	2.680183	-2.276880	3.175765
C	0.967495	4.696434	-0.137148
H	2.943734	4.083982	0.499993
H	-1.098258	4.923370	-0.739111
H	1.199837	5.761777	-0.174760

$TS_{16\text{-}17}$

SCF energy in gas phase: -3508.83608406

Thermal correction to Enthalpy in gas phase: 0.838327

Thermal correction to Gibbs Free Energy in gas phase: 0.721767

SCF energy in solvent: -3509.0838852

Co	-0.444671	0.092126	0.075728
P	-1.427724	-1.865836	0.294567
P	-0.164582	2.252758	0.012379
B	1.363321	-0.453287	-1.125706
H	0.189102	-0.295808	-1.484247
N	-2.078677	0.559498	-1.066916
C	0.433475	-0.027324	1.829831
C	-0.245028	0.491582	2.950665
C	1.685570	-0.581987	2.136587
C	0.282491	0.496678	4.235475
H	-1.239127	0.907731	2.822274
C	2.235877	-0.580971	3.412623
H	2.245414	-1.067707	1.349415
C	1.542585	-0.029614	4.478127
H	-0.295561	0.917045	5.051948
H	3.213993	-1.023017	3.574319
H	1.966180	-0.022106	5.474980
O	2.308315	0.420397	-1.644475
O	1.936442	-1.684641	-0.860267
C	3.609596	-0.167617	-1.521448
C	3.272716	-1.695490	-1.379363
C	4.282243	0.436746	-0.291140
C	4.419567	0.184852	-2.758706
C	4.174191	-2.454091	-0.421166
C	3.209989	-2.424897	-2.719190
H	5.286727	0.035588	-0.149153
H	4.366234	1.515539	-0.431983
H	3.700272	0.264304	0.613132
H	4.590870	1.261610	-2.785964
H	5.391520	-0.312702	-2.736209
H	3.902256	-0.098868	-3.673075
H	3.851110	-3.494090	-0.362828
H	5.208175	-2.436863	-0.772533
H	4.141091	-2.032468	0.581666
H	4.195993	-2.523000	-3.175631
H	2.805058	-3.423668	-2.552580
H	2.550126	-1.905806	-3.415553
C	-1.093995	-3.212941	-0.946456
C	-3.165437	-1.370002	-0.088923
C	-1.535713	-2.672290	1.954380
C	1.507868	3.034612	0.008858
C	-1.213236	3.280727	1.149310
C	-0.854726	2.557948	-1.673922
C	-2.066635	1.677838	-1.824401
C	-3.166742	-0.235649	-1.075338

H	-0.019184	-3.415299	-0.806807
C	-1.284886	-2.684746	-2.374129
C	-1.877860	-4.517573	-0.779950
H	-3.822344	-2.190099	-0.412916
H	-3.574538	-0.977580	0.857767
H	-1.484249	-1.792664	2.616840
C	-0.268968	-3.494384	2.220872
C	-2.810946	-3.444377	2.303978
H	2.099566	2.234307	-0.455996
C	2.025451	3.214596	1.440768
C	1.705268	4.286983	-0.850097
H	-0.751191	3.087914	2.132085
C	-2.652777	2.754949	1.210040
C	-1.209050	4.791431	0.902531
H	-0.067374	2.215197	-2.366574
H	-1.090822	3.603040	-1.919071
C	-3.125799	1.997185	-2.668653
C	-4.254946	0.027749	-1.905200
H	-0.896894	-3.417951	-3.098252
H	-2.352448	-2.532713	-2.604372
H	-0.761206	-1.735163	-2.543313
H	-1.641651	-5.039093	0.156033
H	-2.966725	-4.346690	-0.808164
H	-1.637466	-5.204381	-1.607679
H	-0.260825	-4.434233	1.647325
H	0.635933	-2.925467	1.966775
H	-0.209790	-3.754872	3.288732
H	-2.769729	-3.754236	3.360797
H	-3.717499	-2.832806	2.183309
H	-2.937406	-4.354207	1.701417
H	3.099815	3.456832	1.418708
H	1.515454	4.038803	1.964751
H	1.898319	2.298827	2.037496
H	1.140203	5.155991	-0.484857
H	2.771773	4.566047	-0.845730
H	1.421723	4.115024	-1.899038
H	-3.192981	3.237297	2.039520
H	-3.204131	2.979230	0.282494
H	-2.679370	1.666551	1.360369
H	-1.911724	5.285285	1.592843
H	-0.220877	5.239752	1.067642
H	-1.530283	5.041662	-0.121730
C	-4.230107	1.152148	-2.721851
H	-3.078447	2.902590	-3.274032
H	-5.116070	-0.640719	-1.892906
H	-5.070421	1.378364	-3.380109

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SCF energy in gas phase: -3508.86065378

Thermal correction to Enthalpy in gas phase: 0.83876

Thermal correction to Gibbs Free Energy in gas phase: 0.722965

SCF energy in solvent: -3509.1080468

Co	-0.363447	-0.085269	-0.240656
P	-0.396367	-2.253416	-0.266670
P	-0.685236	2.066490	-0.433271
B	1.552353	0.084228	-0.196757
H	0.073314	-0.037894	-1.681826
N	-2.363147	-0.237874	-0.776861
C	-0.715558	-0.131018	1.751339
C	-2.002085	-0.238914	2.307231
C	0.306349	-0.013630	2.707410

C	-2.251895	-0.248686	3.674910
H	-2.870104	-0.292518	1.657103
C	0.081116	-0.020984	4.077289
H	1.328611	0.114378	2.375262
C	-1.206075	-0.145806	4.577337
H	-3.272299	-0.332254	4.034111
H	0.919902	0.076813	4.758453
H	-1.390099	-0.153386	5.644765
O	2.249374	1.224974	0.219538
O	2.492978	-0.865187	-0.596760
C	3.652455	0.960517	0.273513
C	3.793866	-0.283654	-0.663967
C	4.009952	0.659834	1.726623
C	4.399159	2.200555	-0.189367
C	4.817081	-1.313106	-0.212686
C	4.055340	0.087259	-2.122196
H	5.085504	0.530095	1.857434
H	3.681840	1.493123	2.349205
H	3.508198	-0.241402	2.079914
H	4.232339	3.011997	0.520748
H	5.473607	2.012049	-0.243584
H	4.053064	2.529611	-1.168105
H	4.829870	-2.144623	-0.918988
H	5.818628	-0.878361	-0.180838
H	4.576786	-1.710899	0.771397
H	5.059715	0.490302	-2.263004
H	3.954720	-0.809218	-2.735145
H	3.332379	0.820909	-2.477553
C	-0.076843	-3.211951	-1.822597
C	-2.213570	-2.549496	-0.068244
C	0.244078	-3.294675	1.127090
C	0.467463	3.184299	-1.358772
C	-1.161409	2.981501	1.106524
C	-2.190897	2.065325	-1.498551
C	-3.017282	0.835278	-1.251767
C	-3.009722	-1.405574	-0.629325
H	-0.465401	-4.226144	-1.626679
C	1.405210	-3.319057	-2.184472
C	-0.870080	-2.616540	-2.990663
H	-2.547771	-3.504600	-0.498199
H	-2.399778	-2.591232	1.016496
H	-0.342894	-2.899361	1.973456
C	1.716165	-3.062936	1.473061
C	-0.057030	-4.788983	0.978475
H	1.342784	3.225748	-0.693940
C	-0.051765	4.606214	-1.593756
C	0.929539	2.567555	-2.681943
H	-1.567438	2.165626	1.721882
C	-2.251457	4.051484	1.011065
C	0.100781	3.475385	1.823575
H	-1.809429	1.995839	-2.530495
H	-2.796820	2.978449	-1.436349
C	-4.376190	0.782914	-1.556425
C	-4.362669	-1.532187	-0.942741
H	1.519414	-3.919993	-3.100927
H	1.836861	-2.323394	-2.353155
H	1.993919	-3.799693	-1.390542
H	-1.956953	-2.633908	-2.817864
H	-0.572955	-1.571144	-3.164160
H	-0.672439	-3.193709	-3.907604
H	2.389905	-3.364684	0.659136
H	1.908953	-2.006360	1.689213

H	1.973653	-3.650314	2.368550
H	0.180718	-5.312422	1.917768
H	-1.114278	-4.991096	0.748647
H	0.556451	-5.246567	0.186398
H	0.679905	5.172896	-2.191557
H	-1.001268	4.611701	-2.153491
H	-0.205028	5.158358	-0.657931
H	0.124080	2.566766	-3.434952
H	1.758924	3.162265	-3.096921
H	1.263840	1.530922	-2.557101
H	-2.435081	4.469839	2.013690
H	-1.988921	4.889163	0.349409
H	-3.206649	3.630222	0.662409
H	-0.144265	3.756159	2.859088
H	0.868906	2.688841	1.855948
H	0.535628	4.359611	1.330073
C	-5.057557	-0.418831	-1.399224
H	-4.882420	1.674131	-1.927669
H	-4.859853	-2.493435	-0.811688
H	-6.120529	-0.487913	-1.636380

$TS_{17\text{-}18}$

SCF energy in gas phase: -3508.85716935

Thermal correction to Enthalpy in gas phase: 0.837107

Thermal correction to Gibbs Free Energy in gas phase: 0.72107

SCF energy in solvent: -3509.10465325

Co	-0.390614	-0.097143	-0.134492
P	-0.221870	-2.272199	-0.114690
P	-0.868112	2.039309	-0.346512
B	1.496949	0.179766	-0.211515
H	0.104440	-0.066736	-1.552973
N	-2.365986	-0.418035	-0.741141
C	-0.769435	-0.090421	1.833960
C	-2.055244	-0.283320	2.364327
C	0.220541	0.159995	2.798278
C	-2.335700	-0.241099	3.725772
H	-2.891548	-0.456881	1.692739
C	-0.037238	0.207090	4.161088
H	1.238648	0.346851	2.474652
C	-1.323466	0.002734	4.639718
H	-3.352398	-0.395591	4.071765
H	0.772367	0.408597	4.854550
H	-1.532047	0.037931	5.702067
O	2.151556	1.404152	-0.016769
O	2.476780	-0.774697	-0.509517
C	3.565502	1.204777	0.008952
C	3.713286	-0.121908	-0.794378
C	3.985393	1.063670	1.469813
C	4.244788	2.413617	-0.610534
C	4.859570	-1.016311	-0.356759
C	3.773752	0.107155	-2.303972
H	5.069074	0.986735	1.572569
H	3.647027	1.942482	2.020113
H	3.529580	0.183313	1.924872
H	4.078766	3.288751	0.019617
H	5.322168	2.254002	-0.693853
H	3.846600	2.628469	-1.601027
H	4.877106	-1.917008	-0.972392
H	5.817834	-0.505348	-0.474795
H	4.749757	-1.320328	0.682694
H	4.718449	0.561347	-2.607535

