

Supplementary Information for

**A Strategy for Developing Metal-Free Hydrogenation
Catalysts: A DFT Proof-of-Principle Study**

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1. Energetic Results for Acetone Hydrogenation Catalyzed by Computed Molecules.

Table S1: Energetic results (in kcal/mol) for acetone hydrogenation catalyzed by various computed molecules.

Molecule	Ring-size	$\Delta G^\ddagger(\text{TS1})$	$\Delta G(\text{H}_2\text{PR})$	$\Delta G^\ddagger(\text{TS2})$	$\Delta G^\ddagger(\text{rds})$
M12OL3	665	25.8	1.0	24.2	25.8
M5OL3	565	24.2	-7.9	18.2	26.1
M6NHL2	665	26.3	2.0	25.9	26.3
M12OL2	665	24.1	-4.2	22.6	26.8
M6OL3	665	23.2	-7.5	19.9	27.4
M6NHL3	665	26.9	2.6	27.6	27.6
M10OL2	065	25.3	-5.9	21.8	27.7
M4OL3	065	23.9	-8.0	19.7	27.7
M11OL2	565	27.9	-5.4	20.7	27.9
M10OL3	065	28.0	1.3	23.8	28.0
M4NHL3	065	28.0	2.7	28.2	28.2
M4NHL2	065	28.5	0.9	28.1	28.5
M5NHL2	565	28.6	1.2	25.3	28.6
M5CH ₂ L2	565	28.7	6.9	25.3	28.7
M6CH ₂ L2	665	25.7	7.8	28.9	28.9
M6CH ₂ L3	665	28.2	11.9	29.5	29.5
M12NHL2	665	27.9	8.3	29.9	29.9
M15OL2	565	27.6	1.8	29.9	29.9
M8OL2	566	27.5	-4.0	26.0	30.0
M5OL2	565	23.1	-14.6	16.7	31.3
M6OL2	665	21.4	-12.4	20.3	32.7
M4OL2	065	23.7	-13.7	19.1	32.8
M7OL2	066	26.8	-3.2	31.1	34.3
M13OL2	666	27.9	1.7	36.0	36.0

2. Energetic Results of H₂ Activation and Acetone Hydrogenation Catalyzed by Computed Molecules with P^{III}-site or O-site as Lewis Basic Site.

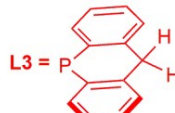
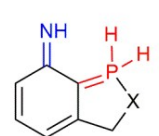
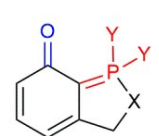
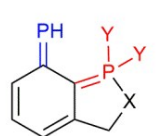
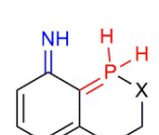
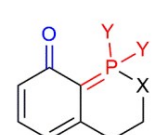
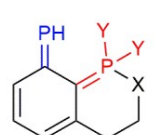
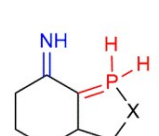
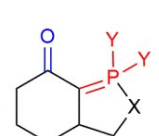
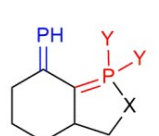
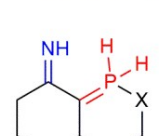
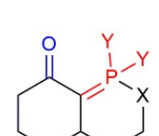
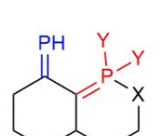
($\Delta G^\ddagger$ / ΔG)									
									
	M4XL1	M4XL2	M4XL3	M4X-OL1	M4X-OL2	M4X-OL3	M4X-PL1	M4X-PL2	M4X-PL3
X=CH ₂	25.6/6.6	29.5/9.4		26.8/20.9			32.2/13.2		
X=NH	21.8/-4.1	28.5/0.9	28.0/2.7	21.9/10.4			28.2/-1.1		
X=O	17.2/-18.2	23.7/-13.7	23.9/-8.0	16.0/-3.3	23.6/1.9	22.4/6.8	22.3/-12.0	29.9/-6.2	29.1/-0.6
									
	M7XL1	M7XL2	M7XL3	M7X-OL1	M7X-OL2	M7X-OL3	M7X-PL1	M7X-PL2	M7X-PL3
X=CH ₂	31.3/15.0			34.3/30.9			35.9/21.6		
X=NH	23.6/0.5	29.3/10.6		29.4/20.3			31.2/7.1		
X=O	23.5/-5.7	26.8/-3.2	31.2/5.0	21.3/4.9	29.6/12.5	35.0/20.3	30.6/3.0		
									
	M10XL1	M10XL2	M10XL3	M10X-OL1	M10X-OL2	M10X-OL3	M10X-PL1	M10X-PL2	M10X-PL3
X=CH ₂	28.7/13.6			30.8/26.8			38.5/18.4		
X=NH	23.7/1.8	30.0/6.7		24.9/16.1			34.2/6.8		
X=O	20.2/-9.2	25.3/-5.9	28.0/1.3	21.0/4.9	27.8/10.7	26.3/13.4	29.2/-4.2		
									
	M13XL1	M13XL2	M13XL3	M13X-OL1	M13X-OL2	M13X-OL3	M13X-PL1	M13X-PL2	M13X-PL3
X=CH ₂	31.1/18.2			35.5/33.9			40.1/28.2		
X=NH	26.8/8.0	31.3/11.6		29.8/22.9			33.8/15.1		
X=O	23.6/-1.9	27.9/1.7	32.3/10.3	22.1/9.2	30.0/17.3		30.0/8.1		

Fig. S1 Energetic results of H₂ activations by computed molecules which P^{III}-site or O-site acts as Lewis basic site. The two values separated by a slash are H₂ activation barrier ($\Delta G^\ddagger$) and endergonicity/exergonicity (ΔG) of the activation, respectively.

Table S2. Energetic results (in kcal/mol) for acetone hydrogenation catalyzed by computed molecules with P^{III}-site or O-site as Lewis basic site. The three numbers in the ring size column are the sizes of the N-contained, middle, and P-contained rings, respectively.

Molecule	Ring-size	$\Delta G^\ddagger(\text{TS1})$	$\Delta G(\text{H}_2\text{PR})$	$\Delta G^\ddagger(\text{TS2})$	$\Delta G^\ddagger(\text{rds})$
M4O-OL2	065	23.6	1.9	29.0	29.0
M4O-OL3	065	22.4	6.8	29.8	29.8
M10O-OL2	065	27.8	10.7	33.8	33.8
M10O-OL3	065	26.3	13.4	33.1	33.1

From the hydrogen activation energetic results of Fig S1, one can observe that most molecules with a P^{III}-site or an O-site as Lewis basic site have higher barriers and larger endergonicities than their counterparts with a N Lewis basic site. We also chose the molecules with hydrogen activation barriers lower than 29.0 kcal/mol to perform acetone hydrogenation. As shown in Table S2, all hydrogenations catalyzed by these molecules have barriers higher than 29.0 kcal/mol, indicating that they may not perform catalytic hydrogenation well.

3. Energetic and Geometric Results for Catalysts Dimerization

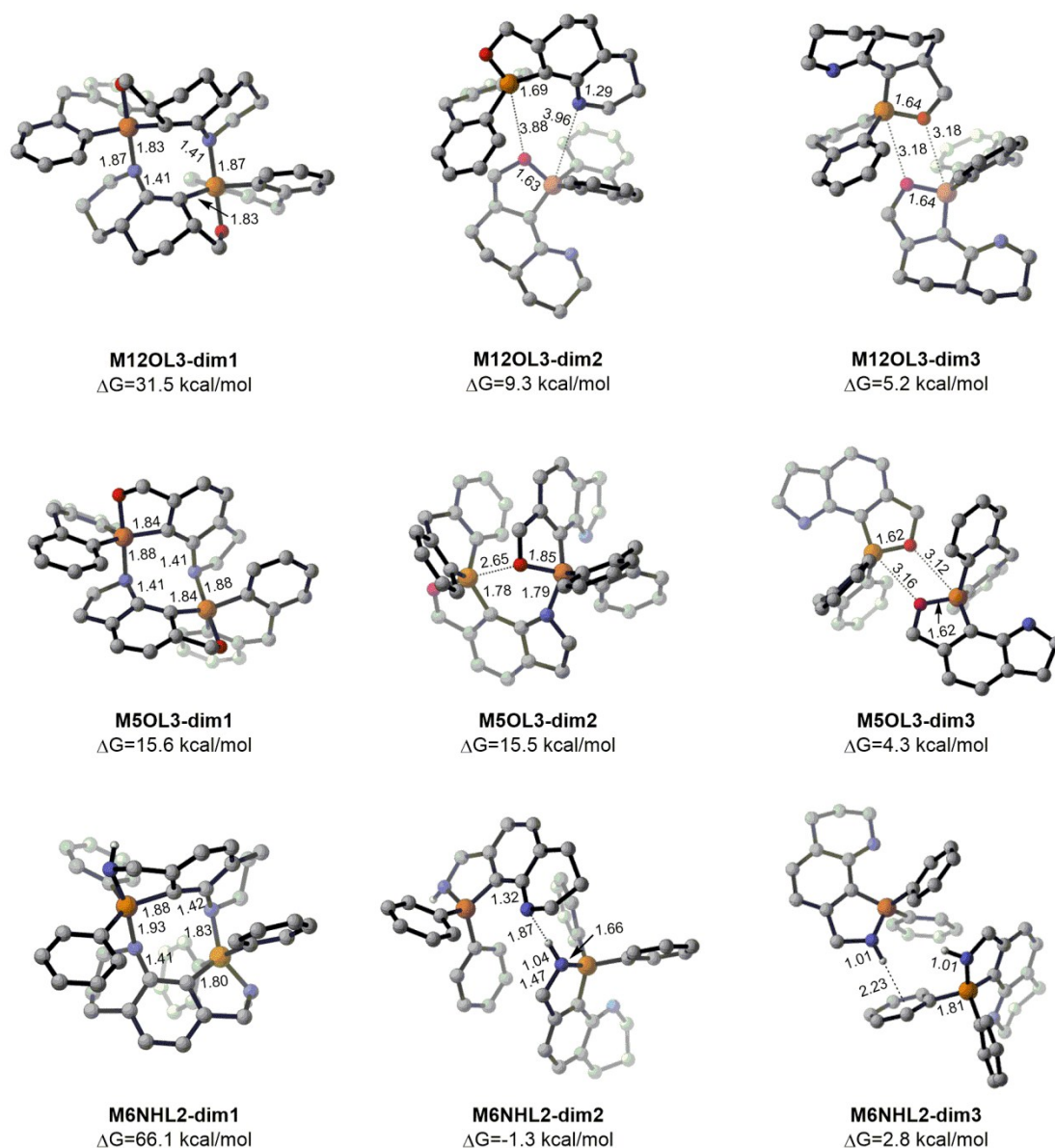


Fig. S2 Energetic and geometric results of three possible dimers for **M5OL3**, **M6NHL2** and **M12OL3**. Hydrogen atoms except which forming dimers are omitted for clarity.

