SUPPORTING INFORMATION PART 2

Integrating Metal-Catalyzed C–H and C–O Functionalization to Achieve Sterically Controlled Regioselectivity in Arene Acylation

*Nicholas A. Serratore, Constance B. Anderson, Grant B. Frost, Truong-Giang Hoang, Steven J. Underwood, Philipp M. Gemmel, Melissa A. Hardy, Christopher J. Douglas**

*E-mail: cdouglas@umn.edu

Department of Chemistry, University of Minnesota - Twin Cities, 207 Pleasant Street SE, Minneapolis, MN 55455, USA

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Computations: All computed structures were optimized in the gas phase and verified as minima or first-order saddle points by calculations of the full Hessian using Gaussian 09[1] and 16[2]. All geometries reported are M06, M06-L, and M15-L (closed-shell species) with the SDD basis set for iridium and 6-31G(d,p) basis set for H, C, O, and P atoms. Electronic energies were further evaluated with the SDD basis set for iridium and 6-311+G(2df,2pd) basis set on H, C, O, and P atoms and SMD solvation for structures below (solvent was toluene unless otherwise specified). All ZPE, enthalpic, and entropic free energy corrections (unscaled) utilize values computed at the lower basis set level at 443.15 K and 1 atm.

1. Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

2. Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

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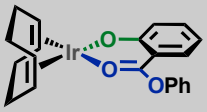
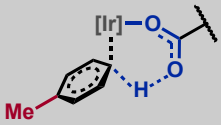
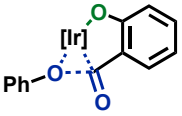
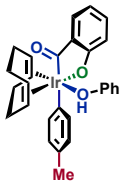
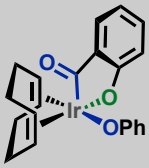
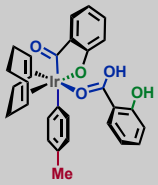
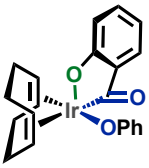
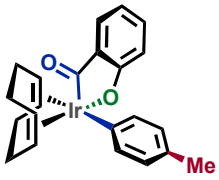
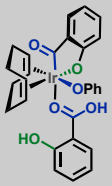
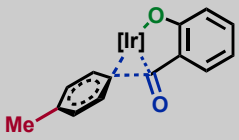
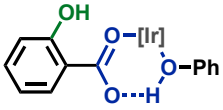
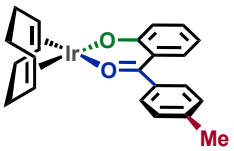
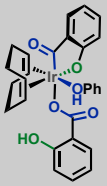
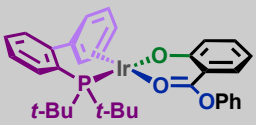
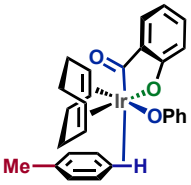
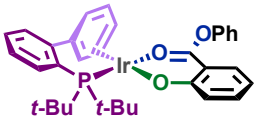
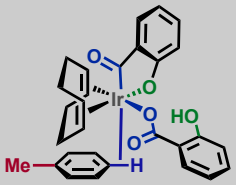
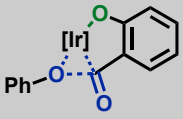
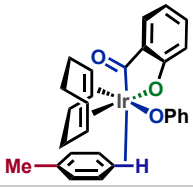
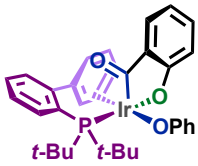
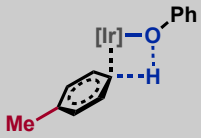
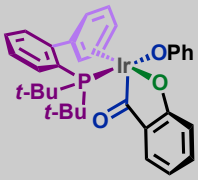
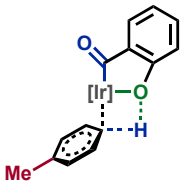
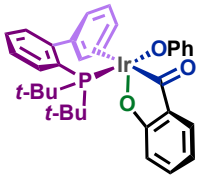
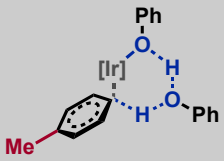
I		N	
C		XV	
III[1]		XVI	
III[2]		VII	
X		H	
L		VIII	
XIV		XIII[1]	
XI		XIII[2]	

XII		**C_{JP}**	 with JohnPhos
VI		**V_{JP}^1**	
G		**V_{JP}^2**	
G^2		**V_{JP}^3**	
G-phenol			

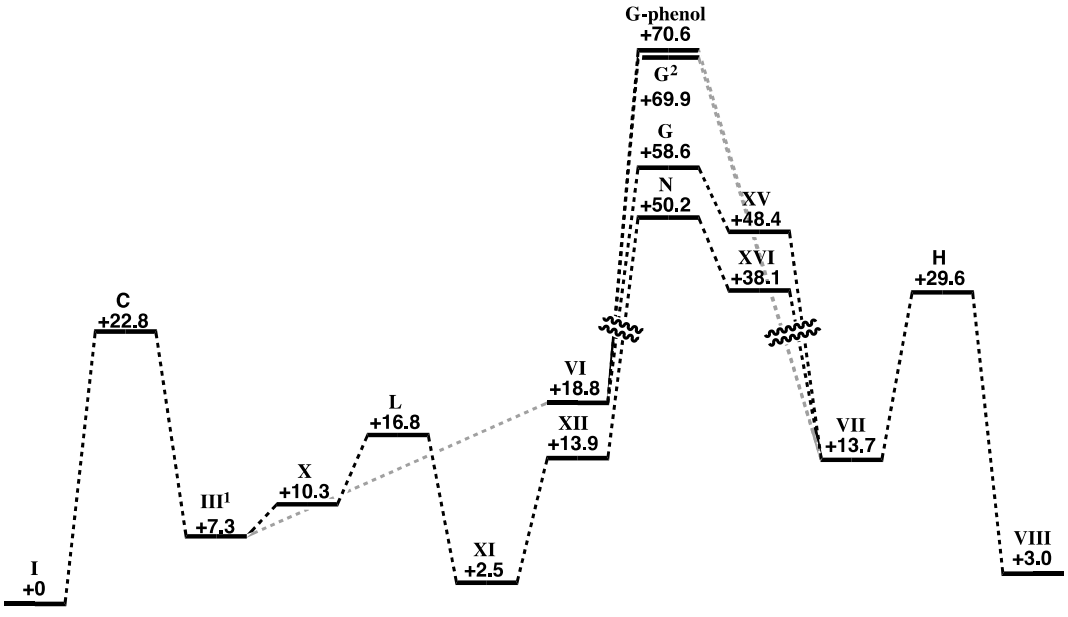


Table 1. Relative Energies of Catalytic Intermediates and Transition States Using M06-L Functional

Structure	Relative Gibbs Energy (kcal)	Structure	Relative Gibbs Energy (kcal)
I	0	**N**	+50.2
C	+22.8	**XV**	+48.4
III^1	+7.3	**XVI**	+38.1
III^2	+26.3	**VII**	+13.7
X	+10.4	**H**	+29.6
L	+16.8	**VIII**	+3.0
XIV	–	**XIII^1**	+11.3
XI	+2.5	**XIII^2**	+15.2
XII	+13.9	**C$_{JP}$**	+44.7
VI	+18.8	**V$_{JP}^1$**	+16.4
G	+58.6	**V$_{JP}^2$**	+16.6
G^2	+69.9	**V$_{JP}^3$**	+22.0
G-phenol	+70.6		

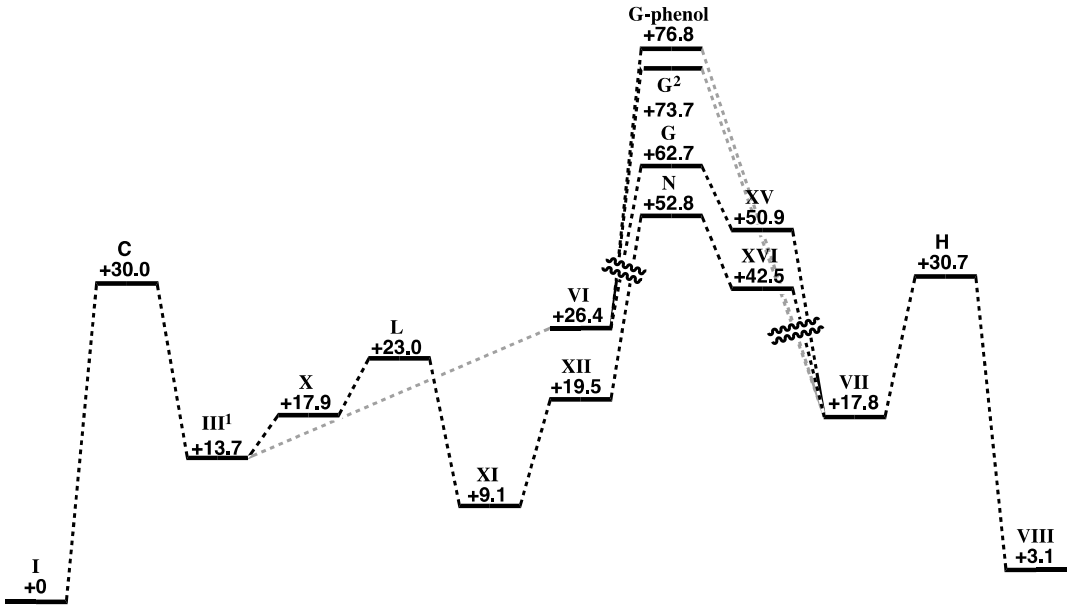


Table 2. Relative Energies of Catalytic Intermediates and Transition States Using M06 Functional

Structure	Relative Gibbs Energy (kcal)	Structure	Relative Gibbs Energy (kcal)
I	0	**N**	+52.8
C	+30.0	**XV**	+50.9
III^1	+13.7	**XVI**	+42.5
III^2	+32.6	**VII**	+17.8
X	+17.9	**H**	+30.7
L	+23.0	**VIII**	+3.1
XIV	–	**XIII^1**	+14.3
XI	+9.1	**XIII^2**	+15.0
XII	+19.5	**C$_{JP}$**	+50.3
VI	+26.4	**V$_{JP}^1$**	+25.0
G	+62.7	**V$_{JP}^2$**	+23.5
G^2	+73.7	**V$_{JP}^3$**	+31.6
G-phenol	+76.8		

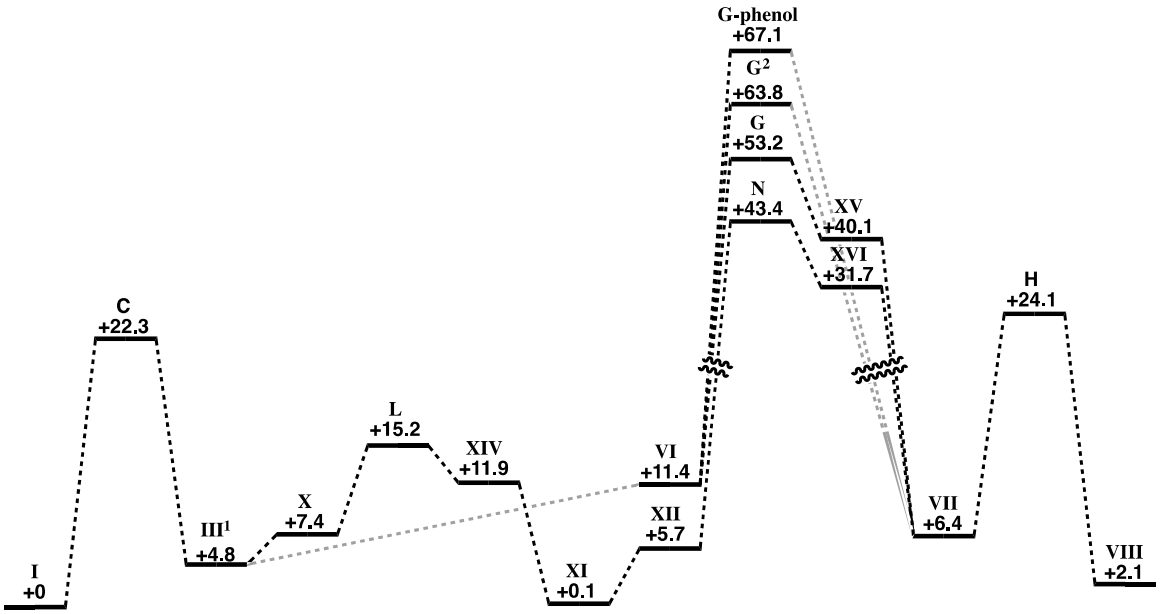


Table 3. Relative Energies of Catalytic Intermediates and Transition States Using M15-L Functional

Structure	Relative Gibbs Energy (kcal)	Structure	Relative Gibbs Energy (kcal)
I	0	**N**	+43.4
C	+22.3	**XV**	+40.1
III^1	+4.8	**XVI**	+31.7
III^2	+23.6	**VII**	+6.4
X	+7.4	**H**	+24.1
L	+15.2	**VIII**	+2.1
XIV	+11.9	**XIII^1**	+9.6
XI	+0.1	**XIII^2**	+14.0
XII	+5.7	**C$_{JP}$**	+44.6
VI	+11.4	**V$_{JP}^1$**	+15.1
G	+53.2	**V$_{JP}^2$**	+15.8
G^2	+63.8	**V$_{JP}^3$**	+20.8
G-phenol	+67.1		

1: M06L/6-311+G(2df,2pd) SCF= -727.2545534 hartree (solvent=toluene)
SCF= -727.2540142 hartree (solvent=*m*-xylene)
SCF= -727.2542687 hartree (solvent=anisole)
Gibbs correction= 0.131871 hartree
Total Gibbs Energy= -727.1226824 hartree (solvent=toluene)
Total Gibbs Energy= -727.1221432 hartree (solvent=*m*-xylene)
Total Gibbs Energy= -727.1223977 hartree (solvent=anisole)

C	3.27969	-1.84868	0.37616
C	1.96693	-1.42654	0.28687
C	1.65388	-0.08442	0.00788
C	2.70773	0.84565	-0.18372
C	4.03521	0.40538	-0.09178
C	4.31171	-0.92144	0.18420
H	3.50759	-2.88703	0.59281
H	1.15055	-2.12589	0.43211
H	4.82502	1.13373	-0.24251
H	5.34720	-1.24433	0.25221
O	2.50241	2.14024	-0.45182
H	1.52971	2.27875	-0.47961
C	0.27668	0.38891	-0.08791
O	-0.04753	1.55026	-0.31573
O	-0.63175	-0.60551	0.09440
C	-1.99645	-0.32000	0.06002
C	-2.78087	-1.18681	-0.69116
C	-2.55999	0.71096	0.80455
C	-4.16136	-1.01388	-0.70341
H	-2.30210	-1.98308	-1.25194
C	-3.94179	0.87276	0.77901
H	-1.92917	1.37528	1.38226
C	-4.74470	0.01681	0.02875
H	-4.77999	-1.68816	-1.28831
H	-4.39182	1.67649	1.35445
H	-5.82195	0.15201	0.01683

2am1: M06L/6-311+G(2df,2pd) SCF= -691.3283533 hartree
Gibbs correction= 0.15372 hartree
Total Gibbs Energy= -691.1746333 hartree

C	-3.71778	0.34692	0.07952
C	-2.72500	1.10469	0.70583
C	-1.38851	0.72560	0.65078
C	-1.00944	-0.44171	-0.02266
C	-2.00771	-1.22548	-0.61789
C	-3.33387	-0.82792	-0.58135
H	-3.00635	2.00304	1.25088
H	-0.63945	1.31854	1.16819
H	-1.71475	-2.15096	-1.10487
H	-4.09419	-1.43972	-1.06248
C	-5.15243	0.77475	0.10735
H	-5.32929	1.55202	0.85470

H	-5.46489	1.17797	-0.86268
H	-5.81942	-0.06443	0.32644
C	0.38376	-0.95824	-0.04202
O	0.54571	-2.19375	-0.00089
C	1.53757	-0.05443	-0.09684
C	1.43001	1.30018	-0.47009
C	2.83344	-0.56974	0.19077
C	2.53281	2.13316	-0.50563
H	0.45795	1.68405	-0.76373
C	3.94075	0.28989	0.18572
C	3.78838	1.62127	-0.15628
H	2.42610	3.16986	-0.80759
H	4.91091	-0.12881	0.43235
H	4.66032	2.26993	-0.17138
O	3.04891	-1.85493	0.48035
H	2.18423	-2.31564	0.34132

Phenol: M06L/6-311+G(2df,2pd) SCF= -307.5365093 hartree (solvent=toluene)
SCF= -307.5361959 hartree (solvent=*m*-xylene)
SCF= -307.5369823 hartree (solvent=anisole)
Gibbs correction= 0.057576 hartree
Total Gibbs Energy= -307.4789333 hartree (solvent=toluene)
Total Gibbs Energy= -307.4786199 hartree (solvent=*m*-xylene)
Total Gibbs Energy= -307.4794063 hartree (solvent=anisole)

C	-1.85230	0.02702	0.00005
C	-1.12897	1.21578	0.00005
C	0.26288	1.19710	-0.00012
C	0.94005	-0.02405	-0.00025
C	0.22129	-1.22148	-0.00007
C	-1.16712	-1.18767	0.00006
H	-2.93749	0.04555	0.00010
H	-1.64721	2.17079	0.00009
H	0.82589	2.12889	-0.00007
H	0.76784	-2.15911	-0.00012
H	-1.72027	-2.12291	0.00012
O	2.29933	-0.11059	0.00013
H	2.66165	0.78127	0.00054

***m*-xylene**: M06L/6-311+G(2df,2pd) SCF= -310.9401098 hartree
Gibbs correction= 0.099063 hartree
Total Gibbs Energy= -310.8410468 hartree

C	0.00067	-0.94803	-0.01771
C	-1.22135	-0.27248	-0.00876
C	-1.20700	1.12566	0.00068
C	-0.00123	1.81836	0.00449
C	1.20628	1.12674	-0.00163
C	1.22272	-0.27028	-0.01011
C	-2.51670	-1.02720	0.00856
H	-2.14872	1.67076	-0.00185

H	2.14757	1.67248	-0.00552
C	2.51749	-1.02591	0.00966
H	0.00072	-2.03797	-0.03536
H	-2.39127	-2.05457	-0.34341
H	-3.27457	-0.54666	-0.61720
H	-2.93342	-1.08242	1.02111
H	3.32468	-0.45824	-0.46142
H	2.43421	-1.98646	-0.50655
H	2.83755	-1.24335	1.03549
H	-0.00200	2.90524	0.00364

2aa1: M06L/6-311+G(2df,2pd) SCF= -730.6517722 hartree
Gibbs correction= 0.173938 hartree
Total Gibbs Energy= -730.4778342 hartree

C	3.49761	0.53975	-0.01472
C	2.49410	1.38983	-0.47625
C	1.17807	0.91651	-0.49641
C	0.87975	-0.38427	-0.08357
C	1.91609	-1.22574	0.34154
C	3.22908	-0.77174	0.39931
C	2.80913	2.77792	-0.94754
H	0.38599	1.55815	-0.87626
H	1.67097	-2.24635	0.62430
C	4.33584	-1.65586	0.88949
C	-0.48728	-0.96500	-0.17845
O	-0.58739	-2.16227	-0.50996
C	-1.68328	-0.16209	0.09653
C	-1.63453	1.07593	0.76826
C	-2.95852	-0.66881	-0.28413
C	-2.77693	1.81610	1.00951
H	-0.67467	1.43653	1.12474
C	-4.10770	0.10370	-0.06535
C	-4.01389	1.32807	0.57089
H	-2.71512	2.76139	1.53864
H	-5.06158	-0.30076	-0.38771
H	-4.91700	1.90662	0.74704
O	-3.11573	-1.86298	-0.85945
H	-2.22423	-2.29279	-0.84581
H	4.52474	0.90339	0.01288
H	3.87595	2.99907	-0.86411
H	2.26732	3.53314	-0.36852
H	2.52161	2.92119	-1.99439
H	4.00025	-2.68792	1.01461
H	4.72105	-1.31585	1.85721
H	5.18434	-1.65962	0.19810

2aa2: M06L/6-311+G(2df,2pd) SCF= -730.6509883 hartree
Gibbs correction= 0.176724 hartree
Total Gibbs Energy= -730.4742643 hartree

C	-3.54230	-0.73471	-0.17476
C	-2.49958	-1.44816	-0.76960
C	-1.20453	-0.95121	-0.73791
C	-0.91058	0.27906	-0.13482
C	-1.95541	1.02803	0.44966
C	-3.24073	0.48715	0.43276
H	-2.70407	-2.39943	-1.25550
H	-0.40179	-1.51176	-1.21000
C	-1.73020	2.35960	1.10055
H	-4.04358	1.04793	0.91064
C	-4.94882	-1.24792	-0.20770
H	-5.48005	-0.88734	-1.09625
H	-4.98100	-2.34029	-0.23949
H	-5.52202	-0.91486	0.66168
C	0.46852	0.83063	-0.21188
O	0.61419	2.03434	-0.50368
C	1.63646	-0.02587	0.02517
C	1.53732	-1.29935	0.62130
C	2.93260	0.45711	-0.31332
C	2.65106	-2.08994	0.83380
H	0.55960	-1.65046	0.93695
C	4.05323	-0.36292	-0.12060
C	3.91023	-1.61749	0.44342
H	2.55001	-3.06327	1.30260
H	5.02433	0.02698	-0.40760
H	4.79140	-2.23468	0.59830
O	3.13699	1.67411	-0.82248
H	2.25703	2.12721	-0.80824
H	-2.58257	2.62869	1.72980
H	-1.59276	3.14513	0.35289
H	-0.82757	2.37444	1.71709

1,2-Dimethoxybenzene: M06L/6-311+G(2df,2pd) SCF= -461.3853036 hartree
Gibbs correction= 0.108249 hartree
Total Gibbs Energy= -461.2770546 hartree

C	0.70703	-0.13818	-0.00001
C	1.39256	1.07124	0.00030
C	0.69260	2.28190	0.00023
C	-0.69193	2.28209	-0.00013
C	-1.39226	1.07166	-0.00039
C	-0.70713	-0.13797	-0.00028
H	2.47715	1.07743	0.00071
H	1.24493	3.21666	0.00049
H	-2.47686	1.07820	-0.00072
O	1.28962	-1.36806	0.00003
O	-1.28999	-1.36770	-0.00068
C	2.69915	-1.39636	-0.00005
H	2.98228	-2.44902	-0.00055
H	3.11734	-0.90906	-0.89141

H	3.11735	-0.90981	0.89173
C	-2.69954	-1.39588	0.00069
H	-3.11852	-0.90932	-0.89071
H	-2.98274	-2.44852	0.00128
H	-3.11685	-0.90858	0.89242
H	-1.24398	3.21703	-0.00021

2ag: M06L/6-311+G(2df,2pd) SCF= -881.100121 hartree
Gibbs correction= 0.18436 hartree
Total Gibbs Energy= -880.915761 hartree

C	-2.85974	-0.73244	-0.16487
C	-1.80234	-1.57024	-0.50603
C	-0.49046	-1.09863	-0.48483
C	-0.22095	0.22514	-0.13681
C	-1.29468	1.08195	0.17011
C	-2.59806	0.61906	0.17747
H	-1.99692	-2.59587	-0.79898
H	0.31480	-1.75960	-0.78809
H	-1.06500	2.11752	0.39410
C	1.13049	0.82799	-0.19099
O	1.22202	2.03848	-0.48363
C	2.34045	0.03845	0.07582
C	2.31844	-1.18911	0.76652
C	3.60367	0.55476	-0.32978
C	3.47285	-1.91618	0.99430
H	1.37095	-1.55099	1.15312
C	4.76381	-0.20573	-0.12839
C	4.69532	-1.42430	0.52274
H	3.43043	-2.85318	1.54003
H	5.70725	0.20512	-0.47286
H	5.60744	-1.99208	0.68726
O	3.73936	1.74808	-0.91439
H	2.84809	2.17577	-0.86731
O	-4.16246	-1.09515	-0.13833
O	-3.69141	1.36063	0.48498
C	-4.46006	-2.43507	-0.47763
H	-5.54137	-2.53507	-0.39019
H	-4.15572	-2.66879	-1.50583
H	-3.97255	-3.14244	0.20536
C	-3.45883	2.71737	0.80744
H	-4.43621	3.14843	1.02219
H	-2.81398	2.81839	1.69003
H	-2.99685	3.25834	-0.02823

Toluene: M06L/6-311+G(2df,2pd) SCF= -271.6160472 hartree
Gibbs correction= 0.078037 hartree
Total Gibbs Energy= -271.5380102 hartree

C	-0.91280	0.00012	-0.01064
C	-0.19480	-1.19968	-0.00843

C	1.19676	-1.20268	0.00212
C	1.89862	-0.00008	0.00822
C	1.19696	1.20258	0.00212
C	-0.19466	1.19975	-0.00843
H	-0.73813	-2.14278	-0.01781
H	1.73466	-2.14703	0.00082
H	2.98498	-0.00018	0.01276
H	1.73495	2.14687	0.00082
H	-0.73785	2.14292	-0.01781
C	-2.41215	0.00006	0.00825
H	-2.82353	-0.88128	-0.49208
H	-2.79931	-0.00702	1.03414
H	-2.82341	0.88810	-0.48012

1,5-COD: M06L/6-311+G(2df,2pd) SCF= -312.0836913 hartree
Gibbs correction= 0.126543 hartree
Total Gibbs Energy= -311.9571483 hartree

C	-0.87337	-1.63240	-0.20553
C	0.38687	-1.81077	0.20178
C	-0.38687	1.81077	-0.20178
C	1.23043	-0.79727	0.92077
C	0.87337	1.63240	0.20553
C	1.68805	0.38396	0.02243
H	-1.35117	-2.44733	-0.74834
H	0.67943	-0.38735	1.77846
H	-0.86565	2.76120	0.03168
H	1.35117	2.44733	0.74834
H	0.86565	-2.76120	-0.03168
H	2.11036	-1.29705	1.33850
H	2.73926	0.61005	0.22829
H	1.64811	0.05763	-1.02599
C	-1.68805	-0.38396	-0.02243
H	-1.64811	-0.05763	1.02599
H	-2.73926	-0.61005	-0.22829
C	-1.23043	0.79727	-0.92077
H	-0.67943	0.38735	-1.77846
H	-2.11036	1.29705	-1.33850

JohnPhos: M06L/6-311+G(2df,2pd) SCF= -1119.901881 hartree
Gibbs correction= 0.329089 hartree
Total Gibbs Energy= -1119.572792 hartree

C	0.99116	3.63977	0.06180
C	1.80302	2.51888	-0.03907
C	1.26918	1.22648	-0.16627
C	-0.13776	1.05742	-0.15335
C	-0.93374	2.20825	-0.04157
C	-0.39127	3.48421	0.05225
H	1.43548	4.62800	0.14264
H	2.88479	2.63170	-0.04782

H	-2.01348	2.09960	-0.00664
H	-1.04557	4.34811	0.13165
C	2.24112	0.11050	-0.28694
C	3.26977	-0.01243	0.65572
C	2.20742	-0.79568	-1.35443
C	4.22070	-1.02317	0.55209
H	3.30458	0.68517	1.49038
C	3.16273	-1.79886	-1.46601
H	1.42573	-0.70353	-2.10334
C	4.16898	-1.92127	-0.50973
H	5.00134	-1.10879	1.30309
H	3.12153	-2.48863	-2.30448
H	4.91023	-2.71104	-0.59478
P	-0.85304	-0.65072	-0.17339
C	-2.46771	-0.52260	-1.18732
C	-1.27601	-0.86471	1.67219
C	-2.07821	-2.15783	1.82922
H	-2.16309	-2.41531	2.89259
H	-3.09693	-2.06618	1.43826
H	-1.59472	-2.99945	1.32082
C	0.08437	-1.04849	2.35686
H	0.66122	-1.86591	1.91106
H	0.69187	-0.13872	2.29424
H	-0.06350	-1.27377	3.42080
C	-2.00522	0.28657	2.36047
H	-2.99335	0.48178	1.93619
H	-2.15033	0.04289	3.42151
H	-1.42796	1.21480	2.31766
C	-2.77793	-1.96856	-1.60541
H	-3.01021	-2.60796	-0.74802
H	-3.64966	-1.98377	-2.27246
H	-1.93518	-2.42116	-2.13650
C	-3.72887	0.05538	-0.54469
H	-4.54880	0.02948	-1.27520
H	-4.05653	-0.52838	0.32071
H	-3.62238	1.09531	-0.22510
C	-2.13699	0.26516	-2.45890
H	-2.95517	0.15687	-3.18210
H	-1.99879	1.33266	-2.26742
H	-1.22394	-0.10706	-2.93844

II: M06L/6-311+G(2df,2pd) SCF= -535.4814154 hartree
Gibbs correction= 0.089398 hartree
Total Gibbs Energy= -535.3920174 hartree

C	-2.89659	-0.66942	-0.00009
C	-1.98426	-1.73172	0.00007
C	-0.62925	-1.45805	0.00013
C	-0.15735	-0.13445	0.00007
C	-1.09009	0.93299	-0.00003

C	-2.46160	0.64388	-0.00014
H	-3.96395	-0.87440	-0.00015
H	-2.33631	-2.75803	0.00014
H	0.09820	-2.26311	0.00025
H	-3.15826	1.47561	-0.00025
C	1.26971	0.17792	0.00014
O	1.73458	1.31858	0.00025
O	2.06257	-0.90924	-0.00002
O	-0.72599	2.22086	-0.00005
H	0.25760	2.24039	0.00001
C	3.46426	-0.62343	-0.00024
H	3.74139	-0.04868	0.88637
H	3.96200	-1.59155	-0.00055
H	3.74101	-0.04822	-0.88668

Methanol: M06L/6-311+G(2df,2pd) SCF= -115.7493009 hartree
Gibbs correction= 0.015199 hartree
Total Gibbs Energy= -115.7341019 hartree

O	-0.74563	0.12120	0.00000
C	0.65521	-0.01898	0.00000
H	1.03884	-0.54042	-0.89053
H	1.03884	-0.54041	0.89053
H	1.07700	0.98854	-0.00000
H	-1.12086	-0.76342	0.00000

[Ir(cod)OMe]$_2$: M06L/6-311+G(2df,2pd)(SDD) SCF= -1063.519213 hartree
Gibbs correction= 0.354631 hartree
Total Gibbs Energy= -1063.164582 hartree

C	-2.24731	-1.57942	0.72429
C	-3.06785	-1.31240	-0.41711
C	-2.44603	1.10833	1.25575
C	-4.44853	-0.68258	-0.30305
C	-3.06159	1.41220	0.00085
C	-4.38693	0.84317	-0.45426
H	-1.54339	-2.41311	0.64019
H	-5.10645	-1.10266	-1.07040
H	-1.76313	1.85825	1.66334
H	-2.81508	2.37747	-0.45055
H	-2.92803	-1.96238	-1.28437
H	-4.90233	-0.96138	0.65576
H	-4.51052	1.10459	-1.51135
H	-5.22271	1.32458	0.07621
C	-2.62032	-1.24192	2.14961
H	-1.72283	-1.38512	2.76337
H	-3.37053	-1.94742	2.53814
C	-3.09996	0.20713	2.29200
H	-4.19086	0.26835	2.19841
H	-2.87099	0.57588	3.29698
C	2.24688	-1.57896	0.72533

C	3.06733	-1.31303	-0.41639
C	2.44656	1.10906	1.25503
C	4.44824	-0.68359	-0.30293
C	3.06203	1.41185	-0.00017
C	4.38711	0.84207	-0.45513
H	1.54262	-2.41244	0.64193
H	4.90207	-0.96192	0.65600
H	1.76404	1.85954	1.66223
H	2.81576	2.37687	-0.45223
H	2.92715	-1.96359	-1.28316
H	5.10592	-1.10438	-1.07010
H	5.22313	1.32357	0.07490
H	4.51060	1.10276	-1.51241
C	2.62027	-1.24067	2.15037
H	3.37033	-1.94616	2.53918
H	1.72284	-1.38321	2.76439
C	3.10036	0.20833	2.29177
H	2.87165	0.57778	3.29655
H	4.19127	0.26915	2.19800
Ir	1.48280	0.07146	-0.30352
Ir	-1.48283	0.07145	-0.30360
O	-0.00001	-0.98786	-1.38986
O	0.00001	1.51893	-0.80647
C	0.00007	-2.36502	-1.65515
H	-0.88866	-2.63196	-2.24154
H	0.88717	-2.63122	-2.24434
H	0.00177	-2.98376	-0.74393
C	-0.00003	2.83618	-0.32171
H	0.88653	3.37142	-0.68648
H	-0.88534	3.37207	-0.68855
H	-0.00129	2.89102	0.77814

4-CN-Phenol: M06L/6-311+G(2df,2pd)(SDD) SCF= -399.8041429 hartree
Gibbs correction= 0.05112 hartree
Total Gibbs Energy= -399.7530229 hartree

O	-3.06402	0.08689	-0.00002
C	-1.71204	0.01431	-0.00012
C	-1.01930	-1.20078	-0.00005
C	-1.00809	1.22340	-0.00001
C	0.36639	-1.20757	0.00002
H	-1.56819	-2.13977	0.00000
C	0.37461	1.21391	0.00002
H	-1.56526	2.15397	0.00010
C	1.08103	-0.00106	0.00001
H	0.90621	-2.14907	0.00008
H	0.92488	2.14935	0.00009
C	2.50488	-0.00864	0.00003
N	3.67392	-0.01512	-0.00002
H	-3.42778	-0.80520	0.00060

4-CN-Phenyl Salicylate: M06L/6-311+G(2df,2pd)(SDD) SCF= -819.5191559 hartree
Gibbs correction= 0.124986 hartree
Total Gibbs Energy= -819.3941699 hartree

C	3.95720	-1.82504	0.37562
C	2.64176	-1.41610	0.27877
C	2.31803	-0.07428	0.00456
C	3.36463	0.86765	-0.17403
C	4.69531	0.43920	-0.07449
C	4.98175	-0.88619	0.19629
H	4.19402	-2.86203	0.58840
H	1.83231	-2.12519	0.41436
H	5.47922	1.17564	-0.21521
H	6.01953	-1.19974	0.27036
O	3.15133	2.16153	-0.43622
H	2.18020	2.29850	-0.47134
C	0.94157	0.38733	-0.09798
O	0.59900	1.54313	-0.31850
O	0.03595	-0.62455	0.06537
C	-1.32297	-0.36005	0.04339
C	-2.10422	-1.27581	-0.65624
C	-1.89922	0.69630	0.74662
C	-3.48286	-1.13455	-0.66385
H	-1.61951	-2.08902	-1.18550
C	-3.27869	0.83622	0.73429
H	-1.27896	1.39886	1.28739
C	-4.08189	-0.07325	0.03022
H	-4.10328	-1.84057	-1.20570
H	-3.74520	1.65289	1.27526
C	-5.49974	0.07742	0.02488
N	-6.66179	0.19952	0.02122

Salicylic Acid: M06L/6-311+G(2df,2pd)(SDD) SCF= -496.1771106 hartree
Gibbs correction= 0.066832 hartree
Total Gibbs Energy= -496.1102786 hartree

C	-1.89199	-1.46601	0.00009
C	-0.51001	-1.45564	-0.00011
C	0.20392	-0.24486	-0.00023
C	-0.50746	0.98115	-0.00016
C	-1.90877	0.95839	0.00009
C	-2.58489	-0.24865	0.00023
H	-2.43354	-2.40610	0.00015
H	0.05094	-2.38461	-0.00020
H	-2.43492	1.90717	0.00018
H	-3.67169	-0.24694	0.00044
O	0.09611	2.17487	-0.00043
H	3.19849	-1.25615	0.00018
C	1.66054	-0.21227	0.00003
O	2.24537	-1.42637	-0.00027

O	2.34068	0.81473	0.00062
H	1.06543	2.00803	0.00026

I: M06L/6-311+G(2df,2pd)(SDD) SCF= -1143.251047 hartree
Gibbs correction= 0.278996 hartree
Total Gibbs Energy= -1142.972051 hartree