H	3.675452	-0.853051	-2.811829
H	2.953683	0.747433	-2.632959
C	0.305989	-3.286462	-1.585205
C	-2.019116	-2.713936	-0.086320
C	0.368136	-3.187943	1.381183
C	0.032104	3.069429	-1.602366
C	-1.005286	3.069466	1.195079
C	-2.600249	1.989370	-1.002874
C	-3.094210	0.587895	-1.241447
C	-2.837237	-1.676077	-0.796221
H	-0.195374	-4.258053	-1.430823
C	1.806535	-3.554065	-1.716523
C	-0.240832	-2.670222	-2.876537
H	-2.229068	-3.719866	-0.474643
H	-2.312842	-2.695654	0.976117
H	-0.289071	-2.765684	2.160193
C	1.803250	-2.843798	1.787895
C	0.145407	-4.702170	1.326075
H	1.061434	3.070524	-1.213605
C	-0.445267	4.517866	-1.740970
C	0.054229	2.386513	-2.973638
H	-1.365785	2.313958	1.910730
C	-1.995951	4.237965	1.238812
C	0.385462	3.503214	1.670386
H	-2.694755	2.589888	-1.919022
H	-3.276637	2.450202	-0.268749
C	-4.299817	0.354112	-1.905337
C	-4.035544	-1.978921	-1.438197
H	1.989013	-4.170362	-2.611655
H	2.363903	-2.614238	-1.808568
H	2.210610	-4.099041	-0.852084
H	-1.329589	-2.512693	-2.844747
H	0.227098	-1.692736	-3.064430
H	-0.023538	-3.333704	-3.728616
H	2.541513	-3.188193	1.050608
H	1.929536	-1.761237	1.902662
H	2.031720	-3.321835	2.753466
H	0.375936	-5.148263	2.306254
H	-0.894119	-4.968563	1.082030
H	0.801268	-5.185696	0.585744
H	0.093275	5.007035	-2.568197
H	-1.521485	4.585126	-1.971306
H	-0.255135	5.107747	-0.835530
H	-0.951997	2.340058	-3.424020
H	0.692148	2.961987	-3.662918
H	0.437990	1.360645	-2.911729
H	-2.023486	4.636174	2.265752
H	-1.718171	5.067494	0.575213
H	-3.025295	3.940008	0.992092
H	0.316516	3.909836	2.691024
H	1.086450	2.659849	1.675707
H	0.810252	4.288594	1.023927
C	-4.768267	-0.948182	-2.017865
H	-4.859502	1.192790	-2.320357
H	-4.383283	-3.011209	-1.478486
H	-5.704229	-1.158064	-2.538318

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SCF energy in gas phase: -3508.85919426

Thermal correction to Enthalpy in gas phase: 0.837822

Thermal correction to Gibbs Free Energy in gas phase: 0.720104

SCF energy in solvent: -3509.10630407

Co	-0.331482	-0.161376	-0.072234
P	0.297336	-2.273790	-0.136157
P	-1.301295	1.808821	-0.207422
B	1.424528	0.534434	-0.251841
H	0.377294	0.121530	-1.403064
N	-2.191465	-0.882417	-0.804561
C	-0.807502	-0.313613	1.851939
C	-2.040764	-0.800906	2.310812
C	0.069432	0.101176	2.868246
C	-2.377846	-0.875069	3.658383
H	-2.783460	-1.135265	1.591275
C	-0.247630	0.036213	4.217393
H	1.040286	0.501057	2.595265
C	-1.479644	-0.455827	4.626083
H	-3.348603	-1.261093	3.951362
H	0.471624	0.373714	4.956015
H	-1.733392	-0.509135	5.677772
O	1.786989	1.897205	-0.270293
O	2.615637	-0.211960	-0.321585
C	3.200856	2.020772	-0.138542
C	3.691945	0.649022	-0.689230
C	3.522496	2.207829	1.342909
C	3.667367	3.234095	-0.924283
C	4.977653	0.129540	-0.070685
C	3.800544	0.635718	-2.213894
H	4.590015	2.363097	1.507454
H	2.987413	3.082419	1.713780
H	3.201985	1.341367	1.923337
H	3.273054	4.141387	-0.463977
H	4.757757	3.300438	-0.925603
H	3.318349	3.197856	-1.954994
H	5.246194	-0.825424	-0.525371
H	5.800043	0.828279	-0.240380
H	4.864632	-0.026888	1.000657
H	4.640272	1.237693	-2.564984
H	3.949842	-0.390538	-2.551318
H	2.883801	1.011610	-2.671389
C	1.211996	-3.042530	-1.569982
C	-1.347458	-3.090708	-0.386280
C	0.887483	-3.131289	1.388706
C	-0.843105	2.858910	-1.664874
C	-1.482442	2.865490	1.299664
C	-3.053381	1.348191	-0.560909
C	-3.144258	-0.018369	-1.179374
C	-2.318385	-2.185929	-1.087760
H	0.821500	-4.074233	-1.610111
C	2.734826	-3.137220	-1.446690
C	0.816397	-2.336492	-2.870936
H	-1.275139	-4.068969	-0.880387
H	-1.752638	-3.259500	0.625967
H	0.098966	-2.849475	2.107188
C	2.197854	-2.544042	1.921713
C	0.934987	-4.658744	1.296585
H	0.248499	2.945950	-1.561520
C	-1.450075	4.261165	-1.722581
C	-1.139244	2.097825	-2.964010
H	-1.700825	2.087108	2.050040
C	-2.631795	3.878865	1.343483
C	-0.149947	3.504414	1.695695
H	-3.597873	2.104318	-1.142871
H	-3.547630	1.273386	0.422376

C	-4.196277	-0.412099	-2.005429
C	-3.343793	-2.653542	-1.908365
H	3.151730	-3.527288	-2.389466
H	3.173971	-2.153728	-1.243813
H	3.043993	-3.821805	-0.645001
H	-0.274497	-2.239802	-2.984948
H	1.239485	-1.321956	-2.900663
H	1.198932	-2.900403	-3.736461
H	3.055862	-2.796010	1.283204
H	2.142039	-1.450753	1.985340
H	2.393600	-2.941319	2.930024
H	1.182465	-5.083959	2.281989
H	-0.028196	-5.091750	0.986882
H	1.703412	-5.006277	0.589385
H	-1.158937	4.750966	-2.665720
H	-2.552057	4.239720	-1.694249
H	-1.099973	4.899793	-0.900797
H	-2.222667	2.047120	-3.164534
H	-0.676003	2.619882	-3.815708
H	-0.745559	1.072011	-2.935109
H	-2.761868	4.225328	2.381190
H	-2.436147	4.766237	0.727308
H	-3.593754	3.451603	1.024275
H	-0.257686	4.017138	2.664181
H	0.636848	2.746493	1.785389
H	0.186341	4.246207	0.953583
C	-4.276080	-1.744002	-2.398679
H	-4.942894	0.316369	-2.322231
H	-3.409762	-3.714914	-2.148125
H	-5.079882	-2.078174	-3.056961

$TS_{18\text{-}19}$

SCF energy in gas phase: -3508.83557264

Thermal correction to Enthalpy in gas phase: 0.836332

Thermal correction to Gibbs Free Energy in gas phase: 0.7211

SCF energy in solvent: -3509.0837128

Co	0.341711	-0.021034	-0.094114
P	0.840096	2.080469	-0.400746
P	0.826121	-2.068618	-0.608362
B	-1.573985	-0.012885	-0.192415
H	0.112138	0.012420	-1.561122
N	2.155407	-0.067186	0.874135
C	-0.708413	-0.073434	1.684549
C	-1.009026	1.069969	2.440040
C	-0.843468	-1.280372	2.388449
C	-1.364623	1.027766	3.780879
H	-1.006191	2.039538	1.959127
C	-1.191332	-1.347619	3.729215
H	-0.706681	-2.218493	1.866677
C	-1.449650	-0.187217	4.441774
H	-1.587344	1.949136	4.307545
H	-1.275955	-2.313167	4.215468
H	-1.730191	-0.230263	5.487025
O	-2.402961	-1.134731	-0.359474
O	-2.374011	1.136437	-0.324186
C	-3.764339	-0.723960	-0.262465
C	-3.683052	0.759746	-0.740647
C	-4.193715	-0.853011	1.198240
C	-4.615369	-1.632153	-1.133284
C	-4.694236	1.693555	-0.098275
C	-3.742794	0.892581	-2.261484

H	-5.252034	-0.618502	1.326785
H	-4.024875	-1.880765	1.522278
H	-3.604622	-0.201977	1.845101
H	-4.611366	-2.642150	-0.720228
H	-5.649930	-1.282620	-1.164560
H	-4.231153	-1.681235	-2.150955
H	-4.560912	2.703270	-0.490678
H	-5.715212	1.374619	-0.320937
H	-4.565050	1.728653	0.982088
H	-4.734801	0.658254	-2.651493
H	-3.501893	1.920651	-2.534560
H	-3.012474	0.234842	-2.735404
C	2.047133	2.415396	-1.781529
C	1.934379	2.339141	1.060250
C	-0.367569	3.483240	-0.340813
C	1.834789	-2.294722	-2.155840
C	-0.413540	-3.445429	-0.615220
C	2.031866	-2.489427	0.722826
C	2.764348	-1.239992	1.134872
C	2.723964	1.080825	1.293761
H	2.864523	1.728086	-1.495875
C	2.641258	3.825882	-1.848819
C	1.553149	1.974734	-3.162736
H	2.590930	3.218155	1.008811
H	1.261398	2.473765	1.921911
H	-1.161861	3.063608	0.292668
C	-1.009532	3.705729	-1.713881
C	0.111989	4.794068	0.287119
H	1.136302	-1.988383	-2.952862
C	2.338629	-3.709547	-2.454717
C	3.012149	-1.314970	-2.168013
H	-1.157177	-3.075688	0.105275
C	0.057524	-4.825804	-0.150055
C	-1.141946	-3.492171	-1.964015
H	2.732936	-3.298692	0.474375
H	1.437378	-2.824062	1.587207
C	3.999761	-1.294191	1.776998
C	3.961001	1.092497	1.933557
H	1.899743	4.558057	-2.201739
H	3.028719	4.176218	-0.881051
H	3.479692	3.843629	-2.563394
H	1.092104	0.978437	-3.123558
H	0.810777	2.676369	-3.569583
H	2.398127	1.940802	-3.869045
H	-0.337219	4.246043	-2.398051
H	-1.295336	2.751284	-2.177770
H	-1.923750	4.309794	-1.603290
H	-0.726261	5.508450	0.329578
H	0.469966	4.654456	1.317897
H	0.918157	5.269022	-0.289805
H	1.526161	-4.423711	-2.637879
H	2.971948	-3.695222	-3.356217
H	2.958424	-4.103883	-1.633029
H	3.789450	-1.614695	-1.445750
H	3.480208	-1.294201	-3.164407
H	2.682840	-0.300816	-1.913886
H	-0.798724	-5.519637	-0.135844
H	0.822535	-5.262657	-0.806757
H	0.467532	-4.799441	0.870697
H	-2.044933	-4.115858	-1.875181
H	-1.467514	-2.487064	-2.266592
H	-0.518732	-3.922203	-2.762863