4. Energies and Cartesian Coordinates of All the Structures

All energies are given in Hartree.

H₂

SCF energy in gas phase: -1.167212

SCF energy in solution: -1.167846

Free energy in solution: -1.169171

H	0.000000	0.000000	0.368377
H	0.000000	0.000000	-0.368377

Acetone

SCF energy in gas phase: -193.062279

SCF energy in solution: -193.128853

Free energy in solution: -193.072467

C	0.000015	0.186282	-0.000053
O	-0.000116	1.395367	0.000001
C	-1.286722	-0.613328	0.000108
H	-1.329459	-1.257751	-0.883517
H	-1.324599	-1.266983	0.877084
H	-2.140122	0.063731	0.005670
C	1.286821	-0.613170	-0.000137
H	1.329533	-1.257278	0.883771
H	1.324710	-1.267284	-0.876757
H	2.140178	0.063930	-0.005769

Isopropanol

SCF energy in gas phase: -194.262771

SCF energy in solution: -194.329321

Free energy in solution: -194.247130

C	0.001374	0.046565	0.368610
O	-0.049835	1.359603	-0.166277
C	-1.188574	-0.780976	-0.102834
H	-1.194366	-0.828244	-1.195711
H	-1.143183	-1.799462	0.292995
H	-2.133439	-0.335513	0.226670
C	1.322035	-0.547050	-0.088919
H	1.457971	-1.552373	0.317841
H	1.341174	-0.602453	-1.181246
H	2.152389	0.082470	0.237813
H	-0.006126	0.088490	1.470173

H	-0.884748	1.759025	0.100540
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M1

SCF energy in gas phase: -328.950920

SCF energy in solution: -329.049480

Free energy in solution: -328.961466

C	1.831590	-0.649056	0.062345
C	1.774272	0.787633	-0.058666
C	0.569097	1.382741	-0.080734
C	-0.626506	-0.754160	-0.019181
C	0.696894	-1.372019	0.097694
H	2.796362	-1.142902	0.125730
H	2.675938	1.383010	-0.111934
H	0.451513	2.457950	-0.141275
H	0.717113	-2.453494	0.183857
N	-0.636897	0.682200	-0.005160
B	-1.857142	1.421162	0.132910
H	-1.763732	2.607257	0.081859
H	-2.878268	0.858504	0.314248
H	-1.571293	-2.374474	-0.108079
N	-1.736533	-1.369700	-0.140227

M1-TS1

SCF energy in gas phase: -330.114509

SCF energy in solution: -330.213640

Free energy in solution: -330.109036

C	-1.978583	0.511427	-0.002065
C	-1.809974	-0.908312	0.078320
C	-0.549349	-1.402071	0.040386
C	0.451016	0.802690	-0.037529
C	-0.902951	1.331224	-0.064484
H	-2.979877	0.931816	-0.005916
H	-2.656948	-1.576467	0.153257
H	-0.336996	-2.464900	0.073027
H	-1.012787	2.409366	-0.112906
N	0.559540	-0.600133	-0.078739
B	1.910156	-1.190559	-0.240966
H	2.009456	-2.334159	0.086529

H	2.641242	-0.718407	-1.046966
H	1.373448	2.461623	0.084895
H	2.724969	-0.755739	1.166039
H	2.618534	-0.040883	0.886484
N	1.555777	1.461676	0.054827

M1-Pr

SCF energy in gas phase: -330.172710

SCF energy in solution: -330.275034

Free energy in solution: -330.165924

C	1.968892	0.545260	-0.002415
C	1.841462	-0.850430	-0.000595
C	0.572836	-1.382258	0.000666
C	-0.430093	0.723310	0.002924
C	0.842314	1.333715	-0.000928
H	2.950794	1.007540	-0.004815
H	2.704322	-1.503003	-0.001419
H	0.383306	-2.448507	-0.000218
H	0.905439	2.415907	0.000719
N	-0.543128	-0.624378	0.001106
B	-2.001806	-1.303586	-0.001377
H	-1.824523	-2.495087	-0.036861
H	-2.567289	-0.882667	-0.993428
H	-2.552284	-0.930257	1.014147
N	-1.568845	1.444580	0.026889
H	-1.532817	2.441215	-0.093048
H	-2.446572	0.953787	-0.072075

M2

SCF energy in gas phase: -629.306727

SCF energy in solution: -629.425131

Free energy in solution: -629.332450

C	0.211552	-0.508685	0.000052
C	-1.369128	1.326915	-0.000146
C	-2.100956	-1.024796	-0.000086
C	-2.361435	0.360555	-0.000160
C	-0.785980	-1.473477	0.000020
C	-0.019763	0.892905	-0.000046
H	-3.398063	0.688160	-0.000240
H	-0.548438	-2.533501	0.000095
H	-1.617432	2.382951	-0.000220
H	-2.923872	-1.729375	-0.000104

N	1.182264	1.475060	-0.000048
H	1.277591	2.481063	0.000003
P	1.983683	-0.466284	0.000157
H	2.321367	-1.857038	0.000299
H	2.705925	-0.101860	1.140721
H	2.706083	-0.102055	-1.140373

M2-TS1

SCF energy in gas phase: -630.444695

SCF energy in solution: -630.568817

Free energy in solution: -630.461502

C	0.314261	-0.322054	-0.011290
C	-1.663125	1.071993	-0.009857
C	-1.876790	-1.351095	0.039409
C	-2.441805	-0.056667	0.025985
C	-0.506619	-1.468083	0.022622
C	-0.233651	1.005296	-0.054117
H	-3.522936	0.050349	0.042111
H	-0.048823	-2.455490	0.017798
H	-2.122143	2.056877	-0.016690
H	-2.508265	-2.231227	0.046870
N	0.591314	2.047499	-0.127361
H	0.103759	2.934327	-0.040609
P	2.056715	-0.558966	-0.041119
H	2.831723	-0.970140	1.051508
H	2.753876	0.379398	-0.797571
H	2.202852	-1.734966	-0.831791
H	1.614114	1.652743	0.736048
H	2.152288	1.093789	1.224133

M2-Pr

SCF energy in gas phase: -630.488984

SCF energy in solution: -630.603497

Free energy in solution: -630.490518

C	0.344206	-0.266206	-0.033002
C	-1.748528	0.946560	0.022564
C	-1.775071	-1.467923	0.009958
C	-2.449279	-0.247795	0.038690
C	-0.388658	-1.456895	-0.036176
C	-0.343517	0.969340	-0.012710
H	-3.534420	-0.224897	0.069758
H	0.159874	-2.394957	-0.078448

H	-2.284679	1.892135	0.024948
H	-2.320900	-2.404446	0.016456
N	0.300096	2.191369	-0.122712
H	-0.251987	2.986469	0.162988
P	2.180060	-0.430097	0.023298
H	2.959988	-0.997008	1.073268
H	3.016438	0.043528	-1.018167
H	2.070852	-1.751960	-0.618752
H	1.250925	2.222495	0.217028
H	2.297415	0.878027	0.724496

M3

SCF energy in gas phase: -631.717387

SCF energy in solution: -631.838035

Free energy in solution: -631.699763

C	-0.429187	-0.405701	-0.010434
C	1.402868	1.326689	0.126140
C	1.913472	-1.133464	0.336161
C	2.324252	0.187269	-0.318189
C	0.526160	-1.565216	-0.150450
C	-0.066784	0.970136	0.007412
H	3.362570	0.433106	-0.073623
H	0.624148	-1.901442	-1.194495
H	2.646288	-1.915300	0.111245
N	-1.039259	1.835000	-0.021626
H	-0.713247	2.795717	0.056874
P	-2.132966	-0.482949	0.003918
H	-2.902386	0.005697	-1.072331
H	-2.804675	0.100772	1.090919
H	-2.520215	-1.834508	0.053761
H	2.270775	0.075823	-1.408939
H	1.893097	-1.004383	1.425753
H	0.190365	-2.436871	0.424248
H	1.599635	1.561853	1.180457
H	1.598268	2.240487	-0.445103