C	3.10525	0.29360	0.76826
C	3.16291	0.14303	-0.64877
C	1.50204	-1.96113	0.73012
C	3.67293	-1.12050	-1.32436
C	1.37238	-1.96310	-0.68945
C	2.52851	-2.08804	-1.65585
H	3.16570	1.31396	1.15307
H	4.20725	-0.85356	-2.24175
H	0.62564	-2.27816	1.29921
H	0.40900	-2.29101	-1.08985
H	3.25909	1.06150	-1.23072
H	4.41758	-1.60477	-0.68148
H	2.14644	-1.86095	-2.65789
H	2.89381	-3.12536	-1.70027
C	3.48503	-0.78078	1.76099
H	3.14717	-0.44889	2.74935
H	4.57930	-0.87503	1.83220
C	2.83831	-2.13414	1.43519
H	3.50539	-2.74430	0.81457
H	2.69473	-2.70471	2.35839
Ir	1.17430	0.00351	0.02007
O	0.90126	2.06043	-0.03755
C	-0.22528	2.71007	-0.05510
C	-1.55006	2.14527	-0.04743
C	-0.13177	4.12918	-0.09155
C	-2.67254	3.01382	-0.08631
C	-1.24318	4.93580	-0.12595
H	0.87057	4.54534	-0.09455
C	-2.53604	4.37968	-0.12510
H	-3.66123	2.56955	-0.08373
H	-1.11877	6.01581	-0.15518
H	-3.41277	5.01821	-0.15415
C	-1.78197	0.72700	-0.00052
O	-0.94389	-0.19976	0.04394
O	-3.09393	0.38728	0.01046
C	-3.46366	-0.95786	-0.00486
C	-4.33159	-1.37502	0.99537
C	-3.06385	-1.81298	-1.02629
C	-4.80548	-2.68400	0.97665
H	-4.62491	-0.67397	1.77000
C	-3.54231	-3.11903	-1.02980
H	-2.38888	-1.45928	-1.79802
C	-4.41051	-3.55833	-0.03190

H	-5.48454	-3.01813	1.75557
H	-3.23427	-3.79603	-1.82136
H	-4.77965	-4.57938	-0.04324

C: M06L/6-311+G(2df,2pd)(SDD) SCF= -1143.214579 hartree
Gibbs correction= 0.278913 hartree
Total Gibbs Energy= -1142.935666 hartree

C	-2.34105	0.01696	1.66484
C	-2.24453	-1.21768	0.96227
C	-2.54052	1.20054	-0.84990
C	-3.30376	-1.69686	-0.01479
C	-2.21074	0.00893	-1.54457
C	-2.98136	-1.28684	-1.45915
H	-1.79931	0.07861	2.61103
H	-3.38709	-2.78619	0.04560
H	-2.15840	2.13235	-1.27171
H	-1.59387	0.11155	-2.43835
H	-1.63050	-1.99472	1.42148
H	-4.28111	-1.30654	0.29231
H	-2.36146	-2.06031	-1.92507
H	-3.90064	-1.22900	-2.06013
C	-3.46794	1.01071	1.50317
H	-3.16889	1.93274	2.01446
H	-4.37249	0.66075	2.02241
C	-3.77290	1.32690	0.03141
H	-4.56197	0.66891	-0.35095
H	-4.17406	2.34192	-0.04855
Ir	-0.92566	0.20601	0.12757
O	0.58782	-0.30964	1.48367
C	1.57975	-1.04198	1.05935
C	1.63747	-1.56746	-0.26328
C	2.63970	-1.38435	1.93107
C	2.65014	-2.46860	-0.65187
C	3.63915	-2.24550	1.52372
H	2.62483	-0.96718	2.93287
C	3.64966	-2.80899	0.23596
H	2.64039	-2.85602	-1.66724
H	4.43313	-2.49951	2.22211
H	4.44000	-3.48979	-0.06203
C	0.72061	-1.13103	-1.28105
O	0.32298	-1.55130	-2.31626
O	0.65003	0.68666	-1.27128
C	1.75614	1.34270	-0.80560
C	3.01074	1.06418	-1.35537
C	1.63047	2.31424	0.19064
C	4.12946	1.75186	-0.89972
H	3.09408	0.30524	-2.12859
C	2.75467	3.00045	0.63524
H	0.64502	2.50927	0.61236

C	4.00856	2.71931	0.09634
H	5.10340	1.52771	-1.32596
H	2.64972	3.75434	1.41051
H	4.88634	3.25206	0.44971

III[1]: M06L/6-311+G(2df,2pd)(SDD) SCF= -1143.24065 hartree
Gibbs correction= 0.280348 hartree
Total Gibbs Energy= -1142.960302 hartree

C	-1.27882	2.18050	0.35051
C	-0.59065	2.55107	-0.82663
C	1.25400	1.26469	1.22129
C	0.60885	3.48210	-0.82190
C	1.88091	1.42496	-0.02715
C	1.93761	2.71497	-0.81234
H	-2.32477	1.89244	0.23805
H	0.56716	4.12401	-1.70684
H	1.55146	0.39194	1.79779
H	2.63300	0.68006	-0.29605
H	-1.15114	2.48253	-1.76051
H	0.54330	4.15657	0.03850
H	2.22154	2.46985	-1.84202
H	2.74912	3.34750	-0.42451
C	-0.86603	2.61314	1.73450
H	-1.45544	2.04417	2.45853
H	-1.13449	3.66812	1.88906
C	0.62799	2.39349	2.02070
H	1.19592	3.31290	1.83634
H	0.75620	2.17030	3.08350
Ir	-0.04879	0.52010	-0.38735
O	-1.67370	-0.13982	-1.50964
C	-2.46340	-0.92108	-0.82434
C	-2.24970	-1.10559	0.56708
C	-3.56318	-1.58006	-1.41928
C	-3.09403	-1.93109	1.33743
C	-4.37943	-2.38204	-0.64718
H	-3.73590	-1.44690	-2.48213
C	-4.15668	-2.56683	0.73183
H	-2.88721	-2.04929	2.39706
H	-5.21761	-2.88875	-1.11979
H	-4.81663	-3.20569	1.30954
C	-1.12465	-0.42031	1.16671
O	-0.77326	-0.39409	2.31894
O	0.82817	-1.21373	-0.95279
C	1.96976	-1.70425	-0.44243
C	3.05297	-1.95270	-1.30209
C	2.10249	-2.01949	0.92028
C	4.23167	-2.49858	-0.80657
H	2.94067	-1.71443	-2.35620
C	3.28858	-2.56252	1.40342

H	1.25602	-1.84852	1.58155
C	4.36172	-2.80320	0.54767
H	5.05955	-2.68410	-1.48677
H	3.37079	-2.80503	2.46023
H	5.28541	-3.22749	0.92969

III^{2}: M06L/6-311+G(2df,2pd)(SDD) SCF= -1143.209816 hartree
Gibbs correction= 0.279677 hartree
Total Gibbs Energy= -1142.930139 hartree

C	0.53346	-1.15452	-1.78063
C	-0.47260	-1.82938	-1.03998
C	2.17431	-1.41562	0.66617
C	-0.26649	-3.10781	-0.24310
C	1.12374	-1.76629	1.45677
C	0.18311	-2.91537	1.21598
H	0.19486	-0.56786	-2.63603
H	-1.21340	-3.65604	-0.23244
H	2.82663	-0.61349	1.00550
H	0.99988	-1.23762	2.40197
H	-1.49573	-1.67971	-1.38644
H	0.43501	-3.75295	-0.78467
H	-0.70336	-2.74412	1.83041
H	0.63812	-3.84675	1.58218
C	1.97746	-1.58716	-1.87375
H	2.56692	-0.72527	-2.20555
H	2.06841	-2.33507	-2.67592
C	2.59474	-2.14370	-0.58049
H	2.36155	-3.20774	-0.47647
H	3.68500	-2.08559	-0.66899
Ir	0.06475	-0.02649	-0.01338
O	-1.58863	-0.58230	1.12765
C	-2.69895	-0.02172	0.67842
C	-2.65658	0.83204	-0.44402
C	-3.93805	-0.26488	1.30180
C	-3.82311	1.43417	-0.93595
C	-5.07794	0.34429	0.80328
H	-3.97562	-0.91685	2.16879
C	-5.03569	1.19274	-0.31456
H	-3.74350	2.08545	-1.80217
H	-6.03030	0.15557	1.29353
H	-5.94677	1.65329	-0.68347
C	-1.32950	1.03591	-1.02848
O	-1.08442	1.72292	-2.00757
O	0.39156	1.56520	1.37737
C	1.58908	1.77382	0.90254
C	2.73165	1.87777	1.74079
C	1.77308	1.71206	-0.52139
C	3.98989	1.83603	1.18331
H	2.57969	1.95201	2.81315

C	3.08335	1.62970	-1.04570
H	0.95725	2.00573	-1.17777
C	4.17766	1.66928	-0.20873
H	4.86218	1.90509	1.82919
H	3.21917	1.59166	-2.12401
H	5.18405	1.62510	-0.61362

X: M06L/6-311+G(2df,2pd)(SDD) SCF= -1639.445276 hartree
Gibbs correction= 0.379458 hartree
Total Gibbs Energy= -1639.065818 hartree

C	1.14075	-1.18006	2.33427
C	-0.11598	-0.55464	2.47599
C	2.02190	1.35805	1.44653
C	-0.33658	0.67642	3.33724
C	0.73619	1.91962	1.38673
C	-0.22235	1.99238	2.55122
H	1.13614	-2.23790	2.06821
H	-1.32811	0.61374	3.79664
H	2.71783	1.64011	0.65975
H	0.53327	2.61436	0.56942
H	-0.99267	-1.17101	2.27258
H	0.37683	0.66101	4.16913
H	-1.20487	2.26970	2.15877
H	0.07830	2.81074	3.22066
C	2.40958	-0.66825	2.96736
H	3.24905	-1.23644	2.55923
H	2.39034	-0.88520	4.04495
C	2.64808	0.82975	2.72477
H	2.27227	1.42010	3.56903
H	3.72469	1.01486	2.68174
Ir	0.63242	-0.06897	0.52155
O	-0.22873	-1.78875	-0.27733
C	0.65814	-2.57250	-0.84294
C	2.03679	-2.25915	-0.75737
C	0.27949	-3.74681	-1.52797
C	3.00932	-3.08941	-1.34538
C	1.25063	-4.54969	-2.09581
H	-0.77507	-3.99298	-1.59833
C	2.61918	-4.23310	-2.01226
H	4.05468	-2.80637	-1.26038
H	0.94571	-5.45029	-2.62374
H	3.35796	-4.88230	-2.47098
C	2.40838	-1.04215	-0.05152
O	3.52630	-0.61996	0.13032
O	0.60551	0.64240	-1.45768
C	1.13090	1.84011	-1.80339
C	0.28640	2.92060	-2.10235
C	2.51943	2.01477	-1.90030
C	0.82275	4.14242	-2.49702

H	-0.79022	2.78463	-2.02770
C	3.04356	3.24382	-2.28724
H	3.16949	1.17390	-1.67313
C	2.20228	4.31405	-2.58756
H	0.15471	4.96780	-2.73032
H	4.12162	3.36333	-2.36114
H	2.61745	5.27020	-2.89198
C	-6.61630	-0.45316	-0.40901
C	-5.98623	-0.49220	-1.65882
C	-2.44362	0.30903	-0.68410
C	-5.90191	-0.16607	0.74127
C	-4.62965	-0.24020	-1.73921
C	-4.52757	0.09277	0.67037
C	-3.87787	0.05457	-0.58893
O	-1.76724	0.61111	0.33386
O	-1.91584	0.22144	-1.87690
O	-3.88351	0.36602	1.81576
H	-7.68258	-0.65043	-0.33516
H	-2.94840	0.53643	1.56533
H	-0.91324	0.37835	-1.80177
H	-6.55569	-0.71907	-2.55404
H	-6.37874	-0.13333	1.71532
H	-4.11274	-0.26710	-2.69289

L: M06L/6-311+G(2df,2pd)(SDD) SCF= -1639.432528 hartree
Gibbs correction= 0.377014 hartree
Total Gibbs Energy= -1639.055514 hartree

C	-1.27003	1.26215	2.23759
C	0.03855	0.76712	2.41680
C	-1.90001	-1.40252	1.52602
C	0.37257	-0.37626	3.35746
C	-0.56781	-1.84394	1.49983
C	0.38953	-1.74673	2.66213
H	-1.36337	2.29460	1.89858
H	1.35173	-0.18680	3.80747
H	-2.56589	-1.80085	0.76470
H	-0.29609	-2.56899	0.73048
H	0.85608	1.44177	2.16019
H	-0.34301	-0.37241	4.18746
H	1.39469	-1.95221	2.28543
H	0.16484	-2.54250	3.38617
C	-2.48750	0.67634	2.90521
H	-3.37514	1.13194	2.45956
H	-2.49419	0.96858	3.96481
C	-2.57922	-0.85053	2.76661
H	-2.15206	-1.34293	3.64815
H	-3.63275	-1.14083	2.73853
Ir	-0.65029	0.09074	0.50273
O	0.03008	1.83606	-0.39621

C	-0.93035	2.50393	-0.98965
C	-2.27194	2.06211	-0.88256
C	-0.66710	3.67618	-1.73002
C	-3.32147	2.76584	-1.50360
C	-1.71248	4.35380	-2.32783
H	0.35875	4.01824	-1.81827
C	-3.04428	3.91022	-2.22276
H	-4.33434	2.38706	-1.40044
H	-1.49719	5.25449	-2.89787
H	-3.84260	4.46371	-2.70636
C	-2.51845	0.84972	-0.11964
O	-3.58640	0.31557	0.07448
O	-0.57339	-0.72343	-1.43514
C	-0.92670	-2.02012	-1.71385
C	0.05099	-2.98028	-1.98779
C	-2.28029	-2.36427	-1.73736
C	-0.33487	-4.28440	-2.28489
H	1.09926	-2.69459	-1.97493
C	-2.64884	-3.67450	-2.02604
H	-3.02424	-1.59902	-1.53332
C	-1.68148	-4.63972	-2.29950
H	0.42759	-5.02754	-2.50175
H	-3.70262	-3.93879	-2.04529
H	-1.97548	-5.65971	-2.52753
C	6.62236	0.71418	-0.38666
C	6.02214	0.60682	-1.64581
C	2.46581	-0.19836	-0.69500
C	5.88545	0.52463	0.77057
C	4.67347	0.30763	-1.72730
C	4.52092	0.21930	0.69516
C	3.90075	0.10971	-0.57309
O	1.79402	-0.42236	0.36785
O	1.96246	-0.24514	-1.87051
O	3.85230	0.04428	1.84822
H	7.68085	0.94933	-0.30931
H	2.93031	-0.17618	1.57788
H	0.65668	-0.48553	-1.73688
H	6.60644	0.75778	-2.54781
H	6.33827	0.60532	1.75356
H	4.17473	0.22099	-2.68749

XI: M06L/6-311+G(2df,2pd)(SDD) SCF= -1331.888178 hartree
Gibbs correction= 0.28882 hartree
Total Gibbs Energy= -1331.599358 hartree

C	3.11420	0.03660	-0.04213
C	2.92125	-0.68234	-1.23921
C	1.37958	-1.88482	1.09974
C	3.20177	-2.16705	-1.37255
C	0.99505	-2.44903	-0.12705

C	1.94282	-3.02014	-1.15617
H	3.27771	1.11113	-0.13707
H	3.60515	-2.36418	-2.37004
H	0.58603	-1.77516	1.83194
H	-0.04323	-2.77255	-0.19728
H	2.91666	-0.09953	-2.16214
H	3.99053	-2.45293	-0.66916
H	1.40109	-3.11088	-2.10445
H	2.21752	-4.04686	-0.87530
C	3.57482	-0.58259	1.25151
H	3.45063	0.15792	2.04620
H	4.65316	-0.78883	1.19584
C	2.80118	-1.85612	1.62447
H	3.33193	-2.74839	1.27288
H	2.76358	-1.93877	2.71426
Ir	0.98019	-0.29940	-0.39388
O	0.90575	1.50297	-1.42802
C	0.62365	2.50970	-0.64394
C	0.59954	2.32877	0.76358
C	0.36785	3.80312	-1.15042
C	0.31883	3.39762	1.63869
C	0.09672	4.83805	-0.27734
H	0.38287	3.95360	-2.22481
C	0.06882	4.64964	1.11826
H	0.30293	3.21061	2.70827
H	-0.10429	5.82741	-0.68130
H	-0.14910	5.48403	1.77663
C	0.86393	0.99921	1.27225
O	0.96941	0.61228	2.40346
O	-1.07834	-0.18948	-0.51034
C	-1.93405	-0.82750	0.24554
O	-1.60495	-1.58348	1.18235
C	-3.35222	-0.58980	-0.08409
C	-3.72318	0.28130	-1.12017
C	-4.36528	-1.25043	0.65468
C	-5.05374	0.50026	-1.43262
H	-2.93062	0.78142	-1.66809
C	-5.71040	-1.02444	0.33015
C	-6.04506	-0.16149	-0.69924
H	-5.32478	1.17816	-2.23593
H	-6.46861	-1.54206	0.90917
H	-7.09374	0.00225	-0.93520
O	-4.09744	-2.09180	1.66106
H	-3.11226	-2.10757	1.74288

XII: M06L/6-311+G(2df,2pd)(SDD) SCF= -1603.517516 hartree
Gibbs correction= 0.39831 hartree
Total Gibbs Energy= -1603.119206 hartree

C	3.11325	-0.35990	-0.35450

C	2.79421	0.90818	0.17109
C	1.18722	0.24042	-2.33731
C	2.88043	2.19202	-0.63114
C	0.70060	1.38637	-1.69034
C	1.54375	2.57154	-1.28666
H	3.40778	-1.12657	0.36393
H	3.19006	3.00222	0.03667
H	0.44219	-0.39071	-2.80998
H	-0.37216	1.56681	-1.76547
H	2.83758	1.00746	1.25646
H	3.67352	2.09561	-1.38119
H	0.96112	3.17319	-0.58184
H	1.71536	3.21371	-2.16285
C	3.53413	-0.60502	-1.77983
H	3.52825	-1.68389	-1.95679
H	4.57601	-0.28068	-1.91332
C	2.62001	0.07958	-2.80559
H	3.01820	1.06335	-3.08042
H	2.61497	-0.51189	-3.72543
Ir	0.94536	-0.14354	-0.16932
O	1.07051	-0.96315	1.74818
C	0.99277	-2.26967	1.73125
C	1.00271	-2.96557	0.49591
C	0.92572	-3.02813	2.92046
C	0.93911	-4.37191	0.44566
C	0.86479	-4.40649	2.85080
H	0.91830	-2.50605	3.87179
C	0.87030	-5.09112	1.62070
H	0.94221	-4.86143	-0.52379
H	0.80871	-4.97767	3.77447
H	0.81881	-6.17473	1.59936
C	1.07560	-2.17829	-0.72078
O	1.15448	-2.55272	-1.85972
C	-0.32550	1.94607	1.85088
C	-1.30625	2.56609	1.07226
C	-1.21810	3.92515	0.79068
C	-0.14867	4.69419	1.26950
C	0.83130	4.06081	2.04215
C	0.74465	2.70129	2.33263
H	-0.41506	0.89479	2.10904
H	-2.14310	1.97969	0.69881
H	-1.98985	4.40498	0.19171
H	1.50253	2.22562	2.95146
H	1.66470	4.64672	2.42610
C	-0.03877	6.14869	0.92699
H	0.59564	6.68626	1.63659
H	0.40056	6.28953	-0.06814
H	-1.01751	6.63641	0.90985
O	-1.09352	-0.47688	0.05912

C	-1.99254	-0.47395	-0.88584
O	-1.72887	-0.42843	-2.10474
C	-3.39163	-0.51507	-0.41033
C	-3.69592	-0.54238	0.95994
C	-4.45332	-0.51155	-1.34926
C	-5.00637	-0.56479	1.40603
H	-2.86723	-0.54789	1.66242
C	-5.77771	-0.53610	-0.88897
C	-6.04566	-0.56212	0.46896
H	-5.22432	-0.58633	2.46917
H	-6.57380	-0.53373	-1.62681
H	-7.07913	-0.58084	0.80625
O	-4.25015	-0.48298	-2.67172
H	-3.26780	-0.46826	-2.79141

VI: M06L/6-311+G(2df,2pd)(SDD) SCF= -1414.867185 hartree
Gibbs correction= 0.387137 hartree
Total Gibbs Energy= -1414.480048 hartree

C	0.54805	-1.94927	1.65800
C	-0.75830	-1.96605	1.12491
C	0.03607	0.78594	2.17542
C	-1.98197	-1.54899	1.91970
C	-1.16597	0.82287	1.44831
C	-2.35330	-0.07583	1.70087
H	1.27034	-2.63215	1.20832
H	-2.82873	-2.17460	1.61694
H	0.67328	1.66415	2.10846
H	-1.38125	1.73807	0.89080
H	-0.93201	-2.64185	0.28675
H	-1.81227	-1.75971	2.98198
H	-3.01933	-0.00207	0.83497
H	-2.92590	0.30998	2.55721
C	0.88328	-1.46833	3.04713
H	1.97083	-1.39892	3.13247
H	0.56891	-2.22341	3.78203
C	0.26399	-0.10373	3.38360
H	-0.68926	-0.23312	3.90959
H	0.92279	0.42368	4.07915
Ir	0.27133	-0.27729	0.26318
O	0.94133	-1.47689	-1.30668
C	2.24442	-1.47346	-1.40930
C	3.03239	-0.82722	-0.42225
C	2.91227	-2.12544	-2.46987
C	4.43956	-0.82132	-0.49525
C	4.29213	-2.10981	-2.52247
H	2.31968	-2.62189	-3.23138
C	5.06836	-1.46184	-1.54219
H	5.00148	-0.30739	0.27920
H	4.79249	-2.61085	-3.34789

H	6.15111	-1.46620	-1.61345
C	2.33702	-0.15986	0.66021
O	2.79942	0.41572	1.61277
O	0.48227	1.26545	-1.05779
C	0.36852	2.56513	-0.74153
C	-0.63040	3.33849	-1.35913
C	1.25193	3.20040	0.14869
C	-0.74227	4.69746	-1.08705
H	-1.29910	2.85173	-2.06439
C	1.12681	4.55954	0.41651
H	2.04349	2.61338	0.60775
C	0.12887	5.31767	-0.19311
H	-1.52032	5.27711	-1.57839
H	1.82405	5.03204	1.10440
H	0.03650	6.37872	0.01877
C	-2.34538	0.03784	-2.01125
C	-3.51468	0.75670	-1.76279
C	-4.63526	0.11424	-1.24407
C	-4.61205	-1.25622	-0.95421
C	-3.43749	-1.96724	-1.21774
C	-2.31360	-1.33105	-1.74334
H	-1.45950	0.52815	-2.40436
H	-3.55328	1.82286	-1.97314
H	-5.54469	0.68084	-1.05210
H	-1.40773	-1.89472	-1.95342
H	-3.40682	-3.03641	-1.00959
C	-5.79784	-1.93003	-0.33307
H	-5.81271	-3.00270	-0.54443
H	-5.78847	-1.81901	0.75882
H	-6.74102	-1.50231	-0.68447

G: M06L/6-311+G(2df,2pd)(SDD) SCF= -1414.804557 hartree
Gibbs correction= 0.387874 hartree
Total Gibbs Energy= -1414.416683 hartree

C	1.25471	-1.38825	1.93966
C	-0.13311	-1.71110	1.87662
C	0.38787	1.26131	2.00875
C	-1.12160	-1.27315	2.94621
C	-0.96503	0.97017	1.75526
C	-1.79731	0.07245	2.64113
H	1.93424	-2.08096	1.44115
H	-1.88860	-2.04588	3.05213
H	0.79652	2.15637	1.54620
H	-1.51628	1.69604	1.15505
H	-0.39387	-2.61298	1.32251
H	-0.60074	-1.23466	3.91111
H	-2.75146	-0.11101	2.13967
H	-2.03642	0.60201	3.57501
C	1.86695	-0.55033	3.03342

H	2.90529	-0.34079	2.76420
H	1.90360	-1.13391	3.96489
C	1.12277	0.77218	3.24550
H	0.40195	0.68172	4.06758
H	1.83518	1.54340	3.54990
Ir	0.26560	-0.23183	0.42023
O	0.88785	-1.69233	-0.94661
C	2.12476	-1.54199	-1.35918
C	2.93740	-0.52142	-0.81566
C	2.68094	-2.39445	-2.33748
C	4.26609	-0.34651	-1.24388
C	3.98971	-2.20813	-2.74118
H	2.06304	-3.18093	-2.75922
C	4.79425	-1.18684	-2.20331
H	4.85073	0.45544	-0.80131
H	4.40618	-2.86972	-3.49741
H	5.81776	-1.06332	-2.54271
C	2.34077	0.32520	0.20578
O	2.88719	1.25522	0.76188
O	-0.05101	1.04934	-1.40935
C	-0.40032	2.36570	-1.30287
C	-1.65444	2.80494	-1.74107
C	0.52174	3.28491	-0.79087
C	-1.98427	4.15398	-1.64699
H	-2.35293	2.08650	-2.16116
C	0.17841	4.62997	-0.70618
H	1.49863	2.93122	-0.47213
C	-1.07544	5.07183	-1.12590
H	-2.96004	4.48799	-1.98997
H	0.90067	5.33876	-0.30974
H	-1.33824	6.12301	-1.05494
C	-1.86561	-0.65044	-0.63191
C	-3.07943	0.00988	-0.34412
C	-4.31906	-0.58361	-0.54934
C	-4.41366	-1.89245	-1.03579
C	-3.22355	-2.57064	-1.31799
C	-1.98594	-1.96460	-1.12800
H	-0.96515	0.30167	-1.25169
H	-3.06242	1.03424	0.02835
H	-5.23114	-0.03084	-0.32702
H	-1.08346	-2.51956	-1.36939
H	-3.27398	-3.59136	-1.69566
C	-5.74590	-2.53298	-1.27276
H	-5.69132	-3.62235	-1.19618
H	-6.49984	-2.17773	-0.56448
H	-6.12174	-2.30300	-2.27688

G^2: M06L/6-311+G(2df,2pd)(SDD) SCF= -1414.785241 hartree
Gibbs correction= 0.386612 hartree

Total Gibbs Energy= -1414.398629 hartree

C	0.14558	-1.35572	2.42956
C	-1.22960	-1.17581	2.13583
C	0.40836	1.35877	1.87115
C	-2.10776	-0.17248	2.86590
C	-0.91764	1.50212	1.37167
C	-2.17140	1.18294	2.15185
H	0.56180	-2.33916	2.20182
H	-3.11872	-0.58290	2.95238
H	1.17855	1.95218	1.37784
H	-1.05645	2.21115	0.55567
H	-1.73859	-2.04438	1.72471
H	-1.74389	-0.05645	3.89420
H	-3.00544	1.17468	1.44119
H	-2.38150	1.99338	2.86560
C	0.89837	-0.56124	3.46846
H	1.96029	-0.80196	3.38197
H	0.58761	-0.89101	4.47066
C	0.71298	0.94996	3.30363
H	-0.09028	1.31731	3.95406
H	1.62204	1.46351	3.62744
Ir	-0.06993	-0.25975	0.56346
O	0.02410	-2.10380	-0.63086
C	1.28998	-2.24684	-1.13519
C	2.32905	-1.57908	-0.47452
C	1.55360	-3.10986	-2.19374
C	3.65183	-1.81557	-0.86347
C	2.87350	-3.30933	-2.58591
H	0.73218	-3.62085	-2.68544
C	3.92397	-2.67120	-1.92180
H	4.44212	-1.28872	-0.33523
H	3.08529	-3.97789	-3.41580
H	4.94853	-2.83400	-2.24173
C	2.02943	-0.58786	0.60208
O	2.89484	-0.03722	1.24140
O	0.62092	0.69833	-1.20252
C	1.24048	1.88801	-1.22270
C	0.51527	3.09482	-1.28334
C	2.64593	1.96594	-1.26412
C	1.16904	4.32010	-1.36508
H	-0.57158	3.05399	-1.29268
C	3.29053	3.19389	-1.34710
H	3.21766	1.04242	-1.24327
C	2.56032	4.38086	-1.38960
H	0.58344	5.23524	-1.41571
H	4.37714	3.22423	-1.37933
H	3.06861	5.33877	-1.45066
C	-2.26811	0.56711	-1.65766
C	-3.54323	0.80353	-2.15561

C	-4.62134	-0.01741	-1.80173
C	-4.36911	-1.09268	-0.94503
C	-3.09142	-1.31747	-0.44111
C	-1.99602	-0.49732	-0.77511
H	-1.44505	1.20793	-1.96200
H	-3.71367	1.63966	-2.83326
H	-0.80061	-1.48342	-1.07831
H	-5.18776	-1.75759	-0.67201
H	-2.94776	-2.18051	0.20869
C	-5.99313	0.23822	-2.34494
H	-6.04110	0.02829	-3.41956
H	-6.74634	-0.38483	-1.85579
H	-6.28789	1.28509	-2.22009

G-phenol: M06L/6-311+G(2df,2pd)(SDD) SCF= -1722.350049 hartree
Gibbs correction= 0.473621 hartree
Total Gibbs Energy= -1721.876428 hartree

C	-0.60023	-1.21951	-2.62549
C	-1.28541	0.02182	-2.47393
C	-2.05585	-2.03037	-0.40379
C	-2.80213	0.13319	-2.49202
C	-2.59872	-0.76327	-0.11396
C	-3.44938	0.00089	-1.10338
H	0.40329	-1.16206	-3.05030
H	-3.07376	1.10168	-2.92224
H	-1.77262	-2.65524	0.43835
H	-2.74251	-0.50906	0.93836
H	-0.74141	0.90180	-2.81194
H	-3.20015	-0.62366	-3.17993
H	-3.63434	0.99834	-0.69717
H	-4.43243	-0.48543	-1.18556
C	-1.29426	-2.54800	-2.77754
H	-0.54316	-3.34023	-2.72846
H	-1.73913	-2.60864	-3.78161
C	-2.35045	-2.77710	-1.69352
H	-3.34324	-2.48041	-2.05344
H	-2.41593	-3.84511	-1.46897
Ir	-0.49279	-0.52235	-0.59169
O	1.32469	0.37316	-1.09629
C	2.34141	-0.45783	-1.11415
C	2.13835	-1.83851	-0.88333
C	3.65335	0.00230	-1.35381
C	3.22188	-2.73908	-0.87947
C	4.70043	-0.89755	-1.34567
H	3.81524	1.06710	-1.49344
C	4.49882	-2.27184	-1.11217
H	3.02299	-3.79019	-0.68922
H	5.71021	-0.52815	-1.51093
H	5.34346	-2.95361	-1.10897

C	0.77888	-2.28209	-0.63470
O	0.41150	-3.40584	-0.38004
O	0.27075	-0.82693	1.55408
C	-0.56586	-1.18745	2.58782
C	-1.06408	-0.22847	3.47243
C	-0.88797	-2.53599	2.74111
C	-1.91182	-0.63019	4.50122
H	-0.76693	0.81054	3.35813
C	-1.74664	-2.91777	3.76767
H	-0.45098	-3.26207	2.06131
C	-2.26648	-1.96946	4.64648
H	-2.29661	0.11406	5.19314
H	-2.00055	-3.96747	3.88662
H	-2.93279	-2.27423	5.44785
C	-0.89841	1.80978	0.05872
C	-2.00675	2.15423	0.86650
C	-2.79572	3.26827	0.61791
C	-2.52312	4.10883	-0.47051
C	-1.42467	3.79964	-1.28151
C	-0.63487	2.68674	-1.01697
H	0.19208	1.61850	0.82982
H	-2.24985	1.52861	1.72719
H	-3.63878	3.49924	1.26820
H	0.23309	2.48584	-1.64480
H	-1.18970	4.44972	-2.12367
C	-3.36117	5.32099	-0.73252
H	-3.05781	6.15646	-0.09055
H	-3.26942	5.66226	-1.76702
H	-4.41943	5.13590	-0.52582
H	0.71702	0.10217	1.74402
O	1.05305	1.49695	1.73997
C	2.31171	1.87493	1.43141
C	2.55674	3.05567	0.71536
C	3.39885	1.09807	1.85606
C	3.86216	3.44053	0.43075
H	1.71207	3.65891	0.39222
C	4.70015	1.50092	1.57761
H	3.20613	0.17540	2.39949
C	4.94330	2.67083	0.86087
H	4.03697	4.35770	-0.12709
H	5.53102	0.88415	1.91217
H	5.96095	2.98083	0.64136

N: M06L/6-311+G(2df,2pd)(SDD) SCF= -1603.460105 hartree
Gibbs correction= 0.3987 hartree
Total Gibbs Energy= -1603.061405 hartree

2 Imaginary Frequencies (–804.7 and –23.7 cm^{-1})

C	1.77355	-2.44159	0.31111
C	2.62262	-1.30398	0.43327

C	1.13837	-1.42716	-2.20228
C	3.74273	-1.01415	-0.55549
C	1.82929	-0.20889	-2.03102
C	3.30944	-0.12919	-1.73466
H	1.34057	-2.81891	1.23890
H	4.56241	-0.52382	-0.02149
H	0.19062	-1.39436	-2.73438
H	1.39294	0.67643	-2.49290
H	2.77186	-0.92931	1.44454
H	4.14892	-1.96800	-0.91622
H	3.55094	0.91335	-1.50760
H	3.87995	-0.38712	-2.63919
C	1.86485	-3.44102	-0.81505
H	1.02124	-4.13082	-0.73357
H	2.77248	-4.04905	-0.68664
C	1.84329	-2.77404	-2.19390
H	2.86487	-2.63557	-2.56966
H	1.34296	-3.43301	-2.90829
Ir	0.72045	-0.64223	-0.22653
O	0.03483	-0.57392	1.76227
C	-0.99421	-1.35489	1.99536
C	-1.48485	-2.21471	0.98468
C	-1.63509	-1.36533	3.25397
C	-2.58590	-3.05701	1.22216
C	-2.71441	-2.20259	3.46630
H	-1.26464	-0.70673	4.03329
C	-3.20161	-3.05418	2.45813
H	-2.92842	-3.69729	0.41357
H	-3.20003	-2.19889	4.43959
H	-4.05407	-3.69741	2.65226
C	-0.79895	-2.19789	-0.30144
O	-1.09984	-2.85398	-1.27329
C	1.46467	1.51694	0.39724
C	1.79659	2.52237	-0.53514
C	2.74852	3.49830	-0.27211
C	3.43421	3.51633	0.94999
C	3.10925	2.54107	1.89812
C	2.14548	1.57448	1.62848
H	0.01779	1.58937	0.58257
H	1.27710	2.55089	-1.49498
H	2.97130	4.26039	-1.01816
H	1.89475	0.84411	2.39663
H	3.61985	2.54850	2.86050
C	4.45446	4.57274	1.24167
H	5.08082	4.78397	0.36971
H	3.97638	5.51924	1.52029
H	5.10864	4.28685	2.06944
O	-1.05834	0.34630	-1.05726
C	-1.66866	1.24287	-0.40758

O	-1.11790	1.86266	0.58965
C	-3.03275	1.60992	-0.78116
C	-3.68677	0.85243	-1.76957
C	-3.71633	2.69292	-0.17524
C	-4.97506	1.15375	-2.16631
H	-3.14402	0.01834	-2.20442
C	-5.02013	2.99403	-0.59196
C	-5.63605	2.23531	-1.57119
H	-5.46880	0.55748	-2.92643
H	-5.52367	3.83025	-0.11825
H	-6.64970	2.48366	-1.87479
O	-3.19380	3.47026	0.78464
H	-2.30684	3.12759	1.00252

XV: M06L/6-311+G(2df,2pd)(SDD) SCF= -1414.824617 hartree
Gibbs correction= 0.391675 hartree
Total Gibbs Energy= -1414.432942 hartree

C	1.51268	-1.38465	1.79963
C	0.14635	-1.81678	1.90205
C	0.45104	1.15922	2.06290
C	-0.72909	-1.49228	3.10529
C	-0.90451	0.77180	1.97654
C	-1.55533	-0.21235	2.92007
H	2.17209	-2.02211	1.20902
H	-1.40285	-2.33516	3.28547
H	0.73071	2.09633	1.58606
H	-1.58543	1.47456	1.49397
H	-0.09762	-2.74188	1.37919
H	-0.09398	-1.42202	3.99721
H	-2.53221	-0.47350	2.50108
H	-1.75086	0.26815	3.89014
C	2.19138	-0.53273	2.84179
H	3.16802	-0.22989	2.45616
H	2.38818	-1.13870	3.73893
C	1.37362	0.71426	3.18741
H	0.77099	0.54607	4.08839
H	2.05027	1.53927	3.42529
Ir	0.22735	-0.29572	0.46878
O	0.77065	-1.66343	-1.03555
C	1.96383	-1.45955	-1.55116
C	2.78779	-0.41371	-1.07387
C	2.45300	-2.27816	-2.59271
C	4.06036	-0.18850	-1.62695
C	3.70966	-2.04012	-3.11872
H	1.82541	-3.08280	-2.96342
C	4.52571	-0.99662	-2.64581
H	4.65444	0.63014	-1.22826
H	4.07397	-2.67875	-3.92056
H	5.50688	-0.83190	-3.08024