C	4.613419	-0.111647	2.171589
H	4.468775	-2.261198	1.959702
H	4.397757	2.041957	2.243488
H	5.585550	-0.128468	2.666829

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SCF energy in gas phase: -3508.8740588

Thermal correction to Enthalpy in gas phase: 0.839508

Thermal correction to Gibbs Free Energy in gas phase: 0.724091

SCF energy in solvent: -3509.12167641

Co	-0.358813	-0.065214	-0.024713
P	-1.227620	-1.995167	-0.650407
P	-0.373306	2.058646	-0.591871
B	1.844898	-0.331188	0.559169
C	0.875552	-0.274602	1.845799
H	1.059322	-0.326178	-0.618721
N	-2.165608	0.312490	0.707557
O	2.630929	-1.534529	0.447495
O	2.754840	0.778111	0.383208
C	3.871652	-1.184057	-0.140556
C	4.077244	0.270193	0.389639
C	3.734738	-1.224881	-1.665383
C	4.928080	-2.180606	0.305754
C	4.956410	1.148294	-0.485899
C	4.594954	0.291478	1.828848
H	4.684908	-1.020287	-2.161902
H	3.400092	-2.218745	-1.965033
H	2.995997	-0.500060	-2.011050
H	4.712046	-3.161447	-0.121592
H	5.920970	-1.873383	-0.031624
H	4.939165	-2.279209	1.389899
H	5.043587	2.140916	-0.039950
H	5.960779	0.727398	-0.575118
H	4.534886	1.262153	-1.483113
H	5.640462	-0.016630	1.892372
H	4.511418	1.309108	2.213633
H	3.995035	-0.361788	2.463491
C	0.635708	0.917996	2.543393
C	0.271733	-1.432675	2.353927
C	-0.223782	0.971509	3.628051
H	1.158513	1.812916	2.227699
C	-0.589221	-1.392536	3.443660
H	0.531599	-2.383835	1.907921
C	-0.861414	-0.183951	4.064680
H	-0.395444	1.910255	4.142147
H	-1.042221	-2.305277	3.813954
H	-1.537572	-0.145718	4.910218
C	-2.175853	-2.108839	-2.247819
C	-2.601713	-2.080571	0.580708
C	-0.496006	-3.694427	-0.462329
C	-1.295778	2.461322	-2.155886
C	1.071765	3.204068	-0.456838
C	-1.545490	2.670183	0.689177
C	-2.533477	1.581324	0.996684
C	-3.033041	-0.692358	0.956451
H	-2.780796	-3.029301	-2.197371
C	-1.232053	-2.210488	-3.449444
C	-3.136679	-0.927972	-2.400064
H	-3.467687	-2.678430	0.259047
H	-2.177713	-2.563744	1.474635
H	-0.353262	-3.761631	0.629256

C	-1.405953	-4.852824	-0.879589
C	0.893763	-3.801850	-1.096608
H	-2.272029	1.991680	-1.935889
C	-0.701141	1.730535	-3.364047
C	-1.555498	3.934956	-2.474918
H	1.630104	2.749824	0.374920
C	1.979355	3.071816	-1.683375
C	0.790640	4.668763	-0.111544
H	-0.942130	2.851213	1.591789
H	-2.063783	3.608167	0.444348
C	-3.775950	1.874812	1.552697
C	-4.285376	-0.457016	1.519721
H	-0.714287	-3.179159	-3.483514
H	-1.794537	-2.102328	-4.390469
H	-0.462731	-1.423186	-3.421788
H	-3.884180	-0.887260	-1.593399
H	-2.588501	0.023248	-2.396011
H	-3.682259	-1.005126	-3.353812
H	-1.524742	-4.901071	-1.973364
H	-0.962463	-5.809642	-0.561337
H	-2.409715	-4.788212	-0.431281
H	1.561338	-3.019609	-0.709371
H	1.337108	-4.781847	-0.856240
H	0.853289	-3.721601	-2.193417
H	-0.439388	0.695470	-3.103927
H	-1.421846	1.710544	-4.197290
H	0.210917	2.226803	-3.725772
H	-0.632282	4.445467	-2.787393
H	-2.271368	4.018550	-3.308558
H	-1.976574	4.487679	-1.621888
H	2.149324	2.015632	-1.937610
H	1.560218	3.589465	-2.560503
H	2.961715	3.520016	-1.469890
H	0.268308	5.201848	-0.918140
H	0.194069	4.776655	0.806571
H	1.745422	5.191671	0.061103
C	-4.663878	0.842785	1.826274
H	-4.033274	2.912359	1.765353
H	-4.953580	-1.298246	1.703827
H	-5.641488	1.050108	2.264240

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SCF energy in gas phase: -2865.86863335

Thermal correction to Enthalpy in gas phase: 0.545416

Thermal correction to Gibbs Free Energy in gas phase: 0.456848

SCF energy in solvent: -2866.11337465

Co	-0.000023	-0.566115	-0.170522
P	2.114887	-0.461625	-0.039496
P	-2.114833	-0.461544	-0.039654
H	-0.000386	-2.082241	0.050713
N	-0.000002	1.385837	-0.385516
C	2.911940	-0.563612	1.627720
C	2.439717	1.291767	-0.529683
C	3.230394	-1.451543	-1.131515
C	-2.912218	-0.563023	1.627429
C	-3.229927	-1.452031	-1.131521
C	-2.439711	1.291696	-0.530353
C	-1.166025	2.083525	-0.374401
C	1.166008	2.083571	-0.373945
H	3.950028	-0.199986	1.534729
C	2.928087	-2.008957	2.131794

C	2.162617	0.347588	2.604171
H	3.273396	1.770649	0.005340
H	2.705250	1.288449	-1.599957
H	3.122606	-2.474643	-0.733344
C	2.668570	-1.461381	-2.556410
C	4.708157	-1.059085	-1.100904
H	-3.950293	-0.199442	1.534055
C	-2.163167	0.348500	2.603793
C	-2.928488	-2.008190	2.132005
H	-3.121811	-2.475000	-0.733104
C	-4.707815	-1.060026	-1.101170
C	-2.667940	-1.461970	-2.556354
H	-2.705111	1.288229	-1.600653
H	-3.273467	1.770623	0.004515
C	-1.193744	3.470554	-0.253426
C	1.193637	3.470576	-0.252868
H	3.566997	-2.656860	1.512749
H	3.314522	-2.050402	3.162777
H	1.910554	-2.430508	2.123218
H	2.139721	1.395571	2.266494
H	1.119471	0.012817	2.712506
H	2.641791	0.324854	3.595997
H	2.741833	-0.467397	-3.028689
H	3.233042	-2.165127	-3.188666
H	1.608898	-1.757326	-2.555498
H	5.142660	-1.146456	-0.093965
H	5.293635	-1.710228	-1.769945
H	4.856276	-0.021641	-1.443909
H	-2.140024	1.396354	2.265736
H	-2.642722	0.326191	3.595444
H	-1.120097	0.013672	2.712681
H	-1.910947	-2.429732	2.123871
H	-3.315203	-2.049266	3.162896
H	-3.567205	-2.656338	1.513018
H	-5.142398	-1.147203	-0.094248
H	-4.856195	-0.022728	-1.444514
H	-5.293027	-1.711554	-1.770067
H	-2.741304	-0.468051	-3.028755
H	-1.608219	-1.757742	-2.555268
H	-3.232228	-2.165891	-3.188577
C	-0.000086	4.178095	-0.174253
H	-2.154893	3.984858	-0.225367
H	2.154756	3.984913	-0.224346
H	-0.000117	5.264015	-0.068567

PhBPin

SCF energy in gas phase: -642.972712553

Thermal correction to Enthalpy in gas phase: 0.289602

Thermal correction to Gibbs Free Energy in gas phase: 0.233969

SCF energy in solvent: -642.985893393

B	0.122213	0.000186	0.000565
C	1.675542	0.000196	0.000627
O	-0.637353	1.117115	-0.225266
O	-0.637327	-1.116934	0.226154
C	-2.004006	0.779429	0.080041
C	-2.003773	-0.779516	-0.080182
C	-2.923080	1.516134	-0.876111
C	-2.265023	1.232934	1.512717
C	-2.263725	-1.232978	-1.513124
C	-2.923459	-1.516425	0.875218
H	-3.958953	1.205869	-0.724086

H	-2.859105	2.588958	-0.692458
H	-2.651552	1.332269	-1.913717
H	-2.054974	2.299969	1.587232
H	-3.303104	1.063599	1.801325
H	-1.617299	0.709536	2.217238
H	-2.053534	-2.299997	-1.587503
H	-3.301596	-1.063709	-1.802541
H	-1.615510	-0.709553	-2.217175
H	-3.959252	-1.206321	0.722359
H	-2.859163	-2.589232	0.691587
H	-2.652811	-1.332549	1.913060
C	2.390850	-1.187942	0.160949
C	2.390977	1.188169	-0.160171
C	3.776451	-1.190891	0.161157
H	1.849698	-2.118325	0.286293
C	3.776588	1.190815	-0.161458
H	1.849958	2.118711	-0.284916
C	4.470099	-0.000117	-0.000477
H	4.317705	-2.120445	0.286648
H	4.317934	2.120258	-0.287373
H	5.553296	-0.000256	-0.001016