M3-TS1

SCF energy in gas phase: -632.852270

SCF energy in solution: -632.970431

Free energy in solution: -632.817172

C	-0.426155	-0.301855	-0.005319
C	1.581095	1.211388	0.100092

C	1.871381	-1.263929	0.315899
C	2.389164	0.001741	-0.362301
C	0.436211	-1.541939	-0.129680
C	0.077815	0.997927	0.071128
H	3.450287	0.158934	-0.145339
H	0.462390	-1.912981	-1.165515
H	2.507394	-2.122305	0.077951
N	-0.734889	2.045171	0.156439
H	-0.254610	2.936156	0.078630
P	-2.151567	-0.556832	0.017587
H	-2.959081	-0.958838	-1.061468
H	-2.884757	0.295526	0.843752
H	-2.251948	-1.782321	0.752733
H	-1.756762	1.704833	-0.609761
H	-2.345277	1.133921	-1.119044
H	2.296100	-0.110457	-1.449765
H	1.896662	-1.127258	1.404262
H	0.014566	-2.358393	0.473337
H	1.855429	1.466796	1.131994
H	1.810260	2.092666	-0.509552

M3-Pr

SCF energy in gas phase: -632.886498

SCF energy in solution: -632.998973

Free energy in solution: -632.841424

C	-0.453745	-0.241120	-0.010566
C	1.671368	1.107960	-0.009215
C	1.799502	-1.343482	0.380231
C	2.394232	-0.175579	-0.397454
C	0.338773	-1.535295	-0.015372
C	0.162210	0.970195	0.033813
H	3.466197	-0.069079	-0.206129
H	0.294461	-1.999725	-1.011957
H	2.361173	-2.264815	0.197414
N	-0.457361	2.189048	0.232238
H	0.040759	2.987840	-0.132584
P	-2.275189	-0.439034	-0.064714
H	-2.981805	-0.932729	-1.198351
H	-3.188680	-0.124043	0.981951
H	-2.146445	-1.814860	0.460204
H	-1.452762	2.220667	0.060710
H	-2.457036	0.937044	-0.613997
H	2.272822	-0.358618	-1.472103

H	1.863945	-1.130011	1.454860
H	-0.139814	-2.249885	0.663064
H	2.001990	1.446727	0.981391
H	1.920524	1.917592	-0.708043

M4CH₂L1

SCF energy in gas phase: -706.705206

SCF energy in solution: -706.856680

Free energy in solution: -706.728617

C	0.040047	0.273257	-0.041570
C	2.427663	0.096501	0.039516
C	0.998655	-1.918740	0.015130
C	2.267566	-1.262813	0.053024
C	-0.120917	-1.126899	-0.034814
C	1.283967	0.993004	-0.017289
H	3.159441	-1.883793	0.095812
H	3.423686	0.529711	0.073102
H	0.933696	-3.000672	0.019178
N	1.227530	2.294742	-0.038606
H	2.162817	2.699005	-0.004355
P	-1.460828	1.098233	-0.015429
C	-1.563010	-1.585879	-0.148127
H	-1.768665	-2.431755	0.512998
C	-2.509189	-0.398785	0.183953
H	-1.857576	1.854940	-1.134586
H	-1.695144	2.005082	1.030026
H	-1.752799	-1.925786	-1.171616
H	-2.834197	-0.431315	1.226883
H	-3.400244	-0.369983	-0.444712

M4CH₂L1-TS1

SCF energy in gas phase: -707.854309

SCF energy in solution: -707.996759

Free energy in solution: -707.853918

C	-0.034927	0.264795	-0.029120
C	-2.432644	0.003439	0.026853
C	-0.984128	-1.962218	-0.049115
C	-2.261467	-1.357226	-0.014089
C	0.119324	-1.140256	-0.066169
C	-1.317330	0.907407	0.060737
H	-3.142864	-1.993153	-0.010778
H	-3.431211	0.429799	0.063647

H	-0.876614	-3.041262	-0.052706
N	-1.391789	2.221718	0.189161
H	-2.341636	2.575670	0.131728
P	1.539893	1.034954	-0.106685
C	1.553717	-1.629161	-0.128930
C	2.455920	-0.495578	0.390792
H	3.472332	-0.528729	-0.006818
H	-0.238441	2.713087	-0.439516
H	0.582199	2.752868	-0.839470
H	1.852268	2.023390	0.825994
H	2.176655	1.375868	-1.308358
H	2.504532	-0.516545	1.483287
H	1.681723	-2.547131	0.450765
H	1.814383	-1.867409	-1.167385

M4CH₂L1-Pr

SCF energy in gas phase: -707.900141

SCF energy in solution: -708.033332

Free energy in solution: -707.884225

C	-0.019958	0.263717	-0.020680
C	-2.421453	0.050741	0.043854
C	-1.042195	-1.937086	-0.059976
C	-2.295625	-1.328947	-0.007225
C	0.088836	-1.130769	-0.062434
C	-1.287268	0.881070	0.037942
H	-3.193124	-1.940469	0.002054
H	-3.405581	0.507370	0.107368
H	-0.945895	-3.017949	-0.090939
N	-1.449919	2.247583	0.175081
H	-2.361006	2.600012	-0.075990
P	1.622483	1.091910	-0.148865
C	1.507190	-1.664549	-0.126682
H	1.582383	-2.618798	0.404716
C	2.401236	-0.569737	0.437229
H	3.443270	-0.643412	0.109837
H	2.286600	1.827806	0.874400
H	2.363404	1.065895	-1.367528
H	-0.684867	2.821970	-0.147298
H	1.002372	2.357625	-0.619300
H	2.377252	-0.590006	1.533675
H	1.762803	-1.868407	-1.175757

M4NHL1

SCF energy in gas phase: -722.741104

SCF energy in solution: -722.901400

Free energy in solution: -722.784592

C	0.031933	0.264340	0.022177
C	2.411261	0.151139	-0.007987
C	1.034371	-1.904575	-0.005077
C	2.282349	-1.214914	-0.013334
C	-0.102629	-1.130799	0.014398
C	1.247501	1.020292	0.009443
H	3.190581	-1.812924	-0.027430
H	3.398801	0.604217	-0.019476
H	0.996269	-2.987399	-0.014165
N	1.138131	2.320852	0.014393
H	2.054145	2.767033	-0.001634
P	-1.499388	1.029022	-0.003455
C	-1.545731	-1.593681	0.032811
H	-1.799323	1.881637	-1.076131
H	-1.881417	1.812476	1.102538
H	-1.752960	-2.277657	-0.796176
H	-1.772159	-2.112489	0.971556
N	-2.387829	-0.380956	-0.099919
H	-3.349554	-0.440308	0.196841

M4NHL1-TS1

SCF energy in gas phase: -723.894899

SCF energy in solution: -724.047487

Free energy in solution: -723.915978

C	0.022125	0.267953	0.025946
C	2.423791	0.038255	0.028153
C	1.006743	-1.949966	0.033054
C	2.274362	-1.323929	0.054701
C	-0.103174	-1.138236	0.028295
C	1.298953	0.934263	-0.046455
H	3.165672	-1.945373	0.079414
H	3.416705	0.479196	0.028604
H	0.913666	-3.029890	0.005721
N	1.369999	2.241319	-0.189075
H	2.320967	2.593041	-0.133293
P	-1.574764	0.977896	0.068108
C	-1.525068	-1.649026	-0.022677
H	0.092406	2.762329	0.319059

H	-0.724626	2.815214	0.627209
H	-1.918057	1.882107	-0.937268
H	-2.176620	1.464751	1.238097
H	-1.641405	-2.365786	-0.842499
H	-1.778452	-2.164272	0.913313
N	-2.383389	-0.478626	-0.238757
H	-3.341464	-0.574498	0.068736

M4NHL1-Pr

SCF energy in gas phase: -723.948601

SCF energy in solution: -724.094767

Free energy in solution: -723.957250

C	0.005081	0.262068	-0.010589
C	2.407463	0.077107	-0.013309
C	1.054656	-1.929704	0.054796
C	2.300053	-1.304274	0.038995
C	-0.079207	-1.130874	0.024322
C	1.265164	0.896632	-0.042437
H	3.206164	-1.902592	0.056644
H	3.387190	0.545791	-0.049921
H	0.969070	-3.011535	0.078827
N	1.425059	2.262558	-0.177790
H	2.324779	2.623430	0.099500
P	-1.645532	1.045431	0.128601
C	-1.495745	-1.658682	0.030502
H	0.644801	2.841176	0.092653
H	-1.067294	2.367117	0.442002
H	-2.488323	1.672042	-0.820291
H	-2.239307	1.075225	1.417825
H	-1.579594	-2.509003	-0.659199
H	-1.724683	-2.042715	1.041952
N	-2.309926	-0.541223	-0.382908
H	-3.300540	-0.663384	-0.197799

M4OL1

SCF energy in gas phase: -742.606615

SCF energy in solution: -742.769727

Free energy in solution: -742.664951

C	-0.028005	0.269613	0.002102
C	-2.406744	0.159770	-0.000182
C	-1.029863	-1.900333	-0.000111
C	-2.278257	-1.205460	-0.000351

C	0.104859	-1.126561	0.000875
C	-1.241074	1.028620	0.000481
H	-3.186961	-1.802558	-0.000975
H	-3.394291	0.612636	-0.000756
H	-0.995820	-2.983008	-0.001056
N	-1.123634	2.326894	-0.000329
H	-2.035539	2.781692	-0.001713
P	1.516222	0.986088	-0.000029
H	1.923198	1.763079	1.094622
H	1.919704	1.763535	-1.095675
O	2.399725	-0.367135	-0.001001
C	1.554881	-1.560324	-0.000036
H	1.820495	-2.134717	0.890635
H	1.818754	-2.135109	-0.890992