C	2.25560	0.39727	0.01307
O	2.81791	1.36971	0.49096
O	-0.23840	1.18859	-1.30144
C	-0.56852	2.53076	-1.16325
C	-1.82441	3.00027	-1.53888
C	0.40987	3.38791	-0.66812
C	-2.10582	4.35734	-1.40352
H	-2.56832	2.31195	-1.93341
C	0.10719	4.73939	-0.53549
H	1.38514	2.99202	-0.40064
C	-1.14614	5.22948	-0.89790
H	-3.08350	4.72828	-1.69704
H	0.86560	5.41454	-0.15001
H	-1.37123	6.28619	-0.79261
C	-1.77943	-0.94551	-0.13348
C	-2.88261	-0.08856	-0.26843
C	-4.10489	-0.51982	-0.79181
C	-4.28963	-1.84431	-1.18461
C	-3.20118	-2.71447	-1.04628
C	-1.98108	-2.27429	-0.54431
H	-1.00616	0.69679	-1.64473
H	-2.81207	0.95286	0.04847
H	-4.93170	0.18474	-0.88357
H	-1.15399	-2.97972	-0.49670
H	-3.31310	-3.75547	-1.34916
C	-5.59936	-2.32515	-1.73169
H	-6.03303	-3.11417	-1.10730
H	-6.33165	-1.51571	-1.79473
H	-5.48757	-2.74988	-2.73532

XVI: M06L/6-311+G(2df,2pd)(SDD) SCF= -1603.477414 hartree
Gibbs correction= 0.396801 hartree
Total Gibbs Energy= -1603.080613 hartree

C	3.12857	0.56025	0.12425
C	2.43904	1.77213	0.43848
C	1.72839	0.66957	-2.27057
C	2.54935	3.01934	-0.42875
C	0.91005	1.76190	-1.89479
C	1.44361	3.11392	-1.48652
H	3.38828	-0.08000	0.96901
H	2.50809	3.90061	0.21823
H	1.27019	-0.12042	-2.86213
H	-0.11227	1.76277	-2.27290
H	2.24532	1.95011	1.49524
H	3.54164	3.03964	-0.89701
H	0.60486	3.68657	-1.07884
H	1.79520	3.66269	-2.37285
C	3.98137	0.38286	-1.10858
H	4.28017	-0.66664	-1.17188

H	4.91053	0.96116	-0.99599
C	3.24113	0.77660	-2.39065
H	3.49609	1.80250	-2.68411
H	3.56945	0.13453	-3.21191
Ir	1.01985	0.36904	-0.25855
O	0.77540	-0.56263	1.66050
C	1.28901	-1.79726	1.73456
C	1.82744	-2.40873	0.58748
C	1.26676	-2.50920	2.94512
C	2.33667	-3.71399	0.65141
C	1.78008	-3.79701	2.98931
H	0.84883	-2.03490	3.82816
C	2.31775	-4.40931	1.84824
H	2.73986	-4.14959	-0.25936
H	1.76384	-4.34008	3.93129
H	2.71357	-5.41861	1.90687
C	1.84255	-1.62170	-0.65710
O	2.19843	-2.07841	-1.72696
C	-0.45229	1.75429	0.59842
C	-1.60380	2.16702	-0.08760
C	-2.60372	2.91789	0.52852
C	-2.49811	3.30026	1.86803
C	-1.35561	2.89647	2.56244
C	-0.36143	2.14070	1.94216
H	-0.78527	-0.76179	1.36616
H	-1.75016	1.88803	-1.13193
H	-3.48266	3.21540	-0.04310
H	0.49184	1.82376	2.54003
H	-1.24348	3.17587	3.60997
C	-3.58235	4.08673	2.54110
H	-4.10856	4.73749	1.83653
H	-4.33737	3.42986	2.98980
H	-3.18822	4.71249	3.34717
O	-0.80346	-0.64082	-1.01277
C	-1.77329	-0.96873	-0.29484
O	-1.70331	-1.03115	1.02394
C	-3.06251	-1.30930	-0.88275
C	-3.17896	-1.24982	-2.28524
C	-4.19553	-1.68205	-0.11563
C	-4.36424	-1.55242	-2.92312
H	-2.29769	-0.95940	-2.84850
C	-5.39368	-1.98800	-0.77660
C	-5.47476	-1.92502	-2.15510
H	-4.43360	-1.50263	-4.00455
H	-6.24620	-2.27079	-0.16818
H	-6.41520	-2.16668	-2.64304
O	-4.22153	-1.76631	1.22230
H	-3.34880	-1.51766	1.56964

VII: M06L/6-311+G(2df,2pd)(SDD) SCF= -1107.308363 hartree
Gibbs correction= 0.299009 hartree
Total Gibbs Energy= -1107.009354 hartree

C	2.65374	0.74998	-0.25170
C	2.62262	-0.16242	-1.29676
C	1.55558	-1.42460	1.30143
C	3.28615	-1.52254	-1.25232
C	1.30382	-2.25761	0.19396
C	2.31659	-2.64702	-0.85897
H	2.41274	1.78662	-0.48610
H	3.70704	-1.74454	-2.23800
H	0.84621	-1.48463	2.12204
H	0.44608	-2.92653	0.26826
H	2.34995	0.22348	-2.27956
H	4.13903	-1.49159	-0.56729
H	1.76625	-2.97446	-1.74959
H	2.87561	-3.53204	-0.52060
C	3.25265	0.49931	1.10450
H	2.87928	1.27175	1.78371
H	4.34309	0.63650	1.06509
C	2.91935	-0.88080	1.69406
H	3.68798	-1.61299	1.42227
H	2.95288	-0.80595	2.78493
Ir	0.57942	-0.28783	-0.29261
O	-0.09660	1.26727	-1.50539
C	-0.54689	2.28186	-0.81032
C	-0.44309	2.26622	0.60302
C	-1.12021	3.41663	-1.42358
C	-0.90202	3.34314	1.38206
C	-1.56451	4.46645	-0.64116
H	-1.20541	3.43848	-2.50548
C	-1.46100	4.44335	0.76139
H	-0.80861	3.28443	2.46266
H	-2.00849	5.33291	-1.12596
H	-1.81859	5.28303	1.34865
C	0.13659	1.07628	1.21493
O	0.34522	0.88139	2.38763
C	-1.35168	-0.95328	-0.02814
C	-1.80733	-1.67736	1.08710
C	-3.10310	-2.17440	1.15426
C	-4.00871	-1.97772	0.10416
C	-3.56844	-1.25286	-1.00381
C	-2.27483	-0.73569	-1.06543
H	-1.14309	-1.84640	1.93420
H	-3.42396	-2.72413	2.03851
H	-1.97783	-0.15219	-1.93379
H	-4.25606	-1.07748	-1.83037
C	-5.40192	-2.52457	0.17730
H	-5.40493	-3.61937	0.22839

H	-5.92961	-2.17042	1.06956
H	-5.99435	-2.23497	-0.69463

H: M06L/6-311+G(2df,2pd)(SDD) SCF= -1107.286886 hartree
Gibbs correction= 0.302929 hartree
Total Gibbs Energy= -1106.983957 hartree

C	2.42510	1.15767	-0.11116
C	2.61101	0.27842	-1.21292
C	1.71911	-1.14326	1.30874
C	3.52884	-0.93019	-1.18218
C	1.63786	-1.97760	0.17026
C	2.77842	-2.21537	-0.79409
H	2.08135	2.16607	-0.34779
H	3.98071	-1.06373	-2.16995
H	0.98264	-1.29715	2.09322
H	0.87414	-2.75816	0.18144
H	2.40253	0.69969	-2.19732
H	4.36652	-0.74735	-0.50039
H	2.36012	-2.67090	-1.69911
H	3.47373	-2.96124	-0.38061
C	3.05839	0.99943	1.24511
H	2.52563	1.66029	1.93799
H	4.09975	1.35349	1.22436
C	2.98309	-0.44029	1.76589
H	3.86117	-1.01679	1.45513
H	3.00467	-0.42984	2.85984
Ir	0.70845	-0.10895	-0.30139
O	-0.12920	1.42066	-1.44801
C	-0.92616	2.22157	-0.76711
C	-1.21465	1.95992	0.59315
C	-1.48875	3.37017	-1.35835
C	-1.99390	2.84555	1.34913
C	-2.27294	4.22488	-0.60029
H	-1.27813	3.57234	-2.40419
C	-2.52750	3.97822	0.75643
H	-2.17137	2.61435	2.39598
H	-2.69235	5.11166	-1.07015
H	-3.13439	4.66777	1.33463
C	-0.68985	0.72595	1.19691
O	-0.54570	0.53034	2.38996
C	-1.27130	-0.81327	0.26973
C	-1.51248	-1.83895	1.20482
C	-2.48266	-2.79931	0.98652
C	-3.28493	-2.76996	-0.16590
C	-3.08120	-1.73362	-1.07809
C	-2.10633	-0.76231	-0.86443
H	-0.95033	-1.84143	2.13533
H	-2.64221	-3.58265	1.72559
H	-1.97431	0.02704	-1.59815

H	-3.70028	-1.68148	-1.97167
C	-4.34456	-3.80338	-0.38400
H	-3.94231	-4.81733	-0.28913
H	-5.14505	-3.71612	0.35919
H	-4.80168	-3.71282	-1.37219

VIII: M06L/6-311+G(2df,2pd)(SDD) SCF= -1107.327864 hartree
Gibbs correction= 0.301592 hartree
Total Gibbs Energy= -1107.026272 hartree

C	3.19731	0.31205	1.05847
C	3.41792	0.47380	-0.33942
C	1.95040	-2.06577	0.36827
C	4.17149	-0.54517	-1.17966
C	1.96637	-1.77701	-1.02733
C	3.21956	-1.54986	-1.84238
H	3.06802	1.22610	1.64210
H	4.75322	-0.02595	-1.94819
H	1.07776	-2.60274	0.74538
H	1.10736	-2.12523	-1.60704
H	3.43492	1.49899	-0.71366
H	4.90823	-1.06254	-0.55362
H	2.91060	-1.15995	-2.81914
H	3.73481	-2.50099	-2.04637
C	3.62734	-0.89578	1.85906
H	3.14853	-0.82517	2.84244
H	4.71125	-0.87205	2.04926
C	3.21869	-2.21780	1.19382
H	4.02699	-2.59869	0.55807
H	3.06580	-2.98305	1.96169
Ir	1.40697	-0.05032	0.02939
O	0.83380	1.91038	0.39388
C	-0.33012	2.42200	0.13111
C	-1.54372	1.69130	-0.15925
C	-0.41278	3.84204	0.16497
C	-2.71000	2.43763	-0.49094
C	-1.57061	4.51519	-0.13857
H	0.50033	4.37105	0.41873
C	-2.73587	3.81070	-0.49463
H	-3.59852	1.89223	-0.79136
H	-1.57855	5.60257	-0.12112
H	-3.63873	4.34152	-0.77822
C	-1.62209	0.25283	-0.16272
O	-0.62654	-0.53489	-0.23558
C	-2.92594	-0.45129	-0.08193
C	-3.08166	-1.66317	-0.77042
C	-4.25743	-2.38850	-0.66770
C	-5.30772	-1.95209	0.15091
C	-5.13500	-0.76263	0.86365
C	-3.96860	-0.01637	0.74625

H	-2.26284	-2.01978	-1.38816
H	-4.36701	-3.31764	-1.22322
H	-3.84952	0.89618	1.32376
H	-5.92637	-0.41997	1.52667
C	-6.57795	-2.73813	0.24992
H	-7.19199	-2.61479	-0.64954
H	-6.38249	-3.80996	0.35046
H	-7.18431	-2.42307	1.10263

XIII[1]: M06L/6-311+G(2df,2pd)(SDD) SCF= -1951.051324 hartree
Gibbs correction= 0.48171 hartree
Total Gibbs Energy= -1950.569614 hartree

C	-3.09968	4.68544	-0.96798
C	-3.38654	3.35293	-0.77842
C	-2.39468	2.42618	-0.37971
C	-1.05286	2.87628	-0.14950
C	-0.80214	4.26258	-0.33983
C	-1.78800	5.13549	-0.74022
H	-3.87461	5.37571	-1.28484
H	-4.39419	2.98547	-0.93918
H	0.21096	4.60804	-0.15470
H	-1.54434	6.18618	-0.88092
O	-0.04642	2.14766	0.24582
C	-2.75888	1.05126	-0.15240
O	-2.01641	0.09417	0.10875
O	-4.09910	0.82187	-0.23958
C	-4.58453	-0.44085	0.09071
C	-4.56012	-0.87949	1.41010
C	-5.17761	-1.19415	-0.91314
C	-5.15435	-2.09637	1.72613
H	-4.07751	-0.27256	2.16971
C	-5.76818	-2.41247	-0.58502
H	-5.17324	-0.81985	-1.93197
C	-5.76079	-2.86434	0.73255
H	-5.14057	-2.44690	2.75432
H	-6.23628	-3.00764	-1.36390
H	-6.22484	-3.81309	0.98525
Ir	0.15527	0.06893	0.20090
P	2.37961	0.23644	0.25662
C	3.07690	1.47289	-1.01938
C	3.11411	0.58475	1.97033
C	4.52176	1.18449	-1.43289
H	4.61765	0.23074	-1.95808
H	4.84739	1.97218	-2.12362
H	5.22223	1.18459	-0.59293
C	2.19068	1.33410	-2.26284
H	1.16332	1.64996	-2.05988
H	2.59837	1.96101	-3.06615
H	2.15788	0.30060	-2.62765

C	2.97655	2.91012	-0.50438
H	1.97183	3.13267	-0.13878
H	3.69862	3.11987	0.29078
H	3.20168	3.59674	-1.33037
C	2.32228	1.73416	2.60362
H	2.47694	2.68817	2.09437
H	1.24798	1.52424	2.59254
H	2.64346	1.85689	3.64547
C	4.60515	0.91968	1.98989
H	4.92031	1.06900	3.03029
H	5.22557	0.11535	1.58309
H	4.83878	1.84089	1.44959
C	2.87377	-0.67063	2.81306
H	3.25132	-0.50135	3.82863
H	1.80410	-0.89001	2.88862
H	3.38236	-1.55219	2.40852
C	3.01164	-1.37694	-0.31508
C	4.34737	-1.79389	-0.38042
C	1.99822	-2.22024	-0.79843
C	4.68218	-3.01251	-0.96012
H	5.13898	-1.15185	-0.00437
C	2.34993	-3.43387	-1.40254
C	3.68030	-3.82444	-1.48991
H	5.72255	-3.32107	-1.01106
H	1.55924	-4.08048	-1.77752
H	3.93748	-4.77139	-1.95710
C	0.55754	-1.89730	-0.57707
C	0.07783	-1.99976	0.80023
C	-0.37526	-2.24834	-1.63124
C	-1.23870	-2.53753	1.03405
H	0.81482	-2.18208	1.58248
C	-1.64086	-2.66979	-1.35114
H	-0.02456	-2.18790	-2.66045
C	-2.07109	-2.84331	-0.00090
H	-1.55679	-2.70495	2.06117
H	-2.32663	-2.90911	-2.16060
H	-3.06682	-3.23405	0.19232

XIII[2]: M06L/6-31G(2df,2pd)(SDD) SCF= -1951.046237 hartree
Gibbs correction= 0.48274 hartree
Total Gibbs Energy= -1950.563497 hartree

C	4.71780	3.58505	-0.53853
C	4.38665	2.25490	-0.48175
C	3.06057	1.82526	-0.20651
C	2.03054	2.80488	0.02529
C	2.42470	4.17688	-0.03347
C	3.71506	4.55131	-0.30868
H	5.73649	3.88916	-0.75607
H	5.14556	1.49945	-0.65250

H	1.64329	4.91008	0.14413
H	3.96711	5.60877	-0.35139
O	0.79631	2.56257	0.29122
C	2.77384	0.42817	-0.13304
O	1.67624	-0.14545	0.06630
O	3.87202	-0.35713	-0.31873
C	3.77828	-1.73365	-0.16478
C	4.12498	-2.52218	-1.25511
C	3.43820	-2.29814	1.06004
C	4.11903	-3.90762	-1.11800
H	4.38971	-2.04349	-2.19249
C	3.43187	-3.68411	1.18209
H	3.16960	-1.65817	1.89435
C	3.76808	-4.49141	0.09674
H	4.38551	-4.53076	-1.96687
H	3.15799	-4.13277	2.13327
H	3.75997	-5.57241	0.19945
Ir	-0.26958	0.74440	0.25920
P	-1.35210	-1.22302	0.09963
C	-0.79383	-2.27220	-1.39604
C	-1.37676	-2.30025	1.66461
C	-1.85189	-3.25120	-1.90933
H	-2.73042	-2.73763	-2.30794
H	-1.41460	-3.83459	-2.72929
H	-2.18771	-3.96504	-1.15181
C	-0.49790	-1.26832	-2.51675
H	0.34185	-0.61424	-2.26281
H	-0.24774	-1.81581	-3.43457
H	-1.36209	-0.62872	-2.73155
C	0.48757	-3.04192	-1.07588
H	1.25553	-2.40182	-0.63592
H	0.31320	-3.88559	-0.40069
H	0.89624	-3.45798	-2.00565
C	0.05425	-2.36633	2.20694
H	0.72660	-2.92937	1.55517
H	0.47091	-1.36005	2.32954
H	0.04797	-2.86032	3.18713
C	-1.91865	-3.71828	1.49019
H	-1.90162	-4.22693	2.46257
H	-2.95594	-3.73522	1.14275
H	-1.31625	-4.31926	0.80393
C	-2.23458	-1.56221	2.69544
H	-2.25293	-2.13727	3.62916
H	-1.81200	-0.57834	2.92173
H	-3.26979	-1.42878	2.36377
C	-3.08041	-0.79932	-0.30977
C	-4.16344	-1.67637	-0.44992
C	-3.25980	0.56739	-0.57626
C	-5.39763	-1.21589	-0.89538

H	-4.03810	-2.73504	-0.24146
C	-4.49987	1.01621	-1.04732
C	-5.55825	0.13167	-1.21374
H	-6.22688	-1.90875	-1.00735
H	-4.62970	2.07682	-1.25224
H	-6.51620	0.49523	-1.57596
C	-2.19669	1.56163	-0.24388
C	-1.93122	1.76052	1.17811
C	-2.07037	2.72064	-1.10707
C	-1.67180	3.09181	1.65943
H	-2.41705	1.08528	1.88146
C	-1.74275	3.94515	-0.60771
H	-2.27003	2.58846	-2.16911
C	-1.56626	4.13998	0.79537
H	-1.57294	3.24625	2.73079
H	-1.63764	4.79352	-1.27923
H	-1.36129	5.13935	1.17065

C$_{JP}$: M06L/6-311+G(2df,2pd)(SDD) SCF= -1951.001626 hartree
Gibbs correction= 0.485174 hartree
Total Gibbs Energy= -1950.516452 hartree

C	5.03665	-1.51248	1.48354
C	3.88781	-0.79653	1.79394
C	2.95187	-0.51802	0.79461
C	3.10968	-1.00135	-0.52734
C	4.30022	-1.69431	-0.82928
C	5.23463	-1.94326	0.16593
H	5.77566	-1.72437	2.24967
H	3.70382	-0.43028	2.80084
H	4.44191	-2.05803	-1.84298
H	6.13350	-2.50347	-0.08286
O	2.15536	-0.85470	-1.41134
C	1.76567	0.27337	1.10943
O	1.33459	0.62877	2.17857
O	1.61762	1.36350	-0.18105
C	1.60358	2.71466	-0.02911
C	2.12973	3.34493	1.10238
C	1.13268	3.47767	-1.10140
C	2.13495	4.73518	1.16290
H	2.50696	2.75053	1.92684
C	1.14778	4.86556	-1.02630
H	0.78619	2.95903	-1.99184
C	1.63731	5.50312	0.11234
H	2.53474	5.22204	2.04853
H	0.78057	5.44993	-1.86613
H	1.64368	6.58711	0.17441
Ir	0.28264	-0.28944	-0.61016
P	-1.85832	0.42373	-0.05865
C	-2.17467	1.46806	1.50929

C	-2.71783	1.22069	-1.56142
C	-3.59940	2.01060	1.62319
H	-4.35988	1.22562	1.61211
H	-3.69061	2.52460	2.58783
H	-3.84038	2.74430	0.84897
C	-1.90018	0.54900	2.70731
H	-0.92804	0.05350	2.62399
H	-1.87421	1.16071	3.61657
H	-2.67756	-0.20994	2.83568
C	-1.18865	2.63264	1.57324
H	-0.17131	2.26695	1.69955
H	-1.21874	3.29048	0.70041
H	-1.42495	3.24449	2.45242
C	-2.36024	2.70512	-1.63923
H	-2.84649	3.29487	-0.85743
H	-1.28314	2.87792	-1.56567
H	-2.69617	3.10441	-2.60388
C	-4.23864	1.06471	-1.59138
H	-4.62292	1.57185	-2.48509
H	-4.53925	0.01586	-1.66075
H	-4.73778	1.51310	-0.72852
C	-2.15899	0.51855	-2.80392
H	-2.58713	0.97755	-3.70347
H	-1.06630	0.59388	-2.86711
H	-2.42570	-0.54389	-2.82145
C	-2.77180	-1.10594	0.35856
C	-4.13206	-1.22064	0.67896
C	-1.92497	-2.19999	0.58618
C	-4.63295	-2.38382	1.25357
H	-4.81016	-0.39335	0.50399
C	-2.43331	-3.35909	1.18450
C	-3.77636	-3.44765	1.52711
H	-5.68813	-2.45095	1.50249
H	-1.76364	-4.19893	1.35489
H	-4.15867	-4.35180	1.99265
C	-0.52170	-2.20930	0.08756
C	-0.35577	-2.22487	-1.35696
C	0.47039	-2.91160	0.87091
C	0.66226	-3.05922	-1.93730
H	-1.24238	-2.04259	-1.96576
C	1.47095	-3.62168	0.27325
H	0.38635	-2.87091	1.95538
C	1.53985	-3.73940	-1.14613
H	0.71228	-3.14284	-3.01897
H	2.21843	-4.12113	0.88439
H	2.30919	-4.36424	-1.59037

V_{JP}[1]: M06L/6-311+G(2df,2pd)(SDD) SCF= -1951.04452 hartree
Gibbs correction= 0.482915 hartree

Total Gibbs Energy= -1950.561605 hartree

C	-4.44817	1.79296	1.98608
C	-3.11069	1.53074	2.20486
C	-2.28863	1.16959	1.12195
C	-2.80285	1.08090	-0.19601
C	-4.17355	1.36209	-0.39835
C	-4.96665	1.70299	0.67931
H	-5.09788	2.06631	2.81176
H	-2.67306	1.58698	3.19792
H	-4.57967	1.27617	-1.40151
H	-6.02308	1.90343	0.51418
O	-2.00384	0.75931	-1.17506
C	-0.87619	0.87498	1.29929
O	-0.21268	1.08405	2.28991
O	-0.96684	-1.77330	-0.26191
C	-2.30208	-1.96297	-0.23149
C	-2.97156	-2.07828	0.99550
C	-3.03191	-2.11288	-1.41990
C	-4.33701	-2.34047	1.03052
H	-2.40210	-1.94481	1.91317
C	-4.39505	-2.37792	-1.37645
H	-2.50746	-1.99829	-2.36511
C	-5.05629	-2.49095	-0.15333
H	-4.84305	-2.41865	1.98973
H	-4.94921	-2.48957	-2.30552
H	-6.12375	-2.69083	-0.12427
Ir	-0.13500	0.08479	-0.45415
P	1.88962	-0.92344	0.10010
C	1.91791	-2.11088	1.60065
C	2.62669	-1.85832	-1.40500
C	3.30293	-2.29445	2.22643
H	3.67062	-1.36746	2.67422
H	3.20971	-3.02817	3.03608
H	4.06146	-2.67311	1.53759
C	1.00975	-1.52257	2.67784
H	-0.02600	-1.46739	2.33632
H	1.04652	-2.18190	3.55348
H	1.31518	-0.52211	2.98787
C	1.33189	-3.47228	1.20991
H	0.34821	-3.36126	0.74650
H	1.97803	-4.05187	0.54647
H	1.21003	-4.05987	2.12777
C	1.53514	-2.73141	-2.03463
H	1.16830	-3.51755	-1.37401
H	0.66529	-2.13529	-2.32951
H	1.94180	-3.20842	-2.93488
C	3.84944	-2.71270	-1.06269
H	4.21243	-3.18342	-1.98444
H	4.67581	-2.11417	-0.66607

H	3.63431	-3.51637	-0.35702
C	3.06533	-0.84646	-2.46878
H	3.59798	-1.38367	-3.26194
H	2.20786	-0.36493	-2.94417
H	3.73811	-0.07425	-2.08252
C	3.02721	0.46938	0.40957
C	4.37564	0.32979	0.76921
C	2.49099	1.76186	0.23333
C	5.17614	1.43937	1.01170
H	4.80616	-0.65993	0.87707
C	3.31106	2.86888	0.49723
C	4.63374	2.71529	0.89078
H	6.21482	1.30597	1.29961
H	2.89680	3.86504	0.36197
H	5.24503	3.59204	1.08528
C	1.12216	2.04734	-0.29596
C	0.78456	1.72702	-1.66473
C	0.41170	3.14935	0.29808
C	-0.17148	2.52074	-2.36841
H	1.52687	1.20250	-2.25898
C	-0.56206	3.83031	-0.38223
H	0.65813	3.41970	1.32101
C	-0.84971	3.52576	-1.73606
H	-0.36043	2.29853	-3.41444
H	-1.09811	4.63531	0.11250
H	-1.59845	4.10274	-2.27065

V_{JP}^2: M06L/6-311+G(2df,2pd)(SDD) SCF= -1951.044223 hartree
Gibbs correction= 0.482944 hartree
Total Gibbs Energy= -1950.561279 hartree

C	-2.41607	4.38286	-1.90133
C	-1.68432	3.27847	-2.30010
C	-1.25690	2.34964	-1.33967
C	-1.55341	2.52559	0.02897
C	-2.29095	3.65786	0.42271
C	-2.71116	4.56060	-0.53950
H	-2.76132	5.10676	-2.63268
H	-1.43304	3.10669	-3.34291
H	-2.52387	3.79624	1.47368
H	-3.28662	5.42971	-0.22921
O	-1.08720	1.65969	0.90698
C	-0.44992	1.17826	-1.68556
O	0.04782	0.94293	-2.76039
O	-2.41338	-0.35199	-0.49782
C	-3.12400	-0.97804	0.42681
C	-2.68068	-1.17799	1.75377
C	-4.37944	-1.52141	0.07567
C	-3.43162	-1.91816	2.66309
H	-1.74428	-0.71681	2.07414

C	-5.12347	-2.24677	0.99389
H	-4.73077	-1.37038	-0.94164
C	-4.65722	-2.46469	2.29357
H	-3.05540	-2.05635	3.67480
H	-6.08234	-2.66089	0.68874
H	-5.24471	-3.03816	3.00415
Ir	-0.38393	-0.03075	-0.04405
P	1.78095	0.33247	0.70280
C	2.62724	2.00637	0.35995
C	1.85161	-0.03921	2.57603
C	4.15070	1.99661	0.52589
H	4.63920	1.40945	-0.25565
H	4.50393	3.02927	0.42006
H	4.49762	1.63734	1.49660
C	2.34440	2.38508	-1.09712
H	1.32113	2.73576	-1.23666
H	3.00976	3.21006	-1.37694
H	2.52313	1.56102	-1.79521
C	2.01780	3.07566	1.27045
H	0.92411	3.03757	1.27499
H	2.37342	2.99352	2.30208
H	2.32049	4.06350	0.90373
C	0.74626	0.74038	3.29830
H	0.90610	1.81958	3.29311
H	-0.24108	0.56008	2.86596
H	0.72190	0.41472	4.34533
C	3.18938	0.27186	3.24685
H	3.12878	-0.03275	4.29876
H	4.02848	-0.27450	2.80622
H	3.42306	1.33941	3.23850
C	1.54766	-1.52993	2.75693
H	1.64571	-1.78693	3.81785
H	0.51612	-1.76331	2.46999
H	2.22698	-2.17816	2.19279
C	2.81870	-0.91170	-0.14360
C	4.18645	-1.10842	0.09857
C	2.18797	-1.66213	-1.15563
C	4.94002	-1.97705	-0.68127
H	4.67898	-0.55759	0.89250
C	2.96916	-2.51138	-1.95312
C	4.33116	-2.66105	-1.72973
H	5.99910	-2.10695	-0.47886
H	2.47872	-3.08578	-2.73523
H	4.91184	-3.32951	-2.35908
C	0.71005	-1.72841	-1.35256
C	-0.08757	-2.32280	-0.31926
C	0.19948	-1.80912	-2.68633
C	-1.28815	-3.00943	-0.63662
H	0.39105	-2.54339	0.63216

C	-1.00671	-2.40462	-2.95337
H	0.79029	-1.38115	-3.48900
C	-1.75527	-3.01972	-1.92657
H	-1.84430	-3.49250	0.16125
H	-1.37597	-2.42839	-3.97461
H	-2.69270	-3.51534	-2.16099

V_{JP}^3: M06L/6-311+G(2df,2pd)(SDD) SCF= -1951.030452 hartree
Gibbs correction= 0.477892 hartree
Total Gibbs Energy= -1950.55256 hartree

C	-4.22314	-2.83656	-0.98025
C	-3.41046	-2.49141	0.08640
C	-2.29338	-1.67433	-0.12692
C	-1.98991	-1.18846	-1.41862
C	-2.81310	-1.55341	-2.49797
C	-3.91107	-2.36661	-2.26477
H	-5.09998	-3.45743	-0.82609
H	-3.62401	-2.82338	1.09866
H	-2.58101	-1.18162	-3.49118
H	-4.55003	-2.63761	-3.10212
O	-0.93175	-0.40793	-1.59956
C	-1.39160	-1.23097	0.94344
O	-1.45149	-1.55906	2.11620
O	-1.61339	1.56296	0.76859
C	-2.94225	1.40929	0.72158
C	-3.63339	1.49681	-0.50055
C	-3.67518	1.17334	1.89689
C	-5.01323	1.33854	-0.54097
H	-3.05730	1.65739	-1.40928
C	-5.05720	1.03421	1.84575
H	-3.13331	1.09491	2.83540
C	-5.73570	1.11091	0.63000
H	-5.52922	1.38781	-1.49741
H	-5.60977	0.85193	2.76466
H	-6.81460	0.98957	0.59449
Ir	-0.19693	0.18920	0.22890
P	1.83323	-0.90256	0.14472
C	2.35609	-1.11517	1.96660
C	2.00180	-2.52154	-0.82658
C	3.86223	-1.22545	2.19572
H	4.39842	-0.31826	1.90543
H	4.04273	-1.38797	3.26523
H	4.30958	-2.07036	1.66250
C	1.84269	0.16203	2.64657
H	0.74371	0.24283	2.59210
H	2.09313	0.14558	3.71452
H	2.28774	1.06669	2.21510
C	1.65846	-2.32352	2.59250
H	0.57389	-2.28568	2.47292

H	2.02987	-3.27125	2.19228
H	1.86695	-2.32862	3.66925
C	0.70735	-3.31227	-0.60717
H	0.51058	-3.52963	0.44704
H	-0.15532	-2.78113	-1.00904
H	0.78396	-4.27048	-1.13420
C	3.17385	-3.43709	-0.45974
H	3.09488	-4.34900	-1.06389
H	4.15801	-3.01358	-0.66873
H	3.15382	-3.74755	0.58812
C	2.07750	-2.12932	-2.30561
H	2.02312	-3.03438	-2.92204
H	1.23423	-1.48673	-2.58329
H	3.00871	-1.61075	-2.55357
C	3.15377	0.24360	-0.45731
C	4.45730	-0.22250	-0.68820
C	2.92749	1.63625	-0.51361
C	5.52084	0.63868	-0.92350
H	4.65808	-1.28597	-0.64409
C	4.02053	2.49649	-0.70510
C	5.30554	2.01271	-0.90401
H	6.51422	0.23548	-1.09729
H	3.83057	3.56661	-0.73749
H	6.12855	2.70381	-1.06187
C	1.59276	2.28728	-0.50767
C	0.71444	2.05111	-1.58475
C	1.30275	3.34624	0.37277
C	-0.40135	2.86584	-1.78170
H	0.95358	1.27334	-2.30593
C	0.17197	4.12847	0.18887
H	1.98412	3.54866	1.19681
C	-0.67622	3.89724	-0.89543
H	-1.06013	2.66724	-2.62205
H	-0.05019	4.92656	0.89101
H	-1.56036	4.51255	-1.03426

1: M06/6-311+G(2df,2pd) SCF= -726.8597914 hartree (solvent=toluene)
SCF= -727.2540142 hartree (solvent=*m*-xylene)
SCF= -727.2542687 hartree (solvent=anisole)
Gibbs correction= 0.131313 hartree
Total Gibbs Energy= -726.7284784 hartree (solvent=toluene)
Total Gibbs Energy= -726.7279334 hartree (solvent=*m*-xylene)
Total Gibbs Energy= -726.7285541 hartree (solvent=anisole)

C	3.28711	-1.83403	0.38223
C	1.97347	-1.41953	0.30055
C	1.65280	-0.08282	0.01398
C	2.69490	0.85046	-0.19325
C	4.02400	0.41861	-0.10841
C	4.31059	-0.90252	0.17495
H	3.52307	-2.87052	0.60478
H	1.16113	-2.12303	0.45744
H	4.80640	1.15430	-0.27218
H	5.34941	-1.21914	0.23667
O	2.48248	2.13802	-0.46957
H	1.51214	2.28362	-0.49589
C	0.26817	0.37932	-0.07583
O	-0.06444	1.52984	-0.31478
O	-0.62923	-0.60866	0.12993
C	-1.99135	-0.33021	0.07779
C	-2.75286	-1.11561	-0.77433
C	-2.57105	0.62439	0.90220
C	-4.13119	-0.93752	-0.80641
H	-2.25630	-1.85569	-1.39595
C	-3.94945	0.79482	0.85655
H	-1.95024	1.22487	1.55951
C	-4.73109	0.01828	0.00632
H	-4.73629	-1.54948	-1.47049
H	-4.41531	1.54178	1.49430
H	-5.80865	0.15780	-0.02088

Phenol: M06/6-311+G(2df,2pd) SCF= -307.3610449 hartree (solvent=toluene)
SCF= -307.3607256 hartree (solvent=*m*-xylene)
SCF= -307.3616898 hartree (solvent=anisole)
Gibbs correction= 0.057062 hartree
Total Gibbs Energy= -307.3039829 hartree (solvent=toluene)
Total Gibbs Energy= -307.3036636 hartree (solvent=*m*-xylene)
Total Gibbs Energy= -307.3046278 hartree (solvent=anisole)

C	-1.84960	0.02861	-0.00001
C	-1.12577	1.21503	0.00001
C	0.26488	1.19483	0.00000
C	0.93821	-0.02520	-0.00003
C	0.22021	-1.22027	-0.00002
C	-1.16681	-1.18560	-0.00001
H	-2.93606	0.04809	-0.00001
H	-1.64429	2.17113	0.00003

H	0.83059	2.12677	0.00002
H	0.76984	-2.15782	-0.00002
H	-1.72179	-2.12103	-0.00001
O	2.29364	-0.11112	0.00002
H	2.66581	0.77738	0.00018

2am1: M06/6-311+G(2df,2pd) SCF= -690.9262895 hartree
Gibbs correction= 0.152768 hartree
Total Gibbs Energy= -690.7735215 hartree

C	3.70908	-0.34404	0.08096
C	2.72351	-1.08341	0.73485
C	1.38895	-0.70210	0.68296
C	1.00988	0.44631	-0.01686
C	2.00018	1.21239	-0.64062
C	3.32490	0.81283	-0.60467
H	3.00882	-1.96968	1.29961
H	0.64253	-1.28053	1.22249
H	1.70581	2.12691	-1.14935
H	4.08503	1.41018	-1.10651
C	5.14300	-0.77678	0.10076
H	5.34369	-1.47257	0.92162
H	5.41400	-1.28490	-0.83344
H	5.81808	0.07955	0.20628
C	-0.38399	0.96451	-0.03827
O	-0.54729	2.19193	-0.00155
C	-1.53693	0.05519	-0.09559
C	-1.42159	-1.29544	-0.47349
C	-2.82985	0.56482	0.19248
C	-2.51898	-2.13207	-0.51467
H	-0.44541	-1.67563	-0.76288
C	-3.93249	-0.29819	0.17973
C	-3.77569	-1.62549	-0.16764
H	-2.40722	-3.16876	-0.81886
H	-4.90399	0.12038	0.42769
H	-4.64624	-2.27748	-0.18718
O	-3.05417	1.84297	0.49011
H	-2.20326	2.32217	0.35240