$TS_{13\text{-}20}$

SCF energy in gas phase: -3508.81440183

Thermal correction to Enthalpy in gas phase: 0.83745

Thermal correction to Gibbs Free Energy in gas phase: 0.721102

SCF energy in solvent: -3509.06266645

Co	-0.025007	0.181771	-0.204091
P	-0.647078	2.236923	0.091772
P	-1.234023	-1.440095	0.941295
B	1.961112	-0.110829	-0.334209
C	1.206393	-1.301299	-1.278005
H	0.920630	1.079904	-0.863897
N	-1.946283	0.191603	-1.292999
O	3.014866	0.592172	-1.015042
O	2.526754	-0.601697	0.884160
C	4.246505	0.314671	-0.369918
C	3.785901	0.015943	1.090676
C	5.164455	1.518132	-0.512417
C	4.882288	-0.901441	-1.044537
C	3.562052	1.292179	1.902468
C	4.684596	-0.935209	1.863141
H	6.080938	1.378875	0.066035
H	5.439640	1.647499	-1.560286
H	4.673696	2.430511	-0.176992
H	4.980028	-0.695635	-2.111117
H	5.873023	-1.118201	-0.640304
H	4.254730	-1.785744	-0.929591
H	3.017346	1.035800	2.812008
H	4.503078	1.770817	2.180092
H	2.960090	2.002961	1.335745
H	5.696297	-0.531671	1.949842
H	4.288342	-1.078948	2.869853
H	4.736984	-1.908417	1.377309
C	1.488828	-2.631754	-0.952156
C	0.684028	-1.060681	-2.552946
C	1.219749	-3.672491	-1.825026
H	1.955210	-2.835752	0.003855
C	0.362566	-2.097623	-3.418545
H	0.532374	-0.038509	-2.874922
C	0.627747	-3.407973	-3.053606

H	1.466608	-4.691072	-1.549737
H	-0.073371	-1.880624	-4.386169
H	0.398538	-4.219951	-3.733321
C	-1.983900	2.922586	1.204479
C	-1.424006	2.511258	-1.582537
C	0.647385	3.583462	0.219954
C	-2.539971	-0.916125	2.159833
C	-0.536729	-3.045422	1.562188
C	-2.203333	-2.062712	-0.525874
C	-2.724918	-0.894260	-1.317690
C	-2.328688	1.337670	-1.864682
H	-2.013142	4.006436	1.024842
C	-1.578508	2.702562	2.664183
C	-3.397901	2.415351	0.888448
H	-1.963038	3.465705	-1.677760
H	-0.593928	2.512992	-2.304662
H	1.203615	3.290428	1.126848
C	1.640754	3.578548	-0.948978
C	0.119165	5.008847	0.425632
H	-2.687520	0.133010	1.879079
C	-1.993566	-0.898413	3.591742
C	-3.908811	-1.595440	2.078057
H	-0.094042	-3.446390	0.638940
C	0.616052	-2.826713	2.549637
C	-1.530562	-4.096071	2.065356
H	-1.457337	-2.601085	-1.134813
H	-3.007899	-2.769086	-0.280451
C	-3.943050	-0.884168	-1.997894
C	-3.519305	1.414041	-2.586654
H	-0.619830	3.193766	2.894491
H	-2.337098	3.114874	3.348762
H	-1.452451	1.634985	2.891206
H	-3.794580	2.882901	-0.024217
H	-3.458179	1.329308	0.738117
H	-4.081526	2.675342	1.712737
H	1.154094	3.899308	-1.884687
H	2.442867	4.304975	-0.741412
H	2.112500	2.601620	-1.113462
H	-0.394318	5.147964	1.386858
H	0.963133	5.715867	0.407370
H	-0.571505	5.308178	-0.380276
H	-0.989847	-0.448667	3.639789
H	-2.659104	-0.307573	4.241054
H	-1.928975	-1.909628	4.019386
H	-3.858391	-2.675423	2.277084
H	-4.587055	-1.152811	2.826037
H	-4.377422	-1.451783	1.092588
H	1.312596	-2.055456	2.187832
H	0.251018	-2.523953	3.542188
H	1.175291	-3.767646	2.682906
H	-1.997769	-3.804073	3.017333
H	-2.333208	-4.298688	1.340617
H	-1.002346	-5.046621	2.244241
C	-4.327514	0.281554	-2.656939
H	-4.577271	-1.771336	-2.004575
H	-3.819561	2.350366	-3.058252
H	-5.270990	0.315169	-3.204934

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SCF energy in gas phase: -3688.53305402

Thermal correction to Enthalpy in gas phase: 0.935489

Thermal correction to Gibbs Free Energy in gas phase: 0.808896

SCF energy in solvent: -3688.77800161

Co	-0.501167	0.378305	0.315540
P	-0.945202	2.118300	-0.946314
P	-1.187298	-0.811398	2.014813
B	0.819887	-0.900978	-0.716604
H	0.504037	1.146211	1.181378
B	1.524803	0.438753	0.467062
N	-1.957806	-0.528262	-0.683816
O	0.802074	-2.251347	-0.378191
O	1.094141	-0.779428	-2.072955
O	2.375394	-0.254005	1.378685
O	2.331533	1.418276	-0.181372
C	1.244298	-3.047463	-1.478211
C	1.085779	-2.069079	-2.696068
C	3.588757	0.471450	1.522645
C	3.692630	1.220040	0.154817
C	2.688447	-3.447316	-1.192240
C	0.379270	-4.296871	-1.549505
C	2.218408	-2.124270	-3.707682
C	-0.250770	-2.220710	-3.416274
C	4.717782	-0.506367	1.800971
C	3.434667	1.432950	2.701202
C	4.331178	0.369558	-0.942453
C	4.391157	2.569483	0.218349
H	2.721118	-3.981955	-0.242629
H	3.090464	-4.095892	-1.972236
H	3.329358	-2.571923	-1.099878
H	0.545980	-4.902831	-0.657718
H	-0.680200	-4.047823	-1.597664
H	0.635546	-4.901228	-2.422137
H	2.296397	-3.119435	-4.150961
H	2.025589	-1.408956	-4.508286
H	3.172141	-1.867775	-3.250127
H	-1.085748	-2.197427	-2.717419
H	-0.370835	-1.392173	-4.115729
H	-0.299113	-3.154025	-3.979360
H	5.682241	0.006845	1.818754
H	4.564243	-0.977082	2.773349
H	4.751766	-1.291774	1.047507
H	3.203800	0.857421	3.597854
H	4.348510	2.000482	2.884554
H	2.616825	2.134492	2.526239
H	4.179225	0.866172	-1.901364
H	5.402122	0.231342	-0.783164
H	3.852521	-0.606950	-0.997380
H	5.418909	2.460359	0.572823
H	4.421067	3.011941	-0.778692
H	3.864394	3.258605	0.876178
C	-2.249205	3.371085	-0.502965
C	-1.698207	1.199634	-2.357069
C	0.363254	3.087944	-1.829111
C	-2.532820	-0.290626	3.196341
C	0.035105	-1.692805	3.084259
C	-1.935882	-2.203823	1.067641
C	-2.517104	-1.662920	-0.202672
C	-2.415628	-0.010270	-1.844391
H	-2.317239	4.106655	-1.322402
C	-1.878363	4.094647	0.795940
C	-3.609320	2.686914	-0.341792
H	-2.339498	1.794315	-3.022550

H	-0.829478	0.845401	-2.937758
H	1.089668	2.294549	-2.066731
C	1.072711	4.088034	-0.910771
C	-0.081628	3.771091	-3.124770
H	-2.520087	-0.987270	4.051592
C	-2.260999	1.128125	3.705458
C	-3.917379	-0.349139	2.544091
H	0.819194	-1.956232	2.356677
C	0.657669	-0.737023	4.104209
C	-0.472653	-2.967534	3.760848
H	-1.071504	-2.829719	0.796154
H	-2.660871	-2.823501	1.611851
C	-3.571185	-2.290822	-0.860964
C	-3.477603	-0.588366	-2.535300
H	-2.692976	4.769746	1.103837
H	-1.711184	3.365128	1.603320
H	-0.964055	4.693534	0.702005
H	-3.538819	1.870687	0.395099
H	-4.359414	3.406334	0.022448
H	-3.987429	2.261653	-1.283161
H	1.281244	3.655723	0.076865
H	2.038854	4.377174	-1.352831
H	0.479467	5.008238	-0.788733
H	0.775993	4.286853	-3.586430
H	-0.471708	3.061374	-3.868690
H	-0.856295	4.533921	-2.943505
H	-1.258659	1.238674	4.141267
H	-2.336880	1.843504	2.873034
H	-3.000132	1.410418	4.472516
H	-3.933567	0.219530	1.600271
H	-4.239831	-1.376716	2.322774
H	-4.671637	0.097504	3.211140
H	-0.039615	-0.518111	4.929327
H	1.559373	-1.190649	4.544868
H	0.956592	0.209090	3.632302
H	0.338757	-3.429198	4.346495
H	-1.299883	-2.763753	4.460405
H	-0.819150	-3.718701	3.036053
C	-4.067203	-1.743779	-2.038723
H	-3.999300	-3.198274	-0.435197
H	-3.825385	-0.128330	-3.460118
H	-4.900805	-2.213586	-2.562924

$TS_{21\text{-}22}$

SCF energy in gas phase: -3688.51970618

Thermal correction to Enthalpy in gas phase: 0.932539

Thermal correction to Gibbs Free Energy in gas phase: 0.804684

SCF energy in solvent: -3688.7647234

Co	-0.501890	-0.003111	-0.361623
P	-0.669683	-1.847031	-1.486187
P	-1.347204	1.955646	0.058704
B	0.672434	-0.390855	1.226654
H	-0.196601	0.616856	-1.701227
B	1.322109	0.479113	-0.765021
N	-2.126264	-0.691792	0.611798
O	0.312597	0.135382	2.478689
O	1.682393	-1.329933	1.446608
O	1.939007	1.721938	-0.530529
O	2.216731	-0.306188	-1.511811
C	1.224528	-0.322156	3.480793
C	1.766179	-1.632112	2.839199