M5CH₂L1

SCF energy in gas phase: -784.088599

SCF energy in solution: -784.255206

Free energy in solution: -784.094529

C	0.477696	-0.226730	-0.084645
C	-1.744579	0.776490	0.019390
C	0.255539	2.182776	0.020554
C	-1.178347	2.008295	0.055566
C	-0.936588	-0.433391	-0.055213
H	-1.805880	2.894846	0.115235
H	0.680946	3.180193	0.044474
N	-1.566286	-1.566213	-0.065438
P	1.678361	-1.437062	-0.022378
C	2.569323	1.078173	-0.166161
H	1.918870	-2.274435	-1.132753
H	1.599485	-2.395429	1.004779
C	-3.175148	0.292946	0.038256
C	1.056691	1.081467	-0.052909
C	-2.999899	-1.261251	0.025064
H	-3.532980	-1.716878	-0.818324
H	-3.717205	0.639295	0.923577
C	3.105466	-0.315682	0.250811
H	3.340533	-0.347917	1.317664
H	3.022931	1.859825	0.448466
H	3.991871	-0.625313	-0.304651
H	2.855452	1.274937	-1.205247
H	-3.417105	-1.713429	0.934212
H	-3.729248	0.645170	-0.837981

M5CH₂L1-TS1

SCF energy in gas phase: -785.238838

SCF energy in solution: -785.395227

Free energy in solution: -785.219164

C	0.481577	-0.182220	0.026172
C	-1.741822	0.820706	0.024673
C	0.236025	2.230139	-0.064439
C	-1.180445	2.064097	-0.028641
C	-0.923343	-0.355944	0.074365
H	-1.814423	2.947431	-0.044513
H	0.666565	3.225187	-0.103019
N	-1.588292	-1.498163	0.144459
P	1.715287	-1.413413	-0.070964
C	2.559488	1.140099	-0.150426
H	2.148894	-1.992746	-1.273335
H	1.769266	-2.413053	0.900016
C	-3.169147	0.330902	0.114469
C	1.045603	1.120793	-0.048709
C	-3.005248	-1.203598	-0.096955
H	-3.276957	-1.480748	-1.125404
H	-3.580876	0.538423	1.109018
C	3.088450	-0.225835	0.328124
H	3.215552	-0.227349	1.414588
H	2.985976	1.961929	0.431191
H	4.037957	-0.507851	-0.131548
H	2.850153	1.305159	-1.194944
H	-3.643373	-1.784007	0.575331
H	-3.835235	0.790197	-0.620437
H	-0.659503	-2.394716	-0.335267
H	0.177924	-2.714359	-0.620238

M5CH₂L1-Pr

SCF energy in gas phase: -785.286948

SCF energy in solution: -785.435306

Free energy in solution: -785.252475

C	0.492916	-0.176996	0.001495
C	-1.739772	0.774581	0.047672
C	0.176809	2.231032	-0.081981
C	-1.211947	2.049486	-0.014979
C	-0.892468	-0.348828	0.054662
H	-1.872961	2.912239	-0.016419
H	0.597456	3.230294	-0.142721

N	-1.639021	-1.511893	0.173949
P	1.773481	-1.487697	-0.092572
C	2.527166	1.189578	-0.172658
H	2.428334	-1.765655	-1.325482
H	2.234913	-2.348533	0.945046
C	-3.164579	0.287400	0.180300
C	1.014584	1.124102	-0.070441
C	-3.027069	-1.204470	-0.186242
H	-3.197782	-1.344444	-1.263687
H	-3.507718	0.395701	1.216101
C	3.057374	-0.124516	0.388296
H	3.095572	-0.076772	1.483727
H	2.910781	2.077124	0.341351
H	4.055498	-0.383654	0.020676
H	2.805185	1.295817	-1.230340
H	-3.723053	-1.843330	0.361685
H	-3.872725	0.810267	-0.466107
H	-1.229329	-2.363090	-0.185352
H	0.748670	-2.505473	-0.444294

M5NHL1

SCF energy in gas phase: -800.123515

SCF energy in solution: -800.299406

Free energy in solution: -800.149669

C	0.480968	-0.226162	-0.068668
C	-1.734267	0.773108	-0.001929
C	0.263809	2.183965	0.019253
C	-1.167785	2.006808	0.024219
C	-0.929080	-0.438499	-0.039332
H	-1.797224	2.893267	0.057528
H	0.689611	3.180552	0.056737
N	-1.557359	-1.573058	-0.035508
P	1.707022	-1.405460	0.006277
C	2.575302	1.057347	-0.042760
H	2.987640	1.668590	0.765498
H	1.898792	-2.289605	-1.077024
H	1.689776	-2.312102	1.080789
C	1.060402	1.075693	-0.029373
H	2.958909	1.440667	-0.995544
C	-2.991674	-1.264442	0.033222
C	-3.165539	0.290438	-0.001887
H	-3.519898	-1.744058	-0.799829
H	-3.697699	0.617306	-0.901392

H	-3.417658	-1.686862	0.952723
H	-3.728673	0.662687	0.859396
N	2.995621	-0.353875	0.142493
H	3.910457	-0.609555	-0.198403

M5NHL1-TS1

SCF energy in gas phase: -801.279871

SCF energy in solution: -801.445795

Free energy in solution: -801.281181

C	0.487747	-0.182941	0.032727
C	-1.734544	0.815581	-0.005488
C	0.240323	2.232220	-0.053216
C	-1.175705	2.059684	-0.054722
C	-0.919030	-0.364960	0.070397
H	-1.812416	2.940543	-0.088343
H	0.669903	3.228179	-0.066708
N	-1.583347	-1.501995	0.149687
P	1.743689	-1.384542	-0.033238
C	2.557385	1.137553	0.001196
H	2.922275	1.752420	0.831674
H	-0.569658	-2.447293	-0.209387
H	0.254869	-2.760705	-0.402778
H	2.104515	-2.093618	-1.190870
H	1.836833	-2.307765	1.009864
C	1.044411	1.120126	-0.017600
H	2.945761	1.568363	-0.930491
C	-3.000281	-1.211411	-0.092256
C	-3.164326	0.329887	0.068446
H	-3.280693	-1.524768	-1.107915
H	-3.812492	0.767001	-0.695614
H	-3.634699	-1.768077	0.603776
H	-3.598208	0.571368	1.045703
N	2.995677	-0.255098	0.163617
H	3.916482	-0.472311	-0.190382

M5NHL1-Pr

SCF energy in gas phase: -801.341677

SCF energy in solution: -801.500356

Free energy in solution: -801.327511

C	0.504625	-0.142261	-0.034228
C	-1.755331	0.746324	-0.046150
C	0.111930	2.263747	0.033319

C	-1.268578	2.043807	-0.006021
C	-0.872371	-0.341281	-0.062800
H	-1.955377	2.885679	0.005235
H	0.507054	3.274735	0.077935
N	-1.577252	-1.548973	-0.147567
P	1.852885	-1.450618	-0.040683
C	2.479716	1.241484	0.060471
H	2.815774	1.759761	0.968515
H	-1.143654	-2.349649	0.293566
H	1.352902	-2.112740	-1.197943
H	3.031399	-2.308366	0.002836
H	1.228772	-2.218734	0.995041
C	0.968749	1.166369	0.017980
H	2.861210	1.802779	-0.803186
C	-2.963012	-1.271428	0.257998
C	-3.164178	0.206096	-0.136882
H	-3.660356	-1.945778	-0.244082
H	-3.533514	0.279278	-1.166939
H	-3.088868	-1.384162	1.344982
H	-3.879309	0.714158	0.514085
N	2.934099	-0.134153	0.039367
H	3.923461	-0.332956	0.075480

M5OL1

SCF energy in gas phase: -819.989304

SCF energy in solution: -820.168115

Free energy in solution: -820.031964

C	0.482942	-0.239282	-0.000406
C	-1.730343	0.769919	-0.000049
C	0.272146	2.176978	-0.000084
C	-1.161728	2.001914	-0.000039
C	-0.929502	-0.446944	-0.000175
H	-1.788903	2.890273	0.000145
H	0.699330	3.173459	-0.000020
N	-1.562204	-1.576990	-0.000108
P	1.740423	-1.375505	0.000136
C	2.573895	1.022528	0.000000
H	3.007181	1.482554	0.891493
H	1.899508	-2.251529	-1.087339
H	1.899228	-2.251028	1.088068
O	3.002492	-0.375219	0.000118
C	1.062246	1.065435	-0.000170
H	3.007480	1.482462	-0.891391

C	-2.997146	-1.262918	-0.000222
C	-3.163381	0.292884	0.000476
H	-3.475537	-1.713173	-0.878852
H	-3.709536	0.646022	-0.879798
H	-3.476000	-1.714080	0.877674
H	-3.708384	0.645211	0.881804

M5OL1-TS1

SCF energy in gas phase: -821.151360

SCF energy in solution: -821.321788

Free energy in solution: -821.169233

C	0.489518	-0.190504	-0.041791
C	-1.731183	0.814472	0.006120
C	0.251971	2.228314	0.043003
C	-1.168733	2.054589	0.047663
C	-0.920989	-0.376660	-0.054644
H	-1.803194	2.937013	0.081714
H	0.681502	3.223821	0.060936
N	-1.581448	-1.507342	-0.103263
P	1.769535	-1.348125	0.032845
C	2.558089	1.097469	-0.031196
H	2.994351	1.585113	0.845922
H	-0.467131	-2.502656	0.108226
H	0.338528	-2.806119	0.210641
H	2.005179	-2.220133	-1.031338
H	2.081464	-2.064599	1.193366
O	3.000285	-0.273502	-0.042073
C	1.047176	1.113971	0.001427
H	2.948736	1.579892	-0.932208
C	-3.008952	-1.214650	0.058024
C	-3.164603	0.335678	-0.041034
H	-3.594549	-1.732600	-0.708151
H	-3.637846	0.622828	-0.986319
H	-3.359030	-1.582484	1.031514
H	-3.776953	0.745134	0.767008