Toluene: M06/6-311+G(2df,2pd) SCF= -271.4333762 hartree
Gibbs correction= 0.077331 hartree
Total Gibbs Energy= -271.3560452 hartree

C	-0.91036	0.00015	-0.01085
C	-0.19490	-1.19813	-0.00887
C	1.19497	-1.20124	0.00201
C	1.89595	-0.00012	0.00823
C	1.19523	1.20110	0.00200
C	-0.19470	1.19825	-0.00886
H	-0.73984	-2.14175	-0.01784
H	1.73313	-2.14657	0.00120

H	2.98334	-0.00024	0.01337
H	1.73355	2.14634	0.00120
H	-0.73943	2.14197	-0.01781
C	-2.40930	0.00007	0.00928
H	-2.81874	-0.88289	-0.49347
H	-2.79464	-0.00701	1.03724
H	-2.81870	0.88971	-0.48151

2aa1: M06/6-311+G(2df,2pd) SCF= -730.2228341 hartree
Gibbs correction= 0.173112 hartree
Total Gibbs Energy= -730.0497221 hartree

C	3.49408	0.52428	-0.01762
C	2.49875	1.37205	-0.50213
C	1.18564	0.90592	-0.53239
C	0.87833	-0.38634	-0.09995
C	1.90031	-1.22297	0.35104
C	3.21508	-0.77261	0.41632
C	2.83433	2.75828	-0.96595
H	0.40196	1.54499	-0.93676
H	1.65081	-2.24087	0.64513
C	4.30621	-1.65427	0.94562
C	-0.49069	-0.96414	-0.20361
O	-0.59515	-2.14948	-0.54671
C	-1.68370	-0.15832	0.08907
C	-1.62148	1.06833	0.77596
C	-2.95905	-0.65448	-0.28790
C	-2.75637	1.80903	1.03890
H	-0.65505	1.42291	1.12433
C	-4.10164	0.11767	-0.04453
C	-3.99803	1.33029	0.60793
H	-2.68531	2.74879	1.57889
H	-5.05929	-0.28287	-0.36545
H	-4.89823	1.90948	0.80172
O	-3.13029	-1.83404	-0.88072
H	-2.25134	-2.28188	-0.88566
H	4.52523	0.88123	0.00952
H	3.80172	2.78630	-1.47900
H	2.89778	3.45601	-0.12131
H	2.07545	3.14695	-1.65274
H	4.06133	-2.71374	0.81929
H	4.46942	-1.48344	2.01725
H	5.25846	-1.46201	0.43961

2aa2: M06/6-311+G(2df,2pd) SCF= -730.2217552 hartree
Gibbs correction= 0.175089 hartree
Total Gibbs Energy= -730.0466662 hartree

C	-3.53890	-0.71199	-0.19262
C	-2.51294	-1.40520	-0.83139
C	-1.21523	-0.91612	-0.80010

C	-0.91102	0.28578	-0.15493
C	-1.93965	1.01828	0.46984
C	-3.22642	0.48735	0.44915
H	-2.73244	-2.33397	-1.35534
H	-0.42277	-1.46033	-1.31000
C	-1.69617	2.32939	1.15649
H	-4.02467	1.03880	0.94826
C	-4.93893	-1.24484	-0.17220
H	-5.67684	-0.43673	-0.21915
H	-5.12292	-1.92455	-1.01055
H	-5.13410	-1.80531	0.75098
C	0.47044	0.83540	-0.23566
O	0.62027	2.02828	-0.53489
C	1.63340	-0.02677	0.01734
C	1.51709	-1.29232	0.62182
C	2.93053	0.44505	-0.31335
C	2.62112	-2.08771	0.85374
H	0.53155	-1.63558	0.92566
C	4.04222	-0.37900	-0.09889
C	3.88602	-1.62532	0.47501
H	2.50847	-3.05814	1.32841
H	5.01824	0.00606	-0.38114
H	4.76258	-2.24655	0.64566
O	3.15057	1.65038	-0.83395
H	2.28421	2.12237	-0.83740
H	-2.55686	2.60407	1.77442
H	-1.52168	3.12693	0.42757
H	-0.80880	2.30172	1.79785

***m*-xylene**: M06/6-311+G(2df,2pd) SCF= -310.7307118 hartree
Gibbs correction= 0.097228 hartree
Total Gibbs Energy= -310.6334838 hartree

C	0.00091	-0.94755	-0.01892
C	-1.21848	-0.27182	-0.00957
C	-1.20543	1.12393	-0.00036
C	-0.00140	1.81684	0.00467
C	1.20461	1.12553	-0.00072
C	1.21999	-0.26923	-0.00986
C	-2.51483	-1.02606	0.01003
H	-2.14967	1.66736	-0.00372
H	2.14769	1.67084	-0.00418
C	2.51531	-1.02521	0.01022
H	0.00211	-2.03905	-0.03732
H	-2.40573	-2.02608	-0.42312
H	-3.29554	-0.49807	-0.54863
H	-2.88486	-1.15535	1.03532
H	3.32310	-0.45165	-0.45698
H	2.43087	-1.98235	-0.51600
H	2.83003	-1.24899	1.03772

H	-0.00214	2.90478	0.00395

2ag: M06/6-311+G(2df,2pd) SCF= -880.6307319 hartree
Gibbs correction= 0.182822 hartree
Total Gibbs Energy= -880.4479099 hartree

C	-2.85483	-0.72818	-0.17001
C	-1.80265	-1.56068	-0.52923
C	-0.49067	-1.08952	-0.51720
C	-0.22113	0.22639	-0.15715
C	-1.28858	1.08005	0.17027
C	-2.59037	0.61866	0.18456
H	-1.99735	-2.58547	-0.82972
H	0.31272	-1.74916	-0.83307
H	-1.05495	2.11415	0.40406
C	1.13222	0.83000	-0.21483
O	1.22610	2.02846	-0.52011
C	2.34000	0.03929	0.07115
C	2.30584	-1.17526	0.78002
C	3.60273	0.54426	-0.33436
C	3.45365	-1.90187	1.02926
H	1.35201	-1.52983	1.16126
C	4.75717	-0.21506	-0.10860
C	4.68023	-1.42017	0.56187
H	3.40332	-2.83187	1.58824
H	5.70373	0.19086	-0.45484
H	5.59006	-1.98816	0.74340
O	3.75120	1.72091	-0.94090
H	2.87241	2.16754	-0.91283
O	-4.15108	-1.09319	-0.13578
O	-3.67452	1.35660	0.50911
C	-4.46801	-2.41894	-0.48575
H	-5.55096	-2.51234	-0.38879
H	-4.17924	-2.64425	-1.52197
H	-3.98284	-3.14182	0.18513
C	-3.45908	2.70606	0.84496
H	-4.44040	3.12840	1.06829
H	-2.81428	2.80571	1.72965
H	-3.00700	3.26381	0.01286

1,2-Dimethoxybenzene: M06/6-311+G(2df,2pd) SCF= -461.1355502 hartree
Gibbs correction= 0.107085 hartree
Total Gibbs Energy= -461.0284652 hartree

C	0.70676	-0.13563	-0.00001
C	1.39023	1.07219	0.00009
C	0.69086	2.28236	0.00006
C	-0.69085	2.28236	-0.00008
C	-1.39023	1.07220	-0.00017
C	-0.70676	-0.13563	-0.00012
H	2.47620	1.08160	0.00021

H	1.24345	3.21834	0.00014
H	-2.47620	1.08161	-0.00032
O	1.29036	-1.35862	0.00002
O	-1.29036	-1.35862	-0.00022
C	2.69315	-1.40533	-0.00011
H	2.96834	-2.46200	-0.00027
H	3.11809	-0.92515	-0.89390
H	3.11826	-0.92538	0.89372
C	-2.69315	-1.40533	0.00041
H	-3.11858	-0.92553	-0.89336
H	-2.96834	-2.46199	0.00084
H	-3.11777	-0.92498	0.89427
H	-1.24344	3.21835	-0.00013

4-CN-Phenyl Salicylate: M06/6-311+G(2df,2pd) SCF= -819.0748187 hartree
Gibbs correction= 0.124872 hartree
Total Gibbs Energy= -818.9499467 hartree

C	3.96063	-1.81244	0.38271
C	2.64500	-1.40946	0.29217
C	2.31565	-0.07311	0.00791
C	3.35193	0.87025	-0.18745
C	4.68366	0.44844	-0.09408
C	4.97814	-0.87106	0.18664
H	4.20394	-2.84742	0.60360
H	1.83855	-2.12140	0.44056
H	5.46131	1.19093	-0.24884
H	6.01882	-1.17954	0.25551
O	3.13344	2.15696	-0.45981
H	2.16457	2.30225	-0.49282
C	0.93238	0.37923	-0.08868
O	0.58403	1.52550	-0.31892
O	0.03671	-0.62434	0.09811
C	-1.32041	-0.36684	0.06347
C	-2.08652	-1.22585	-0.71447
C	-1.90386	0.63549	0.83115
C	-3.46404	-1.08117	-0.73401
H	-1.58898	-1.99910	-1.29239
C	-3.28138	0.78049	0.80627
H	-1.28659	1.29401	1.43194
C	-4.06804	-0.07405	0.02572
H	-4.08006	-1.74359	-1.33547
H	-3.75987	1.55742	1.39585
C	-5.49008	0.07887	0.00886
N	-6.64621	0.20124	-0.00431

4-CN-Phenol: M06/6-311+G(2df,2pd) SCF= -399.5793369 hartree
Gibbs correction= 0.050721 hartree
Total Gibbs Energy= -399.5286159 hartree

O	-3.05674	0.08613	0.00004

C	-1.70886	0.01507	0.00000
C	-1.01947	-1.19898	0.00000
C	-1.00679	1.22261	0.00001
C	0.36540	-1.20573	-0.00001
H	-1.57121	-2.13806	0.00001
C	0.37480	1.21250	-0.00001
H	-1.56846	2.15218	0.00004
C	1.07621	-0.00134	-0.00002
H	0.90823	-2.14718	-0.00001
H	0.92861	2.14755	-0.00001
C	2.50438	-0.00924	-0.00003
N	3.66753	-0.01575	-0.00005
H	-3.42999	-0.80264	0.00031

1,5-COD: M06/6-311+G(2df,2pd) SCF= -311.8774299 hartree
Gibbs correction= 0.125668 hartree
Total Gibbs Energy= -311.7517619 hartree

C	-0.87180	-1.62825	-0.20369
C	0.38594	-1.80649	0.20308
C	-0.38594	1.80649	-0.20308
C	1.23538	-0.79657	0.92254
C	0.87180	1.62825	0.20369
C	1.69213	0.38177	0.02399
H	-1.34914	-2.44607	-0.74545
H	0.69032	-0.38832	1.78669
H	-0.86279	2.75965	0.03001
H	1.34914	2.44607	0.74545
H	0.86279	-2.75965	-0.03001
H	2.11733	-1.30381	1.33162
H	2.74192	0.61547	0.23803
H	1.66047	0.05398	-1.02578
C	-1.69213	-0.38177	-0.02399
H	-1.66047	-0.05398	1.02578
H	-2.74192	-0.61547	-0.23803
C	-1.23538	0.79657	-0.92254
H	-0.69032	0.38832	-1.78669
H	-2.11733	1.30381	-1.33162

JohnPhos: M06/6-311+G(2df,2pd) SCF= -1119.378626 hartree
Gibbs correction= 0.326213 hartree
Total Gibbs Energy= -1119.052413 hartree

C	1.04207	3.63443	-0.02039
C	1.83708	2.50045	-0.07873
C	1.28150	1.21620	-0.15694
C	-0.12301	1.06666	-0.14250
C	-0.90305	2.22991	-0.07990
C	-0.34079	3.49856	-0.02971
H	1.50015	4.61965	0.02565
H	2.92156	2.59596	-0.09035

H	-1.98623	2.14322	-0.05645
H	-0.98252	4.37564	0.01266
C	2.24021	0.08304	-0.24089
C	3.20034	-0.08555	0.76028
C	2.26024	-0.78365	-1.33730
C	4.14320	-1.10473	0.68061
H	3.19222	0.58639	1.61787
C	3.20690	-1.79532	-1.42395
H	1.52815	-0.65079	-2.13140
C	4.14904	-1.96243	-0.41297
H	4.87554	-1.22671	1.47545
H	3.21077	-2.45680	-2.28716
H	4.88712	-2.75826	-0.48017
P	-0.84477	-0.64883	-0.11571
C	-2.37566	-0.57625	-1.26326
C	-1.39925	-0.77225	1.70719
C	-2.17481	-2.07863	1.87261
H	-2.32722	-2.28403	2.94207
H	-3.16713	-2.03641	1.40672
H	-1.62992	-2.92970	1.44338
C	-0.08691	-0.89016	2.48844
H	0.52976	-1.72260	2.12692
H	0.50970	0.02855	2.41664
H	-0.30583	-1.06176	3.55238
C	-2.20340	0.38238	2.29396
H	-3.17355	0.51757	1.80466
H	-2.40008	0.18068	3.35775
H	-1.65500	1.32963	2.23820
C	-2.66528	-2.04135	-1.61459
H	-2.97991	-2.62489	-0.74137
H	-3.47658	-2.09193	-2.35548
H	-1.78223	-2.53093	-2.04203
C	-3.67387	0.05483	-0.76679
H	-4.43196	-0.01292	-1.56182
H	-4.08068	-0.46782	0.10683
H	-3.57479	1.11567	-0.51301
C	-1.92691	0.12476	-2.54684
H	-2.69264	-0.00928	-3.32455
H	-1.77304	1.20011	-2.40626
H	-0.99005	-0.30123	-2.93148

[Ir(cod)OMe]$_2$: M06/6-311+G(2df,2pd) SCF= -1062.861165 hartree
Gibbs correction= 0.354007 hartree
Total Gibbs Energy= -1062.507158 hartree

C	-2.38710	-1.53960	0.78926
C	-3.11775	-1.33066	-0.41590
C	-2.60995	1.18157	1.15818
C	-4.49449	-0.68514	-0.45268
C	-3.11722	1.41569	-0.15200

C	-4.39592	0.82453	-0.70216
H	-1.68023	-2.37694	0.80006
H	-5.09388	-1.15007	-1.24426
H	-1.95295	1.95053	1.57498
H	-2.82162	2.35123	-0.63855
H	-2.91210	-2.01904	-1.24096
H	-5.02967	-0.89326	0.48320
H	-4.39677	1.00803	-1.78482
H	-5.27764	1.34924	-0.29973
C	-2.84089	-1.11497	2.16751
H	-1.97215	-1.20737	2.83376
H	-3.60765	-1.80219	2.56065
C	-3.33548	0.33535	2.19314
H	-4.41895	0.38272	2.02226
H	-3.17537	0.76129	3.19076
C	2.38707	-1.53957	0.78933
C	3.11773	-1.33070	-0.41585
C	2.60998	1.18162	1.15813
C	4.49447	-0.68520	-0.45266
C	3.11724	1.41566	-0.15207
C	4.39592	0.82446	-0.70221
H	1.68019	-2.37690	0.80017
H	5.02965	-0.89329	0.48323
H	1.95300	1.95061	1.57490
H	2.82165	2.35118	-0.63866
H	2.91205	-2.01911	-1.24087
H	5.09385	-1.15019	-1.24422
H	5.27765	1.34917	-0.29981
H	4.39677	1.00791	-1.78487
C	2.84089	-1.11489	2.16756
H	3.60764	-1.80211	2.56071
H	1.97215	-1.20724	2.83382
C	3.33551	0.33542	2.19312
H	3.17542	0.76140	3.19071
H	4.41898	0.38276	2.02221
Ir	1.52042	0.05341	-0.26608
Ir	-1.52042	0.05341	-0.26609
O	-0.00000	-1.06833	-1.19045
O	0.00000	1.45237	-0.73462
C	0.00000	-2.45030	-1.40191
H	-0.88771	-2.74248	-1.98116
H	0.88761	-2.74244	-1.98134
H	0.00011	-3.03174	-0.46408
C	0.00000	2.78099	-0.29522
H	0.88536	3.30911	-0.67821
H	-0.88525	3.30917	-0.67837
H	-0.00009	2.86717	0.80461

Methanol: M06/6-311+G(2df,2pd) SCF= -115.6994043 hartree

Gibbs correction= 0.014923 hartree
Total Gibbs Energy= -115.6844813 hartree

O	0.74282	0.12181	0.00000
C	-0.65401	-0.01982	0.00000
H	-1.03449	-0.54284	0.89145
H	-1.03449	-0.54283	-0.89145
H	-1.08163	0.98716	0.00000
H	1.13208	-0.75705	-0.00000

II: M06/6-311+G(2df,2pd) SCF= -535.2118099 hartree
Gibbs correction= 0.089783 hartree
Total Gibbs Energy= -535.1220269 hartree

C	2.89134	-0.67350	-0.00045
C	1.97782	-1.73326	-0.00007
C	0.62554	-1.45557	0.00030
C	0.15908	-0.13209	0.00034
C	1.09008	0.93113	-0.00003
C	2.45918	0.63871	-0.00043
H	3.95914	-0.88102	-0.00075
H	2.32752	-2.76153	-0.00008
H	-0.10487	-2.25956	0.00058
H	3.15515	1.47297	-0.00070
C	-1.27107	0.18151	0.00069
O	-1.73054	1.31823	-0.00016
O	-2.06167	-0.89671	0.00026
O	0.73312	2.21685	0.00006
H	-0.24825	2.25371	0.00053
C	-3.46089	-0.62718	-0.00030
H	-3.74434	-0.05501	-0.88847
H	-3.95304	-1.59998	-0.00052
H	-3.74505	-0.05505	0.88768

Salicylic Acid: M06/6-311+G(2df,2pd) SCF= -495.9350214 hartree
Gibbs correction= 0.066659 hartree
Total Gibbs Energy= -495.8683624 hartree

C	-1.88924	-1.46556	0.00017
C	-0.50944	-1.45383	-0.00011
C	0.20171	-0.24334	-0.00034
C	-0.50645	0.98004	-0.00024
C	-1.90621	0.95607	0.00009
C	-2.58118	-0.24908	0.00033
H	-2.43110	-2.40672	0.00031
H	0.05251	-2.38358	-0.00021
H	-2.42953	1.90808	0.00020
H	-3.66895	-0.24764	0.00063
O	0.09249	2.17148	-0.00068
H	3.19838	-1.25255	0.00020
C	1.66092	-0.21262	0.00006
O	2.24357	-1.41928	-0.00052

O	2.33835	0.80936	0.00102
H	1.06270	2.01977	0.00051

I: M06/6-311+G(2df,2pd) SCF= -1142.578371 hartree
Gibbs correction= 0.27753 hartree
Total Gibbs Energy= -1142.300841 hartree

C	3.11763	0.29799	0.71591
C	3.14090	0.12068	-0.69289
C	1.49273	-1.95503	0.75688
C	3.61340	-1.15782	-1.36743
C	1.32534	-1.97885	-0.65310
C	2.44495	-2.10827	-1.66150
H	3.18787	1.32742	1.07915
H	4.12638	-0.90683	-2.30341
H	0.62428	-2.24811	1.35335
H	0.34412	-2.29861	-1.02105
H	3.21882	1.03031	-1.29432
H	4.36751	-1.65044	-0.73964
H	2.02425	-1.86088	-2.64542
H	2.79660	-3.15046	-1.73124
C	3.49253	-0.75610	1.73240
H	3.14853	-0.39662	2.71126
H	4.58765	-0.85358	1.80898
C	2.84092	-2.11502	1.44251
H	3.49986	-2.74060	0.82594
H	2.70911	-2.66461	2.38213
Ir	1.15574	0.00979	0.02363
O	0.90056	2.05355	-0.05922
C	-0.21904	2.70732	-0.06016
C	-1.54205	2.15012	-0.03503
C	-0.12192	4.12609	-0.10102
C	-2.66380	3.02002	-0.06286
C	-1.22986	4.93330	-0.12254
H	0.88418	4.53724	-0.11817
C	-2.52576	4.38268	-0.10461
H	-3.65484	2.57703	-0.04696
H	-1.10252	6.01391	-0.15516
H	-3.40107	5.02559	-0.12290
C	-1.78034	0.73185	0.01709
O	-0.94607	-0.19024	0.08086
O	-3.08266	0.38893	0.00387
C	-3.43615	-0.95734	-0.00648
C	-4.17477	-1.43076	1.06619
C	-3.13165	-1.76185	-1.09677
C	-4.61616	-2.75046	1.04920
H	-4.39684	-0.76261	1.89398
C	-3.57440	-3.07894	-1.09919
H	-2.55339	-1.35622	-1.92299
C	-4.31547	-3.57544	-0.02943

H	-5.19759	-3.13238	1.88468
H	-3.34090	-3.72030	-1.94550
H	-4.66071	-4.60615	-0.03926

C: M06/6-311+G(2df,2pd) SCF= -1142.531564 hartree
Gibbs correction= 0.278465 hartree
Total Gibbs Energy= -1142.253099 hartree

C	2.34610	-0.04299	-1.66410
C	2.28091	-1.23914	-0.91078
C	2.51620	1.26177	0.82283
C	3.34286	-1.65278	0.09216
C	2.22067	0.09658	1.55864
C	3.00725	-1.19189	1.51770
H	1.79341	-0.03196	-2.60756
H	3.44567	-2.74379	0.07880
H	2.09861	2.19801	1.20297
H	1.59834	0.21966	2.44697
H	1.67281	-2.04585	-1.32864
H	4.31596	-1.25715	-0.22698
H	2.39098	-1.95557	2.00771
H	3.92471	-1.10070	2.12006
C	3.42203	1.01135	-1.53834
H	3.06396	1.90273	-2.07011
H	4.33927	0.69571	-2.06053
C	3.73142	1.38975	-0.08200
H	4.54737	0.77164	0.31447
H	4.09947	2.42155	-0.04711
Ir	0.91038	0.20092	-0.13340
O	-0.53573	-0.35436	-1.52017
C	-1.53077	-1.07148	-1.08229
C	-1.57138	-1.56309	0.24521
C	-2.61116	-1.41031	-1.92599
C	-2.60073	-2.41346	0.68959
C	-3.62481	-2.22759	-1.47034
H	-2.60531	-1.01821	-2.93967
C	-3.62804	-2.74924	-0.16541
H	-2.57755	-2.76925	1.71786
H	-4.44186	-2.47850	-2.14446
H	-4.43404	-3.39676	0.16751
C	-0.60730	-1.11141	1.22345
O	-0.21913	-1.51474	2.26462
O	-0.62777	0.74054	1.23656
C	-1.76422	1.34397	0.78902
C	-2.98261	1.04082	1.40135
C	-1.72047	2.27953	-0.24599
C	-4.14826	1.65339	0.96073
H	-2.99766	0.31754	2.21461
C	-2.89136	2.89217	-0.67521
H	-0.76202	2.50550	-0.71322

C	-4.10979	2.57798	-0.07999
H	-5.09496	1.40648	1.43601
H	-2.84995	3.61852	-1.48383
H	-5.02482	3.05458	-0.42278

III[1]: M06/6-311+G(2df,2pd) SCF= -1142.556675 hartree
Gibbs correction= 0.277701 hartree
Total Gibbs Energy= -1142.278974 hartree

C	-1.23772	2.20153	0.39671
C	-0.57662	2.56958	-0.78934
C	1.30601	1.24522	1.22182
C	0.64457	3.47187	-0.81673
C	1.90722	1.39711	-0.03156
C	1.95525	2.67439	-0.83926
H	-2.29134	1.92598	0.30585
H	0.59697	4.10991	-1.70627
H	1.59387	0.35861	1.78584
H	2.63700	0.63618	-0.32227
H	-1.15933	2.50856	-1.71208
H	0.61800	4.15301	0.04246
H	2.19277	2.40171	-1.87606
H	2.79491	3.29762	-0.49409
C	-0.79119	2.60994	1.77891
H	-1.36823	2.02828	2.50564
H	-1.05199	3.66478	1.95597
C	0.70650	2.37930	2.03319
H	1.27897	3.29532	1.83775
H	0.85305	2.15246	3.09483
Ir	-0.05217	0.51710	-0.38039
O	-1.67831	-0.08942	-1.49429
C	-2.47586	-0.87276	-0.82516
C	-2.26128	-1.08114	0.55724
C	-3.58318	-1.50947	-1.42645
C	-3.10947	-1.90581	1.32129
C	-4.40507	-2.31048	-0.66271
H	-3.75534	-1.35692	-2.48840
C	-4.18144	-2.51847	0.71285
H	-2.89669	-2.04116	2.37915
H	-5.25218	-2.80032	-1.13967
H	-4.84843	-3.15869	1.28324
C	-1.11730	-0.42334	1.15836
O	-0.74771	-0.43036	2.29843
O	0.77146	-1.23925	-0.91401
C	1.92371	-1.73139	-0.43438
C	3.01745	-1.88344	-1.29969
C	2.05803	-2.13976	0.90128
C	4.21046	-2.42609	-0.83777
H	2.89757	-1.57468	-2.33657
C	3.25821	-2.67782	1.35228

H	1.20340	-2.04203	1.56915
C	4.34221	-2.82304	0.49072
H	5.04742	-2.53854	-1.52455
H	3.34301	-2.99386	2.39043
H	5.27746	-3.24611	0.84891

III^{2}: M06/6-311+G(2df,2pd) SCF= -1142.528706 hartree
Gibbs correction= 0.279867 hartree
Total Gibbs Energy= -1142.248839 hartree

C	0.66027	1.10730	1.77851
C	-0.37700	1.80489	1.11633
C	2.16133	1.38864	-0.74575
C	-0.19195	3.10567	0.34991
C	1.07448	1.78386	-1.45950
C	0.19251	2.96023	-1.13361
H	0.36738	0.48899	2.63087
H	-1.13333	3.66449	0.39899
H	2.77951	0.58918	-1.15227
H	0.87779	1.28530	-2.41105
H	-1.38400	1.65706	1.51291
H	0.54264	3.72444	0.88279
H	-0.72399	2.85052	-1.71973
H	0.67770	3.88705	-1.47654
C	2.10734	1.54049	1.80642
H	2.71007	0.67943	2.11973
H	2.23019	2.29713	2.59819
C	2.67362	2.08711	0.48553
H	2.47193	3.16160	0.40151
H	3.76604	1.98966	0.51483
Ir	0.08248	0.02680	0.00170
O	-1.57455	0.65670	-1.06950
C	-2.68326	0.07956	-0.64847
C	-2.64515	-0.79753	0.45029
C	-3.92000	0.33093	-1.27050
C	-3.80862	-1.41191	0.93009
C	-5.05828	-0.28941	-0.78759
H	-3.95369	1.00322	-2.12406
C	-5.01893	-1.16102	0.31248
H	-3.72551	-2.08180	1.78338
H	-6.01097	-0.09313	-1.27678
H	-5.93119	-1.63248	0.66810
C	-1.32001	-1.01422	1.03566
O	-1.08863	-1.69765	2.01463
O	0.29607	-1.56097	-1.40746
C	1.47664	-1.79417	-0.92303
C	2.63185	-1.90460	-1.74840
C	1.63519	-1.72690	0.50660
C	3.87659	-1.88792	-1.17295
H	2.48793	-1.97622	-2.82359

C	2.95156	-1.68069	1.04464
H	0.83951	-2.09799	1.15177
C	4.05068	-1.73547	0.22739
H	4.75799	-1.97184	-1.80641
H	3.07252	-1.66241	2.12676
H	5.05425	-1.72003	0.64427

X: M06/6-311+G(2df,2pd) SCF= -1638.519577 hartree
Gibbs correction= 0.378831 hartree
Total Gibbs Energy= -1638.140746 hartree

C	1.21901	-1.20364	2.29918
C	-0.06620	-0.66307	2.47180
C	1.94534	1.41333	1.47902
C	-0.35432	0.53167	3.36472
C	0.63531	1.89697	1.44852
C	-0.32334	1.87345	2.61519
H	1.27494	-2.25348	2.00196
H	-1.34019	0.39880	3.82549
H	2.61320	1.75534	0.68939
H	0.38131	2.59848	0.64961
H	-0.90692	-1.32692	2.25585
H	0.36266	0.53739	4.19561
H	-1.32327	2.09817	2.22757
H	-0.07333	2.69056	3.30907
C	2.46647	-0.63648	2.92976
H	3.33093	-1.14349	2.48938
H	2.47592	-0.88757	4.00157
C	2.61842	0.87911	2.73092
H	2.22824	1.42345	3.60107
H	3.68487	1.12124	2.67346
Ir	0.62499	-0.08117	0.50905
O	-0.13301	-1.82177	-0.30518
C	0.78841	-2.54836	-0.88785
C	2.14111	-2.15616	-0.81035
C	0.47357	-3.73352	-1.58235
C	3.15760	-2.91525	-1.41409
C	1.48602	-4.46896	-2.16592
H	-0.56737	-4.03961	-1.64532
C	2.83336	-4.07244	-2.09025
H	4.18484	-2.56694	-1.33305
H	1.23135	-5.38159	-2.70204
H	3.60629	-4.67178	-2.56333
C	2.43913	-0.92030	-0.09356
O	3.52707	-0.42803	0.06236
O	0.58766	0.66773	-1.44458
C	1.03641	1.90381	-1.75717
C	0.12709	2.94922	-1.96644
C	2.40651	2.15256	-1.90642
C	0.58213	4.21509	-2.31922

H	-0.93852	2.74976	-1.85726
C	2.85005	3.42428	-2.25110
H	3.10659	1.33389	-1.75079
C	1.94470	4.46214	-2.45877
H	-0.13684	5.01518	-2.48395
H	3.91724	3.60323	-2.36639
H	2.29817	5.45333	-2.73185
C	-6.59747	-0.54671	-0.42949
C	-5.97202	-0.51874	-1.68080
C	-2.42686	0.22727	-0.67715
C	-5.87953	-0.32479	0.73103
C	-4.61650	-0.26535	-1.74995
C	-4.50621	-0.06514	0.67102
C	-3.86320	-0.03529	-0.58774
O	-1.75250	0.47844	0.35069
O	-1.90458	0.20462	-1.86686
O	-3.86414	0.14257	1.82692
H	-7.66501	-0.74579	-0.36347
H	-2.92805	0.32587	1.59927
H	-0.89844	0.36536	-1.79794
H	-6.54486	-0.69525	-2.58662
H	-6.35043	-0.34385	1.71011
H	-4.10150	-0.24037	-2.70633

L: M06/6-311+G(2df,2pd) SCF= -1638.507574 hartree
Gibbs correction= 0.375049 hartree
Total Gibbs Energy= -1638.132525 hartree

C	-1.29634	1.26380	2.23599
C	0.01593	0.79833	2.42386
C	-1.88515	-1.42299	1.53929
C	0.37349	-0.33740	3.36582
C	-0.55274	-1.83921	1.52162
C	0.40783	-1.71244	2.67925
H	-1.40762	2.29464	1.89191
H	1.35596	-0.13133	3.80565
H	-2.54033	-1.83137	0.77122
H	-0.26213	-2.55927	0.75223
H	0.82165	1.48888	2.16332
H	-0.33444	-0.34069	4.20449
H	1.41538	-1.90151	2.29509
H	0.20048	-2.50712	3.41203
C	-2.51080	0.66083	2.89598
H	-3.40193	1.09886	2.43516
H	-2.53270	0.96292	3.95426
C	-2.57857	-0.86831	2.77093
H	-2.15197	-1.34786	3.66156
H	-3.63003	-1.17253	2.73617
Ir	-0.64733	0.10003	0.49571
O	0.01350	1.84318	-0.38300

C	-0.94394	2.50485	-0.98317
C	-2.27555	2.04765	-0.89036
C	-0.68882	3.68211	-1.71499
C	-3.33044	2.73548	-1.51568
C	-1.73779	4.34695	-2.31710
H	0.33578	4.03597	-1.79131
C	-3.06440	3.88595	-2.22619
H	-4.33903	2.33912	-1.42219
H	-1.53012	5.25423	-2.88166
H	-3.86632	4.43186	-2.71534
C	-2.50622	0.82198	-0.13705
O	-3.56110	0.26398	0.02673
O	-0.57591	-0.72502	-1.43776
C	-0.92567	-2.02300	-1.70377
C	0.05625	-2.99592	-1.89645
C	-2.27711	-2.35722	-1.79338
C	-0.32290	-4.30519	-2.17476
H	1.10602	-2.71427	-1.83676
C	-2.64025	-3.67216	-2.06245
H	-3.02476	-1.57940	-1.65160
C	-1.66852	-4.65106	-2.25274
H	0.44444	-5.06051	-2.32918
H	-3.69464	-3.93009	-2.13293
H	-1.95868	-5.67652	-2.46705
C	6.62128	0.71428	-0.40846
C	6.02267	0.57823	-1.66442
C	2.46699	-0.20761	-0.69671
C	5.88430	0.55133	0.75090
C	4.67540	0.27726	-1.73845
C	4.52117	0.24469	0.68255
C	3.90447	0.10599	-0.58074
O	1.79844	-0.40739	0.36578
O	1.96650	-0.28251	-1.86622
O	3.85669	0.09784	1.83763
H	7.68078	0.95166	-0.33615
H	2.93351	-0.12960	1.58545
H	0.65462	-0.49300	-1.74221
H	6.60781	0.70858	-2.57061
H	6.33346	0.65418	1.73528
H	4.17630	0.16817	-2.69777

XI: M06/6-311+G(2df,2pd) SCF= -1331.138434 hartree
Gibbs correction= 0.287643 hartree
Total Gibbs Energy= -1330.850791 hartree

C	3.11576	0.03134	-0.02155
C	2.93085	-0.66091	-1.22852
C	1.38100	-1.92269	1.09395
C	3.19919	-2.14461	-1.39576
C	0.99850	-2.46180	-0.13565

C	1.93535	-2.99468	-1.19577
H	3.27678	1.10997	-0.09570
H	3.59439	-2.32160	-2.40218
H	0.58177	-1.81730	1.82422
H	-0.04333	-2.77710	-0.21415
H	2.92168	-0.05788	-2.14043
H	3.99059	-2.45477	-0.70325
H	1.37963	-3.04044	-2.14166
H	2.20661	-4.03529	-0.95991
C	3.56732	-0.60546	1.26784
H	3.42706	0.12411	2.07240
H	4.64926	-0.80240	1.21900
C	2.80242	-1.89060	1.61861
H	3.34066	-2.77499	1.25405
H	2.76347	-1.98820	2.70898
Ir	0.97280	-0.29493	-0.38978
O	0.90918	1.49157	-1.41659
C	0.63586	2.50276	-0.63885
C	0.60386	2.32228	0.76324
C	0.39583	3.79767	-1.14457
C	0.32974	3.38791	1.64161
C	0.13184	4.83143	-0.27049
H	0.41795	3.94719	-2.22063
C	0.09496	4.64218	1.12480
H	0.30704	3.19502	2.71150
H	-0.05699	5.82477	-0.67353
H	-0.11906	5.47905	1.78336
C	0.85285	0.98540	1.26887
O	0.93992	0.59128	2.39265
O	-1.07286	-0.19795	-0.49109
C	-1.93264	-0.83382	0.25183
O	-1.61659	-1.59948	1.17820
C	-3.35142	-0.58435	-0.08305
C	-3.70807	0.28985	-1.11941
C	-4.36985	-1.23690	0.64843
C	-5.03351	0.52044	-1.43901
H	-2.90781	0.78395	-1.66408
C	-5.70995	-0.99816	0.31828
C	-6.03272	-0.13261	-0.71069
H	-5.29466	1.20151	-2.24453
H	-6.47316	-1.51240	0.89667
H	-7.07986	0.04048	-0.95159
O	-4.11871	-2.08103	1.65208
H	-3.13812	-2.11746	1.74796

XII: M06/6-311+G(2df,2pd) SCF= -1414.000195 hartree
Gibbs correction= 0.385396 hartree
Total Gibbs Energy= -1413.614799 hartree