C	3.098341	1.829511	-1.351459
C	3.487898	0.332843	-1.552651
C	2.305543	0.743043	3.648078
C	0.473436	-0.510399	4.786934
C	3.201728	-1.979892	3.188608
C	0.858709	-2.835906	3.092124
C	4.137385	2.672744	-0.634258
C	2.676044	2.510069	-2.652679
C	4.326711	-0.220935	-0.402473
C	4.158487	0.019782	-2.879274
H	1.833588	1.687835	3.918370
H	3.016871	0.475260	4.431188
H	2.849774	0.895807	2.714498
H	0.137644	0.458414	5.159992
H	-0.402268	-1.143355	4.652430
H	1.119157	-0.960072	5.544892
H	3.314186	-2.126168	4.265408
H	3.486835	-2.905596	2.686752
H	3.888057	-1.198251	2.867838
H	-0.180752	-2.593001	2.862341
H	1.172107	-3.650544	2.437628
H	0.916927	-3.179941	4.126162
H	5.074635	2.694383	-1.195161
H	3.775543	3.697528	-0.535933
H	4.336118	2.286939	0.364318
H	2.224826	3.474212	-2.412873
H	3.524269	2.682158	-3.317443
H	1.932724	1.909181	-3.179336
H	4.374153	-1.306300	-0.497435
H	5.342853	0.177753	-0.413805
H	3.862311	0.001124	0.558206
H	5.092342	0.577121	-2.983971
H	4.391871	-1.045062	-2.928042
H	3.509107	0.263588	-3.718690
C	-1.821215	-1.825750	-2.944482
C	-1.574052	-2.886588	-0.271051
C	0.710080	-2.924585	-2.099119
C	-2.553561	2.478201	-1.261618
C	-0.442467	3.496027	0.546975
C	-2.379366	1.547279	1.516977
C	-2.871204	0.135998	1.381360
C	-2.473026	-1.998271	0.542851
H	-1.924723	-2.866982	-3.288186
C	-1.216377	-0.987000	-4.072415
C	-3.216853	-1.321935	-2.573660
H	-2.128970	-3.733047	-0.700984
H	-0.799971	-3.293429	0.400113
H	1.316232	-2.219122	-2.688211
C	0.290061	-4.099129	-2.988811
C	1.593769	-3.416035	-0.950186
H	-2.837671	1.495908	-1.666703
C	-3.850562	3.175350	-0.842073
C	-1.817727	3.212125	-2.386408
H	0.199995	3.686469	-0.328217
C	-1.318480	4.725845	0.807256
C	0.487610	3.253165	1.738197
H	-1.670267	1.556463	2.360579
H	-3.197430	2.245135	1.737761
C	-4.010182	-0.307286	2.048578
C	-3.592790	-2.498595	1.200434
H	-1.872096	-0.999562	-4.957351
H	-1.092632	0.057675	-3.745289

H -0.226297 -1.356388 -4.381490
H -3.163863 -0.329171 -2.104443
H -3.842580 -1.240647 -3.476486
H -3.732188 -1.995154 -1.872620
H -0.145199 -3.781527 -3.946675
H 1.173845 -4.713973 -3.222622
H -0.437157 -4.756913 -2.483719
H 2.523183 -3.842401 -1.359882
H 1.855444 -2.607818 -0.258091
H 1.095750 -4.219249 -0.379846
H -4.434101 2.557524 -0.142959
H -3.685403 4.153554 -0.370386
H -4.482604 3.341368 -1.729754
H -1.536766 4.236741 -2.097138
H -0.899358 2.674382 -2.671076
H -2.457774 3.285250 -3.279463
H -2.062583 4.536031 1.597934
H -0.686923 5.560920 1.150368
H -1.852937 5.068997 -0.087735
H 1.118345 4.142899 1.893039
H -0.079516 3.082328 2.667137
H 1.139785 2.393172 1.565906
C -4.385150 -1.641695 1.955409
H -4.588488 0.401165 2.642020
H -3.836734 -3.557025 1.106345
H -5.275964 -2.009285 2.466743

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SCF energy in gas phase: -3688.53805915

Thermal correction to Enthalpy in gas phase: 0.935129

Thermal correction to Gibbs Free Energy in gas phase: 0.808771

SCF energy in solvent: -3688.78214262

Co -0.352972 -0.541848 0.000346
P -0.412861 -0.911276 2.124856
P -0.637518 -0.823827 -2.110210
B -0.221657 1.458545 -0.051697
H -0.282731 -2.049026 -0.028454
B 1.556276 -0.529074 -0.077776
N -2.401451 -0.481447 0.110042
O -1.345144 2.236244 -0.378165
O 0.823799 2.335478 0.237067
O 2.343069 -0.549372 -1.236995
O 2.417396 -0.541315 1.026828
C -1.132882 3.602648 -0.028834
C 0.431676 3.701459 0.099467
C 3.709004 -0.775247 -0.888574
C 3.754768 -0.291621 0.594964
C -1.870788 3.838709 1.288187
C -1.739984 4.486302 -1.107549
C 0.921732 4.469777 1.320394
C 1.125126 4.271901 -1.135032
C 4.596067 0.005026 -1.842774
C 3.976116 -2.271932 -1.031070
C 4.007684 1.208605 0.726142
C 4.713741 -1.059472 1.488458
H -1.792019 4.873881 1.624406
H -2.924957 3.598443 1.143932
H -1.483016 3.187499 2.071705
H -2.818720 4.326743 -1.141009
H -1.558225 5.542664 -0.897924

H	-1.332842	4.253136	-2.090065
H	2.012061	4.442343	1.346072
H	0.608215	5.515063	1.273999
H	0.555367	4.036427	2.248059
H	0.927249	5.339758	-1.243911
H	2.201410	4.131861	-1.024106
H	0.815354	3.767478	-2.045925
H	5.645534	-0.070467	-1.548834
H	4.495778	-0.400484	-2.850943
H	4.314511	1.056320	-1.870183
H	3.744484	-2.576657	-2.052140
H	5.019122	-2.518946	-0.825881
H	3.338878	-2.845046	-0.355902
H	3.301529	1.774896	0.118658
H	3.851292	1.498821	1.766188
H	5.028723	1.471943	0.443895
H	5.741027	-0.963990	1.129144
H	4.670684	-0.654946	2.500990
H	4.456008	-2.116389	1.534024
C	-0.342463	-2.689285	2.661240
C	-2.143175	-0.408743	2.516804
C	0.555226	-0.117390	3.498217
C	-0.690395	-2.566117	-2.748149
C	0.237896	0.024632	-3.508105
C	-2.374399	-0.240312	-2.297323
C	-3.132170	-0.450250	-1.017412
C	-3.019532	-0.533509	1.301641
H	-0.416315	-2.687191	3.759814
C	0.997724	-3.318210	2.268699
C	-1.509931	-3.514445	2.118284
H	-2.578388	-0.921957	3.385846
H	-2.083750	0.665068	2.765553
H	1.515171	-0.655758	3.462705
C	0.845636	1.355448	3.227716
C	-0.062224	-0.281635	4.892485
H	-0.880565	-2.498486	-3.831272
C	0.658704	-3.256433	-2.534131
C	-1.825211	-3.377908	-2.121931
H	1.161235	-0.564664	-3.621679
C	-0.530396	0.014507	-4.834901
C	0.642204	1.449173	-3.142732
H	-2.294948	0.850524	-2.441241
H	-2.906158	-0.662286	-3.161256
C	-4.521087	-0.560764	-0.988516
C	-4.405061	-0.646590	1.400194
H	1.094326	-3.347690	1.172725
H	1.856147	-2.752537	2.658412
H	1.058540	-4.348250	2.653691
H	-1.416328	-4.560792	2.449142
H	-2.486988	-3.144808	2.464580
H	-1.511063	-3.503436	1.019096
H	1.343504	1.501345	2.264375
H	-0.085841	1.946564	3.219307
H	1.480373	1.766317	4.029398
H	-0.271338	-1.325434	5.164793
H	0.628492	0.119690	5.650912
H	-1.002344	0.286385	4.982828
H	1.486696	-2.705756	-3.002864
H	0.881136	-3.330586	-1.459006
H	0.637499	-4.271944	-2.959698
H	-2.818354	-2.969028	-2.361397
H	-1.795939	-4.414755	-2.492157

H	-1.721929	-3.403442	-1.027555
H	-0.849023	-0.989152	-5.150282
H	-1.426741	0.653042	-4.781128
H	0.106952	0.420755	-5.636135
H	-0.244461	2.067254	-2.927784
H	1.292403	1.459771	-2.260292
H	1.182378	1.916480	-3.981613
C	-5.165536	-0.677020	0.237158
H	-5.082765	-0.551687	-1.922776
H	-4.873482	-0.706236	2.382811
H	-6.251249	-0.775537	0.286401

$TS_{22\text{-}23}$

SCF energy in gas phase: -3688.53239341

Thermal correction to Enthalpy in gas phase: 0.93366

Thermal correction to Gibbs Free Energy in gas phase: 0.807998

SCF energy in solvent: -3688.77778608

Co	0.272651	0.220201	-0.600573
P	0.354092	2.347209	-0.329107
P	0.430499	-1.837287	-1.257231
B	0.521800	-0.222724	1.328118
H	-0.148458	0.519480	-2.021646
B	-1.624600	0.173038	-0.364521
N	2.279850	0.373396	-0.995438
O	1.692797	0.076103	2.041714
O	-0.308674	-0.965231	2.169754
O	-2.479476	-0.878258	-0.718682
O	-2.420178	1.206475	0.153647
C	1.755640	-0.676777	3.252403
C	0.265660	-1.135286	3.465480
C	-3.838317	-0.458109	-0.613285
C	-3.732685	0.710036	0.412580
C	2.310364	0.211006	4.356140
C	2.726843	-1.831622	3.008238
C	-0.519010	-0.263865	4.442342
C	0.102853	-2.594093	3.871502
C	-4.686899	-1.633443	-0.160952
C	-4.280465	0.006868	-1.999067
C	-3.757831	0.229506	1.862751
C	-4.737596	1.830651	0.214101
H	2.333097	-0.318723	5.311024
H	3.330932	0.504152	4.105761
H	1.717943	1.116297	4.476532
H	3.694929	-1.417182	2.724451
H	2.860098	-2.448775	3.898323
H	2.387783	-2.469302	2.191541
H	-1.571506	-0.545818	4.391493
H	-0.173842	-0.401175	5.468652
H	-0.444494	0.790735	4.188114
H	0.571944	-2.787346	4.838726
H	-0.959545	-2.826747	3.954864
H	0.535023	-3.268865	3.134281
H	-5.717331	-1.320486	0.022987
H	-4.697985	-2.398932	-0.938504
H	-4.288754	-2.080801	0.748081
H	-4.126674	-0.808267	-2.707585
H	-5.335529	0.285778	-2.017144
H	-3.684832	0.858943	-2.329647
H	-3.015997	-0.554808	2.022651
H	-3.500103	1.067077	2.512798
H	-4.743503	-0.139686	2.151478