M5OL1-Pr

SCF energy in gas phase: -821.219651

SCF energy in solution: -821.388632

Free energy in solution: -821.227866

C	-0.506792	-0.177288	-0.043472
C	1.721724	0.770403	-0.039102

C	-0.195781	2.232375	0.064894	H	-4.450022	-0.524851	0.437384
C	1.193492	2.045915	0.024888	N	-1.204663	-1.481313	-0.173564
C	0.878248	-0.355593	-0.073307	C	3.311648	-0.543044	0.272237
H	1.857001	2.906321	0.048240	H	4.151268	-0.925410	-0.310211
H	-0.616568	3.231447	0.123081	H	3.441953	1.615639	0.607541
N	1.629386	-1.514537	-0.177230	H	-3.361074	1.775739	0.387802
P	-1.800788	-1.445342	0.045022	H	-2.935130	-2.517724	0.328720
C	-2.535362	1.121907	0.077095	H	-3.103370	-0.403920	1.576667
H	-2.945756	1.824872	-0.659361	H	-3.265425	0.942281	-1.161917
H	-2.333874	-1.779050	1.304309	H	3.560831	-0.647662	1.331240
H	-2.440808	-2.125883	-1.007086	H	3.297521	1.157997	-1.085333
O	-2.979904	-0.171802	-0.202230				
C	-1.021396	1.119418	0.025424	M6CH₂L1-TS1			
H	-2.867408	1.462437	1.072506	SCF energy in gas phase: -824.543145			
C	3.009489	-1.206865	0.213324	SCF energy in solution: -824.708963			
C	3.150544	0.287383	-0.141379	Free energy in solution: -824.503923			
H	3.717222	-1.841023	-0.324567				
H	3.517056	0.403137	-1.168179	C	0.726111	-0.145845	-0.077860
H	3.157647	-1.353823	1.293024	C	-1.418929	1.001763	-0.109341
H	3.841923	0.808051	0.524547	C	0.681620	2.271167	-0.045316
H	1.218710	-2.375886	0.153229	C	-0.730057	2.188708	-0.077018
H	-0.824798	-2.530232	0.173190	C	-0.706747	-0.255691	-0.071359
				H	-1.307336	3.111870	-0.068936
M6CH₂L1				H	1.181814	3.232340	0.000704
SCF energy in gas phase: -823.394653				P	1.901302	-1.447772	-0.097661
SCF energy in solution: -823.568054				C	2.912715	1.016110	-0.044321
Free energy in solution: -823.378184				H	2.424605	-1.999753	-1.276706
				H	1.775610	-2.486030	0.826297
C	0.724065	-0.135304	-0.088051	C	1.399093	1.099331	-0.055177
C	-1.410258	0.996365	-0.084447	C	-2.725590	-1.541359	-0.087102
C	0.721272	2.254866	0.018249	C	-2.927351	0.943763	-0.147603
C	-0.707637	2.167442	-0.006292	C	-3.424205	-0.331964	0.533452
C	-0.700933	-0.279371	-0.125396	H	-3.049692	-1.640524	-1.136113
H	-1.275519	3.096086	0.038371	H	-4.510010	-0.429198	0.435560
H	1.212729	3.220089	0.066143	N	-1.280744	-1.445892	-0.004749
P	1.764078	-1.491022	-0.019479	C	3.296229	-0.377520	0.482700
C	2.941255	0.925146	-0.076236	H	4.269876	-0.726348	0.132330
H	1.890437	-2.338615	-1.136479	H	3.346571	1.813256	0.565154
H	1.561905	-2.427306	1.008848	H	-3.349834	1.837300	0.324162
C	1.433136	1.085233	-0.026884	H	-3.037870	-2.459838	0.422251
C	-2.654923	-1.581911	-0.170213	H	-0.341516	-2.337489	-0.550906
C	-2.914762	0.914121	-0.120573	H	0.418347	-2.698820	-0.907486
C	-3.364044	-0.406575	0.511421	H	-3.187278	-0.293952	1.602901
H	-3.027552	-1.669644	-1.204517	H	-3.273520	0.944239	-1.190394

H	3.291779	-0.387370	1.576452
H	3.296798	1.147361	-1.063443

M6CH₂L1-Pr

SCF energy in gas phase: -824.588016

SCF energy in solution: -824.745540

Free energy in solution: -824.534718

C	0.738877	-0.138415	-0.050975
C	-1.422451	0.970397	-0.068024
C	0.636323	2.279036	-0.082957
C	-0.752551	2.188904	-0.082862
C	-0.672610	-0.228515	-0.047322
H	-1.348770	3.099147	-0.085404
H	1.133612	3.244089	-0.085079
P	1.950640	-1.526720	-0.139621
C	2.892708	1.056570	-0.060536
H	2.711620	-1.768720	-1.323309
H	2.224767	-2.471498	0.890726
C	1.377223	1.104512	-0.062706
C	-2.742750	-1.543572	-0.207656
C	-2.936400	0.930231	-0.064604
C	-3.462929	-0.393923	0.485364
H	-2.963263	-1.512231	-1.287338
H	-4.542111	-0.476763	0.329368
N	-1.319814	-1.444855	0.056986
C	3.271351	-0.295517	0.526081
H	4.278584	-0.626071	0.252545
H	3.303674	1.910932	0.487137
H	-3.324100	1.771030	0.519945
H	-3.092724	-2.507081	0.173010
H	-0.762869	-2.248916	-0.193944
H	0.928119	-2.458768	-0.683988
H	-3.270194	-0.458290	1.561415
H	-3.309858	1.065861	-1.088333
H	3.195712	-0.267906	1.620056
H	3.256150	1.141723	-1.094207

M6NHL1

SCF energy in gas phase: -839.430335

SCF energy in solution: -839.613002

Free energy in solution: -839.434060

C	0.724694	-0.130864	-0.004587
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C	-1.397386	0.993040	-0.098366
C	0.732317	2.259211	0.005376
C	-0.693013	2.167890	-0.048977
C	-0.692283	-0.282678	-0.070168
H	-1.261388	3.097142	-0.058503
H	1.223902	3.224839	0.031082
P	1.790763	-1.466410	-0.005599
C	2.939231	0.889794	0.091817
H	3.335767	1.256263	1.045706
H	1.744512	-2.359224	-1.087359
H	1.775214	-2.350600	1.090416
C	1.436786	1.080830	0.027457
C	-2.637519	-1.590162	-0.151399
C	-2.900667	0.909916	-0.175093
C	-3.370024	-0.396642	0.473194
H	-2.968379	-1.699700	-1.198161
H	-3.360804	1.782091	0.302261
H	-4.452833	-0.517191	0.363985
N	-1.188475	-1.490368	-0.092163
H	-2.943425	-2.512554	0.357320
H	-3.146819	-0.367283	1.546475
H	-3.222312	0.916527	-1.226082
H	3.442765	1.427469	-0.717640
N	3.194752	-0.564441	-0.044286
H	4.075596	-0.919991	0.294095

M6NHL1-TS1

SCF energy in gas phase: -840.584329

SCF energy in solution: -840.760306

Free energy in solution: -840.566645

C	0.727413	-0.149702	0.007226
C	-1.408525	1.011456	-0.058585
C	0.695347	2.272086	0.022726
C	-0.717073	2.194325	0.007353
C	-0.705465	-0.253953	-0.112591
H	-1.291397	3.119063	0.029500
H	1.202496	3.230567	0.012931
P	1.912958	-1.429062	0.086240
C	2.908609	1.001499	0.013570
H	3.325887	1.380745	0.955576
H	1.890107	-2.400143	-0.915510
H	2.246189	-2.116449	1.263934
C	1.399565	1.093074	0.030176

C	-2.731044	-1.519494	-0.256712
C	-2.916239	0.958184	-0.107872
C	-3.408923	-0.364129	0.479363
H	-3.108637	-1.554395	-1.290873
H	-3.339459	1.815829	0.425725
H	-4.497084	-0.448268	0.398765
N	-1.282883	-1.428365	-0.266646
H	0.383283	-2.791972	0.618700
H	-0.318495	-2.405141	0.270299
H	-3.009124	-2.475689	0.202637
H	-3.148204	-0.411393	1.543218
H	-3.260617	1.030696	-1.148946
H	3.317137	1.607442	-0.802339
N	3.240899	-0.414626	-0.185591
H	4.145448	-0.704122	0.160514

M6NHL1-Pr

SCF energy in gas phase: -840.636033

SCF energy in solution: -840.806764

Free energy in solution: -840.606730

C	0.749376	-0.142194	-0.002379
C	-1.408579	0.971406	-0.045095
C	0.647520	2.281066	0.028955
C	-0.740927	2.189461	0.001984
C	-0.663514	-0.233073	-0.042449
H	-1.339030	3.098388	0.006091
H	1.147270	3.244439	0.049209
P	1.961893	-1.510621	0.146020
C	2.887189	1.032111	0.043503
H	3.237116	1.293918	1.059476
H	2.512915	-2.420647	-0.792502
H	2.480661	-1.761578	1.443829
C	1.377746	1.102107	0.019992
C	-2.747558	-1.536008	-0.313014
C	-2.920914	0.932124	-0.107128
C	-3.467554	-0.399538	0.402233
H	-2.979598	-1.490999	-1.389493
H	-3.332068	1.764381	0.473523
H	-4.544846	-0.469993	0.228287
N	-1.323789	-1.437962	-0.069980
H	0.917932	-2.505885	0.446677
H	-0.767073	-2.268863	-0.173903
H	-3.090690	-2.506547	0.056320