C	2.77563	1.40117	0.40806

C	2.94155	0.10952	-0.11472
C	1.16179	0.14907	2.38336
C	3.46811	-1.06168	0.69246
C	1.13403	-1.08810	1.73948
C	2.35293	-1.88967	1.35024
H	2.78588	2.22505	-0.31024
H	4.04228	-1.71446	0.02448
H	0.22526	0.46609	2.83627
H	0.19382	-1.64041	1.79574
H	3.03115	0.03228	-1.20063
H	4.17825	-0.69277	1.44353
H	2.03107	-2.67365	0.65391
H	2.74116	-2.41195	2.23876
C	3.05477	1.78386	1.83901
H	2.65910	2.79108	2.00581
H	4.14319	1.85369	1.98903
C	2.43228	0.82286	2.86226
H	3.15638	0.05128	3.15573
H	2.19837	1.38360	3.77370
Ir	0.81981	0.42800	0.18674
O	0.68343	1.22557	-1.72160
C	0.16722	2.42553	-1.72564
C	-0.08868	3.08433	-0.50308
C	-0.12663	3.11141	-2.92267
C	-0.63058	4.38183	-0.46309
C	-0.65589	4.38446	-2.86627
H	0.06829	2.61329	-3.86876
C	-0.91388	5.03277	-1.64379
H	-0.81714	4.84197	0.50442
H	-0.88230	4.90132	-3.79715
H	-1.33453	6.03426	-1.63495
C	0.22126	2.36627	0.72281
O	0.12795	2.73842	1.85509
C	0.27156	-1.90316	-1.89779
C	-0.32564	-2.89115	-1.11316
C	0.35184	-4.07563	-0.84922
C	1.63836	-4.29629	-1.35374
C	2.22575	-3.30261	-2.14108
C	1.54881	-2.11748	-2.41449
H	-0.26511	-0.98741	-2.13143
H	-1.32753	-2.72850	-0.71743
H	-0.11958	-4.84852	-0.24251
H	2.00659	-1.35600	-3.04404
H	3.22188	-3.46936	-2.55136
C	2.38282	-5.55408	-1.01894
H	3.14245	-5.78738	-1.77257
H	2.89971	-5.46113	-0.05389
H	1.70733	-6.41270	-0.93848
O	-1.20154	0.06007	-0.02586

C	-2.04758	-0.27347	0.90012
O	-1.79032	-0.27846	2.11604
C	-3.38329	-0.68190	0.40474
C	-3.67344	-0.70216	-0.96709
C	-4.38340	-1.07223	1.32438
C	-4.91413	-1.09728	-1.43371
H	-2.89134	-0.39195	-1.65643
C	-5.63810	-1.46895	0.84405
C	-5.89559	-1.48043	-0.51452
H	-5.12340	-1.10660	-2.49999
H	-6.38904	-1.76286	1.57293
H	-6.87677	-1.79189	-0.86765
O	-4.19163	-1.08498	2.64519
H	-3.26568	-0.77859	2.79529

VI: M06/6-311+G(2df,2pd) SCF= -1414.000195 hartree
Gibbs correction= 0.385396 hartree
Total Gibbs Energy= -1413.614799 hartree

C	0.46949	-1.84083	1.78798
C	-0.84023	-1.83115	1.28017
C	0.09706	0.94979	2.15686
C	-2.03424	-1.30716	2.05704
C	-1.10938	1.00003	1.45301
C	-2.33321	0.17213	1.77037
H	1.15400	-2.58113	1.36599
H	-2.91533	-1.90165	1.78511
H	0.77554	1.79040	2.01926
H	-1.29015	1.88771	0.83877
H	-1.05925	-2.54050	0.47939
H	-1.87134	-1.47475	3.12957
H	-3.01428	0.23911	0.91287
H	-2.86567	0.62743	2.62031
C	0.86054	-1.29124	3.13756
H	1.95388	-1.26372	3.19043
H	0.53319	-1.98756	3.92505
C	0.31135	0.11780	3.40778
H	-0.63443	0.06335	3.96283
H	1.01382	0.65167	4.05706
Ir	0.25266	-0.24291	0.28862
O	0.82324	-1.56249	-1.20096
C	2.11910	-1.63393	-1.33371
C	2.95727	-0.96914	-0.41068
C	2.72889	-2.38393	-2.36185
C	4.35968	-1.03423	-0.50765
C	4.10474	-2.43991	-2.44021
H	2.09293	-2.89782	-3.07772
C	4.93415	-1.77020	-1.52015
H	4.96064	-0.49723	0.22254
H	4.56253	-3.01807	-3.24096

H	6.01469	-1.83290	-1.61308
C	2.31454	-0.19520	0.63652
O	2.82198	0.42776	1.52671
O	0.55497	1.20679	-1.09987
C	0.48130	2.52433	-0.86615
C	-0.52934	3.27615	-1.48639
C	1.41450	3.19571	-0.05983
C	-0.60979	4.65014	-1.29448
H	-1.23218	2.75548	-2.13549
C	1.32063	4.56982	0.12983
H	2.22026	2.62412	0.39786
C	0.30845	5.30688	-0.47930
H	-1.39925	5.21370	-1.78861
H	2.05652	5.07175	0.75556
H	0.24209	6.38158	-0.32881
C	-2.25441	-0.11746	-1.98920
C	-3.36116	0.68945	-1.72829
C	-4.52812	0.13402	-1.21441
C	-4.61325	-1.23547	-0.94310
C	-3.50410	-2.03683	-1.22179
C	-2.33471	-1.48757	-1.74178
H	-1.33272	0.30955	-2.37994
H	-3.31298	1.75954	-1.92430
H	-5.39138	0.76889	-1.01521
H	-1.47172	-2.11583	-1.95443
H	-3.56220	-3.10914	-1.02976
C	-5.85281	-1.82237	-0.33587
H	-5.99405	-2.86613	-0.63687
H	-5.80280	-1.80657	0.76166
H	-6.74842	-1.26130	-0.62403

G: M06/6-311+G(2df,2pd) SCF= -1413.942132 hartree
Gibbs correction= 0.385189 hartree
Total Gibbs Energy= -1413.556943 hartree

C	1.08728	-1.59757	1.87520
C	-0.30502	-1.83139	1.73548
C	0.37772	1.09691	2.12031
C	-1.32170	-1.41917	2.78827
C	-0.97191	0.90638	1.80241
C	-1.88942	-0.00537	2.58435
H	1.74777	-2.29120	1.34988
H	-2.14650	-2.14038	2.77442
H	0.85611	1.99660	1.73718
H	-1.45759	1.70377	1.23589
H	-0.58998	-2.67049	1.09821
H	-0.85837	-1.51086	3.78039
H	-2.83869	-0.07628	2.04334
H	-2.11931	0.45865	3.55635
C	1.70470	-0.87976	3.04936

H	2.76557	-0.71873	2.83297
H	1.66704	-1.53249	3.93548
C	1.03747	0.46943	3.33634
H	0.28470	0.36686	4.12970
H	1.78961	1.16863	3.71611
Ir	0.23503	-0.26853	0.39711
O	0.81279	-1.65180	-1.04046
C	2.06352	-1.53692	-1.41624
C	2.90945	-0.61616	-0.76905
C	2.60036	-2.32897	-2.45131
C	4.25563	-0.47420	-1.14373
C	3.92708	-2.17881	-2.80383
H	1.95166	-3.04095	-2.95509
C	4.76810	-1.25437	-2.15886
H	4.86530	0.25658	-0.61669
H	4.33105	-2.79372	-3.60637
H	5.80688	-1.15703	-2.46245
C	2.32039	0.17968	0.30248
O	2.89841	1.03295	0.93465
O	0.06002	1.12618	-1.30474
C	-0.17876	2.45935	-1.16123
C	-1.37608	3.01111	-1.62575
C	0.79367	3.28702	-0.59294
C	-1.60358	4.37725	-1.49833
H	-2.11180	2.36227	-2.09708
C	0.55258	4.65082	-0.47371
H	1.73315	2.85022	-0.25998
C	-0.64615	5.20344	-0.91787
H	-2.53788	4.79823	-1.86394
H	1.31570	5.28879	-0.03284
H	-0.82794	6.27088	-0.82119
C	-1.89292	-0.49062	-0.73714
C	-3.07633	0.21388	-0.43679
C	-4.33824	-0.32130	-0.65743
C	-4.48341	-1.61260	-1.17248
C	-3.32571	-2.32810	-1.48453
C	-2.06550	-1.77827	-1.27938
H	-0.92774	0.41916	-1.24246
H	-3.01693	1.23187	-0.04718
H	-5.22883	0.26648	-0.43258
H	-1.18301	-2.35436	-1.55051
H	-3.41921	-3.32985	-1.90531
C	-5.84109	-2.21387	-1.37051
H	-5.84076	-2.94913	-2.18237
H	-6.17908	-2.73344	-0.46430
H	-6.59066	-1.44890	-1.60101

G^2: M06/6-311+G(2df,2pd) SCF= -1413.925094 hartree
Gibbs correction= 0.385658 hartree

Total Gibbs Energy= -1413.539436 hartree

C	0.27246	-1.43239	2.35521
C	-1.10967	-1.29147	2.10497
C	0.43216	1.31440	1.91075
C	-2.01333	-0.35262	2.88870
C	-0.90463	1.43752	1.45649
C	-2.12779	1.03767	2.24940
H	0.71631	-2.39026	2.06771
H	-3.01235	-0.79972	2.95360
H	1.17260	1.95172	1.42423
H	-1.08795	2.18043	0.67904
H	-1.59087	-2.16438	1.66587
H	-1.64969	-0.27964	3.92270
H	-2.97973	1.04484	1.55731
H	-2.33958	1.80279	3.01326
C	1.03363	-0.65823	3.40328
H	2.10124	-0.85329	3.26411
H	0.77094	-1.04509	4.40028
C	0.78849	0.85022	3.31447
H	-0.00913	1.15825	4.00382
H	1.69034	1.38111	3.63674
Ir	-0.03126	-0.26774	0.53056
O	0.04745	-2.05918	-0.68502
C	1.30161	-2.21830	-1.20017
C	2.34761	-1.54640	-0.56284
C	1.54959	-3.09463	-2.24940
C	3.66330	-1.78064	-0.96701
C	2.86334	-3.29760	-2.65574
H	0.71860	-3.61064	-2.72283
C	3.92190	-2.64991	-2.01655
H	4.46044	-1.24690	-0.45358
H	3.06530	-3.97826	-3.47975
H	4.94315	-2.81819	-2.34803
C	2.05634	-0.55045	0.51792
O	2.93101	0.00517	1.13243
O	0.56491	0.78756	-1.18677
C	1.12807	2.00341	-1.18214
C	0.34657	3.17292	-1.21500
C	2.52584	2.14927	-1.22003
C	0.94037	4.42954	-1.26364
H	-0.73864	3.08122	-1.22933
C	3.11062	3.40756	-1.26843
H	3.14236	1.25318	-1.21678
C	2.32547	4.55812	-1.28312
H	0.31047	5.31703	-1.29328
H	4.19563	3.49005	-1.29690
H	2.78800	5.54154	-1.31928
C	-2.29311	0.53209	-1.63869
C	-3.58037	0.75315	-2.11014

C	-4.64270	-0.06316	-1.71188
C	-4.36563	-1.12667	-0.85076
C	-3.07603	-1.33688	-0.37703
C	-1.99575	-0.51072	-0.74121
H	-1.47527	1.16244	-1.98103
H	-3.77168	1.56938	-2.80784
H	-0.82449	-1.45394	-1.09225
H	-5.17239	-1.79833	-0.55562
H	-2.91233	-2.19708	0.27343
C	-6.03617	0.20025	-2.19484
H	-6.04097	0.54716	-3.23422
H	-6.66260	-0.69578	-2.13016
H	-6.52117	0.98121	-1.59485

G-phenol: M06/6-311+G(2df,2pd) SCF= -1721.31209 hartree
Gibbs correction= 0.473647 hartree
Total Gibbs Energy= -1720.838443 hartree

C	-0.70945	-1.06467	-2.64852
C	-1.39000	0.15194	-2.39696
C	-2.04804	-2.03751	-0.40732
C	-2.90467	0.27346	-2.33133
C	-2.59400	-0.80175	-0.03391
C	-3.50982	-0.01742	-0.94605
H	0.27326	-0.97180	-3.11693
H	-3.17540	1.29380	-2.62727
H	-1.71623	-2.70215	0.38779
H	-2.69234	-0.60356	1.03649
H	-0.86339	1.05233	-2.71062
H	-3.34247	-0.38902	-3.09199
H	-3.75358	0.93017	-0.45678
H	-4.46075	-0.56280	-1.05167
C	-1.39102	-2.39474	-2.84387
H	-0.62438	-3.17502	-2.88087
H	-1.88706	-2.40105	-3.82719
C	-2.38680	-2.71132	-1.72569
H	-3.40297	-2.41737	-2.02192
H	-2.41615	-3.79378	-1.56304
Ir	-0.49552	-0.49072	-0.56685
O	1.29679	0.42853	-1.07673
C	2.30797	-0.39715	-1.20114
C	2.10751	-1.78209	-1.05101
C	3.60788	0.07036	-1.48005
C	3.17553	-2.68834	-1.16330
C	4.64457	-0.83439	-1.58875
H	3.76767	1.14266	-1.56967
C	4.44365	-2.21828	-1.43312
H	2.97127	-3.74887	-1.03238
H	5.64739	-0.46234	-1.79299
H	5.28121	-2.90496	-1.52245

C	0.74826	-2.22982	-0.76419
O	0.41251	-3.37176	-0.56655
O	0.30657	-0.83270	1.47175
C	-0.45207	-1.35341	2.48210
C	-1.09665	-0.51134	3.39228
C	-0.56015	-2.73887	2.61177
C	-1.85707	-1.06175	4.41888
H	-0.97608	0.56702	3.29823
C	-1.33311	-3.27451	3.63625
H	-0.03134	-3.37275	1.90302
C	-1.98689	-2.44214	4.54087
H	-2.35103	-0.40270	5.12965
H	-1.41617	-4.35492	3.73243
H	-2.58569	-2.86719	5.34254
C	-0.93629	1.81417	0.10972
C	-2.05686	2.16219	0.89343
C	-2.79020	3.32036	0.67656
C	-2.43266	4.20740	-0.34447
C	-1.30920	3.90533	-1.11963
C	-0.58117	2.74527	-0.88948
H	0.13502	1.57817	0.92202
H	-2.36022	1.50441	1.71178
H	-3.65134	3.55168	1.30454
H	0.30948	2.54673	-1.48647
H	-1.00398	4.59821	-1.90453
C	-3.20518	5.47136	-0.56496
H	-2.83271	6.27535	0.08332
H	-3.11816	5.82303	-1.59850
H	-4.26801	5.34002	-0.33398
H	0.75009	0.20912	1.73876
O	0.97536	1.40552	1.81363
C	2.23887	1.82674	1.52899
C	2.44334	3.12922	1.07216
C	3.32465	0.97318	1.72305
C	3.73496	3.56955	0.80880
H	1.58188	3.78005	0.93352
C	4.61249	1.43033	1.46810
H	3.14830	-0.04637	2.06309
C	4.82630	2.72689	1.00964
H	3.89051	4.58574	0.45203
H	5.45470	0.75759	1.61714
H	5.83537	3.07961	0.81054

N: M06/6-311+G(2df,2pd) SCF= -1602.532211 hartree
Gibbs correction= 0.395098 hartree
Total Gibbs Energy= -1602.137113 hartree

C	1.76817	-2.47097	0.20681
C	2.61254	-1.34743	0.39557
C	1.11714	-1.31318	-2.24664

C	3.72679	-0.98214	-0.57457
C	1.80358	-0.11274	-2.00877
C	3.28279	-0.03834	-1.70358
H	1.34244	-2.90651	1.11388
H	4.53472	-0.50303	-0.00971
H	0.16274	-1.24896	-2.76719
H	1.35834	0.79779	-2.41221
H	2.76318	-1.03979	1.43009
H	4.15554	-1.90668	-0.98624
H	3.51308	0.99371	-1.41564
H	3.85752	-0.23965	-2.62141
C	1.84861	-3.40236	-0.97761
H	1.00112	-4.09332	-0.92968
H	2.75661	-4.01946	-0.88979
C	1.81868	-2.65930	-2.31649
H	2.83800	-2.50443	-2.69535
H	1.30571	-3.27765	-3.06044
Ir	0.69474	-0.63800	-0.21010
O	0.04950	-0.69014	1.77321
C	-0.99400	-1.45800	1.96924
C	-1.49855	-2.24781	0.91642
C	-1.63205	-1.52961	3.22525
C	-2.61025	-3.08563	1.10259
C	-2.72283	-2.36026	3.38955
H	-1.24763	-0.92058	4.03947
C	-3.22468	-3.14498	2.33609
H	-2.96204	-3.67200	0.25635
H	-3.20837	-2.40505	4.36303
H	-4.08829	-3.78505	2.49504
C	-0.80954	-2.16571	-0.37042
O	-1.12300	-2.76085	-1.37112
C	1.43397	1.50945	0.49965
C	1.70179	2.55095	-0.41056
C	2.70545	3.48456	-0.19913
C	3.50386	3.41866	0.94840
C	3.23580	2.41639	1.88356
C	2.21500	1.49740	1.66849
H	0.03922	1.53319	0.71181
H	1.08715	2.64243	-1.30979
H	2.88061	4.27972	-0.92454
H	2.00217	0.74967	2.43275
H	3.83169	2.36915	2.79560
C	4.58172	4.43092	1.18863
H	4.17032	5.34183	1.64273
H	5.35032	4.04836	1.86848
H	5.06838	4.73102	0.25394
O	-1.04833	0.38753	-0.98510
C	-1.66305	1.26122	-0.30959
O	-1.13418	1.82070	0.71867

C	-3.01262	1.66044	-0.71666
C	-3.64532	0.94647	-1.74782
C	-3.69151	2.73491	-0.09950
C	-4.91267	1.28487	-2.17679
H	-3.10480	0.11427	-2.19243
C	-4.97313	3.07549	-0.54912
C	-5.57029	2.36074	-1.57041
H	-5.39314	0.72182	-2.97175
H	-5.47318	3.90905	-0.06336
H	-6.56891	2.63996	-1.89996
O	-3.18471	3.46693	0.89769
H	-2.31436	3.09894	1.14143

XV: M06/6-311+G(2df,2pd) SCF= -1413.965022 hartree
Gibbs correction= 0.389287 hartree
Total Gibbs Energy= -1413.575735 hartree

C	1.45023	-1.53017	1.74137
C	0.07665	-1.92599	1.80643
C	0.47287	1.03043	2.15094
C	-0.80541	-1.65448	3.01747
C	-0.88613	0.68690	2.03918
C	-1.57021	-0.32706	2.92640
H	2.09714	-2.15440	1.12097
H	-1.52322	-2.47677	3.11443
H	0.78258	1.98585	1.72853
H	-1.54547	1.43440	1.59384
H	-0.18612	-2.81209	1.22645
H	-0.18581	-1.68812	3.92446
H	-2.56492	-0.51475	2.50716
H	-1.72843	0.10019	3.92931
C	2.14953	-0.76435	2.83622
H	3.14185	-0.47705	2.47463
H	2.31443	-1.43006	3.69851
C	1.37722	0.49121	3.24865
H	0.76846	0.29721	4.14211
H	2.08637	1.27790	3.52642
Ir	0.21874	-0.32221	0.45511
O	0.72340	-1.59664	-1.11644
C	1.92078	-1.39927	-1.62147
C	2.77382	-0.41996	-1.07586
C	2.38313	-2.15897	-2.71557
C	4.05335	-0.19718	-1.60703
C	3.64823	-1.92791	-3.22079
H	1.72678	-2.91475	-3.14004
C	4.49682	-0.94850	-2.67665
H	4.67011	0.57531	-1.15146
H	3.99461	-2.52202	-4.06510
H	5.48570	-0.78710	-3.09772
C	2.25168	0.33948	0.05874

O	2.83588	1.27243	0.57787
O	-0.16096	1.23050	-1.21800
C	-0.45987	2.57487	-1.05548
C	-1.70046	3.07677	-1.43263
C	0.53022	3.39791	-0.53126
C	-1.95516	4.43505	-1.26877
H	-2.45637	2.41218	-1.84907
C	0.25355	4.75069	-0.36875
H	1.49668	2.97440	-0.26605
C	-0.98448	5.27409	-0.73262
H	-2.92247	4.83417	-1.56390
H	1.02191	5.40235	0.04000
H	-1.18923	6.33375	-0.60472
C	-1.80751	-0.88728	-0.16105
C	-2.89000	0.00111	-0.24021
C	-4.12225	-0.36372	-0.78792
C	-4.33979	-1.65198	-1.26575
C	-3.27435	-2.55345	-1.18994
C	-2.04462	-2.17826	-0.66257
H	-0.90352	0.76452	-1.64228
H	-2.79961	1.02175	0.13682
H	-4.93067	0.36800	-0.83122
H	-1.23604	-2.90756	-0.67474
H	-3.41122	-3.56875	-1.56586
C	-5.66229	-2.07073	-1.83501
H	-6.15383	-2.81798	-1.19898
H	-6.34594	-1.22072	-1.93372
H	-5.54672	-2.52561	-2.82638

XVI: M06/6-311+G(2df,2pd) SCF= -1602.551876 hartree
Gibbs correction= 0.398321 hartree
Total Gibbs Energy= -1602.153555 hartree

C	3.14050	0.44560	0.11178
C	2.50841	1.68207	0.42410
C	1.73810	0.59449	-2.28089
C	2.65773	2.92746	-0.43951
C	0.97724	1.72155	-1.91060
C	1.57663	3.05189	-1.52095
H	3.38075	-0.19801	0.96130
H	2.61458	3.80699	0.21280
H	1.24083	-0.18237	-2.86146
H	-0.04700	1.76609	-2.28395
H	2.33263	1.86648	1.48395
H	3.66220	2.93407	-0.88562
H	0.76219	3.67957	-1.14298
H	1.97398	3.55811	-2.41498
C	3.97838	0.21590	-1.12288
H	4.22487	-0.84969	-1.17592
H	4.93593	0.75039	-1.01810

C	3.25351	0.63246	-2.40593
H	3.55564	1.64382	-2.71003
H	3.54935	-0.03418	-3.22240
Ir	1.01548	0.33244	-0.25403
O	0.74272	-0.56500	1.65871
C	1.20182	-1.82056	1.74269
C	1.69355	-2.46330	0.59813
C	1.16061	-2.51753	2.95805
C	2.13927	-3.78870	0.66235
C	1.61200	-3.82731	3.00597
H	0.77667	-2.01297	3.84164
C	2.10326	-4.47307	1.86428
H	2.50737	-4.24937	-0.25228
H	1.58219	-4.36264	3.95319
H	2.45044	-5.50122	1.92579
C	1.72893	-1.67897	-0.65401
O	2.03045	-2.17018	-1.72117
C	-0.36891	1.81275	0.57946
C	-1.50958	2.25772	-0.10453
C	-2.46265	3.07808	0.49456
C	-2.32361	3.49860	1.81674
C	-1.19741	3.06125	2.51226
C	-0.24971	2.23703	1.90894
H	-0.78781	-0.75132	1.39359
H	-1.68844	1.95597	-1.13865
H	-3.33314	3.39968	-0.07928
H	0.58995	1.90093	2.51717
H	-1.06008	3.36769	3.55043
C	-3.36074	4.36039	2.47347
H	-3.85632	5.01663	1.74905
H	-4.14439	3.75482	2.94766
H	-2.92332	4.99036	3.25620
O	-0.82834	-0.59064	-0.97983
C	-1.79077	-0.93025	-0.26442
O	-1.70905	-1.01965	1.04363
C	-3.08692	-1.25042	-0.85474
C	-3.21512	-1.14013	-2.25167
C	-4.20772	-1.65083	-0.09009
C	-4.40544	-1.41914	-2.88785
H	-2.33915	-0.82988	-2.81528
C	-5.41112	-1.93375	-0.74908
C	-5.50641	-1.82021	-2.12185
H	-4.48659	-1.33014	-3.96716
H	-6.25612	-2.24014	-0.13872
H	-6.45264	-2.04495	-2.60914
O	-4.21755	-1.78408	1.23938
H	-3.34526	-1.54512	1.59520

VII: M06/6-311+G(2df,2pd) SCF= -1106.625359 hartree

Gibbs correction= 0.300769 hartree
Total Gibbs Energy= -1106.32459 hartree

C	2.67691	0.71755	-0.25112
C	2.62802	-0.18395	-1.29773
C	1.55394	-1.44855	1.31599
C	3.25170	-1.56324	-1.26744
C	1.27620	-2.26925	0.21442
C	2.25199	-2.66080	-0.87332
H	2.44654	1.76019	-0.47924
H	3.65270	-1.79242	-2.26167
H	0.84768	-1.49552	2.14226
H	0.40193	-2.91883	0.29013
H	2.34306	0.21040	-2.27595
H	4.11455	-1.56465	-0.59156
H	1.66385	-2.94250	-1.75845
H	2.78898	-3.57468	-0.57320
C	3.27420	0.45536	1.10515
H	2.90684	1.23178	1.78613
H	4.36744	0.58065	1.06331
C	2.92813	-0.92170	1.69394
H	3.68594	-1.66460	1.41435
H	2.97184	-0.84686	2.78638
Ir	0.57390	-0.28336	-0.28096
O	-0.07775	1.25284	-1.50169
C	-0.52397	2.27702	-0.82197
C	-0.43401	2.26910	0.58772
C	-1.07716	3.41350	-1.44648
C	-0.88607	3.35186	1.35913
C	-1.51512	4.47077	-0.67332
H	-1.14998	3.42825	-2.53093
C	-1.42559	4.45482	0.72985
H	-0.80179	3.29407	2.44191
H	-1.94389	5.34129	-1.16687
H	-1.77978	5.30292	1.30936
C	0.12863	1.07163	1.20948
O	0.32191	0.87813	2.37979
C	-1.35847	-0.92190	-0.00345
C	-1.86270	-1.53363	1.15470
C	-3.15740	-2.03371	1.20328
C	-4.00659	-1.95160	0.09549
C	-3.51835	-1.33449	-1.05378
C	-2.22654	-0.81217	-1.10028
H	-1.24265	-1.60805	2.04898
H	-3.52383	-2.49621	2.12086
H	-1.89055	-0.30510	-2.00393
H	-4.16572	-1.24539	-1.92679
C	-5.39863	-2.50581	0.15872
H	-5.39207	-3.59198	0.31619
H	-5.96715	-2.06869	0.98897

H	-5.95239	-2.30827	-0.76515

H: M06/6-311+G(2df,2pd) SCF= -1106.604445 hartree
Gibbs correction= 0.300494 hartree
Total Gibbs Energy= -1106.303951 hartree

C	2.47390	1.05495	-0.11073
C	2.62303	0.17921	-1.21054
C	1.67979	-1.23385	1.31518
C	3.48110	-1.07268	-1.19229
C	1.56024	-2.05231	0.17658
C	2.66905	-2.32259	-0.81690
H	2.16055	2.07673	-0.34070
H	3.92215	-1.21919	-2.18504
H	0.94174	-1.36753	2.10363
H	0.76166	-2.79919	0.18189
H	2.41296	0.60761	-2.19351
H	4.32992	-0.93842	-0.51046
H	2.20334	-2.72834	-1.72510
H	3.33183	-3.11670	-0.43703
C	3.08430	0.87022	1.25330
H	2.55505	1.54268	1.94102
H	4.13659	1.19639	1.24870
C	2.96483	-0.56776	1.77065
H	3.82748	-1.17062	1.46101
H	2.98477	-0.55652	2.86639
Ir	0.69173	-0.14379	-0.29446
O	-0.07012	1.40253	-1.44605
C	-0.80793	2.25788	-0.77164
C	-1.11155	2.02072	0.58585
C	-1.29910	3.43509	-1.36622
C	-1.84087	2.94796	1.33943
C	-2.03328	4.33391	-0.61213
H	-1.07387	3.61845	-2.41411
C	-2.30726	4.10612	0.74377
H	-2.03226	2.72822	2.38762
H	-2.40031	5.24322	-1.08520
H	-2.87710	4.83151	1.31812
C	-0.64720	0.76412	1.19511
O	-0.51158	0.56524	2.38131
C	-1.31112	-0.77456	0.26181
C	-1.62830	-1.75280	1.22077
C	-2.64601	-2.66329	1.00781
C	-3.41436	-2.62648	-0.16435
C	-3.13228	-1.63792	-1.10395
C	-2.11148	-0.71440	-0.89363
H	-1.08926	-1.76016	2.16641
H	-2.87070	-3.41266	1.76693
H	-1.91825	0.04532	-1.64730
H	-3.72533	-1.58231	-2.01626

C	-4.52965	-3.60413	-0.36936
H	-5.36533	-3.39680	0.31115
H	-4.91821	-3.56594	-1.39190
H	-4.20252	-4.63075	-0.16641

VIII: M06/6-311+G(2df,2pd) SCF= -1106.647711 hartree
Gibbs correction= 0.299717 hartree
Total Gibbs Energy= -1106.347994 hartree

C	3.20653	0.31757	1.04797
C	3.42300	0.46964	-0.34581
C	1.95429	-2.07459	0.37465
C	4.16386	-0.55230	-1.19331
C	1.96209	-1.79311	-1.01697
C	3.19975	-1.54817	-1.85107
H	3.07186	1.23719	1.62493
H	4.74018	-0.03313	-1.96835
H	1.07823	-2.60389	0.75919
H	1.09561	-2.14071	-1.58902
H	3.42796	1.49413	-0.72703
H	4.90451	-1.07744	-0.57583
H	2.86477	-1.13663	-2.81264
H	3.71389	-2.49473	-2.08466
C	3.61611	-0.88580	1.86620
H	3.10764	-0.80402	2.83603
H	4.69641	-0.86292	2.08355
C	3.22023	-2.21382	1.20613
H	4.03638	-2.59533	0.57825
H	3.06549	-2.97423	1.98089
Ir	1.40168	-0.05215	0.03058
O	0.84355	1.90069	0.37308
C	-0.31752	2.41184	0.11900
C	-1.53204	1.68496	-0.15345
C	-0.39797	3.83251	0.14294
C	-2.70325	2.42849	-0.47486
C	-1.55670	4.50259	-0.15038
H	0.52124	4.36007	0.38451
C	-2.72928	3.79848	-0.48613
H	-3.59879	1.88113	-0.75540
H	-1.56348	5.59107	-0.13882
H	-3.63657	4.33038	-0.75786
C	-1.61059	0.24693	-0.15018
O	-0.62220	-0.53875	-0.21609
C	-2.92045	-0.45086	-0.07149
C	-3.10549	-1.61961	-0.81839
C	-4.28679	-2.33650	-0.72129
C	-5.30599	-1.93180	0.14641
C	-5.10234	-0.78553	0.91603
C	-3.93145	-0.04695	0.80604
H	-2.30859	-1.95331	-1.47846

H	-4.42462	-3.23552	-1.32091
H	-3.78655	0.83588	1.42503
H	-5.87360	-0.46989	1.61727
C	-6.58647	-2.70455	0.23420
H	-7.27436	-2.42025	-0.57247
H	-6.41164	-3.78210	0.14183
H	-7.10313	-2.52258	1.18221

XIII[1]: M06/6-311+G(2df,2pd) SCF= -1950.06313 hartree
Gibbs correction= 0.48441 hartree
Total Gibbs Energy= -1949.57872 hartree

C	-3.08360	4.68037	-0.96969
C	-3.37455	3.35275	-0.77078
C	-2.38871	2.42831	-0.35484
C	-1.05007	2.87071	-0.11925
C	-0.79457	4.25593	-0.31391
C	-1.77260	5.12654	-0.72999
H	-3.85335	5.37175	-1.30055
H	-4.38326	2.98612	-0.93673
H	0.21721	4.60160	-0.11457
H	-1.52459	6.17692	-0.87341
O	-0.05635	2.13949	0.28819
C	-2.76283	1.05669	-0.10954
O	-2.02572	0.10276	0.15037
O	-4.09808	0.84178	-0.17351
C	-4.59464	-0.42476	0.10148
C	-4.63250	-0.88781	1.40971
C	-5.12774	-1.15942	-0.94645
C	-5.22118	-2.11961	1.66903
H	-4.19914	-0.28456	2.20354
C	-5.71632	-2.39118	-0.67546
H	-5.07942	-0.75700	-1.95497
C	-5.76490	-2.87225	0.62987
H	-5.25759	-2.49257	2.68984
H	-6.14189	-2.97404	-1.48881
H	-6.22945	-3.83269	0.83909
Ir	0.14631	0.07317	0.21460
P	2.38759	0.25155	0.23444
C	3.05929	1.44639	-1.09354
C	3.14015	0.63683	1.93405
C	4.50758	1.17578	-1.50326
H	4.62722	0.19450	-1.97462
H	4.80100	1.93349	-2.24363
H	5.21459	1.24927	-0.66975
C	2.17453	1.24033	-2.32739
H	1.13664	1.53663	-2.13671
H	2.56782	1.85298	-3.15169
H	2.17186	0.19348	-2.65968
C	2.93231	2.89963	-0.63597

H	1.92224	3.11633	-0.27499
H	3.65510	3.15350	0.14892
H	3.14268	3.55619	-1.49253
C	2.36806	1.80701	2.55017
H	2.53553	2.74946	2.01920
H	1.28896	1.61532	2.55403
H	2.70468	1.94343	3.58786
C	4.63251	0.96411	1.93485
H	4.94818	1.15199	2.97110
H	5.24902	0.13914	1.55939
H	4.86796	1.86607	1.35944
C	2.90347	-0.59618	2.80889
H	3.29372	-0.39792	3.81688
H	1.83263	-0.81208	2.90347
H	3.40889	-1.48987	2.42241
C	3.02084	-1.38143	-0.30167
C	4.35474	-1.79946	-0.36654
C	2.00572	-2.23873	-0.74365
C	4.68330	-3.03882	-0.90060
H	5.15303	-1.14753	-0.01961
C	2.34898	-3.47655	-1.29862
C	3.67649	-3.87175	-1.38289
H	5.72416	-3.34997	-0.94986
H	1.55323	-4.13797	-1.63868
H	3.92819	-4.83927	-1.81177
C	0.56214	-1.91142	-0.53487
C	0.06615	-2.00544	0.82676
C	-0.35272	-2.26523	-1.60374
C	-1.25218	-2.54498	1.04743
H	0.78926	-2.16399	1.62912
C	-1.61448	-2.70030	-1.34160
H	0.01524	-2.20174	-2.62834
C	-2.06284	-2.86867	0.00479
H	-1.58881	-2.69872	2.07189
H	-2.28714	-2.95044	-2.16018
H	-3.06173	-3.26170	0.18716

XIII[2]: M06/6-311+G(2df,2pd) SCF= -1950.057391 hartree
Gibbs correction= 0.479765 hartree
Total Gibbs Energy= -1949.577626 hartree

C	4.72966	3.57368	-0.51735
C	4.39670	2.24674	-0.46729
C	3.07007	1.81863	-0.19171
C	2.04459	2.79268	0.05092
C	2.43967	4.16558	-0.00070
C	3.72653	4.53885	-0.27772
H	5.74858	3.87972	-0.73709
H	5.15471	1.48978	-0.64531
H	1.65491	4.89568	0.18553

H	3.97993	5.59727	-0.31474
O	0.81803	2.54853	0.32571
C	2.77888	0.42086	-0.12157
O	1.67886	-0.14156	0.05344
O	3.87163	-0.36427	-0.27337
C	3.77767	-1.74026	-0.15150
C	4.06862	-2.50655	-1.27109
C	3.49993	-2.32506	1.07717
C	4.06910	-3.89333	-1.15949
H	4.29177	-2.00708	-2.21023
C	3.49868	-3.71189	1.17508
H	3.28254	-1.69488	1.93609
C	3.78054	-4.49795	0.06029
H	4.29633	-4.50206	-2.03131
H	3.27620	-4.17931	2.13185
H	3.78119	-5.58179	0.14474
Ir	-0.25874	0.75050	0.25137
P	-1.35355	-1.23239	0.09218
C	-0.83870	-2.26434	-1.42903
C	-1.34555	-2.30683	1.66022
C	-1.88240	-3.27823	-1.89952
H	-2.80436	-2.79409	-2.23840
H	-1.46583	-3.82569	-2.75708
H	-2.14033	-4.02208	-1.13784
C	-0.62818	-1.25289	-2.56064
H	0.18947	-0.55692	-2.34097
H	-0.38486	-1.79775	-3.48449
H	-1.53119	-0.65737	-2.75052
C	0.47811	-2.99278	-1.16646
H	1.25112	-2.32692	-0.76895
H	0.35844	-3.83801	-0.47740
H	0.85125	-3.40514	-2.11551
C	0.09307	-2.36803	2.17870
H	0.76319	-2.91126	1.50341
H	0.50193	-1.35913	2.31821
H	0.10162	-2.88467	3.14969
C	-1.88076	-3.72856	1.50124
H	-1.83280	-4.23263	2.47736
H	-2.92910	-3.75438	1.18212
H	-1.28796	-4.32721	0.80124
C	-2.19053	-1.57571	2.70540
H	-2.17081	-2.14742	3.64384
H	-1.78301	-0.57992	2.91631
H	-3.23847	-1.46843	2.39946
C	-3.09843	-0.80693	-0.27174
C	-4.18536	-1.68080	-0.38427
C	-3.28211	0.55786	-0.52190
C	-5.43225	-1.21408	-0.78066
H	-4.05912	-2.74246	-0.18525