H	-5.759501	1.458181	0.316240
H	-4.580863	2.601058	0.970855
H	-4.630090	2.290992	-0.766827
C	0.041912	3.386067	-1.835394
C	2.149613	2.577874	-0.001486
C	-0.439469	3.378439	0.991807
C	-0.526616	-2.376044	-2.758115
C	0.309812	-3.237970	-0.029020
C	2.200722	-1.930334	-1.796386
C	2.938108	-0.634741	-1.585885
C	2.932351	1.519523	-0.722449
H	0.197930	4.435060	-1.535694
C	-1.403520	3.224785	-2.315867
C	1.022842	3.063068	-2.965534
H	2.528084	3.584305	-0.228082
H	2.269265	2.395643	1.079428
H	-1.461191	3.530173	0.612163
C	-0.549220	2.627950	2.316372
C	0.223140	4.744133	1.205818
H	-1.565844	-2.212913	-2.432787
C	-0.266898	-1.465159	-3.961718
C	-0.354209	-3.840640	-3.170087
H	0.804047	-2.766335	0.833914
C	-1.140276	-3.498426	0.389265
C	1.042436	-4.560717	-0.289466
H	2.727162	-2.708005	-1.226028
H	2.268734	-2.232674	-2.851991
C	4.274282	-0.511864	-1.968294
C	4.266483	1.704395	-1.075466
H	-1.574190	2.189938	-2.649850
H	-2.137247	3.443030	-1.526693
H	-1.596394	3.901271	-3.163145
H	0.771182	3.653015	-3.860941
H	2.064275	3.297322	-2.698169
H	0.966705	1.995357	-3.229144
H	-1.095343	1.686678	2.185250
H	0.446011	2.396566	2.728052
H	-1.085173	3.244683	3.055794
H	0.324356	5.329969	0.281115
H	-0.379207	5.343055	1.907039
H	1.225083	4.637296	1.651297
H	-0.401041	-0.407394	-3.704304
H	0.754516	-1.594641	-4.359004
H	-0.964261	-1.722084	-4.774574
H	-0.770935	-4.535630	-2.430521
H	-0.881529	-4.022351	-4.120079
H	0.704157	-4.105938	-3.330800
H	-1.630310	-2.575723	0.716794
H	-1.730407	-3.924574	-0.437652
H	-1.159102	-4.220595	1.221190
H	0.527367	-5.194831	-1.022149
H	2.080044	-4.433943	-0.630398
H	1.085765	-5.129358	0.654096
C	4.947009	0.676070	-1.716770
H	4.772163	-1.349746	-2.457382
H	4.758218	2.649801	-0.845725
H	5.990858	0.797778	-2.010702

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SCF energy in gas phase: -3688.53917086

Thermal correction to Enthalpy in gas phase: 0.935194

Thermal correction to Gibbs Free Energy in gas phase: 0.808561

SCF energy in solvent: -3688.78341302

Co	-0.311375	-0.583344	0.320058
P	-0.708753	0.283179	2.241503
P	-0.236894	-1.954648	-1.335500
B	-0.375614	1.172468	-0.666542
H	-0.033177	-1.881381	1.048606
B	1.583484	-0.314261	0.357246
N	-2.332291	-0.870425	0.299574
O	-1.526027	1.972248	-0.746584
O	0.621553	1.801771	-1.411369
O	2.485059	-0.784796	-0.604377
O	2.321687	0.337864	1.354358
C	-1.339858	3.122910	-1.572658
C	0.173753	3.010218	-2.025026
C	3.824310	-0.596739	-0.151259
C	3.657104	0.550273	0.893343
C	-1.663306	4.364607	-0.746772
C	-2.354137	3.053135	-2.712460
C	1.068593	4.140294	-1.525447
C	0.369108	2.862276	-3.530458
C	4.701674	-0.254996	-1.343117
C	4.286541	-1.909291	0.477511
C	3.706449	1.938349	0.259145
C	4.607484	0.483784	2.076029
H	-1.600479	5.268825	-1.355023
H	-2.684128	4.279860	-0.370762
H	-0.997196	4.479126	0.103742
H	-3.358175	3.043222	-2.286174
H	-2.270371	3.920393	-3.369849
H	-2.239378	2.154384	-3.312485
H	2.094049	3.947100	-1.842768
H	0.761523	5.104750	-1.933797
H	1.065541	4.202459	-0.438753
H	0.051061	3.759676	-4.064264
H	1.427899	2.698511	-3.734991
H	-0.178437	2.008010	-3.923224
H	5.714634	-0.000635	-1.022413
H	4.763194	-1.115818	-2.011081
H	4.289148	0.580560	-1.905775
H	4.169452	-2.710046	-0.254214
H	5.334360	-1.867436	0.780011
H	3.680209	-2.158609	1.349235
H	3.005729	2.002503	-0.573727
H	3.409374	2.676190	1.006129
H	4.709826	2.188633	-0.090053
H	5.645811	0.550961	1.742978
H	4.413075	1.321252	2.748000
H	4.479644	-0.439176	2.639230
C	-0.831384	-0.905580	3.661483
C	-2.448827	0.849414	2.002531
C	0.141456	1.726480	3.027183
C	0.944102	-3.388952	-1.387059
C	-0.285020	-1.446143	-3.117857
C	-1.885011	-2.765420	-1.134155
C	-2.862476	-1.823761	-0.485619
C	-3.132801	-0.096708	1.052318
H	-1.221714	-0.336880	4.520804
C	0.557474	-1.448610	4.011158
C	-1.804946	-2.053443	3.381798
H	-3.024569	0.950881	2.934037

H	-2.383331	1.836202	1.519184
H	1.128130	1.316987	3.289879
C	0.376328	2.854691	2.026058
C	-0.538843	2.262353	4.290994
H	1.875536	-2.919924	-1.739132
C	1.228961	-3.982943	-0.007132
C	0.543492	-4.498940	-2.366360
H	-0.418380	-2.363624	-3.712887
C	-1.498460	-0.552092	-3.378544
C	1.026179	-0.774279	-3.536707
H	-2.288607	-3.194986	-2.061780
H	-1.722293	-3.597700	-0.428498
C	-4.241383	-1.967708	-0.619892
C	-4.520546	-0.197380	0.970325
H	0.986006	-1.974775	3.144116
H	1.259742	-0.653060	4.300155
H	0.487651	-2.158171	4.850504
H	-1.821625	-2.743853	4.239831
H	-2.835163	-1.701227	3.221224
H	-1.489906	-2.616341	2.489982
H	0.905734	2.492164	1.137164
H	-0.575798	3.305000	1.710009
H	0.982838	3.648249	2.490705
H	-0.606183	1.515034	5.093515
H	0.036393	3.113657	4.688249
H	-1.556273	2.629700	4.079625
H	1.619662	-3.226880	0.682238
H	0.321530	-4.410262	0.450775
H	1.968495	-4.794470	-0.100916
H	0.436157	-4.145075	-3.400695
H	1.315169	-5.284706	-2.371768
H	-0.403379	-4.979720	-2.070823
H	-2.448856	-1.096088	-3.269278
H	-1.527375	0.293868	-2.679279
H	-1.465055	-0.152293	-4.405099
H	1.240836	0.096150	-2.901862
H	1.880937	-1.461369	-3.456903
H	0.958736	-0.440806	-4.585166
C	-5.081510	-1.129969	0.106168
H	-4.643812	-2.739874	-1.275883
H	-5.145689	0.453003	1.582314
H	-6.165375	-1.219532	0.015561

$TS_{23\text{-}24}$

SCF energy in gas phase: -3688.53111153

Thermal correction to Enthalpy in gas phase: 0.933971

Thermal correction to Gibbs Free Energy in gas phase: 0.810848

SCF energy in solvent: -3688.77619443

Co	-0.405759	0.262451	-0.492698
P	-0.760029	2.339440	0.092176
P	-0.531649	-1.794950	-1.161088
B	-0.165850	-0.460727	1.348535
B	1.471013	0.410153	-0.755962
N	-2.448319	0.289308	-0.895110
H	0.135431	0.812925	-1.830240
O	-1.076093	-1.262344	2.062737
O	0.983303	-0.336853	2.134930
O	2.301256	-0.524836	-1.403235
O	2.283049	1.464181	-0.316255
C	-0.595697	-1.547571	3.380439
C	0.928238	-1.173020	3.289869

C	3.595329	0.041272	-1.593567
C	3.653338	1.101299	-0.450649
C	-0.875668	-3.011151	3.689079
C	-1.377424	-0.672880	4.356751
C	1.848248	-2.366917	3.040613
C	1.466688	-0.395361	4.483642
C	4.642006	-1.055950	-1.502714
C	3.620754	0.668297	-2.986792
C	4.105099	0.510098	0.883023
C	4.465994	2.343756	-0.773341
H	-0.474597	-3.288907	4.666235
H	-1.953890	-3.177493	3.704745
H	-0.443229	-3.671143	2.937934
H	-2.443277	-0.865765	4.226895
H	-1.108555	-0.889547	5.392073
H	-1.204597	0.384987	4.167203
H	2.855615	-1.996438	2.846549
H	1.887112	-3.031907	3.905185
H	1.537280	-2.944347	2.172867
H	1.412933	-0.995109	5.395060
H	2.512375	-0.143433	4.302090
H	0.921665	0.531974	4.646783
H	4.512577	-1.756616	-2.329332
H	5.648410	-0.635696	-1.566767
H	4.556420	-1.612117	-0.570703
H	4.603886	1.074099	-3.232191
H	3.370462	-0.099047	-3.720839
H	2.881333	1.466411	-3.067192
H	3.924445	1.244738	1.668652
H	3.520471	-0.376997	1.127806
H	5.167306	0.257805	0.875121
H	5.506396	2.084770	-0.983643
H	4.055818	2.872054	-1.632917
H	4.451926	3.022121	0.081345
C	-1.368386	2.817760	1.775337
C	-2.253960	2.694165	-0.931932
C	0.369316	3.747759	-0.345599
C	0.214945	-3.250036	-0.275091
C	-0.255927	-2.039342	-2.979627
C	-2.323817	-2.119844	-0.877966
C	-3.117342	-0.863573	-1.068536
C	-3.094165	1.457370	-1.055810
H	-1.731216	3.855453	1.696746
C	-0.222897	2.777225	2.790395
C	-2.559210	1.947734	2.191927
H	-2.846385	3.548146	-0.572668
H	-1.879712	2.944113	-1.937582
H	1.284808	3.509451	0.214635
C	0.739390	3.754015	-1.832925
C	-0.136541	5.134283	0.068767
H	0.068428	-2.930140	0.766646
C	1.720322	-3.395778	-0.508258
C	-0.500811	-4.601957	-0.402824
H	0.776606	-1.669823	-3.099184
C	-1.183988	-1.118130	-3.781288
C	-0.344477	-3.467692	-3.519478
H	-2.385092	-2.396778	0.187455
H	-2.734385	-2.946699	-1.474219
C	-4.473500	-0.883404	-1.389041
C	-4.451864	1.508904	-1.365442
H	0.271032	1.795364	2.792902
H	0.549525	3.527583	2.562675