H	-3.290771	-0.491449	1.479126
H	-3.253803	1.081202	-1.143088
H	3.307950	1.780489	-0.640967
N	3.200019	-0.315813	-0.365323
H	4.155321	-0.595892	-0.165375

M6OL1

SCF energy in gas phase: -859.296037

SCF energy in solution: -859.481791

Free energy in solution: -859.314978

C	0.725402	-0.139452	-0.034830
C	-1.393922	0.992696	-0.099214
C	0.742582	2.252046	0.012393
C	-0.686033	2.163578	-0.039802
C	-0.692454	-0.287227	-0.087822
H	-1.250984	3.094691	-0.035338
H	1.234995	3.216459	0.052620
P	1.819987	-1.439569	0.000733
C	2.935918	0.848552	0.065765
H	3.385788	1.244707	0.979542
H	1.907800	-2.313633	-1.092825
H	1.818899	-2.322835	1.091216
O	3.193191	-0.590641	0.058268
C	1.440211	1.071975	0.012457
C	-2.641172	-1.590281	-0.151885
C	-2.897262	0.911805	-0.168418
C	-3.363868	-0.395402	0.481042
H	-2.984382	-1.702754	-1.193786
H	-3.354431	1.783928	0.311370
H	-4.447671	-0.513031	0.380773
N	-1.190452	-1.491920	-0.115002
H	-2.938759	-2.511603	0.363048
H	-3.131999	-0.368391	1.552481
H	-3.222270	0.919081	-1.218260
H	3.454447	1.265742	-0.801097

M6OL1-TS1

SCF energy in gas phase: -860.455467

SCF energy in solution: -860.636173

Free energy in solution: -860.454648

C	0.728535	-0.160966	-0.012771
C	-1.406230	1.006850	-0.067651

C	0.703438	2.265032	0.026197
C	-0.713269	2.185189	0.002040
C	-0.710663	-0.271388	-0.107746
H	-1.286214	3.110719	0.024009
H	1.209606	3.223672	0.033598
P	1.948532	-1.390807	0.071151
C	2.905651	0.969759	0.007661
H	3.357304	1.381196	0.915999
H	2.067607	-2.323970	-0.960197
H	2.222354	-2.091100	1.249657
O	3.250817	-0.426329	-0.070659
C	1.400114	1.085538	0.019593
C	-2.739833	-1.520030	-0.228994
C	-2.913615	0.960499	-0.126594
C	-3.418047	-0.348276	0.480030
H	-3.107116	-1.571880	-1.266251
H	-3.336572	1.830519	0.386532
H	-4.505873	-0.428351	0.391703
N	-1.291293	-1.439016	-0.225954
H	0.476452	-2.934788	0.420293
H	-0.209374	-2.521830	0.176594
H	-3.029258	-2.465942	0.244004
H	-3.166864	-0.378110	1.546755
H	-3.247878	1.014759	-1.172066
H	3.343880	1.467720	-0.861531

M6OL1-Pr

SCF energy in gas phase: -860.520516

SCF energy in solution: -860.698700

Free energy in solution: -860.510411

C	0.752125	-0.145389	-0.015740
C	-1.400612	0.972017	-0.051508
C	0.660974	2.277806	0.018435
C	-0.728218	2.188223	-0.008386
C	-0.660504	-0.235308	-0.047969
H	-1.324246	3.098489	-0.004490
H	1.162041	3.240299	0.041937
P	1.970963	-1.497488	0.120422
C	2.891701	0.983024	0.041676
H	3.259664	1.294327	1.034762
H	2.531004	-2.282343	-0.904458
H	2.512057	-1.770379	1.392812
O	3.226853	-0.339338	-0.246275

C	1.383220	1.094629	0.007820
C	-2.748505	-1.534191	-0.295101
C	-2.913320	0.936857	-0.104991
C	-3.459645	-0.390235	0.416767
H	-2.985681	-1.495835	-1.370473
H	-3.318917	1.773688	0.472788
H	-4.538126	-0.459254	0.250477
N	-1.322087	-1.439334	-0.060145
H	-3.092637	-2.500750	0.083387
H	-3.276299	-0.475154	1.493106
H	-3.251630	1.080137	-1.139914
H	3.346836	1.653987	-0.697877
H	-0.768697	-2.268237	-0.195039
H	0.956678	-2.521214	0.361851

M7CH₂L1

SCF energy in gas phase: -746.012618

SCF energy in solution: -746.170200

Free energy in solution: -746.013417

C	1.507379	-0.932480	0.024321
C	2.507002	1.293264	0.028693
C	0.096210	1.164237	-0.100943
C	1.238595	1.932553	-0.045861
C	0.249000	-0.236912	-0.072406
C	2.662563	-0.066344	0.063834
C	-2.595749	-0.396659	-0.152142
C	-2.383171	0.985048	0.487774
C	-1.278785	1.787208	-0.210153
N	1.418193	-2.239450	0.066847
P	-1.052025	-1.374743	-0.059987
H	3.395304	1.919439	0.065652
H	1.172192	3.015231	-0.059720
H	3.651572	-0.511399	0.127330
H	-3.409871	-0.945051	0.329160
H	-3.326827	1.536797	0.437654
H	-1.242869	2.798548	0.205390
H	-1.545103	1.896466	-1.271137
H	2.329135	-2.685574	0.143946
H	-2.854752	-0.283027	-1.210277
H	-2.135804	0.869027	1.549492
H	-1.116224	-2.187520	1.081627
H	-1.081984	-2.305133	-1.105953

M7CH₂L1-TS1

SCF energy in gas phase: -747.147971

SCF energy in solution: -747.300383

Free energy in solution: -747.129634

C	-1.560857	-0.805717	-0.144333
C	-2.384494	1.493197	-0.100499
C	-0.037547	1.122038	0.296552
C	-1.096122	1.998249	0.168319
C	-0.264136	-0.266594	0.142455
C	-2.618566	0.148842	-0.245717
C	2.526346	-0.413052	-0.531048
C	2.288778	1.106635	-0.617074
C	1.372219	1.625406	0.501627
N	-1.692640	-2.128066	-0.280174
P	1.129927	-1.335653	0.293566
H	-3.214480	2.187975	-0.195858
H	-0.931241	3.066390	0.262754
H	-3.621124	-0.220034	-0.443297
H	2.675250	-0.838804	-1.527160
H	3.252658	1.623330	-0.587779
H	1.368012	2.718379	0.508075
H	1.767023	1.307461	1.478007
H	-2.662643	-2.418687	-0.355546
H	1.028781	-2.507182	-0.451555
H	1.724541	-1.583158	1.537352
H	-0.898673	-2.586539	0.692954
H	-0.193518	-2.594627	1.344859
H	3.430784	-0.628969	0.048154
H	1.820484	1.351703	-1.574940

M7CH₂L1-Pr

SCF energy in gas phase: -747.185941

SCF energy in solution: -747.332562

Free energy in solution: -747.155676

C	1.576760	-0.814917	0.062079
C	2.478405	1.429004	0.074273
C	0.104309	1.110591	-0.220065
C	1.204205	1.960078	-0.106301
C	0.296140	-0.276064	-0.136634
C	2.668904	0.058395	0.159049
C	-2.738498	-0.365698	0.218466
C	-2.295561	1.050341	0.622796

C	-1.291797	1.684548	-0.359847
N	1.766052	-2.185342	0.213130
P	-1.207763	-1.311508	-0.232386
H	3.334229	2.092096	0.155030
H	1.058830	3.035041	-0.154334
H	3.664809	-0.350645	0.306278
H	-3.255360	-0.860416	1.044235
H	-3.184815	1.683769	0.700539
H	-1.241004	2.762256	-0.181305
H	-1.656691	1.548608	-1.386614
H	2.715316	-2.500470	0.078867
H	1.099360	-2.782108	-0.255173
H	-1.394163	-0.918019	-1.659140
H	-1.151822	-2.678371	-0.661398
H	-1.031172	-1.770697	1.169398
H	-3.384540	-0.326960	-0.662566
H	-1.836103	1.018263	1.617174

M7NHL1

SCF energy in gas phase: -762.050910

SCF energy in solution: -762.207965

Free energy in solution: -762.062577

C	1.320630	-1.017191	0.001776
C	2.636602	0.981429	0.044546
C	0.237191	1.238306	-0.118894
C	1.506296	1.816443	-0.057256
C	0.223856	-0.141263	-0.083610
C	2.594447	-0.411651	0.085623
C	-2.227003	1.110430	0.450582
C	-1.095401	1.947442	-0.186916
N	0.768790	-2.249489	-0.027668
P	-1.084037	-1.308399	-0.019930
H	3.611725	1.458779	0.105662
H	1.627568	2.894722	-0.063662
H	3.507496	-0.990519	0.172181
H	-3.167327	1.668200	0.400456
H	-1.034694	2.918156	0.317184
H	-1.347883	2.154472	-1.235687
H	1.295176	-3.063201	0.262299
H	-1.345774	-1.916003	1.208802
H	-1.479480	-2.145420	-1.067369
H	-2.000934	0.976266	1.515906
N	-2.447478	-0.223111	-0.125179