C	-4.53649	1.01562	-0.94005
C	-5.60175	0.13644	-1.07537
H	-6.26752	-1.90476	-0.86982
H	-4.67136	2.07946	-1.13032
H	-6.57286	0.50694	-1.39633
C	-2.20593	1.55570	-0.23517
C	-1.92169	1.81272	1.16348
C	-2.08018	2.67089	-1.15376
C	-1.65691	3.16226	1.58597
H	-2.37669	1.15840	1.90861
C	-1.75579	3.91639	-0.71354
H	-2.28994	2.48725	-2.20776
C	-1.56770	4.17216	0.67889
H	-1.54056	3.36150	2.64918
H	-1.66077	4.73553	-1.42328
H	-1.36458	5.18866	1.00970

C_{JP}: M06/6-311+G(2df,2pd) SCF= -1950.00439 hartree
Gibbs correction= 0.483102 hartree
Total Gibbs Energy= -1949.521288 hartree

C	5.08559	-1.44225	1.37152
C	3.91017	-0.78338	1.70451
C	2.94559	-0.56049	0.72376
C	3.10544	-1.02202	-0.59868
C	4.31529	-1.65993	-0.92690
C	5.27656	-1.86546	0.05146
H	5.85068	-1.61880	2.12281
H	3.72449	-0.42597	2.71575
H	4.45538	-2.01077	-1.94711
H	6.19800	-2.38119	-0.21482
O	2.12589	-0.89649	-1.45946
C	1.70555	0.16143	1.03801
O	1.26717	0.48212	2.11396
O	1.60706	1.34418	-0.21806
C	1.60851	2.68250	-0.02167
C	2.07884	3.25653	1.16240
C	1.22716	3.50007	-1.08837
C	2.10169	4.64124	1.28490
H	2.39684	2.61631	1.98049
C	1.25606	4.88235	-0.95115
H	0.93925	3.02412	-2.02464
C	1.67998	5.46168	0.24205
H	2.45695	5.08377	2.21327
H	0.95640	5.51010	-1.78799
H	1.69912	6.54309	0.35166
Ir	0.30583	-0.31625	-0.60820
P	-1.85803	0.46775	-0.05915
C	-2.19980	1.49023	1.51754
C	-2.63227	1.29281	-1.59275

C	-3.61728	2.05672	1.59028
H	-4.39235	1.28481	1.54308
H	-3.72967	2.55935	2.56100
H	-3.81473	2.80835	0.81752
C	-1.97900	0.55135	2.70945
H	-0.98949	0.08027	2.67464
H	-2.02015	1.15184	3.62863
H	-2.74946	-0.22528	2.78267
C	-1.19871	2.63781	1.63539
H	-0.19058	2.25482	1.80200
H	-1.18200	3.30667	0.76734
H	-1.46853	3.24413	2.51146
C	-2.21176	2.75956	-1.65924
H	-2.71277	3.37173	-0.90091
H	-1.13150	2.89220	-1.54013
H	-2.49139	3.16496	-2.64172
C	-4.15546	1.20895	-1.68866
H	-4.47054	1.73978	-2.59819
H	-4.50518	0.17516	-1.78102
H	-4.66920	1.68287	-0.84571
C	-2.05540	0.55799	-2.80665
H	-2.44960	1.01554	-3.72512
H	-0.95796	0.61260	-2.84472
H	-2.34862	-0.50021	-2.81638
C	-2.82614	-1.05169	0.28574
C	-4.20490	-1.13839	0.51955
C	-2.02463	-2.17012	0.53030
C	-4.76945	-2.30244	1.02394
H	-4.85076	-0.28740	0.32833
C	-2.59736	-3.33354	1.05566
C	-3.95935	-3.39758	1.31026
H	-5.84045	-2.34896	1.20574
H	-1.96029	-4.19662	1.24173
H	-4.39282	-4.30750	1.71866
C	-0.58371	-2.21753	0.14827
C	-0.28684	-2.32348	-1.25799
C	0.32486	-2.85618	1.07132
C	0.79377	-3.17056	-1.68590
H	-1.10242	-2.16298	-1.96762
C	1.37982	-3.59210	0.62196
H	0.12761	-2.74939	2.13750
C	1.59163	-3.79131	-0.77390
H	0.95656	-3.30972	-2.75127
H	2.06286	-4.05100	1.33390
H	2.41024	-4.42680	-1.10228

V_{JP}[1]: M06/6-311+G(2df,2pd) SCF= -1950.043999 hartree
Gibbs correction= 0.482333 hartree
Total Gibbs Energy= -1949.561666 hartree

C	-4.52461	1.77429	1.90002
C	-3.18952	1.53802	2.15114
C	-2.34070	1.18208	1.08988
C	-2.81859	1.07065	-0.23376
C	-4.18717	1.32268	-0.47228
C	-5.00934	1.65955	0.58269
H	-5.19985	2.04391	2.70779
H	-2.77336	1.61018	3.15377
H	-4.56567	1.21358	-1.48558
H	-6.06624	1.83824	0.39103
O	-1.98948	0.74741	-1.18367
C	-0.92951	0.88931	1.30041
O	-0.29460	1.06324	2.30840
O	-0.96451	-1.73348	-0.20074
C	-2.29329	-1.94902	-0.21734
C	-3.00170	-2.06812	0.98442
C	-2.97559	-2.12045	-1.42826
C	-4.36282	-2.34932	0.97292
H	-2.46172	-1.92549	1.92046
C	-4.33443	-2.40536	-1.43203
H	-2.41515	-2.00412	-2.35469
C	-5.03659	-2.51895	-0.23340
H	-4.90142	-2.43281	1.91498
H	-4.85300	-2.53553	-2.38028
H	-6.10192	-2.73777	-0.24061
Ir	-0.14611	0.11000	-0.42081
P	1.88955	-0.94740	0.12083
C	1.97877	-2.07307	1.66239
C	2.51493	-1.92623	-1.40866
C	3.39473	-2.30879	2.19313
H	3.83842	-1.38914	2.58960
H	3.32016	-3.01693	3.02991
H	4.08147	-2.74765	1.46312
C	1.19034	-1.38861	2.77468
H	0.12467	-1.33659	2.53845
H	1.30989	-1.98043	3.69283
H	1.53926	-0.37050	2.97535
C	1.30535	-3.41624	1.36933
H	0.30702	-3.27804	0.93872
H	1.90111	-4.05673	0.70942
H	1.19652	-3.95266	2.32220
C	1.41495	-2.85737	-1.93045
H	1.17370	-3.66847	-1.23895
H	0.47964	-2.32374	-2.13264
H	1.76694	-3.30982	-2.86835
C	3.77813	-2.74604	-1.14332
H	4.07142	-3.24039	-2.07993
H	4.62584	-2.12461	-0.83138
H	3.62483	-3.53503	-0.40113

C	2.83206	-0.93095	-2.52807
H	3.29025	-1.47989	-3.36174
H	1.92097	-0.46802	-2.92261
H	3.53285	-0.14375	-2.22411
C	3.07849	0.42952	0.33556
C	4.44113	0.26694	0.61867
C	2.56278	1.72611	0.16309
C	5.28126	1.36074	0.77338
H	4.85576	-0.72968	0.73548
C	3.42381	2.81933	0.33148
C	4.76472	2.64459	0.63952
H	6.33338	1.20919	1.00161
H	3.02595	3.82299	0.19309
H	5.40924	3.51191	0.76144
C	1.16389	2.04603	-0.26774
C	0.74064	1.79026	-1.61582
C	0.52607	3.14200	0.41466
C	-0.24012	2.63126	-2.22856
H	1.42264	1.26042	-2.27906
C	-0.44554	3.89140	-0.18492
H	0.84389	3.36276	1.43128
C	-0.82842	3.64364	-1.52848
H	-0.50934	2.44502	-3.26498
H	-0.91334	4.70420	0.36554
H	-1.58332	4.26932	-1.99779

V_{JP}^2: M06/6-311+G(2df,2pd) SCF= -1950.04431 hartree
Gibbs correction= 0.480337 hartree
Total Gibbs Energy= -1949.563973 hartree

C	-2.29920	4.38495	-1.98440
C	-1.62185	3.24121	-2.36269
C	-1.22803	2.32138	-1.38261
C	-1.49780	2.53840	-0.01960
C	-2.18201	3.70854	0.35473
C	-2.57149	4.60481	-0.62425
H	-2.62093	5.10783	-2.72917
H	-1.38810	3.03098	-3.40400
H	-2.39737	3.87839	1.40649
H	-3.10574	5.50626	-0.32901
O	-1.05578	1.67256	0.86516
C	-0.47887	1.10379	-1.70310
O	-0.02331	0.80180	-2.77314
O	-2.40018	-0.37292	-0.48356
C	-3.16645	-0.92616	0.43974
C	-2.80870	-1.03160	1.79946
C	-4.40111	-1.48515	0.04854
C	-3.62286	-1.70510	2.70606
H	-1.89264	-0.54915	2.14455
C	-5.20681	-2.14423	0.96280

H	-4.68515	-1.39627	-0.99859
C	-4.82460	-2.27382	2.29977
H	-3.31406	-1.77241	3.74848
H	-6.14947	-2.57375	0.62631
H	-5.45956	-2.79685	3.01047
Ir	-0.39330	-0.04565	-0.03200
P	1.80249	0.35803	0.67926
C	2.64181	2.01193	0.23273
C	1.90255	0.06026	2.56705
C	4.16307	2.03109	0.40848
H	4.66442	1.39461	-0.32816
H	4.50346	3.06040	0.22984
H	4.50465	1.74896	1.40790
C	2.37003	2.28555	-1.24890
H	1.34233	2.61096	-1.42729
H	3.02777	3.10277	-1.57464
H	2.57618	1.41707	-1.88674
C	2.02164	3.13558	1.06673
H	0.92668	3.08472	1.08846
H	2.39169	3.13404	2.09908
H	2.30872	4.09832	0.62205
C	0.83294	0.89465	3.27964
H	1.04210	1.96751	3.24501
H	-0.16772	0.74969	2.86147
H	0.81154	0.59532	4.33686
C	3.25671	0.36749	3.20520
H	3.19847	0.11288	4.27266
H	4.07547	-0.22497	2.78126
H	3.51649	1.42949	3.14694
C	1.58302	-1.41687	2.81323
H	1.68096	-1.62313	3.88751
H	0.54936	-1.66048	2.53933
H	2.26215	-2.09467	2.28098
C	2.82813	-0.93854	-0.11738
C	4.19829	-1.11807	0.11653
C	2.18035	-1.76605	-1.05048
C	4.93416	-2.05999	-0.58863
H	4.71016	-0.49983	0.84780
C	2.94127	-2.69868	-1.76885
C	4.30330	-2.84132	-1.55048
H	5.99733	-2.17564	-0.39309
H	2.43653	-3.34051	-2.48853
H	4.86832	-3.57620	-2.11892
C	0.70138	-1.82315	-1.26388
C	-0.13186	-2.35568	-0.23629
C	0.22388	-1.93476	-2.60623
C	-1.34362	-3.02053	-0.55858
H	0.30622	-2.54132	0.74468
C	-0.98014	-2.52280	-2.88652

H	0.84567	-1.54382	-3.40701
C	-1.76925	-3.08228	-1.85828
H	-1.93926	-3.45008	0.24384
H	-1.32062	-2.58030	-3.91743
H	-2.71210	-3.56698	-2.09904

V_{JP}^3: M06/6-311+G(2df,2pd) SCF= -1950.02900023 hartree
Gibbs correction= 0.4778 hartree
Total Gibbs Energy= -1949.5512 hartree

C	-4.17654	-2.85637	-0.94097
C	-3.38219	-2.47295	0.12465
C	-2.27635	-1.64792	-0.10236
C	-1.96368	-1.18864	-1.39596
C	-2.76569	-1.59329	-2.47453
C	-3.85381	-2.41506	-2.23229
H	-5.04698	-3.48716	-0.78227
H	-3.60024	-2.78158	1.14476
H	-2.52431	-1.24286	-3.47490
H	-4.47874	-2.71890	-3.07034
O	-0.91503	-0.39963	-1.57623
C	-1.38671	-1.16092	0.95968
O	-1.43555	-1.45052	2.13698
O	-1.63587	1.58048	0.73260
C	-2.95994	1.39594	0.68093
C	-3.65163	1.51056	-0.53534
C	-3.68502	1.10218	1.84496
C	-5.02571	1.31420	-0.58399
H	-3.08073	1.72909	-1.43669
C	-5.06121	0.92082	1.78689
H	-3.13714	1.00708	2.78032
C	-5.74062	1.02011	0.57496
H	-5.54405	1.38978	-1.53855
H	-5.60896	0.69113	2.69927
H	-6.81678	0.86866	0.53360
Ir	-0.19433	0.23921	0.22056
P	1.82963	-0.92544	0.15548
C	2.33778	-1.22769	1.97042
C	1.97201	-2.50032	-0.89760
C	3.83849	-1.38824	2.20615
H	4.40768	-0.49741	1.92087
H	4.00090	-1.55339	3.28041
H	4.26142	-2.25220	1.68052
C	1.86538	0.02758	2.71375
H	0.77259	0.16446	2.65138
H	2.10226	-0.07183	3.78271
H	2.36613	0.93366	2.34850
C	1.61687	-2.44799	2.54508
H	0.53001	-2.38280	2.44068
H	1.97044	-3.38538	2.09964

H	1.83612	-2.50219	3.62071
C	0.70732	-3.33603	-0.67615
H	0.57178	-3.64083	0.36735
H	-0.19339	-2.81045	-0.99851
H	0.78717	-4.25090	-1.27899
C	3.17234	-3.40924	-0.62210
H	3.07155	-4.30242	-1.25406
H	4.13711	-2.96183	-0.87573
H	3.20990	-3.75551	0.41681
C	1.99024	-2.03571	-2.35632
H	1.94651	-2.91751	-3.01058
H	1.11707	-1.40928	-2.57953
H	2.90064	-1.47797	-2.60564
C	3.16285	0.23301	-0.41227
C	4.47691	-0.21269	-0.61861
C	2.91148	1.61427	-0.51121
C	5.51964	0.66007	-0.89282
H	4.70671	-1.26829	-0.52961
C	3.98018	2.48892	-0.75705
C	5.27236	2.02648	-0.94641
H	6.52341	0.27166	-1.04670
H	3.76673	3.55398	-0.82846
H	6.07872	2.72811	-1.14584
C	1.57319	2.26436	-0.46427
C	0.69262	2.10846	-1.55095
C	1.31790	3.29055	0.46607
C	-0.39449	2.97001	-1.70849
H	0.91514	1.36582	-2.31538
C	0.21676	4.11657	0.32002
H	2.01331	3.43811	1.29172
C	-0.63706	3.96280	-0.77375
H	-1.05618	2.83870	-2.56140
H	0.02197	4.89205	1.05637
H	-1.49946	4.61534	-0.88541

1: M15-L/6-311+G(2df,2pd) SCF= -726.7500227 hartree (solvent=toluene)
SCF= -726.7494708 hartree (solvent=*m*-xylene)
SCF= -726.7500594 hartree (solvent=anisole)
Gibbs correction= 0.131676 hartree
Total Gibbs Energy= -726.6183467 hartree (solvent=toluene)
Total Gibbs Energy= -726.6177948 hartree (solvent=*m*-xylene)
Total Gibbs Energy= -726.6183834 hartree (solvent=anisole)

C	3.30375	-1.85821	0.38585
C	1.97963	-1.43511	0.29621
C	1.66191	-0.08276	0.00905
C	2.72092	0.85582	-0.19038
C	4.05985	0.41382	-0.09734
C	4.34210	-0.92188	0.18638
H	3.53633	-2.90490	0.60858
H	1.15809	-2.14278	0.44751
H	4.85320	1.15256	-0.25456
H	5.38836	-1.24556	0.25458
O	2.52483	2.15610	-0.46594
H	1.55698	2.31047	-0.49873
C	0.26617	0.38841	-0.08785
O	-0.06753	1.54804	-0.32415
O	-0.63537	-0.61331	0.10691
C	-2.00562	-0.32602	0.06598
C	-2.78718	-1.16057	-0.74192
C	-2.57742	0.67610	0.86208
C	-4.17910	-0.98348	-0.75884
H	-2.29601	-1.93549	-1.34089
C	-3.96978	0.84342	0.83035
H	-1.94072	1.31469	1.48171
C	-4.77237	0.01922	0.02413
H	-4.79953	-1.63258	-1.38799
H	-4.42981	1.62621	1.44507
H	-5.85949	0.15821	0.00814

Phenol: M15-L/6-311+G(2df,2pd) SCF= -307.3163541 hartree (solvent=toluene)
SCF= -307.3160342 hartree (solvent=*m*-xylene)
SCF= -307.3169995 hartree (solvent=anisole)
Gibbs correction= 0.057492 hartree
Total Gibbs Energy= -307.2588621 hartree (solvent=toluene)
Total Gibbs Energy= -307.2585422 hartree (solvent=*m*-xylene)
Total Gibbs Energy= -307.2595075 hartree (solvent=anisole)

C	-1.86605	0.02682	-0.00002
C	-1.13731	1.22560	0.00000
C	0.26588	1.20655	0.00002
C	0.94832	-0.02380	0.00003
C	0.22515	-1.23155	-0.00001
C	-1.17470	-1.19752	-0.00003
H	-2.96146	0.04510	-0.00003
H	-1.66062	2.18965	0.00000

H	0.83653	2.14620	0.00003
H	0.77896	-2.17702	-0.00002
H	-1.73347	-2.14157	-0.00006
O	2.31231	-0.11064	0.00001
H	2.67388	0.78616	0.00009

2am1: M15-L/6-311+G(2df,2pd) SCF= -690.8425596 hartree
Gibbs correction= 0.153117 hartree
Total Gibbs Energy= -690.6894426 hartree

C	3.74464	-0.35083	0.10076
C	2.74008	-1.09743	0.74797
C	1.39361	-0.71638	0.67063
C	1.02205	0.44279	-0.04465
C	2.03119	1.21844	-0.65838
C	3.36765	0.81540	-0.60117
H	3.02228	-1.98713	1.32686
H	0.62911	-1.29766	1.20059
H	1.73865	2.13937	-1.17643
H	4.14330	1.41619	-1.09548
C	5.19308	-0.78995	0.14661
H	5.39049	-1.43572	1.01983
H	5.45996	-1.36709	-0.75950
H	5.87426	0.07830	0.19114
C	-0.38410	0.97464	-0.07824
O	-0.54053	2.21202	-0.06495
C	-1.55364	0.06073	-0.11365
C	-1.45161	-1.29531	-0.52543
C	-2.85017	0.57167	0.22309
C	-2.56310	-2.13625	-0.55384
H	-0.47665	-1.67134	-0.85537
C	-3.96390	-0.29753	0.22931
C	-3.81878	-1.63097	-0.15338
H	-2.46287	-3.17445	-0.88789
H	-4.93528	0.11956	0.51694
H	-4.69872	-2.28659	-0.16023
O	-3.07118	1.85218	0.55882
H	-2.23287	2.33895	0.39067

Toluene: M15-L/6-311+G(2df,2pd) SCF= -271.4144819 hartree
Gibbs correction= 0.077605 hartree
Total Gibbs Energy= -271.3368769 hartree

C	-0.91861	0.00014	-0.01040
C	-0.19656	-1.21016	-0.00872
C	1.20654	-1.21307	0.00201
C	1.91399	-0.00010	0.00859
C	1.20678	1.21294	0.00204
C	-0.19639	1.21026	-0.00868
H	-0.74700	-2.16138	-0.01938
H	1.74973	-2.16636	-0.00009

H	3.01068	-0.00021	0.01283
H	1.75010	2.16615	-0.00004
H	-0.74667	2.16156	-0.01930
C	-2.43390	0.00006	0.00914
H	-2.84312	-0.89192	-0.49803
H	-2.82178	-0.00698	1.04628
H	-2.84302	0.89871	-0.48612

2aa1: M15-L/6-311+G(2df,2pd) SCF= -730.1304439 hartree
Gibbs correction= 0.174473 hartree
Total Gibbs Energy= -729.9559709 hartree

C	3.52522	0.55176	-0.02702
C	2.50531	1.40096	-0.49641
C	1.18129	0.92409	-0.49889
C	0.89039	-0.38807	-0.07030
C	1.93776	-1.23175	0.35441
C	3.26091	-0.76465	0.40373
C	2.83121	2.78759	-1.01609
H	0.37529	1.56800	-0.87555
H	1.69658	-2.26088	0.65014
C	4.38003	-1.64740	0.91997
C	-0.48918	-0.98584	-0.16149
O	-0.58317	-2.18557	-0.48801
C	-1.70147	-0.17453	0.11357
C	-1.65655	1.04326	0.84453
C	-2.97922	-0.65774	-0.32198
C	-2.80782	1.78873	1.09362
H	-0.69251	1.38108	1.24098
C	-4.13508	0.12321	-0.09867
C	-4.04690	1.32813	0.59845
H	-2.75111	2.71793	1.67061
H	-5.09152	-0.26346	-0.46743
H	-4.95808	1.91265	0.77809
O	-3.14447	-1.82640	-0.96071
H	-2.27726	-2.29052	-0.93313
H	4.56145	0.92281	-0.00663
H	3.66717	3.24027	-0.45376
H	1.95820	3.45944	-0.94290
H	3.13322	2.75313	-2.08022
H	4.12581	-2.71633	0.81485
H	4.57504	-1.45701	1.99264
H	5.32339	-1.45785	0.37758

2aa2: M15-L/6-311+G(2df,2pd) SCF= -730.1302287 hartree
Gibbs correction= 0.176471 hartree
Total Gibbs Energy= -729.9537577 hartree

C	-3.56787	-0.74526	-0.19905
C	-2.51228	-1.45707	-0.79878
C	-1.20662	-0.95553	-0.74690

C	-0.92173	0.27764	-0.11951
C	-1.98006	1.02596	0.46906
C	-3.27435	0.47897	0.43458
H	-2.71603	-2.41137	-1.30219
H	-0.38776	-1.51308	-1.21886
C	-1.75788	2.36285	1.15016
H	-4.09149	1.03448	0.91876
C	-4.98984	-1.26403	-0.25040
H	-5.54346	-0.81507	-1.09725
H	-5.01370	-2.35964	-0.38412
H	-5.54337	-1.01075	0.67114
C	0.46913	0.84811	-0.19218
O	0.60505	2.05569	-0.47506
C	1.65512	-0.01565	0.03875
C	1.56283	-1.27895	0.68361
C	2.95279	0.45432	-0.35032
C	2.68732	-2.07415	0.89736
H	0.58142	-1.61564	1.03654
C	4.08233	-0.37269	-0.15974
C	3.94781	-1.61760	0.45459
H	2.59373	-3.03950	1.40612
H	5.05528	0.00813	-0.48938
H	4.83863	-2.23975	0.60823
O	3.16180	1.65481	-0.91244
H	2.30371	2.13602	-0.88071
H	-2.62334	2.61200	1.78848
H	-1.62342	3.16574	0.40475
H	-0.84514	2.36286	1.77118

***m*-xylene**: M15-L/6-311+G(2df,2pd) SCF= -310.7030669 hartree
Gibbs correction= 0.098876 hartree
Total Gibbs Energy= -310.6041909 hartree

C	0.00071	-0.95686	-0.01797
C	-1.22976	-0.27372	-0.00873
C	-1.21685	1.13544	0.00008
C	-0.00126	1.83470	0.00460
C	1.21615	1.13667	0.00002
C	1.23110	-0.27146	-0.00879
C	-2.53983	-1.03702	0.00929
H	-2.16940	1.68277	-0.00598
H	2.16775	1.68553	-0.00591
C	2.54034	-1.03614	0.00933
H	0.00156	-2.05756	-0.03908
H	-2.42934	-2.03604	-0.44840
H	-3.33080	-0.49091	-0.53519
H	-2.90087	-1.18780	1.04496
H	3.35676	-0.44571	-0.44301
H	2.45615	-1.99073	-0.54020
H	2.84649	-1.28116	1.04468

H	-0.00183	2.93197	0.00117

2ag: M15-L/6-311+G(2df,2pd) SCF= -880.4705351 hartree
Gibbs correction= 0.184632 hartree
Total Gibbs Energy= -880.2859031 hartree

C	-2.87379	-0.74519	-0.18038
C	-1.80195	-1.58089	-0.52758
C	-0.48214	-1.09704	-0.48819
C	-0.22439	0.23372	-0.11793
C	-1.31115	1.09245	0.19344
C	-2.62100	0.61599	0.18525
H	-1.98538	-2.61332	-0.83876
H	0.33947	-1.75435	-0.79255
H	-1.08186	2.13417	0.43528
C	1.13810	0.85477	-0.16868
O	1.22498	2.06832	-0.45097
C	2.36433	0.05445	0.09220
C	2.34815	-1.15077	0.84332
C	3.62793	0.54446	-0.37385
C	3.51172	-1.88361	1.07665
H	1.39721	-1.48761	1.27109
C	4.79484	-0.22479	-0.16971
C	4.73417	-1.42164	0.54474
H	3.47624	-2.80288	1.67110
H	5.73917	0.16603	-0.56457
H	5.65456	-1.99558	0.71109
O	3.76917	1.70935	-1.02736
H	2.90474	2.17443	-0.96427
O	-4.18201	-1.10612	-0.16450
O	-3.73264	1.33930	0.49333
C	-4.48745	-2.44543	-0.52314
H	-5.58118	-2.53607	-0.43870
H	-4.17537	-2.66635	-1.56396
H	-3.99968	-3.16824	0.16187
C	-3.52619	2.70147	0.83520
H	-4.52564	3.11335	1.04365
H	-2.88712	2.80010	1.73631
H	-3.05816	3.26161	0.00044

1,2-Dimethoxybenzene: M15-L/6-311+G(2df,2pd) SCF= -461.0397716 hartree
Gibbs correction= 0.108718 hartree
Total Gibbs Energy= -460.9310536 hartree

C	0.71324	-0.13486	-0.00000
C	1.40489	1.08374	0.00011
C	0.69742	2.30371	0.00007
C	-0.69744	2.30371	-0.00009
C	-1.40490	1.08373	-0.00020
C	-0.71324	-0.13487	-0.00014
H	2.49905	1.09527	0.00025

H	1.25490	3.24731	0.00016
H	-2.49906	1.09525	-0.00036
O	1.28728	-1.37403	0.00003
O	-1.28727	-1.37404	-0.00027
C	2.70190	-1.41927	-0.00010
H	2.97035	-2.48751	-0.00025
H	3.12634	-0.93119	-0.90222
H	3.12651	-0.93141	0.90206
C	-2.70190	-1.41928	0.00044
H	-3.12687	-0.93154	-0.90162
H	-2.97034	-2.48752	0.00082
H	-3.12596	-0.93107	0.90266
H	-1.25493	3.24730	-0.00014

4-CN-Phenyl Salicylate: M15-L/6-311+G(2df,2pd) SCF= -818.9584335 hartree
Gibbs correction= 0.125099 hartree
Total Gibbs Energy= -818.8333345 hartree

C	3.98795	-1.83038	0.39030
C	2.66038	-1.42304	0.29308
C	2.32948	-0.07266	0.00587
C	3.37937	0.87903	-0.18547
C	4.72230	0.45132	-0.08502
C	5.01702	-0.88141	0.19837
H	4.23133	-2.87445	0.61309
H	1.84702	-2.14119	0.43855
H	5.50839	1.19887	-0.23619
H	6.06623	-1.19361	0.27255
O	3.17272	2.17721	-0.45960
H	2.20575	2.32835	-0.49812
C	0.93373	0.38390	-0.09759
O	0.57901	1.53690	-0.32845
O	0.03679	-0.63595	0.08105
C	-1.32811	-0.36933	0.05252
C	-2.10682	-1.24682	-0.71663
C	-1.91079	0.65233	0.82058
C	-3.49693	-1.10104	-0.72919
H	-1.60966	-2.03376	-1.29355
C	-3.30075	0.79885	0.80309
H	-1.28289	1.32336	1.41258
C	-4.10165	-0.07325	0.02958
H	-4.12276	-1.77546	-1.32361
H	-3.77933	1.58910	1.39177
C	-5.53283	0.08243	0.01954
N	-6.69806	0.20771	0.01209

4-CN-Phenol: M15-L/6-311+G(2df,2pd) SCF= -399.5278451 hartree
Gibbs correction= 0.050965 hartree
Total Gibbs Energy= -399.4768801 hartree

O	-3.08105	0.08743	0.00003

C	-1.72497	0.01406	0.00001
C	-1.02756	-1.21116	0.00001
C	-1.01688	1.23402	0.00002
C	0.36931	-1.21883	-0.00000
H	-1.58418	-2.15801	0.00002
C	0.37705	1.22479	-0.00001
H	-1.58195	2.17214	0.00005
C	1.08709	-0.00118	-0.00002
H	0.91645	-2.16831	-0.00000
H	0.93495	2.16804	-0.00000
C	2.52416	-0.00842	-0.00004
N	3.69676	-0.01477	-0.00006
H	-3.44339	-0.80953	0.00030

1,5-COD: M15-L/6-311+G(2df,2pd) SCF= -311.8311477 hartree
Gibbs correction= 0.12732 hartree
Total Gibbs Energy= -311.7038277 hartree

C	-0.87897	-1.65086	-0.21276
C	0.39071	-1.83038	0.19733
C	-0.39071	1.83038	-0.19733
C	1.22534	-0.79776	0.93391
C	0.87897	1.65086	0.21276
C	1.69211	0.38479	0.00873
H	-1.36436	-2.46209	-0.77522
H	0.64791	-0.37086	1.78028
H	-0.88773	2.78062	0.04779
H	1.36436	2.46209	0.77522
H	0.88773	-2.78062	-0.04779
H	2.11107	-1.29384	1.37266
H	2.75892	0.60402	0.20091
H	1.62101	0.04967	-1.04702
C	-1.69211	-0.38479	-0.00873
H	-1.62101	-0.04967	1.04702
H	-2.75892	-0.60402	-0.20091
C	-1.22534	0.79776	-0.93391
H	-0.64791	0.37086	-1.78028
H	-2.11107	1.29384	-1.37266

JohnPhos: M15-L/6-311+G(2df,2pd) SCF= -1119.270353 hartree
Gibbs correction= 0.330499 hartree
Total Gibbs Energy= -1118.939854 hartree

C	1.01024	3.66832	-0.10632
C	1.82492	2.53024	-0.12438
C	1.27594	1.22772	-0.19440
C	-0.14180	1.06435	-0.20053
C	-0.94076	2.23330	-0.17534
C	-0.38507	3.51923	-0.14343
H	1.46229	4.66708	-0.06952
H	2.91812	2.63274	-0.11374

H	-2.03170	2.12951	-0.15574
H	-1.03977	4.39929	-0.13079
C	2.24674	0.08469	-0.25167
C	3.21860	-0.06185	0.76049
C	2.26267	-0.81123	-1.34224
C	4.17139	-1.09106	0.69638
H	3.20521	0.63247	1.61242
C	3.22030	-1.83106	-1.41326
H	1.51425	-0.69412	-2.13714
C	4.17488	-1.97722	-0.39175
H	4.91152	-1.20011	1.49860
H	3.22311	-2.51644	-2.26953
H	4.92002	-2.78021	-0.44569
P	-0.85532	-0.64812	-0.09393
C	-2.39248	-0.65241	-1.22580
C	-1.36757	-0.70092	1.73599
C	-2.13170	-2.02247	1.98072
H	-2.24061	-2.18287	3.07268
H	-3.14784	-2.00361	1.54468
H	-1.58479	-2.88698	1.55672
C	-0.02460	-0.77172	2.50974
H	0.61224	-1.60204	2.14904
H	0.54644	0.17163	2.40744
H	-0.23647	-0.92704	3.58754
C	-2.17662	0.48019	2.31145
H	-3.14335	0.63411	1.80117
H	-2.39281	0.27147	3.38021
H	-1.60102	1.42198	2.26821
C	-2.63034	-2.15131	-1.56011
H	-2.89942	-2.74182	-0.66497
H	-3.46484	-2.23507	-2.28655
H	-1.72637	-2.60352	-2.00750
C	-3.73980	-0.06634	-0.74897
H	-4.48273	-0.19484	-1.56393
H	-4.13312	-0.59565	0.13765
H	-3.69596	1.01183	-0.51694
C	-1.97854	0.04380	-2.54591
H	-2.72607	-0.19626	-3.32925
H	-1.92427	1.14185	-2.44312
H	-0.99039	-0.31720	-2.89702

[Ir(cod)OMe]$_2$: M15-L/6-311+G(2df,2pd) SCF= -1061.957161 hartree
Gibbs correction= 0.360611 hartree
Total Gibbs Energy= -1061.59655 hartree

C	-2.07522	-1.73618	0.23102
C	-3.02596	-1.14659	-0.67659
C	-2.15963	0.67264	1.56288
C	-4.38750	-0.60996	-0.20872
C	-2.91635	1.34126	0.53545

C	-4.31601	0.90739	0.10175
H	-1.39002	-2.49582	-0.18675
H	-5.13968	-0.78963	-0.99870
H	-1.38438	1.25795	2.08874
H	-2.70248	2.41155	0.36589
H	-2.99796	-1.49661	-1.72331
H	-4.73036	-1.18536	0.67280
H	-4.56296	1.47368	-0.81669
H	-5.07514	1.19215	0.86311
C	-2.26172	-1.84978	1.74083
H	-1.27297	-2.12377	2.16307
H	-2.96047	-2.67503	2.00050
C	-2.71883	-0.51006	2.36500
H	-3.82230	-0.44305	2.41242
H	-2.36366	-0.44541	3.41001
C	1.93307	-1.67098	0.50797
C	2.86799	-1.33748	-0.53843
C	2.31309	0.89224	1.43817
C	4.29976	-0.87481	-0.22808
C	3.05800	1.30358	0.27548
C	4.38167	0.67173	-0.15575
H	1.13576	-2.40040	0.26793
H	4.64646	-1.33972	0.71535
H	1.64914	1.64240	1.90270
H	2.92779	2.34510	-0.06965
H	2.73918	-1.85329	-1.50612
H	4.98266	-1.24279	-1.01562
H	5.20946	0.99624	0.51272
H	4.61627	1.06591	-1.16311
C	2.22315	-1.57193	2.00397
H	2.87534	-2.40813	2.33909
H	1.25310	-1.69381	2.52686
C	2.82631	-0.19961	2.38615
H	2.54839	0.05194	3.42622
H	3.93268	-0.22601	2.36326
Ir	1.41517	0.16362	-0.31738
Ir	-1.42155	0.16318	-0.33093
O	-0.00350	-0.55434	-1.70202
O	0.00337	1.71243	-0.59179
C	0.01897	-1.80682	-2.35052
H	-0.99240	-2.05166	-2.73425
H	0.71877	-1.75323	-3.20800
H	0.34709	-2.63662	-1.68839
C	-0.00644	2.94413	0.09673
H	0.99496	3.41699	0.04262
H	-0.73590	3.62553	-0.38504
H	-0.28001	2.83997	1.16868

Methanol: M15-L/6-311+G(2df,2pd) SCF= -115.6453402 hartree

Gibbs correction= 0.015418 hartree
Total Gibbs Energy= -115.6299222 hartree

O	0.74859	0.12171	0.00000
C	-0.65793	-0.01892	0.00000
H	-1.04247	-0.54708	0.90056
H	-1.04247	-0.54708	-0.90057
H	-1.08093	1.00076	0.00000
H	1.12475	-0.76680	-0.00000

II: M15-L/6-311+G(2df,2pd) SCF= -535.0936185 hartree
Gibbs correction= 0.090239 hartree
Total Gibbs Energy= -535.0033795 hartree

C	2.91544	-0.68126	-0.00005
C	1.99243	-1.74977	-0.00004
C	0.62757	-1.46906	-0.00002
C	0.15645	-0.13205	-0.00001
C	1.09892	0.94084	-0.00002
C	2.48042	0.64383	-0.00004
H	3.99249	-0.89126	-0.00007
H	2.34461	-2.78676	-0.00005
H	-0.10844	-2.27994	-0.00002
H	3.18368	1.48371	-0.00004
C	-1.28736	0.18260	-0.00001
O	-1.75568	1.32488	-0.00002
O	-2.07713	-0.90913	0.00005
O	0.75006	2.23874	0.00002
H	-0.23031	2.28043	0.00006
C	-3.48591	-0.62571	0.00009
H	-3.76310	-0.04553	-0.89690
H	-3.98161	-1.60766	0.00017
H	-3.76303	-0.04540	0.89701

Salicylic Acid: M15-L/6-311+G(2df,2pd) SCF= -495.8249009 hartree
Gibbs correction= 0.066786 hartree
Total Gibbs Energy= -495.7581149 hartree