H	-0.601315	2.986639	3.804355
H	-2.841572	2.169437	3.233825
H	-3.442801	2.142121	1.565080
H	-2.328080	0.875435	2.119448
H	-0.091753	4.129495	-2.452991
H	1.594901	4.428113	-1.995801
H	1.012452	2.754993	-2.191677
H	0.569972	5.902248	-0.284389
H	-1.116556	5.366059	-0.380544
H	-0.225125	5.252439	1.157586
H	2.113356	-4.211639	0.120121
H	1.953587	-3.642352	-1.555811
H	2.252532	-2.469170	-0.265376
H	-0.060526	-5.303080	0.325175
H	-1.574540	-4.540157	-0.176846
H	-0.387189	-5.055175	-1.396118
H	-2.230358	-1.464446	-3.734354
H	-1.139600	-0.084477	-3.411671
H	-0.886439	-1.120557	-4.841676
H	-0.207902	-3.458428	-4.612919
H	0.427137	-4.126421	-3.099915
H	-1.329231	-3.921672	-3.319840
C	-5.153159	0.320356	-1.531205
H	-4.983495	-1.838315	-1.517950
H	-4.942163	2.475425	-1.484354
H	-6.216638	0.332367	-1.775999

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SCF energy in gas phase: -3688.53105763

Thermal correction to Enthalpy in gas phase: 0.934609

Thermal correction to Gibbs Free Energy in gas phase: 0.806343

SCF energy in solvent: -3688.77622751

Co	-0.395405	0.242004	-0.498429
P	-0.816069	2.322113	0.046136
P	-0.473737	-1.834502	-1.116895
B	-0.175995	-0.426928	1.359524
B	1.477008	0.431013	-0.782910
N	-2.427558	0.221950	-0.963003
H	0.243555	0.773189	-1.813389
O	-1.071709	-1.250030	2.068599
O	0.943786	-0.235431	2.173839
O	2.338734	-0.516402	-1.374486
O	2.265685	1.513915	-0.364616
C	-0.614122	-1.487830	3.403567
C	0.895138	-1.055624	3.340573
C	3.626280	0.064893	-1.556766
C	3.642064	1.161605	-0.448316
C	-0.843475	-2.954250	3.739234
C	-1.453977	-0.624375	4.340700
C	1.865201	-2.216493	3.128419
C	1.375649	-0.241290	4.534228
C	4.689323	-1.009988	-1.408674
C	3.671481	0.648623	-2.968144
C	4.063010	0.617371	0.915156
C	4.451618	2.401277	-0.788656
H	-0.455239	-3.193687	4.731517
H	-1.914231	-3.163388	3.734178
H	-0.367623	-3.613505	3.014469
H	-2.507679	-0.862242	4.188836
H	-1.203871	-0.808278	5.386897

H	-1.318610	0.435298	4.132338
H	2.861304	-1.809723	2.950512
H	1.910936	-2.868592	4.002300
H	1.594951	-2.815624	2.261770
H	1.322269	-0.829351	5.453174
H	2.415240	0.047254	4.374019
H	0.792609	0.667056	4.670203
H	4.588927	-1.739676	-2.213862
H	5.689581	-0.574606	-1.466349
H	4.593994	-1.536642	-0.460768
H	4.652620	1.063244	-3.206180
H	3.449339	-0.145317	-3.682600
H	2.920998	1.431186	-3.088729
H	3.850384	1.372893	1.672239
H	3.482823	-0.269560	1.170283
H	5.128008	0.379212	0.945784
H	5.499798	2.146414	-0.961901
H	4.060437	2.897644	-1.675512
H	4.407621	3.106510	0.042845
C	-1.499975	2.806501	1.698149
C	-2.275923	2.626737	-1.042727
C	0.294169	3.752231	-0.371306
C	0.281997	-3.256437	-0.188425
C	-0.157773	-2.112713	-2.924494
C	-2.265434	-2.182675	-0.866774
C	-3.073920	-0.946487	-1.116793
C	-3.090719	1.373540	-1.166382
H	-1.893128	3.830203	1.588964
C	-0.390349	2.819600	2.753312
C	-2.674418	1.903382	2.089269
H	-2.894629	3.479884	-0.728941
H	-1.865220	2.857392	-2.038556
H	1.203676	3.532091	0.205988
C	0.691081	3.764822	-1.851912
C	-0.245508	5.129849	0.029303
H	0.119439	-2.914439	0.843370
C	1.791586	-3.382308	-0.403557
C	-0.413533	-4.620533	-0.290957
H	0.877312	-1.747639	-3.029126
C	-1.065506	-1.205309	-3.764386
C	-0.237142	-3.551354	-3.438130
H	-2.347625	-2.426650	0.205229
H	-2.646810	-3.034551	-1.446535
C	-4.421511	-0.998797	-1.467911
C	-4.440875	1.393218	-1.509930
H	0.134089	1.854598	2.789647
H	0.365888	3.590339	2.540755
H	-0.811068	3.032591	3.749563
H	-2.997051	2.129795	3.118278
H	-3.543369	2.059337	1.432192
H	-2.405729	0.838606	2.039904
H	-0.132395	4.135194	-2.484982
H	1.542941	4.447194	-1.997432
H	0.983086	2.770773	-2.209129
H	0.452641	5.909914	-0.313601
H	-1.221005	5.341286	-0.439203
H	-0.356668	5.250290	1.115548
H	2.193620	-4.171091	0.252820
H	2.039789	-3.656040	-1.440694
H	2.304242	-2.438637	-0.185529
H	0.034623	-5.300443	0.452133
H	-1.488305	-4.568293	-0.067681

H	-0.292103	-5.092503	-1.274460
H	-2.114082	-1.546040	-3.731285
H	-1.025477	-0.164295	-3.415879
H	-0.746461	-1.230983	-4.818036
H	-0.084438	-3.563218	-4.529320
H	0.529026	-4.200819	-2.995023
H	-1.223974	-4.003139	-3.244526
C	-5.117501	0.188448	-1.661059
H	-4.912326	-1.965730	-1.580152
H	-4.944714	2.347599	-1.664354
H	-6.174645	0.175139	-1.931451

$TS_{24\text{-}25}$

SCF energy in gas phase: -3688.52072229

Thermal correction to Enthalpy in gas phase: 0.935004

Thermal correction to Gibbs Free Energy in gas phase: 0.813902

SCF energy in solvent: -3688.76619415

Co	0.446452	0.347359	-0.334021
P	1.573136	-1.391151	-1.114416
P	-0.048158	2.286526	0.520209
B	-0.296551	-0.677034	1.188554
B	-1.286349	0.074658	-1.172824
N	2.353191	1.146574	-0.279329
H	-0.108909	0.682454	-1.799248
O	0.365004	-1.789539	1.744564
O	-1.483677	-0.516255	1.925530
O	-2.397967	0.911418	-0.935402
O	-1.743931	-1.022073	-1.933167
C	-0.183584	-2.123996	3.011022
C	-1.633277	-1.557619	2.897699
C	-3.493059	0.495843	-1.744653
C	-3.165317	-1.011452	-1.989538
C	0.664101	-1.426674	4.075689
C	-0.087317	-3.629012	3.207654
C	-2.191920	-0.970273	4.184596
C	-2.619752	-2.588532	2.359899
C	-4.786081	0.756569	-0.989656
C	-3.483313	1.308927	-3.038776
C	-3.681079	-1.900902	-0.867086
C	-3.608400	-1.561355	-3.334897
H	0.337075	-1.677830	5.086128
H	1.700866	-1.743950	3.957260
H	0.632706	-0.343054	3.958725
H	0.963162	-3.920153	3.260563
H	-0.570786	-3.935419	4.138027
H	-0.545828	-4.168516	2.380869
H	-3.180559	-0.550886	3.992284
H	-2.293894	-1.747042	4.946085
H	-1.561992	-0.178798	4.582918
H	-2.782831	-3.392381	3.079640
H	-3.577767	-2.104424	2.170407
H	-2.266416	-3.021311	1.424524
H	-4.929903	1.832282	-0.874099
H	-5.644489	0.356127	-1.534154
H	-4.758522	0.310928	0.003045
H	-4.317775	1.036306	-3.687039
H	-3.570005	2.368552	-2.800052
H	-2.551748	1.158129	-3.586492
H	-3.238717	-2.893142	-0.969196
H	-3.380804	-1.489659	0.093487
H	-4.767739	-2.001784	-0.889785

H	-4.692011	-1.482172	-3.449409
H	-3.129379	-1.034827	-4.158734
H	-3.336915	-2.616222	-3.402410
C	2.576213	-2.488776	-0.000542
C	2.859538	-0.431430	-2.021644
C	0.820358	-2.483290	-2.394841
C	-1.379889	2.664331	1.762205
C	-0.112661	3.726092	-0.668663
C	1.527137	2.648407	1.413106
C	2.661216	2.143043	0.571215
C	3.300896	0.677064	-1.114341
H	1.802232	-3.061657	0.528257
C	3.326304	-1.671001	1.059009
C	3.532568	-3.465267	-0.690082
H	3.711926	-1.019697	-2.387123
H	2.338349	0.005398	-2.890027
H	0.073380	-1.809804	-2.837951
C	1.717915	-2.993542	-3.525438
C	0.035292	-3.606620	-1.709054
H	-2.187661	1.987114	1.446542
C	-1.905672	4.103141	1.789418
C	-0.952442	2.272168	3.179516
H	-0.168532	4.626997	-0.035972
C	-1.339860	3.681468	-1.580989
C	1.139927	3.847405	-1.544563
H	1.498511	2.060577	2.342528
H	1.667019	3.706245	1.681079
C	3.947048	2.673334	0.644041
C	4.596917	1.185846	-1.114347
H	4.207888	-1.166314	0.632059
H	2.674752	-0.917855	1.518990
H	3.687493	-2.343460	1.853577
H	4.126760	-3.995112	0.071904
H	3.004793	-4.228122	-1.277036
H	4.246677	-2.955581	-1.357176
H	2.496056	-3.689048	-3.183442
H	1.099059	-3.531476	-4.261836
H	2.213470	-2.170808	-4.062134
H	-0.627054	-4.100405	-2.436889
H	0.700902	-4.375427	-1.284785
H	-0.595410	-3.205848	-0.901888
H	-2.689304	4.184117	2.559663
H	-1.114069	4.821955	2.058632
H	-2.349039	4.423517	0.838494
H	-1.836576	2.225343	3.833401
H	-0.475776	1.286485	3.204236
H	-0.261406	3.016450	3.607594
H	-1.230895	2.868697	-2.311830
H	-2.276397	3.497338	-1.040682
H	-1.427799	4.632638	-2.130194
H	0.998064	4.667047	-2.266651
H	2.049965	4.071551	-0.971716
H	1.307880	2.921145	-2.115206
C	4.929594	2.190371	-0.212581
H	4.161793	3.467232	1.359669
H	5.333484	0.784150	-1.810307
H	5.942097	2.595935	-0.181299