H -2.834214 -0.164944 -1.061998

M7NHL1-TS1

SCF energy in gas phase: -763.191151

SCF energy in solution: -763.351751

Free energy in solution: -763.191134

C	-1.525118	-0.826861	-0.135678
C	-2.423999	1.443139	-0.015014
C	-0.045579	1.142973	0.266748
C	-1.133766	1.982446	0.182988
C	-0.227480	-0.263036	0.139378
C	-2.618950	0.098201	-0.166883
C	2.249149	1.034090	-0.677593
C	1.347787	1.724285	0.348553
N	-1.643433	-2.137134	-0.330360
P	1.173449	-1.325763	0.240926
H	-3.277172	2.114130	-0.064264
H	-0.991660	3.056392	0.242142
H	-3.615190	-0.303968	-0.328636
H	3.228103	1.516879	-0.735799
H	1.298518	2.800420	0.158917
H	1.785924	1.589288	1.347038
H	-2.613658	-2.428642	-0.407685
H	-0.771779	-2.641231	0.618418
H	-0.079052	-2.653804	1.216212
H	1.027584	-2.412728	-0.618695
H	1.792108	-1.768771	1.418639
H	1.790576	1.103434	-1.669284
N	2.468345	-0.374805	-0.333490
H	3.317312	-0.512801	0.201061

M7NHL1-Pr

SCF energy in gas phase: -763.241894

SCF energy in solution: -763.395827

Free energy in solution: -763.227977

C	-1.455492	-0.847769	-0.061824
C	-2.551459	1.310886	-0.048288
C	-0.152353	1.169192	0.164715
C	-1.319173	1.932824	0.106116
C	-0.187784	-0.231778	0.059616
C	-2.619449	-0.070196	-0.125196
C	2.236935	1.211361	-0.525274

C	1.170212	1.876070	0.326224
N	-1.589303	-2.241269	-0.179880
P	1.325513	-1.404947	0.150861
H	-3.461613	1.900538	-0.099855
H	-1.255040	3.014871	0.176410
H	-3.581084	-0.566957	-0.231545
H	3.189218	1.740964	-0.424886
H	1.067625	2.928603	0.043666
H	1.494854	1.846577	1.374161
H	-2.544755	-2.551889	-0.067952
H	-0.970857	-2.789211	0.401548
H	0.773751	-1.981654	1.342995
H	0.806669	-2.230989	-0.875302
H	2.505865	-2.263984	0.313235
H	1.941415	1.256221	-1.582393
N	2.449576	-0.162811	-0.089108
H	3.400725	-0.503863	-0.126609

M7OL1

SCF energy in gas phase: -781.927393

SCF energy in solution: -782.089423

Free energy in solution: -781.954776

C	-1.244508	-1.052316	0.010065
C	-2.669962	0.856193	-0.068671
C	-0.293840	1.252481	0.140308
C	-1.596284	1.756153	0.048634
C	-0.212650	-0.118137	0.125581
C	-2.545802	-0.539271	-0.103281
C	2.147196	1.139231	-0.443739
C	1.026138	1.982988	0.196032
N	-0.569887	-2.248610	0.055378
P	1.122243	-1.257608	0.034847
H	-3.669774	1.274131	-0.154169
H	-1.783753	2.824909	0.039014
H	-3.421255	-1.169317	-0.213665
H	3.093769	1.683655	-0.390955
H	0.965885	2.945235	-0.323537
H	1.292121	2.193208	1.238841
H	-0.940627	-3.074271	-0.397174
H	1.459446	-1.758806	-1.228920
H	1.659143	-2.047167	1.049419
O	2.366260	-0.114917	0.193802
H	1.908800	0.988217	-1.509187

M7OL1-TS1

SCF energy in gas phase: -783.065720

SCF energy in solution: -783.232149

Free energy in solution: -783.083524

C	-1.528991	-0.833989	-0.128975
C	-2.398740	1.455555	-0.059885
C	-0.037436	1.138158	0.270771
C	-1.108910	1.993668	0.161113
C	-0.237448	-0.260613	0.144159
C	-2.609443	0.110082	-0.195035
C	2.278244	0.996092	-0.631352
C	1.377206	1.645266	0.415604
N	-1.635101	-2.145439	-0.286397
P	1.181028	-1.273135	0.253988
H	-3.245324	2.132732	-0.133942
H	-0.961156	3.066300	0.226576
H	-3.609504	-0.277559	-0.368012
H	3.296029	1.389194	-0.578622
H	1.402313	2.731235	0.290950
H	1.782741	1.426992	1.413583
H	-2.602414	-2.443583	-0.376851
H	-0.694821	-2.619951	0.733147
H	-0.022111	-2.598125	1.294889
H	1.126979	-2.421392	-0.528500
H	1.796016	-1.553383	1.476878
O	2.397265	-0.420336	-0.434977
H	1.876537	1.180007	-1.633716

M7OL1-Pr

SCF energy in gas phase: -783.121124

SCF energy in solution: -783.284577

Free energy in solution: -783.130021

C	-1.539250	-0.763532	-0.053867
C	-2.353393	1.517552	-0.113987
C	-0.008961	1.114366	0.248917
C	-1.067523	2.005657	0.109802
C	-0.239344	-0.269993	0.170088
C	-2.590568	0.155398	-0.194626
C	2.374775	0.975409	-0.529763
C	1.399677	1.585328	0.491947
N	-1.783009	-2.120719	-0.221237
P	1.197844	-1.371020	0.314546

H	-3.182452	2.209637	-0.225181
H	-0.885194	3.073568	0.174324
H	-3.595479	-0.217459	-0.372868
H	3.405254	1.173617	-0.200804
H	1.455498	2.676307	0.440140
H	1.707185	1.303883	1.506829
H	-2.755027	-2.383788	-0.149352
H	-1.175181	-2.735848	0.302802
H	0.446584	-2.321508	1.152076
H	1.473266	-2.392983	-0.612697
H	2.056222	-1.154818	1.412073
O	2.184369	-0.402734	-0.734194
H	2.235293	1.480484	-1.494378

M8CH₂L1

SCF energy in gas phase: -823.394267

SCF energy in solution: -823.568372

Free energy in solution: -823.378504

C	-3.137110	-1.324846	0.099916
C	-3.408308	0.217134	0.065427
C	-2.011219	0.787791	0.014118
C	-1.133444	-0.361873	-0.046254
C	-1.498319	2.043307	0.015322
C	0.273945	-0.117723	-0.121527
C	0.798871	1.211672	-0.116681
C	-0.075188	2.263360	-0.043512
C	2.292720	1.425514	-0.215751
H	2.536874	2.420350	0.167612
C	3.120895	0.373327	0.533168
C	2.985065	-1.027881	-0.086078
H	-2.155910	2.908225	0.066906
H	-3.659935	-1.839588	-0.715304
H	-3.992142	0.504584	-0.815165
H	0.307029	3.279131	-0.035305
H	4.178941	0.651807	0.512592
H	3.583089	-1.771047	0.447480
N	-1.688237	-1.538549	-0.013787
P	1.230452	-1.535834	-0.079725
H	1.001735	-2.361974	1.037231
H	1.050526	-2.458862	-1.126436
H	3.322321	-1.013912	-1.127391
H	-3.507631	-1.768315	1.033460
H	-3.963210	0.557189	0.945172

H	2.596361	1.414337	-1.272680	C	-3.414434	0.220759	0.295983
H	2.815397	0.346724	1.585322	C	-2.020096	0.760493	0.076378
M8CH₂L1-TS1				C	-1.136423	-0.326762	0.021239
SCF energy in gas phase: -824.534308				C	-1.533042	2.050002	-0.008909
SCF energy in solution: -824.700789				C	0.230640	-0.135074	-0.142527
Free energy in solution: -824.495927				C	0.726911	1.179730	-0.230345
C	-3.217995	-1.219608	0.066214	C	-0.156572	2.255435	-0.156695
C	-3.416642	0.307592	-0.143140	C	2.219998	1.414828	-0.337343
C	-2.003869	0.826493	-0.033626	H	2.419923	2.473202	-0.147594
C	-1.147504	-0.317529	-0.070174	C	3.026429	0.556327	0.657294
C	-1.480132	2.082874	0.044410	C	3.142859	-0.922148	0.247618
C	0.263075	-0.138238	0.006802	H	-2.208847	2.899210	0.040926
C	0.793648	1.190772	0.057104	H	-3.478456	-1.395026	-1.161912
C	-0.073509	2.262405	0.086611	H	-4.183532	0.722263	-0.295546
C	2.278816	1.503549	-0.040518	H	0.235681	3.266695	-0.211664
H	2.498574	2.362435	0.601104	H	4.035622	0.966768	0.763217
C	3.247402	0.366405	0.274846	H	3.525218	-1.522928	1.076475
C	2.920604	-0.880637	-0.553476	N	-1.828860	-1.528947	0.179194
H	-2.130218	2.953885	0.068463	P	1.440548	-1.495544	-0.224786
H	-3.828628	-1.813842	-0.619583	H	1.152816	-1.905443	1.174546
H	-3.818950	0.509893	-1.142614	H	1.042940	-2.800239	-0.661900
H	0.335009	3.268316	0.108831	H	3.792470	-1.026183	-0.625602
H	4.270824	0.697359	0.074573	H	-3.889342	-1.929003	0.485583
H	3.693012	-1.649598	-0.453334	H	-3.690613	0.308057	1.353559
N	-1.789921	-1.483310	-0.146555	H	2.565184	1.203827	-1.358569
P	1.333985	-1.535283	0.105489	H	2.548692	0.624555	1.641259
H	1.852517	-2.031522	1.315177	H	-1.435501	-2.342796	-0.275165
H	-0.219826	-2.509252	1.102766	H	1.732140	-1.155109	-1.648057
H	2.812931	-0.628286	-1.613744	M8NHL1			
H	-3.502545	-1.507547	1.088276	SCF energy in gas phase: -839.430800			
H	-4.101283	0.753098	0.583356	SCF energy in solution: -839.613277			
H	2.476853	1.834277	-1.069505	Free energy in solution: -839.434466			
H	3.207234	0.118102	1.345033	C	-3.128407	-1.312146	0.114634
H	-0.986660	-2.260020	0.619900	C	-3.389729	0.231595	0.105252
H	0.977469	-2.589340	-0.735475	C	-1.990127	0.794161	0.035681
M8CH₂L1-Pr				C	-1.122417	-0.361531	-0.066191
SCF energy in gas phase: -824.571775				C	-1.470735	2.046746	0.024368
SCF energy in solution: -824.733353				C	0.284325	-0.124328	-0.161357
Free energy in solution: -824.523222				C	0.816315	1.204284	-0.168921
C	-3.248035	-1.262268	-0.094712	C	-0.046886	2.260751	-0.069260
				C	2.315637	1.384328	-0.250430
				H	2.586745	2.383169	0.105109