C	-1.90033	-1.48435	0.00002
C	-0.50731	-1.46790	-0.00009
C	0.20747	-0.24341	-0.00012
C	-0.51299	0.98958	-0.00000
C	-1.92557	0.96004	0.00011
C	-2.60310	-0.25917	0.00012
H	-2.44355	-2.43519	0.00003
H	0.06217	-2.40352	-0.00016
H	-2.45755	1.91754	0.00019
H	-3.70041	-0.26125	0.00021
O	0.07724	2.19612	0.00001
H	3.21967	-1.25654	0.00019
C	1.68110	-0.21085	-0.00024
O	2.26280	-1.42816	0.00002

O	2.36448	0.81749	0.00007
H	1.04782	2.05166	-0.00002

I: M15-L/6-311+G(2df,2pd) SCF= -1142.066177 hartree
Gibbs correction= 0.279712 hartree
Total Gibbs Energy= -1141.786465 hartree

C	3.12108	0.26168	0.69729
C	3.10926	0.07810	-0.72590
C	1.44128	-1.95517	0.78755
C	3.56696	-1.22639	-1.39322
C	1.24863	-1.98654	-0.63333
C	2.36847	-2.17582	-1.65428
H	3.21171	1.29938	1.06214
H	4.06643	-0.99160	-2.35121
H	0.56923	-2.21842	1.41006
H	0.24223	-2.27776	-0.98836
H	3.18959	0.99029	-1.34094
H	4.33323	-1.71518	-0.76140
H	1.94358	-1.95023	-2.65157
H	2.70440	-3.23547	-1.68580
C	3.52340	-0.81273	1.70438
H	3.23096	-0.44535	2.70684
H	4.62800	-0.93985	1.72390
C	2.81544	-2.16683	1.43741
H	3.43386	-2.82124	0.79340
H	2.69078	-2.71064	2.39193
Ir	1.16138	-0.00579	0.03801
O	0.96393	2.03980	-0.06576
C	-0.15279	2.71885	-0.06440
C	-1.50022	2.18303	-0.04161
C	-0.02543	4.14577	-0.10858
C	-2.61446	3.08177	-0.08606
C	-1.12738	4.98376	-0.14276
H	0.99690	4.53913	-0.12149
C	-2.44447	4.45410	-0.13446
H	-3.62279	2.65828	-0.07454
H	-0.97719	6.07044	-0.17909
H	-3.31321	5.11952	-0.16362
C	-1.76293	0.75818	0.03194
O	-0.93739	-0.18174	0.13885
O	-3.07840	0.43345	-0.00030
C	-3.45095	-0.91804	-0.01193
C	-4.34327	-1.33198	0.98166
C	-3.02611	-1.78180	-1.03125
C	-4.81940	-2.65277	0.95891
H	-4.65303	-0.61926	1.75343
C	-3.50698	-3.09867	-1.03840
H	-2.32624	-1.42397	-1.79456
C	-4.40137	-3.53715	-0.04670

H	-5.51906	-2.98818	1.73298
H	-3.18051	-3.78584	-1.82750
H	-4.77257	-4.56796	-0.06088

C: M15-L/6-311+G(2df,2pd) SCF= -1142.029877 hartree
Gibbs correction= 0.278922 hartree
Total Gibbs Energy= -1141.750955 hartree

C	2.32640	-0.07602	-1.65632
C	2.18484	-1.27199	-0.87596
C	2.54333	1.26461	0.78673
C	3.23990	-1.72369	0.13949
C	2.17403	0.12658	1.56147
C	2.91706	-1.20582	1.56648
H	1.77703	-0.04881	-2.61318
H	3.28259	-2.82783	0.15333
H	2.16727	2.24255	1.13136
H	1.53339	0.30121	2.44108
H	1.52964	-2.05959	-1.28660
H	4.23705	-1.37960	-0.19580
H	2.25791	-1.93431	2.07528
H	3.84484	-1.13280	2.17385
C	3.50408	0.88874	-1.55012
H	3.23702	1.79492	-2.12694
H	4.40902	0.46332	-2.03566
C	3.80663	1.29461	-0.08351
H	4.57352	0.63318	0.36293
H	4.23583	2.31299	-0.06596
Ir	0.92391	0.23720	-0.14205
O	-0.55528	-0.32518	-1.48684
C	-1.51870	-1.09862	-1.05133
C	-1.58248	-1.57644	0.29835
C	-2.54394	-1.54127	-1.93645
C	-2.57145	-2.50787	0.71719
C	-3.51746	-2.43896	-1.50680
H	-2.52172	-1.16900	-2.96636
C	-3.53821	-2.94252	-0.18185
H	-2.56152	-2.84541	1.76101
H	-4.28489	-2.77085	-2.21785
H	-4.31079	-3.65140	0.13230
C	-0.70032	-1.05924	1.32873
O	-0.32284	-1.42095	2.39680
O	-0.66096	0.75686	1.23227
C	-1.78936	1.37529	0.75248
C	-3.04147	1.07580	1.32396
C	-1.69097	2.33944	-0.26886
C	-4.18641	1.74658	0.87412
H	-3.09804	0.31611	2.11384
C	-2.84221	3.00842	-0.70708
H	-0.70542	2.54931	-0.70798

C	-4.09330	2.71387	-0.14075
H	-5.15962	1.51013	1.32042
H	-2.75989	3.76153	-1.49977
H	-4.99191	3.23536	-0.48893

III[1]: M15-L/6-311+G(2df,2pd) SCF= -1142.060908 hartree
Gibbs correction= 0.282072 hartree
Total Gibbs Energy= -1141.778836 hartree

C	-1.33186	2.15158	0.35409
C	-0.64639	2.54377	-0.82692
C	1.24448	1.27720	1.22412
C	0.53119	3.52227	-0.80145
C	1.86649	1.46588	-0.03139
C	1.88860	2.77636	-0.81399
H	-2.37392	1.80894	0.24204
H	0.47007	4.18100	-1.68661
H	1.56429	0.39611	1.79488
H	2.63610	0.73115	-0.31999
H	-1.19598	2.44150	-1.77767
H	0.44650	4.18129	0.08203
H	2.16211	2.53893	-1.86025
H	2.69912	3.42806	-0.42282
C	-0.92049	2.61926	1.74430
H	-1.52465	2.06868	2.48534
H	-1.17712	3.69361	1.86173
C	0.58835	2.39246	2.04818
H	1.16400	3.32647	1.89675
H	0.69524	2.12658	3.11480
Ir	-0.05226	0.53224	-0.38539
O	-1.64858	-0.11994	-1.51245
C	-2.41443	-0.94575	-0.83687
C	-2.19888	-1.12757	0.56256
C	-3.49303	-1.64885	-1.44243
C	-3.01577	-1.98920	1.34071
C	-4.28557	-2.48988	-0.66510
H	-3.66977	-1.51927	-2.51538
C	-4.05970	-2.67026	0.72553
H	-2.80057	-2.09733	2.41025
H	-5.10970	-3.03363	-1.14465
H	-4.70323	-3.34178	1.30328
C	-1.08560	-0.38984	1.16603
O	-0.75788	-0.34702	2.32970
O	0.80027	-1.19791	-0.94647
C	1.94966	-1.69405	-0.44119
C	3.05778	-1.87827	-1.30237
C	2.06719	-2.08052	0.91510
C	4.24807	-2.43603	-0.81517
H	2.95198	-1.58392	-2.35372
C	3.26490	-2.63465	1.39051

H	1.20170	-1.95094	1.57748
C	4.36308	-2.81445	0.53321
H	5.09666	-2.57339	-1.49726
H	3.33665	-2.93417	2.44376
H	5.29593	-3.24830	0.91014

III^{2}: M15-L/6-311+G(2df,2pd) SCF= -1142.03116 hartree
Gibbs correction= 0.282295 hartree
Total Gibbs Energy= -1141.748865 hartree

C	0.57390	1.15887	1.77600
C	-0.46330	1.81278	1.04135
C	2.11077	1.30095	-0.72269
C	-0.26045	3.10399	0.23850
C	1.02783	1.66686	-1.49249
C	0.16932	2.89796	-1.24302
H	0.26549	0.54694	2.63897
H	-1.21282	3.66403	0.24476
H	2.75883	0.49535	-1.08367
H	0.84825	1.12655	-2.43523
H	-1.49560	1.64162	1.38784
H	0.46868	3.74157	0.77591
H	-0.73492	2.80488	-1.86556
H	0.71542	3.79947	-1.59360
C	2.01043	1.66577	1.83438
H	2.63660	0.86631	2.26943
H	2.05686	2.51692	2.54871
C	2.61670	2.09884	0.46938
H	2.43253	3.17415	0.28788
H	3.71495	1.97723	0.52465
Ir	0.09534	0.03479	0.00914
O	-1.54859	0.59349	-1.11453
C	-2.66891	0.03055	-0.67160
C	-2.63594	-0.81294	0.46730
C	-3.91116	0.26730	-1.31410
C	-3.81112	-1.41476	0.96889
C	-5.06231	-0.34320	-0.81023
H	-3.94390	0.91443	-2.19752
C	-5.02862	-1.18319	0.32910
H	-3.72958	-2.05696	1.85451
H	-6.02051	-0.16180	-1.31425
H	-5.95173	-1.64333	0.69778
C	-1.29463	-0.99438	1.06726
O	-1.07702	-1.63675	2.09023
O	0.30508	-1.60683	-1.34006
C	1.50647	-1.81381	-0.86972
C	2.64825	-1.97216	-1.72264
C	1.70208	-1.67753	0.56597
C	3.92049	-1.89515	-1.17703
H	2.47859	-2.11472	-2.79567

C	3.03786	-1.55455	1.06756
H	0.91384	-2.01062	1.25207
C	4.12711	-1.63046	0.21310
H	4.79547	-2.00683	-1.83067
H	3.18910	-1.46549	2.15096
H	5.14863	-1.55790	0.60237

X: M15-L/6-311+G(2df,2pd) SCF= -1637.915542 hartree
Gibbs correction= 0.382817 hartree
Total Gibbs Energy= -1637.532725 hartree

C	-0.78559	1.17023	2.35911
C	0.40402	0.39515	2.36852
C	-2.05321	-1.24254	1.51115
C	0.55270	-0.87605	3.21103
C	-0.84647	-1.95103	1.33107
C	0.19454	-2.16777	2.42560
H	-0.68862	2.23352	2.08333
H	1.59740	-0.94214	3.56825
H	-2.85021	-1.41860	0.77824
H	-0.78225	-2.64130	0.47538
H	1.33433	0.90707	2.06854
H	-0.07795	-0.78162	4.11572
H	1.10354	-2.57965	1.95100
H	-0.17320	-2.94850	3.12488
C	-2.04176	0.78652	3.12951
H	-2.84936	1.47898	2.83756
H	-1.86368	0.94262	4.21471
C	-2.49993	-0.67427	2.86406
H	-2.13503	-1.34803	3.66435
H	-3.60309	-0.70937	2.89880
Ir	-0.58918	0.04833	0.49981
O	0.41379	1.66171	-0.29736
C	-0.41820	2.57132	-0.77444
C	-1.81927	2.41754	-0.57507
C	0.04409	3.72283	-1.46540
C	-2.74354	3.37679	-1.05659
C	-0.87974	4.65860	-1.93059
H	1.12074	3.84923	-1.62240
C	-2.27484	4.49923	-1.73398
H	-3.81269	3.20670	-0.88216
H	-0.51367	5.54378	-2.46664
H	-2.97236	5.25234	-2.11539
C	-2.26714	1.20904	0.14290
O	-3.41740	0.92789	0.41230
O	-0.82098	-0.49644	-1.49451
C	-1.42278	-1.66290	-1.83698
C	-0.63836	-2.78634	-2.18907
C	-2.83152	-1.76683	-1.87300
C	-1.25518	-3.98442	-2.57870

H	0.45631	-2.69782	-2.14887
C	-3.43677	-2.97278	-2.25649
H	-3.42810	-0.88791	-1.59613
C	-2.65602	-4.08613	-2.61210
H	-0.63517	-4.84687	-2.85364
H	-4.53152	-3.04116	-2.28420
H	-3.13519	-5.02419	-2.91399
C	6.47825	0.29507	-0.35585
C	5.89478	0.45175	-1.63195
C	2.30278	-0.49457	-0.87826
C	5.71843	-0.12243	0.73750
C	4.53715	0.18715	-1.79451
C	4.34382	-0.40143	0.58361
C	3.74204	-0.24364	-0.70261
O	1.60164	-0.95415	0.06449
O	1.79705	-0.23433	-2.06196
O	3.66871	-0.79811	1.68204
H	7.54603	0.50377	-0.21585
H	2.75373	-0.99940	1.39007
H	0.79859	-0.31673	-1.98928
H	6.50113	0.78125	-2.48178
H	6.15863	-0.24632	1.73249
H	4.05234	0.30731	-2.76905

L: M15-L/6-311+G(2df,2pd) SCF= -1637.899997 hartree
Gibbs correction= 0.379637 hartree
Total Gibbs Energy= -1637.52036 hartree

C	-0.76696	1.22225	2.33381
C	0.38619	0.39329	2.36833
C	-2.12745	-1.14747	1.51017
C	0.47404	-0.86979	3.22934
C	-0.95346	-1.91265	1.35367
C	0.06790	-2.15653	2.45958
H	-0.61793	2.27531	2.04258
H	1.51455	-0.97238	3.58848
H	-2.92537	-1.29722	0.77283
H	-0.90718	-2.61601	0.50758
H	1.34119	0.85151	2.05901
H	-0.15725	-0.73374	4.12827
H	0.96164	-2.61146	1.99809
H	-0.34112	-2.90841	3.16740
C	-2.04875	0.90701	3.09235
H	-2.82255	1.62642	2.77501
H	-1.87822	1.07844	4.17626
C	-2.56239	-0.53857	2.84880
H	-2.23108	-1.21201	3.66350
H	-3.66628	-0.52901	2.87444
Ir	-0.59310	0.06825	0.49826
O	0.49126	1.62498	-0.28887

C	-0.28704	2.56579	-0.79384
C	-1.69846	2.47855	-0.62474
C	0.24431	3.68479	-1.48869
C	-2.56780	3.47256	-1.14054
C	-0.62548	4.65446	-1.98581
H	1.32860	3.75670	-1.62428
C	-2.03160	4.56213	-1.81963
H	-3.64737	3.35439	-0.98898
H	-0.20768	5.51443	-2.52491
H	-2.68401	5.34179	-2.22655
C	-2.21277	1.30262	0.09744
O	-3.37860	1.06470	0.34195
O	-0.80629	-0.49190	-1.51790
C	-1.41441	-1.67922	-1.86116
C	-0.64385	-2.80904	-2.19650
C	-2.81986	-1.74072	-1.86640
C	-1.29490	-4.00328	-2.54333
H	0.45056	-2.73785	-2.17952
C	-3.45448	-2.94505	-2.20566
H	-3.38924	-0.84062	-1.60103
C	-2.69737	-4.07914	-2.54534
H	-0.69676	-4.88352	-2.80806
H	-4.55004	-2.99376	-2.21209
H	-3.19808	-5.01623	-2.81305
C	6.40549	0.26196	-0.28092
C	5.84720	0.37269	-1.57174
C	2.25034	-0.64960	-0.90071
C	5.63036	-0.15370	0.80352
C	4.49966	0.06508	-1.75687
C	4.26863	-0.47586	0.62237
C	3.69096	-0.36389	-0.67782
O	1.56209	-1.12695	0.07073
O	1.75055	-0.41831	-2.05816
O	3.57262	-0.87108	1.71217
H	7.46350	0.50430	-0.12066
H	2.67771	-1.10980	1.37663
H	0.42795	-0.46724	-1.88772
H	6.46324	0.70072	-2.41561
H	6.05059	-0.24360	1.81109
H	4.02781	0.14971	-2.74194

XIV: M15-L/6-311+G(2df,2pd) SCF= -1637.909499 hartree
Gibbs correction= 0.383869 hartree
Total Gibbs Energy= -1637.52563 hartree

C	-0.87707	1.27400	2.26490
C	0.34868	0.54757	2.35590
C	-1.99894	-1.22504	1.52449
C	0.52530	-0.66660	3.27491
C	-0.76500	-1.89893	1.42033

C	0.25051	-2.01318	2.55202
H	-0.80771	2.32748	1.94656
H	1.56184	-0.66345	3.65835
H	-2.76512	-1.46343	0.77726
H	-0.64257	-2.62461	0.60094
H	1.26678	1.08493	2.06383
H	-0.13732	-0.54826	4.15346
H	1.19047	-2.40393	2.12358
H	-0.10237	-2.77232	3.28155
C	-2.13678	0.88217	3.02396
H	-2.96514	1.51957	2.67150
H	-1.99124	1.11122	4.10089
C	-2.51739	-0.60973	2.83035
H	-2.14756	-1.22105	3.67660
H	-3.61798	-0.69737	2.83212
Ir	-0.54689	0.07713	0.49914
O	0.38788	1.71190	-0.32287
C	-0.46844	2.57291	-0.84819
C	-1.86728	2.36054	-0.69429
C	-0.02879	3.72297	-1.55565
C	-2.81388	3.26390	-1.23882
C	-0.97499	4.60290	-2.08007
H	1.04651	3.88903	-1.67979
C	-2.36913	4.38689	-1.92980
H	-3.88038	3.05050	-1.09823
H	-0.62825	5.48821	-2.62849
H	-3.08324	5.09781	-2.35857
C	-2.27983	1.15527	0.04620
O	-3.42940	0.81347	0.25622
O	-0.80027	-0.54977	-1.60808
C	-1.27998	-1.82556	-1.86741
C	-0.39984	-2.88511	-2.14565
C	-2.66924	-2.01957	-1.81802
C	-0.93555	-4.16183	-2.37941
H	0.67974	-2.69901	-2.17745
C	-3.18430	-3.30484	-2.04420
H	-3.31778	-1.16227	-1.59754
C	-2.32208	-4.37835	-2.32466
H	-0.25751	-4.99456	-2.60072
H	-4.26836	-3.46479	-2.00820
H	-2.72994	-5.37936	-2.50362
C	6.35581	0.38355	-0.28885
C	5.80706	0.43625	-1.58678
C	2.18157	-0.47783	-0.91837
C	5.56448	0.04127	0.80974
C	4.45435	0.14449	-1.76385
C	4.19739	-0.26073	0.63549
C	3.62802	-0.20703	-0.67107
O	1.48029	-0.88238	0.10821

O	1.69467	-0.34009	-2.06873
O	3.48741	-0.58779	1.74083
H	7.41761	0.61242	-0.13369
H	2.58938	-0.81373	1.40620
H	0.19035	-0.46096	-1.91057
H	6.43403	0.70637	-2.44319
H	5.97637	-0.00511	1.82380
H	3.98724	0.18298	-2.75422

XI: M15-L/6-311+G(2df,2pd) SCF= -1330.574904 hartree
Gibbs correction= 0.289357 hartree
Total Gibbs Energy= -1330.285547 hartree

C	3.12760	0.08845	-0.07933
C	2.91519	-0.66357	-1.26226
C	1.41737	-1.83506	1.14434
C	3.21298	-2.16147	-1.36352
C	1.00244	-2.42740	-0.06804
C	1.94156	-3.01857	-1.11776
H	3.25554	1.17800	-0.19365
H	3.60345	-2.37815	-2.37419
H	0.63794	-1.69518	1.89967
H	-0.04956	-2.75097	-0.12117
H	2.85745	-0.09619	-2.20696
H	4.01839	-2.42793	-0.65566
H	1.37842	-3.10856	-2.06682
H	2.22282	-4.05329	-0.82768
C	3.64479	-0.52021	1.21589
H	3.56430	0.24111	2.01025
H	4.72557	-0.75036	1.10398
C	2.86267	-1.79147	1.64681
H	3.38715	-2.70950	1.31901
H	2.83155	-1.82508	2.75042
Ir	0.99438	-0.29083	-0.38952
O	0.91247	1.46027	-1.46531
C	0.55457	2.47028	-0.70074
C	0.53710	2.31143	0.71761
C	0.22095	3.74541	-1.23281
C	0.18921	3.37688	1.58766
C	-0.12012	4.78199	-0.36616
H	0.23101	3.88247	-2.31925
C	-0.14122	4.61293	1.04311
H	0.18540	3.19651	2.66890
H	-0.38411	5.76011	-0.78829
H	-0.41607	5.45069	1.69218
C	0.89959	0.99169	1.24709
O	1.08230	0.65717	2.38973
O	-1.04379	-0.21442	-0.54639
C	-1.88841	-0.70856	0.32831
O	-1.54190	-1.20821	1.41877

C	-3.32274	-0.62516	-0.07012
C	-3.70641	-0.04388	-1.30264
C	-4.33113	-1.14520	0.79618
C	-5.04648	0.02507	-1.68400
H	-2.91656	0.35480	-1.94819
C	-5.68567	-1.07224	0.40045
C	-6.03401	-0.49594	-0.82154
H	-5.32863	0.47918	-2.63989
H	-6.44001	-1.47912	1.08265
H	-7.09180	-0.44823	-1.10950
O	-4.06533	-1.71123	1.98619
H	-3.08837	-1.66715	2.10203

XII: M15-L/6-311+G(2df,2pd) SCF= -1602.00966 hartree
Gibbs correction= 0.396191 hartree
Total Gibbs Energy= -1601.613469 hartree

C	2.64717	-1.72067	-0.27460
C	2.90260	-0.41768	0.22298
C	1.19191	-0.40042	-2.33710
C	3.56310	0.68740	-0.60423
C	1.23823	0.87013	-1.72610
C	2.52862	1.58705	-1.33877
H	2.53937	-2.52566	0.47231
H	4.15443	1.32492	0.07956
H	0.24821	-0.68639	-2.81055
H	0.33952	1.50402	-1.81042
H	2.94372	-0.31638	1.31980
H	4.27865	0.23184	-1.31521
H	2.26202	2.43079	-0.68007
H	2.98763	2.02675	-2.25043
C	2.97038	-2.16049	-1.69411
H	2.51903	-3.15354	-1.86009
H	4.06939	-2.28778	-1.79290
C	2.44186	-1.17188	-2.76690
H	3.22892	-0.44763	-3.05369
H	2.18987	-1.74264	-3.67851
Ir	0.79936	-0.56061	-0.15898
O	0.56707	-1.25023	1.77369
C	-0.12383	-2.37215	1.80122
C	-0.41990	-3.05094	0.58290
C	-0.56065	-2.96144	3.01842
C	-1.13578	-4.27506	0.56527
C	-1.26367	-4.16447	2.98512
H	-0.33773	-2.45159	3.96183
C	-1.55881	-4.83138	1.76807
H	-1.34148	-4.75061	-0.40079
H	-1.60104	-4.60754	3.93092
H	-2.11590	-5.77385	1.77975
C	0.05185	-2.43172	-0.66442

O	-0.00110	-2.87834	-1.78348
C	0.50572	2.02894	1.77281
C	-0.06826	3.00319	0.93115
C	0.64182	4.17349	0.62585
C	1.94249	4.38837	1.13462
C	2.51599	3.39673	1.95706
C	1.80286	2.22945	2.27905
H	-0.06651	1.13820	2.05622
H	-1.07836	2.84440	0.53001
H	0.18641	4.94049	-0.01555
H	2.24688	1.47591	2.94330
H	3.52533	3.55491	2.36162
C	2.71452	5.64023	0.77107
H	3.51502	5.84564	1.50277
H	3.19120	5.53986	-0.22295
H	2.05030	6.52129	0.72433
O	-1.15245	0.05270	0.06939
C	-2.00120	0.31261	-0.89251
O	-1.80272	0.04771	-2.09586
C	-3.26457	0.96911	-0.43849
C	-3.46822	1.30157	0.92333
C	-4.28237	1.28449	-1.38789
C	-4.63865	1.92991	1.34956
H	-2.67329	1.05208	1.63688
C	-5.46627	1.91786	-0.94656
C	-5.63805	2.23423	0.40136
H	-4.78062	2.18110	2.40601
H	-6.23222	2.14788	-1.69518
H	-6.56452	2.72658	0.72269
O	-4.17911	1.01122	-2.69946
H	-3.30149	0.58082	-2.82377

VI: M15-L/6-311+G(2df,2pd) SCF= -1413.492961 hartree
Gibbs correction= 0.387759 hartree
Total Gibbs Energy= -1413.105202 hartree

C	0.46586	-1.99691	1.62768
C	-0.84801	-1.95151	1.09325
C	0.07534	0.77860	2.17505
C	-2.05412	-1.50059	1.92271
C	-1.13823	0.86443	1.45608
C	-2.36916	0.00481	1.72558
H	1.17838	-2.69066	1.15034
H	-2.93894	-2.08967	1.61322
H	0.75641	1.63601	2.10409
H	-1.32587	1.78989	0.88453
H	-1.04991	-2.59899	0.22479
H	-1.87280	-1.73745	2.98865
H	-3.05036	0.11820	0.86455
H	-2.90556	0.40788	2.61192

C	0.80201	-1.55697	3.04689
H	1.89834	-1.57616	3.16608
H	0.39089	-2.30000	3.76311
C	0.27484	-0.13493	3.39052
H	-0.68406	-0.19808	3.94170
H	0.99763	0.35476	4.06704
Ir	0.25046	-0.29254	0.26721
O	0.83738	-1.50234	-1.30040
C	2.14641	-1.53338	-1.42518
C	2.96649	-0.93935	-0.42082
C	2.78970	-2.17755	-2.51789
C	4.38285	-0.97171	-0.49677
C	4.18146	-2.20099	-2.57799
H	2.17239	-2.63726	-3.29711
C	4.99056	-1.60331	-1.57637
H	4.96428	-0.49286	0.29989
H	4.66682	-2.69512	-3.42953
H	6.08182	-1.63932	-1.65848
C	2.28232	-0.27697	0.69571
O	2.78174	0.23811	1.66987
O	0.58273	1.22179	-1.03769
C	0.54952	2.53168	-0.71325
C	-0.47800	3.35357	-1.23824
C	1.54928	3.13108	0.09071
C	-0.50265	4.72847	-0.96413
H	-1.23958	2.89042	-1.87720
C	1.51159	4.50661	0.36217
H	2.35592	2.50100	0.48518
C	0.48718	5.31499	-0.15842
H	-1.30517	5.34750	-1.38510
H	2.29893	4.95243	0.98319
H	0.46429	6.38929	0.05594
C	-2.38823	0.14879	-2.09095
C	-3.52728	0.92474	-1.81176
C	-4.67194	0.32697	-1.25785
C	-4.69696	-1.05121	-0.95777
C	-3.55436	-1.82150	-1.25535
C	-2.41123	-1.23255	-1.81993
H	-1.48581	0.59955	-2.52003
H	-3.52890	1.99980	-2.03206
H	-5.55973	0.93678	-1.04130
H	-1.52945	-1.84218	-2.05251
H	-3.56311	-2.89954	-1.03458
C	-5.89400	-1.68318	-0.27730
H	-6.09927	-2.69323	-0.67444
H	-5.71317	-1.79210	0.81087
H	-6.80227	-1.06826	-0.40057

G: M15-L/6-311+G(2df,2pd) SCF= -1413.427997 hartree

Gibbs correction= 0.389498 hartree
Total Gibbs Energy= -1413.038499 hartree

C	1.19674	-1.74437	1.70046
C	-0.21230	-1.99054	1.57709
C	0.43003	0.90594	2.22257
C	-1.19459	-1.70388	2.72033
C	-0.93675	0.71854	1.91295
C	-1.82319	-0.28683	2.64250
H	1.86112	-2.36061	1.07180
H	-1.99997	-2.45924	2.68727
H	0.88170	1.85771	1.92003
H	-1.44735	1.56472	1.42717
H	-0.51130	-2.76456	0.85247
H	-0.66919	-1.84962	3.68466
H	-2.78881	-0.34753	2.11245
H	-2.03801	0.09386	3.66434
C	1.82557	-1.14321	2.94963
H	2.89304	-0.95478	2.74576
H	1.78197	-1.88934	3.77170
C	1.14164	0.18119	3.37295
H	0.40702	0.00248	4.18296
H	1.90618	0.86543	3.78047
Ir	0.26754	-0.30442	0.40812
O	0.81470	-1.53764	-1.16209
C	2.05165	-1.33560	-1.58051
C	2.90619	-0.45296	-0.86746
C	2.56732	-2.00206	-2.72481
C	4.24315	-0.22690	-1.27871
C	3.88536	-1.76851	-3.11532
H	1.91501	-2.68434	-3.28078
C	4.73482	-0.88356	-2.40296
H	4.85834	0.46679	-0.69288
H	4.27505	-2.28495	-4.00218
H	5.76401	-0.72096	-2.74030
C	2.33507	0.19439	0.32638
O	2.94323	0.95850	1.05665
O	0.03492	1.18907	-1.26650
C	-0.27493	2.50254	-1.02616
C	-1.47788	3.05216	-1.51545
C	0.64326	3.31986	-0.33601
C	-1.76605	4.40651	-1.28689
H	-2.16739	2.41270	-2.07956
C	0.34312	4.67233	-0.11962
H	1.58876	2.88286	0.00710
C	-0.86428	5.22144	-0.58420
H	-2.70352	4.82768	-1.67016
H	1.06414	5.30339	0.41423
H	-1.09470	6.27830	-0.40969
C	-1.87366	-0.49084	-0.68951

C	-3.06078	0.23297	-0.37528
C	-4.34213	-0.26479	-0.64473
C	-4.51237	-1.54129	-1.22036
C	-3.35578	-2.28640	-1.52447
C	-2.07461	-1.77254	-1.27478
H	-0.90534	0.46055	-1.19813
H	-2.98638	1.23453	0.07134
H	-5.22970	0.33685	-0.40116
H	-1.20281	-2.38105	-1.54081
H	-3.46784	-3.28631	-1.96833
C	-5.89341	-2.07910	-1.52625
H	-5.90857	-3.18291	-1.50794
H	-6.64129	-1.70449	-0.80518
H	-6.22461	-1.76310	-2.53416

G^2: M15-L/6-311+G(2df,2pd) SCF= -1413.411681 hartree
Gibbs correction= 0.390066 hartree
Total Gibbs Energy= -1413.021615 hartree

C	0.08792	-1.54009	2.26600
C	-1.28042	-1.39579	1.89637
C	0.26897	1.23553	1.93668
C	-2.25852	-0.49141	2.65616
C	-1.04198	1.37272	1.37519
C	-2.33868	0.93235	2.04902
H	0.57745	-2.48215	1.96286
H	-3.26307	-0.95210	2.62159
H	1.05170	1.89398	1.52938
H	-1.17073	2.13520	0.59358
H	-1.71386	-2.25423	1.36998
H	-1.96594	-0.45402	3.72428
H	-3.12883	0.94846	1.27239
H	-2.62673	1.67613	2.82342
C	0.72701	-0.80589	3.43807
H	1.80797	-1.02058	3.43946
H	0.31405	-1.21978	4.38290
C	0.50769	0.72440	3.36502
H	-0.35099	1.03002	3.99524
H	1.39722	1.23716	3.77088
Ir	-0.08271	-0.28939	0.48972
O	0.07036	-2.03688	-0.83639
C	1.37988	-2.15008	-1.24132
C	2.36722	-1.52435	-0.45147
C	1.73519	-2.95469	-2.33339
C	3.73029	-1.73570	-0.74656
C	3.09464	-3.13218	-2.62912
H	0.95039	-3.43663	-2.92633
C	4.09389	-2.53204	-1.83757
H	4.47660	-1.23155	-0.12019
H	3.37935	-3.75418	-3.48627

H	5.15088	-2.67729	-2.08652
C	1.97584	-0.57514	0.66205
O	2.80053	-0.04752	1.37971
O	0.63218	0.80622	-1.16057
C	1.30341	1.97381	-1.06719
C	0.62453	3.22165	-1.05073
C	2.72268	1.99991	-1.06693
C	1.33293	4.43175	-1.01117
H	-0.47061	3.23524	-1.10070
C	3.42181	3.21340	-1.02993
H	3.26590	1.04956	-1.11553
C	2.73615	4.43911	-0.99039
H	0.77821	5.37878	-1.00396
H	4.51918	3.20020	-1.03354
H	3.28767	5.38550	-0.95691
C	-2.29206	0.75502	-1.61237
C	-3.60693	1.04575	-2.00088
C	-4.65819	0.13978	-1.74626
C	-4.34049	-1.08211	-1.11889
C	-3.02491	-1.35902	-0.72006
C	-1.95420	-0.44761	-0.93524
H	-1.49528	1.47356	-1.83236
H	-3.83342	1.99499	-2.50829
H	-0.70969	-1.35715	-1.27766
H	-5.13914	-1.81655	-0.93995
H	-2.82577	-2.33626	-0.25714
C	-6.07590	0.45183	-2.17506
H	-6.24373	0.15571	-3.22841
H	-6.81305	-0.09249	-1.55912
H	-6.28829	1.53323	-2.10401

G-phenol: M15-L/6-311+G(2df,2pd) SCF= -1720.753794 hartree
Gibbs correction= 0.478562 hartree
Total Gibbs Energy= -1720.275232 hartree

C	-0.57531	-1.24141	-2.63677
C	-1.31458	-0.02125	-2.47897
C	-1.98139	-2.11004	-0.38241
C	-2.84768	0.02142	-2.49163
C	-2.58284	-0.86455	-0.08724
C	-3.47230	-0.11413	-1.07684
H	0.43651	-1.13958	-3.06363
H	-3.16384	0.98757	-2.92604
H	-1.65583	-2.71851	0.46810
H	-2.71740	-0.61281	0.97692
H	-0.79827	0.88162	-2.83165
H	-3.22131	-0.76961	-3.17232
H	-3.66182	0.89581	-0.67573
H	-4.45649	-0.62662	-1.13857
C	-1.23224	-2.60331	-2.79806

H	-0.44750	-3.37808	-2.79079
H	-1.71714	-2.64486	-3.79702
C	-2.25776	-2.88802	-1.67521
H	-3.28574	-2.65291	-2.01440
H	-2.24138	-3.96555	-1.43426
Ir	-0.49208	-0.52362	-0.60665
O	1.21587	0.49300	-1.16693
C	2.29410	-0.27259	-1.19615
C	2.18109	-1.66910	-0.95298
C	3.57741	0.26963	-1.47104
C	3.32098	-2.51425	-0.95881
C	4.68614	-0.57319	-1.46537
H	3.67267	1.35041	-1.62380
C	4.57345	-1.96633	-1.21400
H	3.18094	-3.58343	-0.75882
H	5.67812	-0.14073	-1.65048
H	5.46807	-2.59831	-1.21622
C	0.83297	-2.19404	-0.69689
O	0.54014	-3.34934	-0.46466
O	0.39669	-0.80093	1.49413
C	-0.30105	-1.24039	2.60412
C	-0.72867	-0.33435	3.59313
C	-0.52976	-2.62057	2.74654
C	-1.42260	-0.82127	4.71213
H	-0.48989	0.73061	3.48873
C	-1.23643	-3.08718	3.86524
H	-0.13307	-3.30411	1.98700
C	-1.69227	-2.19246	4.84745
H	-1.75116	-0.11683	5.48573
H	-1.41708	-4.16314	3.97561
H	-2.23877	-2.56364	5.72157
C	-1.03267	1.74798	0.15095
C	-2.07803	1.97773	1.09601
C	-3.03807	2.98028	0.92942
C	-3.02161	3.80595	-0.21872
C	-1.98720	3.62032	-1.16031
C	-1.00887	2.63458	-0.96281
H	0.14480	1.62681	0.79843
H	-2.13049	1.34843	1.99626
H	-3.82346	3.13118	1.68416
H	-0.17769	2.54736	-1.67805
H	-1.94653	4.27499	-2.04304
C	-4.05772	4.89317	-0.40334
H	-3.77223	5.80579	0.15430
H	-4.16163	5.17496	-1.46557
H	-5.04568	4.57759	-0.02354
H	0.80819	0.14805	1.66312
O	1.06002	1.56047	1.66005
C	2.28462	2.01190	1.30451

C	2.43437	3.16866	0.50566
C	3.43926	1.33580	1.75843
C	3.71556	3.63497	0.17869
H	1.53426	3.69103	0.15745
C	4.71499	1.81433	1.42876
H	3.31392	0.42869	2.36458
C	4.86465	2.96532	0.63719
H	3.81784	4.53611	-0.43967
H	5.60091	1.27458	1.78668
H	5.86300	3.33871	0.38223

N: M15-L/6-311+G(2df,2pd) SCF= -1601.952121 hartree
Gibbs correction= 0.398688 hartree
Total Gibbs Energy= -1601.553433 hartree