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SCF energy in gas phase: -3688.53180242

Thermal correction to Enthalpy in gas phase: 0.936377

Thermal correction to Gibbs Free Energy in gas phase: 0.81079

SCF energy in solvent: -3688.77662265

Co	-0.719432	-0.055227	0.168812
P	-0.915748	-1.864744	-1.040219
P	-1.290015	2.040268	0.479850
B	0.917754	0.559541	-0.716987
B	0.854896	-0.623112	1.309590
N	-2.642472	-0.477316	0.641607
H	-0.391761	-0.444301	1.691674
O	1.812234	-0.147985	-1.535785
O	1.315214	1.904260	-0.743568
O	1.835507	0.176507	1.935709
O	1.273533	-1.967390	1.400279
C	2.613744	0.763095	-2.290433
C	2.560486	2.055079	-1.415690
C	2.684178	-0.673475	2.705605
C	2.601705	-2.017525	1.917113
C	1.951682	0.942963	-3.655277
C	4.001205	0.173094	-2.479146
C	2.537844	3.358383	-2.197839
C	3.650902	2.105783	-0.352183
C	4.074166	-0.070402	2.798456
C	2.077083	-0.771949	4.105717
C	3.568599	-2.074931	0.737917
C	2.751232	-3.264883	2.771420
H	2.529915	1.608326	-4.298176
H	1.879802	-0.027871	-4.147027
H	0.943116	1.343505	-3.552864
H	3.931777	-0.744709	-3.065124
H	4.645671	0.872447	-3.016604
H	4.471303	-0.068621	-1.528227
H	2.496517	4.198218	-1.502213
H	3.439639	3.466528	-2.804660
H	1.667510	3.415682	-2.850118
H	4.640495	2.252697	-0.788362
H	3.441395	2.933096	0.326649
H	3.644979	1.191521	0.237710
H	4.023243	0.889062	3.315072
H	4.737054	-0.728825	3.364550
H	4.512656	0.096516	1.817362
H	2.701978	-1.359373	4.780388
H	1.978966	0.234983	4.513396
H	1.083317	-1.220776	4.068439
H	3.340964	-2.955598	0.135201
H	3.446076	-1.202017	0.098770
H	4.606525	-2.145921	1.067429
H	3.725274	-3.279908	3.265972
H	1.972450	-3.323107	3.529885
H	2.678121	-4.152106	2.140472
C	-1.906804	-1.847147	-2.620232
C	-2.018815	-2.756178	0.153305
C	0.367369	-3.176046	-1.376989
C	-1.220094	3.432593	-0.752172
C	-0.787173	2.892001	2.055200
C	-3.116961	1.893092	0.740334
C	-3.511596	0.475061	1.026435
C	-3.000346	-1.774050	0.717537
H	-1.849064	-2.863390	-3.047732
C	-1.292211	-0.850062	-3.607081
C	-3.383007	-1.497845	-2.411717
H	-2.539689	-3.639022	-0.244758

H	-1.337735	-3.089669	0.953724
H	1.067002	-3.023635	-0.544164
C	-0.170705	-4.610086	-1.305586
C	1.135142	-2.986023	-2.688506
H	-0.158315	3.712698	-0.752797
C	-2.055965	4.666187	-0.401713
C	-1.549290	2.916158	-2.152285
H	-1.451562	3.766937	2.157744
C	0.665165	3.375727	2.019831
C	-1.019091	1.982681	3.265629
H	-3.603993	2.174333	-0.208641
H	-3.502698	2.579248	1.508132
C	-4.745081	0.149382	1.587192
C	-4.221310	-2.162352	1.262626
H	-1.377830	0.169055	-3.202530
H	-0.229069	-1.037795	-3.795321
H	-1.823774	-0.887991	-4.571430
H	-3.897215	-1.462739	-3.385459
H	-3.914018	-2.228676	-1.784965
H	-3.487670	-0.505102	-1.945525
H	-0.988620	-4.782434	-2.025681
H	0.635686	-5.316396	-1.560561
H	-0.532729	-4.882128	-0.304767
H	1.978927	-3.694291	-2.717636
H	0.503464	-3.201174	-3.565774
H	1.541750	-1.971985	-2.769861
H	-1.912226	5.445491	-1.167357
H	-3.134817	4.442497	-0.370477
H	-1.773682	5.105695	0.565622
H	-1.421103	3.716634	-2.898444
H	-0.890500	2.078704	-2.416439
H	-2.590461	2.558721	-2.229598
H	1.349680	2.525871	1.887228
H	0.845770	4.090720	1.203849
H	0.910420	3.879649	2.968940
H	-0.861331	2.551173	4.196085
H	-2.040328	1.570374	3.298259
H	-0.313676	1.140447	3.256266
C	-5.099423	-1.187630	1.721755
H	-5.419934	0.946825	1.898673
H	-4.471255	-3.221792	1.320076
H	-6.058874	-1.466283	2.160653

$TS_{25\text{-}11}$

SCF energy in gas phase: -3688.51713621

Thermal correction to Enthalpy in gas phase: 0.935821

Thermal correction to Gibbs Free Energy in gas phase: 0.807609

SCF energy in solvent: -3688.76308326

Co	1.012325	-0.113931	0.049919
P	0.946990	-1.366837	1.791935
P	1.616880	1.187041	-1.515719
B	-0.313056	1.224982	0.674087
B	-1.575371	-1.779324	-1.020349
N	2.509581	-1.318180	-0.558439
H	-0.396920	-1.835301	-0.844366
O	-1.714957	1.241445	0.514204
O	0.027063	2.416807	1.343423
O	-2.141557	-1.081192	-2.042074
O	-2.486989	-2.458085	-0.264102
C	-2.305100	2.354817	1.193358
C	-1.083158	3.307051	1.423119

C	-3.541983	-1.402993	-2.088561
C	-3.804841	-2.022567	-0.666626
C	-2.921085	1.871516	2.504066
C	-3.408078	2.923367	0.311389
C	-1.049359	4.004196	2.775657
C	-0.937184	4.360669	0.327211
C	-4.311272	-0.126473	-2.377994
C	-3.725109	-2.399358	-3.228161
C	-4.262149	-0.992301	0.355740
C	-4.736560	-3.220577	-0.656438
H	-3.447091	2.682790	3.010268
H	-3.637415	1.075298	2.301187
H	-2.162473	1.478404	3.177477
H	-4.222965	2.200799	0.237598
H	-3.815308	3.844251	0.734727
H	-3.046968	3.128442	-0.695192
H	-0.159269	4.632442	2.832386
H	-1.925399	4.642351	2.912368
H	-1.006192	3.288034	3.593911
H	-1.725004	5.113424	0.388370
H	0.024850	4.861677	0.443542
H	-0.972655	3.907662	-0.662844
H	-4.058849	0.228857	-3.377683
H	-5.387901	-0.304436	-2.339623
H	-4.053296	0.655094	-1.665972
H	-4.774869	-2.662389	-3.365015
H	-3.357545	-1.948661	-4.150322
H	-3.156345	-3.312496	-3.048460
H	-4.275799	-1.455137	1.342811
H	-3.568691	-0.152964	0.382908
H	-5.265993	-0.628479	0.130999
H	-5.726139	-2.936497	-1.020289
H	-4.358200	-4.034214	-1.272355
H	-4.843096	-3.587484	0.364839
C	2.028561	-0.832793	3.199194
C	1.809303	-2.885333	1.167450
C	-0.517908	-2.204625	2.571077
C	2.072590	2.951298	-1.187970
C	0.699571	1.263185	-3.125011
C	3.234406	0.469006	-2.050191
C	3.349954	-0.943289	-1.553685
C	2.705854	-2.527065	0.018843
H	2.147273	-1.690259	3.883090
C	1.393357	0.335675	3.959872
C	3.410768	-0.439041	2.667636
H	2.370039	-3.443370	1.933195
H	1.013265	-3.553506	0.799966
H	-0.881400	-2.830699	1.738496
C	-0.181674	-3.116760	3.753366
C	-1.658063	-1.250000	2.908939
H	1.107921	3.425182	-0.961986
C	2.721250	3.696519	-2.356203
C	2.923017	3.045991	0.082408
H	1.303706	1.866751	-3.823287
C	-0.663249	1.934990	-2.935879
C	0.555154	-0.140930	-3.718342
H	4.031094	1.053222	-1.562094
H	3.417168	0.529767	-3.133023
C	4.334619	-1.793570	-2.051065
C	3.690352	-3.409888	-0.421095
H	1.159260	1.166938	3.275638
H	0.463197	0.040121	4.466806

H	2.086267	0.706077	4.732494
H	4.054509	-0.105847	3.497303
H	3.920597	-1.275764	2.165320
H	3.321175	0.382890	1.939791
H	0.127736	-2.532230	4.634468
H	-1.069963	-3.699535	4.045440
H	0.622148	-3.833041	3.524548
H	-2.557574	-1.822955	3.187334
H	-1.410372	-0.596071	3.758407
H	-1.904671	-0.617946	2.048685
H	2.969383	4.727112	-2.055242
H	3.661299	3.217221	-2.676252
H	2.061115	3.762766	-3.233077
H	3.066140	4.101924	0.363475
H	2.432390	2.528286	0.917212
H	3.926222	2.611210	-0.063682
H	-1.257764	1.408265	-2.173869
H	-0.556089	2.987212	-2.628781
H	-1.229103	1.924229	-3.881257
H	0.009270	-0.091894	-4.674158
H	1.530692	-0.610624	-3.918588
H	-0.011468	-0.796623	-3.045281
C	4.505353	-3.051282	-1.486429
H	4.973674	-1.449724	-2.864836
H	3.801236	-4.374884	0.074250
H	5.272871	-3.732031	-1.858086