C	1.78127	-2.49001	0.22889
C	2.61059	-1.35435	0.51647
C	1.25556	-1.22173	-2.21185
C	3.78616	-0.94986	-0.38558
C	1.92127	-0.01228	-1.88986
C	3.38896	0.07842	-1.47788
H	1.28839	-2.95914	1.09705
H	4.57650	-0.50650	0.24786
H	0.31782	-1.13731	-2.77798
H	1.47775	0.91460	-2.28055
H	2.69496	-1.09414	1.58062
H	4.22180	-1.86317	-0.83823
H	3.56595	1.09840	-1.08844
H	4.03426	-0.04084	-2.37511
C	1.96130	-3.38081	-0.99333
H	1.13097	-4.10639	-1.02105
H	2.89806	-3.96689	-0.87534
C	1.98120	-2.57012	-2.31188
H	3.02271	-2.38207	-2.64014
H	1.49790	-3.16219	-3.10881
Ir	0.75230	-0.64608	-0.18299
O	0.08784	-0.77168	1.79028
C	-0.99770	-1.51204	1.91523
C	-1.48473	-2.25725	0.80410
C	-1.69829	-1.60524	3.14971
C	-2.63821	-3.07360	0.91212
C	-2.83278	-2.41082	3.23606
H	-1.33018	-1.03495	4.00968
C	-3.31540	-3.14998	2.12562
H	-2.96891	-3.62594	0.02407
H	-3.36919	-2.47129	4.19199
H	-4.21348	-3.76864	2.22687
C	-0.71667	-2.16476	-0.45385
O	-0.97653	-2.76089	-1.48053
C	1.34385	1.51924	0.56962

C	1.43047	2.61344	-0.33689
C	2.37978	3.63015	-0.19592
C	3.31110	3.59570	0.86788
C	3.21916	2.54501	1.80291
C	2.24585	1.54245	1.66290
H	-0.08152	1.38900	0.86016
H	0.71489	2.66368	-1.17481
H	2.41695	4.46350	-0.91251
H	2.17014	0.75612	2.42717
H	3.91812	2.52499	2.65158
C	4.34408	4.69157	1.02164
H	4.75745	4.99514	0.04317
H	3.89612	5.59516	1.47773
H	5.17756	4.37120	1.67043
O	-0.96818	0.41656	-1.04446
C	-1.67335	1.15551	-0.28567
O	-1.23652	1.56356	0.86546
C	-3.01491	1.58672	-0.72464
C	-3.54055	1.04337	-1.92540
C	-3.79292	2.52723	0.01592
C	-4.79446	1.41913	-2.39859
H	-2.92642	0.31322	-2.46362
C	-5.06091	2.90523	-0.47922
C	-5.55039	2.35981	-1.66548
H	-5.18991	0.98880	-3.32429
H	-5.63761	3.63139	0.10334
H	-6.53998	2.66608	-2.02658
O	-3.40723	3.10217	1.16974
H	-2.53950	2.73758	1.42362

XV: M15-L/6-311+G(2df,2pd) SCF= -1413.454154 hartree
Gibbs correction= 0.39469 hartree
Total Gibbs Energy= -1413.059464 hartree

C	1.53650	-1.55932	1.65243
C	0.15441	-1.97010	1.74593
C	0.53602	0.98602	2.17923
C	-0.68960	-1.74287	3.01010
C	-0.83519	0.63457	2.08327
C	-1.49734	-0.42066	2.96274
H	2.17159	-2.14319	0.96551
H	-1.38856	-2.59154	3.11929
H	0.82704	1.96612	1.78256
H	-1.50494	1.40450	1.66941
H	-0.12478	-2.83989	1.13334
H	-0.02435	-1.77211	3.89562
H	-2.50005	-0.62313	2.54569
H	-1.64469	-0.01650	3.98759
C	2.25928	-0.83378	2.77824
H	3.25756	-0.53401	2.41820

H	2.41782	-1.54224	3.62002
C	1.48242	0.41921	3.24746
H	0.89153	0.19980	4.15860
H	2.20217	1.21167	3.51700
Ir	0.25201	-0.32236	0.46592
O	0.73133	-1.53559	-1.15375
C	1.91342	-1.27923	-1.69603
C	2.76740	-0.29407	-1.13182
C	2.35657	-1.98446	-2.84777
C	4.03320	-0.01096	-1.69930
C	3.60772	-1.69206	-3.39160
H	1.70258	-2.74621	-3.28697
C	4.45751	-0.70647	-2.82903
H	4.65129	0.76073	-1.22332
H	3.94151	-2.24237	-4.28111
H	5.43252	-0.49862	-3.28307
C	2.26246	0.39267	0.07433
O	2.88017	1.28262	0.64999
O	-0.17791	1.23059	-1.22396
C	-0.57530	2.55052	-1.02098
C	-1.84201	2.99822	-1.42571
C	0.35783	3.41859	-0.43513
C	-2.18469	4.34360	-1.21707
H	-2.54859	2.29912	-1.89164
C	-0.00615	4.75754	-0.22980
H	1.34979	3.03996	-0.16441
C	-1.27448	5.22452	-0.61359
H	-3.17308	4.69880	-1.53072
H	0.71739	5.44293	0.22661
H	-1.54869	6.27254	-0.45109
C	-1.76605	-0.93119	-0.12738
C	-2.88292	-0.05869	-0.16386
C	-4.12150	-0.43356	-0.72020
C	-4.31835	-1.72123	-1.24690
C	-3.22265	-2.60730	-1.21380
C	-1.98428	-2.22021	-0.67949
H	-0.89455	0.72733	-1.65780
H	-2.80763	0.95897	0.24372
H	-4.95256	0.28741	-0.73272
H	-1.15497	-2.93679	-0.72663
H	-3.34083	-3.61847	-1.63095
C	-5.65636	-2.15157	-1.81164
H	-6.21046	-2.78607	-1.09357
H	-6.29354	-1.28002	-2.04334
H	-5.53113	-2.74437	-2.73583

XVI: M15-L/6-311+G(2df,2pd) SCF= -1601.973411 hartree
Gibbs correction= 0.40136 hartree
Total Gibbs Energy= -1601.572051 hartree

C	-3.15596	-0.40132	0.08668
C	-2.53479	-1.66729	0.37334
C	-1.70061	-0.50617	-2.29971
C	-2.71026	-2.88475	-0.54942
C	-0.95411	-1.66479	-1.94853
C	-1.57770	-3.01056	-1.59779
H	-3.38330	0.23878	0.95539
H	-2.73151	-3.79714	0.07345
H	-1.17050	0.28521	-2.84783
H	0.08512	-1.70551	-2.30549
H	-2.37313	-1.88801	1.43734
H	-3.70161	-2.82145	-1.04094
H	-0.77300	-3.64723	-1.18781
H	-1.94928	-3.50533	-2.52122
C	-3.98849	-0.14296	-1.16411
H	-4.25426	0.92749	-1.18961
H	-4.94155	-0.70988	-1.08839
C	-3.22807	-0.51365	-2.46138
H	-3.53539	-1.51461	-2.82433
H	-3.49077	0.20867	-3.25364
Ir	-1.03635	-0.33045	-0.25927
O	-0.83651	0.45218	1.70134
C	-1.22215	1.73363	1.81430
C	-1.65835	2.44593	0.67088
C	-1.17287	2.39729	3.06444
C	-2.03841	3.80437	0.76680
C	-1.55432	3.74013	3.14145
H	-0.83715	1.84381	3.94902
C	-1.98696	4.45465	1.99978
H	-2.36929	4.31224	-0.14770
H	-1.51643	4.24929	4.11306
H	-2.27826	5.50695	2.08973
C	-1.73242	1.68619	-0.60756
O	-2.05785	2.20965	-1.66301
C	0.36036	-1.80699	0.55058
C	1.53434	-2.21629	-0.13091
C	2.49646	-3.04989	0.46332
C	2.33601	-3.52484	1.77885
C	1.18395	-3.11820	2.47557
C	0.22747	-2.27762	1.87824
H	0.82407	0.60346	1.39043
H	1.73494	-1.86176	-1.15343
H	3.39064	-3.34048	-0.10779
H	-0.62859	-1.95998	2.48779
H	1.03318	-3.46274	3.50947
C	3.38175	-4.40759	2.42922
H	3.88266	-5.05279	1.68545
H	4.16964	-3.80469	2.92078
H	2.93478	-5.05532	3.20418

O	0.79951	0.62072	-0.98943
C	1.78070	0.90919	-0.26168
O	1.72035	0.91508	1.05990
C	3.08149	1.26157	-0.85143
C	3.17532	1.26692	-2.26964
C	4.24012	1.57930	-0.07759
C	4.36568	1.57870	-2.91628
H	2.27176	1.02167	-2.83768
C	5.44276	1.89517	-0.74979
C	5.50350	1.89554	-2.14162
H	4.41881	1.57988	-4.00954
H	6.31586	2.13467	-0.13388
H	6.45040	2.14437	-2.63608
O	4.30145	1.60532	1.26624
H	3.43870	1.35756	1.63669

VII: M15-L/6-311+G(2df,2pd) SCF= -1106.154749 hartree
Gibbs correction= 0.300413 hartree
Total Gibbs Energy= -1105.854336 hartree

C	2.63418	0.70996	-0.25107
C	2.60193	-0.21588	-1.29670
C	1.49562	-1.46267	1.32729
C	3.26915	-1.58703	-1.22433
C	1.24297	-2.29679	0.21224
C	2.25933	-2.70295	-0.85170
H	2.38015	1.75611	-0.48547
H	3.71213	-1.82221	-2.20961
H	0.76677	-1.51918	2.14368
H	0.35462	-2.94537	0.27403
H	2.31091	0.15860	-2.29137
H	4.10983	-1.55540	-0.50857
H	1.69538	-2.99334	-1.76112
H	2.79532	-3.61905	-0.52114
C	3.25134	0.45248	1.11404
H	2.91446	1.25813	1.79064
H	4.35694	0.53822	1.04818
C	2.86901	-0.91921	1.74311
H	3.63908	-1.68241	1.52056
H	2.85972	-0.79788	2.84130
Ir	0.57418	-0.30889	-0.28456
O	-0.04537	1.21778	-1.52708
C	-0.47879	2.26112	-0.85013
C	-0.37689	2.26580	0.57213
C	-1.02362	3.40962	-1.48640
C	-0.81120	3.36933	1.34679
C	-1.44463	4.48900	-0.71024
H	-1.10706	3.41945	-2.57863
C	-1.34449	4.48364	0.70432
H	-0.71825	3.31625	2.43796

H	-1.86891	5.36871	-1.21130
H	-1.68550	5.34921	1.28198
C	0.17347	1.04985	1.20108
O	0.36327	0.86804	2.38440
C	-1.36473	-0.89394	-0.00282
C	-1.92346	-1.37108	1.20816
C	-3.24254	-1.84302	1.26438
C	-4.05838	-1.86961	0.11389
C	-3.51766	-1.37809	-1.08866
C	-2.20468	-0.87932	-1.14581
H	-1.33256	-1.33662	2.13433
H	-3.65665	-2.19209	2.22145
H	-1.82597	-0.46658	-2.09046
H	-4.14386	-1.36582	-1.99242
C	-5.46993	-2.41627	0.17370
H	-5.47931	-3.51841	0.06721
H	-5.95280	-2.17959	1.13875
H	-6.09518	-2.00274	-0.63713

H: M15-L/6-311+G(2df,2pd) SCF= -1106.12783 hartree
Gibbs correction= 0.30171 hartree
Total Gibbs Energy= -1105.82612 hartree

C	2.43772	0.98472	-0.08153
C	2.58221	0.10991	-1.21038
C	1.59652	-1.30817	1.30647
C	3.44598	-1.15480	-1.19876
C	1.46571	-2.11423	0.14411
C	2.60926	-2.41053	-0.82585
H	2.14086	2.02450	-0.30061
H	3.88102	-1.30233	-2.20411
H	0.84284	-1.42237	2.09280
H	0.63394	-2.83914	0.12508
H	2.39530	0.56830	-2.19524
H	4.30427	-1.02443	-0.51399
H	2.16075	-2.82506	-1.74932
H	3.26174	-3.20973	-0.41119
C	3.05267	0.77020	1.29127
H	2.51004	1.43103	1.99543
H	4.11607	1.09356	1.29662
C	2.91494	-0.69158	1.77856
H	3.76455	-1.31487	1.44425
H	2.93493	-0.70629	2.88338
Ir	0.67745	-0.17911	-0.30367
O	-0.00343	1.39155	-1.46267
C	-0.70807	2.28804	-0.78594
C	-1.01349	2.07722	0.58823
C	-1.15255	3.49082	-1.39415
C	-1.69102	3.05564	1.34832
C	-1.84129	4.44033	-0.63463

H	-0.92688	3.65763	-2.45354
C	-2.11088	4.23941	0.73855
H	-1.87980	2.85230	2.40944
H	-2.17199	5.36904	-1.11745
H	-2.64046	5.00531	1.31505
C	-0.61078	0.79039	1.21215
O	-0.45583	0.60697	2.41028
C	-1.34513	-0.69928	0.31295
C	-1.69231	-1.69474	1.26824
C	-2.72471	-2.59937	1.02793
C	-3.48339	-2.54366	-0.16624
C	-3.18012	-1.53401	-1.09586
C	-2.14635	-0.61198	-0.85940
H	-1.16783	-1.71487	2.23038
H	-2.97055	-3.35990	1.78239
H	-1.94569	0.16431	-1.60501
H	-3.76889	-1.45966	-2.02024
C	-4.61089	-3.52348	-0.40279
H	-4.27070	-4.56506	-0.25640
H	-5.43918	-3.35342	0.31060
H	-5.01820	-3.43063	-1.42373

VIII: M15-L/6-311+G(2df,2pd) SCF= -1106.162136 hartree
Gibbs correction= 0.301059 hartree
Total Gibbs Energy= -1105.861077 hartree

C	3.15305	0.25195	1.12079
C	3.41002	0.47476	-0.27177
C	1.88960	-2.09465	0.29939
C	4.19064	-0.52437	-1.13599
C	1.94541	-1.74234	-1.08932
C	3.23492	-1.49974	-1.87074
H	2.99900	1.14802	1.74643
H	4.79632	0.02806	-1.87795
H	0.98608	-2.62814	0.64001
H	1.08143	-2.04008	-1.71013
H	3.42908	1.52472	-0.60877
H	4.91200	-1.07473	-0.50167
H	2.94810	-1.05536	-2.84338
H	3.74950	-2.45867	-2.10017
C	3.56311	-1.00524	1.88395
H	3.05155	-0.97152	2.86508
H	4.65481	-1.00007	2.09621
C	3.15176	-2.30683	1.14626
H	3.97226	-2.67595	0.50097
H	2.96609	-3.10556	1.88791
Ir	1.39905	-0.06164	0.03140
O	0.87089	1.87747	0.47124
C	-0.27568	2.41955	0.16369
C	-1.50341	1.71037	-0.16390

C	-0.33063	3.85132	0.19769
C	-2.66043	2.48217	-0.52079
C	-1.47755	4.55214	-0.13502
H	0.59546	4.36420	0.47978
C	-2.65862	3.86624	-0.52229
H	-3.55829	1.94683	-0.84651
H	-1.46529	5.64953	-0.11532
H	-3.55125	4.42113	-0.82859
C	-1.60089	0.25980	-0.19511
O	-0.61183	-0.53833	-0.30817
C	-2.92533	-0.43491	-0.10438
C	-3.10956	-1.64046	-0.81894
C	-4.30188	-2.35879	-0.69899
C	-5.33104	-1.92120	0.16290
C	-5.12683	-0.73962	0.90317
C	-3.94712	0.00267	0.76775
H	-2.30341	-1.99510	-1.47108
H	-4.44211	-3.28481	-1.27245
H	-3.79594	0.91124	1.36288
H	-5.90415	-0.40293	1.60162
C	-6.62510	-2.69769	0.27725
H	-7.33094	-2.40805	-0.52443
H	-6.45094	-3.78378	0.18135
H	-7.12495	-2.50632	1.24240

XIII[1]: M15-L/6-311+G(2df,2pd) SCF= -1949.492907 hartree
Gibbs correction= 0.485708 hartree
Total Gibbs Energy= -1949.007199 hartree

C	-2.73615	4.66403	-1.33039
C	-3.11309	3.35463	-1.06643
C	-2.22275	2.43574	-0.44000
C	-0.89715	2.85560	-0.05033
C	-0.56261	4.22414	-0.30591
C	-1.44673	5.09324	-0.93304
H	-3.42591	5.35308	-1.82824
H	-4.11145	3.00258	-1.34492
H	0.42827	4.56495	0.01309
H	-1.13556	6.12896	-1.12212
O	0.00570	2.11375	0.54702
C	-2.68658	1.10028	-0.09578
O	-2.01287	0.14973	0.33535
O	-4.02807	0.93110	-0.25675
C	-4.59549	-0.29837	0.09297
C	-4.61613	-0.71986	1.42942
C	-5.21822	-1.03397	-0.92068
C	-5.29177	-1.90501	1.75261
H	-4.10057	-0.12613	2.19218
C	-5.89158	-2.22035	-0.58400
H	-5.17282	-0.66848	-1.95257

C	-5.93372	-2.65479	0.75072
H	-5.31695	-2.24465	2.79462
H	-6.38752	-2.80265	-1.36932
H	-6.46376	-3.57805	1.01094
Ir	0.16222	0.04894	0.32613
P	2.37939	0.15499	0.28846
C	3.04749	1.43805	-0.95505
C	3.17466	0.38873	1.99195
C	4.46102	1.11418	-1.49423
H	4.46274	0.20605	-2.12157
H	4.77971	1.96540	-2.12890
H	5.21659	0.99400	-0.69698
C	2.07131	1.41315	-2.16007
H	1.08692	1.83690	-1.88978
H	2.51246	2.02169	-2.97616
H	1.91370	0.38267	-2.53800
C	3.05719	2.87000	-0.37437
H	2.09860	3.11468	0.10743
H	3.87736	3.02378	0.34978
H	3.22150	3.57617	-1.21380
C	2.44768	1.54520	2.72405
H	2.63835	2.53035	2.26692
H	1.35551	1.37784	2.74208
H	2.82286	1.57603	3.76739
C	4.69531	0.65608	2.01155
H	5.00697	0.76456	3.07020
H	5.27901	-0.17987	1.58729
H	4.97439	1.58658	1.48935
C	2.89387	-0.90519	2.79404
H	3.34350	-0.79560	3.80117
H	1.80576	-1.05459	2.91737
H	3.33197	-1.80156	2.31481
C	2.94710	-1.43789	-0.42244
C	4.26888	-1.92065	-0.55208
C	1.87942	-2.18346	-0.97436
C	4.52872	-3.10069	-1.26224
H	5.10954	-1.35623	-0.13480
C	2.15330	-3.35498	-1.71321
C	3.47039	-3.80614	-1.86272
H	5.55916	-3.46150	-1.36225
H	1.31373	-3.92177	-2.13686
H	3.67511	-4.72082	-2.43242
C	0.45452	-1.81782	-0.65549
C	0.04133	-2.06542	0.73221
C	-0.55224	-1.99484	-1.70358
C	-1.29082	-2.59441	0.97886
H	0.82364	-2.35517	1.45027
C	-1.82490	-2.41608	-1.40098
H	-0.24613	-1.80479	-2.74257

C	-2.18725	-2.76012	-0.04833
H	-1.56070	-2.88109	2.00382
H	-2.57565	-2.52495	-2.19492
H	-3.19033	-3.15605	0.14786

XIII[2]: M15-L/6-311+G(2df,2pd) SCF= -1949.487518 hartree
Gibbs correction= 0.487308 hartree
Total Gibbs Energy= -1949.00021 hartree

C	3.92333	4.04070	-1.15449
C	3.83737	2.67032	-0.96934
C	2.71720	2.08393	-0.30609
C	1.65643	2.91974	0.21736
C	1.80253	4.33619	0.02957
C	2.89001	4.87176	-0.64278
H	4.77492	4.47794	-1.68571
H	4.62605	2.01097	-1.34676
H	1.00368	4.96654	0.43853
H	2.95296	5.95887	-0.78465
O	0.63460	2.49097	0.88668
C	2.67783	0.66166	-0.05878
O	1.69605	-0.03745	0.29868
O	3.87738	0.04488	-0.24119
C	3.95383	-1.34418	-0.11155
C	4.34901	-2.06801	-1.24228
C	3.69239	-1.97209	1.11364
C	4.45862	-3.46457	-1.15104
H	4.54864	-1.53271	-2.17699
C	3.80169	-3.36864	1.18906
H	3.37355	-1.37445	1.97495
C	4.17471	-4.11731	0.05940
H	4.75845	-4.04308	-2.03251
H	3.58136	-3.87392	2.13710
H	4.25219	-5.20837	0.12601
Ir	-0.33283	0.66749	0.47279
P	-1.22050	-1.34945	0.05887
C	-0.48798	-2.21606	-1.47394
C	-1.21804	-2.52162	1.55008
C	-1.44305	-3.21620	-2.16615
H	-2.30735	-2.70690	-2.62659
H	-0.87408	-3.71772	-2.97494
H	-1.81876	-4.00338	-1.48794
C	-0.18415	-1.08555	-2.49103
H	0.63247	-0.42984	-2.13726
H	0.11834	-1.55132	-3.45148
H	-1.07486	-0.45138	-2.67470
C	0.83522	-2.94002	-1.14302
H	1.51163	-2.30699	-0.54939
H	0.67268	-3.89032	-0.60184
H	1.34667	-3.18795	-2.09578

C	0.20841	-2.55781	2.15671
H	0.91720	-3.13526	1.54031
H	0.61035	-1.53558	2.29606
H	0.14508	-3.04904	3.14947
C	-1.68352	-3.97198	1.29932
H	-1.62116	-4.52169	2.26066
H	-2.73375	-4.02864	0.96330
H	-1.04625	-4.50487	0.57328
C	-2.14936	-1.87973	2.60741
H	-2.17977	-2.54153	3.49600
H	-1.75675	-0.89532	2.92214
H	-3.18399	-1.75418	2.23407
C	-2.95539	-1.04359	-0.45407
C	-3.98456	-1.97845	-0.70553
C	-3.18695	0.32636	-0.71597
C	-5.20600	-1.56159	-1.25277
H	-3.82431	-3.04518	-0.51699
C	-4.40756	0.73447	-1.29537
C	-5.40829	-0.20619	-1.56895
H	-5.99449	-2.29732	-1.45037
H	-4.56958	1.80212	-1.49392
H	-6.35755	0.11708	-2.01331
C	-2.20625	1.36364	-0.23750
C	-2.15358	1.53983	1.21964
C	-1.98445	2.54604	-1.07096
C	-2.03244	2.88321	1.75700
H	-2.69682	0.80905	1.83778
C	-1.78524	3.78304	-0.50556
H	-2.01209	2.41494	-2.16215
C	-1.84520	3.95954	0.92369
H	-2.09973	3.02197	2.84303
H	-1.59891	4.65496	-1.14522
H	-1.74429	4.96952	1.34050

C$_{JP}$: M15-L/6-311+G(2df,2pd) SCF= -1949.439081 hartree
Gibbs correction= 0.487624 hartree
Total Gibbs Energy= -1948.951457 hartree

C	5.08872	-1.40064	1.41616
C	3.91857	-0.71574	1.76648
C	2.98478	-0.38366	0.76785
C	3.15312	-0.78386	-0.58886
C	4.36749	-1.43576	-0.93123
C	5.30465	-1.74034	0.06300
H	5.83186	-1.65734	2.17840
H	3.71186	-0.42056	2.80273
H	4.51473	-1.74620	-1.97251
H	6.21968	-2.27921	-0.21608
O	2.17705	-0.63305	-1.45649
C	1.74577	0.32721	1.13495

O	1.29980	0.58859	2.22778
O	1.53331	1.46435	-0.10497
C	1.44599	2.81667	0.06067
C	1.84415	3.47114	1.24218
C	1.01387	3.56285	-1.05262
C	1.73640	4.86845	1.31388
H	2.19909	2.88991	2.09809
C	0.91280	4.95739	-0.96456
H	0.77437	3.01971	-1.97638
C	1.25880	5.61786	0.22656
H	2.02949	5.37613	2.24097
H	0.57067	5.53051	-1.83507
H	1.17360	6.70763	0.30049
Ir	0.30085	-0.24463	-0.61386
P	-1.89514	0.30877	-0.10005
C	-2.30049	1.25988	1.50152
C	-2.75633	1.10257	-1.59898
C	-3.76478	1.72871	1.64255
H	-4.49202	0.90148	1.58059
H	-3.86766	2.17491	2.65204
H	-4.03848	2.50902	0.91131
C	-1.98657	0.29239	2.67657
H	-1.00229	-0.19714	2.55059
H	-1.94832	0.89240	3.60697
H	-2.76528	-0.48393	2.79413
C	-1.36627	2.48002	1.64979
H	-0.33386	2.14176	1.79949
H	-1.39391	3.18423	0.79913
H	-1.67333	3.03614	2.55819
C	-2.48060	2.62053	-1.64402
H	-3.02818	3.17270	-0.86071
H	-1.40667	2.84708	-1.53966
H	-2.82077	3.00570	-2.62607
C	-4.28064	0.86754	-1.69419
H	-4.64684	1.41072	-2.58858
H	-4.51601	-0.20196	-1.83620
H	-4.84076	1.24977	-0.82367
C	-2.13058	0.46232	-2.86332
H	-2.60026	0.92089	-3.75674
H	-1.03589	0.62497	-2.91703
H	-2.32782	-0.62593	-2.90026
C	-2.72526	-1.28989	0.25709
C	-4.09205	-1.51637	0.54220
C	-1.78611	-2.29723	0.57681
C	-4.50280	-2.69738	1.17715
H	-4.84689	-0.76342	0.30345
C	-2.20227	-3.47268	1.23574
C	-3.55387	-3.66421	1.54924
H	-5.56498	-2.85222	1.39980

H	-1.45723	-4.24175	1.47522
H	-3.87190	-4.57721	2.06667
C	-0.36705	-2.19339	0.09761
C	-0.18986	-2.22176	-1.35406
C	0.68972	-2.77602	0.91649
C	0.90845	-2.99099	-1.91546
H	-1.09796	-2.13397	-1.97006
C	1.75956	-3.41472	0.33529
H	0.60250	-2.68054	2.00853
C	1.83821	-3.58010	-1.09420
H	0.97111	-3.09890	-3.00451
H	2.57430	-3.80119	0.96218
H	2.67110	-4.15352	-1.51757

V_{JP}[1]: M15-L/6-311+G(2df,2pd) SCF= -1949.487048 hartree
Gibbs correction= 0.488598 hartree
Total Gibbs Energy= -1948.99845 hartree

C	-4.36726	1.43762	2.21596
C	-2.99288	1.28358	2.37306
C	-2.18112	1.12239	1.22326
C	-2.73263	1.13183	-0.09337
C	-4.13664	1.31958	-0.23188
C	-4.92389	1.45286	0.90885
H	-5.01898	1.54832	3.08951
H	-2.51842	1.26213	3.36201
H	-4.57403	1.29346	-1.23626
H	-6.01057	1.56122	0.79528
O	-1.93614	0.95694	-1.12040
C	-0.73457	0.88352	1.31811
O	-0.02243	1.11025	2.27643
O	-1.02266	-1.66937	-0.33143
C	-2.36870	-1.81149	-0.31651
C	-3.04719	-1.99470	0.90980
C	-3.10859	-1.83201	-1.52079
C	-4.43466	-2.19473	0.92990
H	-2.46502	-1.94755	1.84036
C	-4.49367	-2.04070	-1.49346
H	-2.56927	-1.65533	-2.46060
C	-5.16488	-2.21967	-0.27024
H	-4.94947	-2.32050	1.89065
H	-5.05825	-2.05389	-2.43453
H	-6.25025	-2.37271	-0.25360
Ir	-0.11544	0.14460	-0.47518
P	1.84137	-0.97231	0.07092
C	1.79229	-2.21805	1.53011
C	2.57172	-1.89348	-1.44740
C	3.16527	-2.47861	2.19984
H	3.53491	-1.57408	2.71389
H	3.00128	-3.25468	2.97349

H	3.95022	-2.85128	1.52228
C	0.89198	-1.63327	2.63972
H	-0.14754	-1.51140	2.29034
H	0.89831	-2.35513	3.48075
H	1.26257	-0.66224	3.00496
C	1.14937	-3.56681	1.11641
H	0.15102	-3.41313	0.67481
H	1.76637	-4.16751	0.42902
H	1.03008	-4.15846	2.04595
C	1.43500	-2.68468	-2.14519
H	0.95708	-3.44210	-1.50551
H	0.63612	-2.00176	-2.49156
H	1.86739	-3.19207	-3.03143
C	3.75240	-2.83917	-1.11969
H	4.07457	-3.31167	-2.06872
H	4.62211	-2.28329	-0.72266
H	3.49797	-3.64856	-0.42062
C	3.10990	-0.88935	-2.49893
H	3.68477	-1.46467	-3.25050
H	2.28633	-0.40053	-3.04486
H	3.78214	-0.12282	-2.07068
C	3.00283	0.38831	0.47669
C	4.35267	0.21049	0.86164
C	2.48991	1.70966	0.34348
C	5.16544	1.30402	1.18794
H	4.77297	-0.79727	0.92702
C	3.31961	2.79929	0.69360
C	4.63705	2.60259	1.12530
H	6.20420	1.14007	1.49690
H	2.92312	3.81670	0.58725
H	5.25956	3.46615	1.38807
C	1.15031	2.03692	-0.27116
C	0.92446	1.73009	-1.67359
C	0.40718	3.16803	0.26672
C	0.02990	2.53240	-2.46369
H	1.71427	1.18662	-2.19776
C	-0.50687	3.86088	-0.49922
H	0.58292	3.44314	1.31363
C	-0.69417	3.55179	-1.88319
H	-0.06853	2.30943	-3.53245
H	-1.07301	4.68441	-0.04828
H	-1.39638	4.14398	-2.48089

V_{JP}^2: M15-L/6-311+G(2df,2pd) SCF= -1949.485162 hartree
Gibbs correction= 0.487839 hartree
Total Gibbs Energy= -1948.997323 hartree

C	-2.35608	4.42199	-1.90448
C	-1.64015	3.29486	-2.30844
C	-1.22357	2.35892	-1.33580

C	-1.50649	2.54280	0.04243
C	-2.22729	3.69582	0.44278
C	-2.64117	4.60882	-0.53008
H	-2.69744	5.15785	-2.64035
H	-1.39480	3.10764	-3.36065
H	-2.45344	3.84353	1.50436
H	-3.20485	5.49712	-0.21700
O	-1.03798	1.66604	0.91824
C	-0.43459	1.15328	-1.67791
O	0.04497	0.90954	-2.76342
O	-2.39851	-0.26273	-0.49019
C	-3.13469	-0.88589	0.42620
C	-2.75731	-1.01826	1.79235
C	-4.34200	-1.51808	0.01680
C	-3.51274	-1.80471	2.67856
H	-1.87714	-0.47417	2.16010
C	-5.09070	-2.28749	0.91150
H	-4.63672	-1.41371	-1.03510
C	-4.67775	-2.45648	2.24865
H	-3.18644	-1.89578	3.72316
H	-6.00640	-2.78016	0.55848
H	-5.26449	-3.06928	2.94159
Ir	-0.37551	-0.01614	-0.03290
P	1.80057	0.31548	0.69002
C	2.70627	1.93102	0.23675
C	1.87231	0.04562	2.58149
C	4.24709	1.89304	0.40372
H	4.71528	1.25781	-0.36802
H	4.60959	2.92781	0.24383
H	4.60088	1.56962	1.39497
C	2.45055	2.21650	-1.26454
H	1.45675	2.66038	-1.42851
H	3.20449	2.95520	-1.60038
H	2.54514	1.31194	-1.89509
C	2.12907	3.11202	1.05095
H	1.02375	3.11838	1.03642
H	2.47644	3.10871	2.09984
H	2.48794	4.05138	0.58534
C	0.77737	0.88754	3.28578
H	0.89332	1.97291	3.14014
H	-0.23406	0.61569	2.94675
H	0.84728	0.67608	4.37189
C	3.22301	0.36544	3.26064
H	3.12304	0.10830	4.33389
H	4.06271	-0.22989	2.86197
H	3.47856	1.43696	3.20458
C	1.53408	-1.43969	2.86081
H	1.63289	-1.61649	3.94981
H	0.48516	-1.66637	2.58980

H	2.21011	-2.14065	2.33490
C	2.79269	-0.99738	-0.12361
C	4.15866	-1.26516	0.12969
C	2.12868	-1.72091	-1.14896
C	4.87721	-2.17545	-0.65582
H	4.68102	-0.73352	0.92991
C	2.87480	-2.61138	-1.95550
C	4.23787	-2.82784	-1.72232
H	5.93656	-2.36166	-0.44504
H	2.35404	-3.16856	-2.74410
H	4.79525	-3.52839	-2.35536
C	0.63185	-1.74081	-1.31576
C	-0.13827	-2.32316	-0.24127
C	0.07304	-1.83750	-2.64377
C	-1.36991	-3.00067	-0.50423
H	0.38254	-2.53140	0.70222
C	-1.16150	-2.42034	-2.85823
H	0.65135	-1.42863	-3.47849
C	-1.88671	-3.01655	-1.78748
H	-1.91652	-3.45930	0.32925
H	-1.57287	-2.45362	-3.87385
H	-2.85284	-3.49743	-1.98060

V_{JP}^3: M15-L/6-311+G(2df,2pd) SCF= -1949.473758 hartree
Gibbs correction= 0.484461 hartree
Total Gibbs Energy= -1948.989297 hartree

C	-4.42360	-2.47971	-0.94665
C	-3.54032	-2.25286	0.11077
C	-2.33475	-1.56232	-0.13001
C	-2.02613	-1.05264	-1.41887
C	-2.91153	-1.30767	-2.49276
C	-4.09111	-2.01518	-2.24051
H	-5.37379	-2.99772	-0.77818
H	-3.76435	-2.56850	1.13733
H	-2.67320	-0.92305	-3.49071
H	-4.78616	-2.19594	-3.07073
O	-0.91624	-0.33127	-1.59205
C	-1.37634	-1.17873	0.93641
O	-1.45208	-1.50419	2.11400
O	-1.55958	1.56450	0.80752
C	-2.88855	1.36092	0.77660
C	-3.60747	1.49788	-0.43666
C	-3.58852	0.98171	1.94725
C	-4.97805	1.21294	-0.48310
H	-3.04710	1.75726	-1.34541
C	-4.96544	0.72583	1.89427
H	-3.01696	0.86361	2.87590
C	-5.66740	0.82882	0.68066
H	-5.51115	1.27835	-1.44073

H	-5.49378	0.42398	2.80778
H	-6.74004	0.60657	0.64039
Ir	-0.15441	0.20102	0.22298
P	1.84301	-0.94390	0.09758
C	2.35821	-1.27554	1.90078
C	1.97846	-2.48968	-0.98563
C	3.87728	-1.41957	2.13817
H	4.42239	-0.48117	1.93641
H	4.02776	-1.67786	3.20531
H	4.32891	-2.22837	1.53447
C	1.86390	-0.02690	2.68028
H	0.75352	0.04462	2.68186
H	2.17695	-0.11912	3.74025
H	2.29907	0.91066	2.27896
C	1.64630	-2.52058	2.47693
H	0.55478	-2.47744	2.34532
H	2.03344	-3.45988	2.04494
H	1.85121	-2.55082	3.56585
C	0.64914	-3.27251	-0.83415
H	0.41304	-3.52898	0.21464
H	-0.19054	-2.69837	-1.24977
H	0.73773	-4.21702	-1.40633
C	3.13499	-3.48188	-0.71396
H	3.01832	-4.32057	-1.42892
H	4.14076	-3.06467	-0.88050
H	3.09774	-3.91089	0.30149
C	2.06115	-1.98399	-2.44743
H	1.92899	-2.85070	-3.12536
H	1.25030	-1.25888	-2.65709
H	3.03569	-1.51374	-2.67163
C	3.17562	0.23123	-0.43191
C	4.50112	-0.19966	-0.67878
C	2.92400	1.62944	-0.40411
C	5.55754	0.70480	-0.83985
H	4.72619	-1.26825	-0.70119
C	4.00618	2.53360	-0.52188
C	5.31375	2.08245	-0.73030
H	6.57064	0.33075	-1.02740
H	3.78811	3.60870	-0.49417
H	6.13387	2.80301	-0.83079
C	1.55766	2.24525	-0.40891
C	0.72803	2.02256	-1.54284
C	1.21952	3.29318	0.48969
C	-0.39078	2.84568	-1.77856
H	1.02004	1.25617	-2.27446
C	0.09044	4.08318	0.26150
H	1.86897	3.47502	1.35717
C	-0.70835	3.86937	-0.88058
H	-1.01532	2.65804	-2.65982

H	-0.17431	4.87342	0.97311
H	-1.59372	4.49298	-1.05205