C	3.067252	0.329135	0.569476
H	-2.122435	2.914880	0.093171
H	-3.688952	-1.817874	-0.680488
H	-3.983437	0.532039	-0.764367
H	0.341726	3.273985	-0.053405
H	4.144121	0.513595	0.555150
N	-1.687155	-1.533439	-0.065228
P	1.258541	-1.521870	-0.104392
H	0.859386	-2.398229	0.917482
H	1.312833	-2.397927	-1.207525
H	-3.460079	-1.760172	1.060707
H	-3.929831	0.565603	0.996220
H	2.651743	1.312783	-1.294522
H	2.743563	0.372057	1.614242
N	2.858241	-1.049683	0.082154
H	3.457541	-1.301983	-0.693886

M8NHL1-TS1

SCF energy in gas phase: -840.576588

SCF energy in solution: -840.752589

Free energy in solution: -840.558080

C	-3.221430	-1.215927	0.056607
C	-3.415686	0.316928	-0.119258
C	-1.999296	0.827374	-0.018707
C	-1.149003	-0.327042	-0.073568
C	-1.470166	2.078810	0.064860
C	0.265088	-0.148807	-0.011489
C	0.799931	1.182791	0.043402
C	-0.059036	2.256590	0.091401
C	2.288945	1.473593	-0.079504
H	2.539150	2.341496	0.539157
C	3.224272	0.315138	0.258017
H	-2.117149	2.951747	0.102631
H	-3.830039	-1.792378	-0.646384
H	-3.831654	0.541937	-1.108165
H	0.351630	3.261540	0.112987
H	4.262036	0.581387	0.038440
N	-1.794192	-1.483312	-0.154053
P	1.372424	-1.504656	0.095990
H	1.856033	-1.960679	1.329933
H	1.120155	-2.568142	-0.766588
H	-3.514414	-1.528164	1.068977
H	-4.087538	0.751136	0.625834

H	2.486813	1.772418	-1.118768
H	3.180308	0.084777	1.331068
H	-0.895388	-2.312357	0.590970
H	-0.145366	-2.554409	1.006502
N	2.878292	-0.917814	-0.466751
H	2.868643	-0.749275	-1.471373

M8NHL1-Pr

SCF energy in gas phase: -840.628643

SCF energy in solution: -840.798245

Free energy in solution: -840.596584

C	3.254380	-1.181006	-0.196813
C	3.400668	0.306626	0.171859
C	1.979832	0.799470	0.038375
C	1.116099	-0.309269	0.030730
C	1.467403	2.077522	-0.010101
C	-0.281898	-0.153951	-0.019721
C	-0.792703	1.169614	-0.039663
C	0.083214	2.254238	-0.053360
C	-2.274553	1.507308	0.006104
H	-2.469917	2.337922	-0.681909
C	-3.220091	0.344379	-0.274874
H	2.130119	2.938642	-0.013842
H	3.940916	-1.827376	0.354288
H	3.740618	0.412782	1.208977
H	-0.330380	3.258110	-0.086754
H	-4.256951	0.649790	-0.091875
N	1.862543	-1.477610	0.154800
P	-1.384392	-1.616479	-0.095171
H	-2.067338	-1.828917	-1.322817
H	-1.426431	-2.457948	1.049835
H	3.429983	-1.321677	-1.273357
H	4.111757	0.829661	-0.471248
H	-2.489244	1.892639	1.013092
H	-3.166023	0.072956	-1.339678
H	1.458714	-2.322881	-0.224068
H	-0.292376	-2.442729	-0.635512
N	-2.878601	-0.838371	0.493463
H	-2.829265	-0.621503	1.489379

M8OL1

SCF energy in gas phase: -859.298138

SCF energy in solution: -859.484546

Free energy in solution: -859.317589

C	-3.112684	-1.312274	0.120543
C	-3.375781	0.231858	0.110111
C	-1.977332	0.798007	0.037420
C	-1.111716	-0.357555	-0.075399
C	-1.456449	2.050613	0.035280
C	0.291362	-0.116229	-0.176369
C	0.826196	1.208456	-0.169454
C	-0.031933	2.267018	-0.059131
C	2.327453	1.353211	-0.251560
H	2.635849	2.335134	0.120197
C	3.047167	0.278663	0.557081
H	-2.107708	2.918102	0.114110
H	-3.679078	-1.819929	-0.668838
H	-3.970348	0.529809	-0.759694
H	0.357699	3.279533	-0.035025
H	4.130360	0.396760	0.510547
N	-1.671839	-1.531073	-0.071118
P	1.267974	-1.505589	-0.120521
H	0.922354	-2.375489	0.927668
H	1.339794	-2.378085	-1.217078
H	-3.435306	-1.758439	1.070498
H	-3.915666	0.566013	1.000996
H	2.667031	1.277632	-1.292754
H	2.729089	0.301964	1.605365
O	2.806438	-1.047783	0.019816

M8OL1-TS1

SCF energy in gas phase: -860.448744

SCF energy in solution: -860.630693

Free energy in solution: -860.447993

C	-3.218441	-1.221676	0.010095
C	-3.411194	0.319850	-0.082200
C	-1.992119	0.824774	0.004632
C	-1.143267	-0.337091	-0.068314
C	-1.465831	2.074316	0.091786
C	0.274101	-0.146952	-0.014355
C	0.804268	1.188715	0.031804
C	-0.051453	2.259268	0.096365
C	2.288466	1.457168	-0.143582
H	2.574874	2.343569	0.431154
C	3.194168	0.300110	0.237627

H	-2.115296	2.944741	0.142770
H	-3.795566	-1.753096	-0.753065
H	-3.860394	0.600832	-1.041228
H	0.356179	3.265408	0.103394
H	4.233407	0.499238	-0.028961
N	-1.785641	-1.485705	-0.159071
P	1.390002	-1.477806	0.077653
H	1.853563	-1.962922	1.312991
H	1.176578	-2.543126	-0.789222
H	-3.554180	-1.599907	0.985197
H	-4.055122	0.715909	0.707799
H	2.471314	1.685444	-1.200571
H	3.152761	0.102413	1.320793
H	-0.818162	-2.371594	0.602239
H	-0.098879	-2.607792	0.992485
O	2.807023	-0.882872	-0.477528

M8OL1-Pr

SCF energy in gas phase: -860.512116

SCF energy in solution: -860.689555

Free energy in solution: -860.499874

C	-3.240710	-1.186435	0.210456
C	-3.392125	0.303141	-0.145153
C	-1.969789	0.795630	-0.029016
C	-1.103574	-0.313092	-0.042400
C	-1.462138	2.074405	0.020566
C	0.294486	-0.150420	-0.010945
C	0.799039	1.176530	0.012814
C	-0.077518	2.257556	0.046021
C	2.279642	1.497429	-0.042865
H	2.493527	2.347158	0.614701
C	3.168879	0.315139	0.295173
H	-2.128932	2.932149	0.039841
H	-3.933490	-1.829415	-0.336662
H	-3.746824	0.416836	-1.176391
H	0.333111	3.262270	0.081371
H	4.222301	0.554204	0.116618
N	-1.853904	-1.478356	-0.162760
P	1.396409	-1.603793	0.060562
H	2.064289	-1.851309	1.285644
H	1.570276	-2.435068	-1.062665
H	-3.401454	-1.336068	1.288127
H	-4.093370	0.821606	0.512223

H	2.513700	1.816375	-1.066054
H	3.071833	0.065862	1.369689
O	2.803143	-0.773751	-0.506889
H	-1.449196	-2.334659	0.186648
H	0.313134	-2.453842	0.545007

M9CH₂L1

SCF energy in gas phase: -862.702098

SCF energy in solution: -862.882219

Free energy in solution: -862.662881

C	3.536667	-0.490504	0.570906
C	3.184413	0.840032	-0.102886
C	1.688048	1.015971	-0.101899
C	0.901021	-0.201397	-0.129788
C	2.770980	-1.637975	-0.098117
C	1.042727	2.220831	-0.052899
C	-0.523375	-0.021051	-0.140751
C	-1.170125	1.234944	-0.098200
C	-0.376371	2.357154	-0.049195
C	-2.680118	1.320356	-0.124222
H	-2.989896	2.269989	0.321967
C	-3.380138	0.163161	0.598956
C	-3.120281	-1.192800	-0.077337
H	1.646351	3.126520	-0.009627
H	4.614477	-0.677224	0.524010
H	3.672041	1.684178	0.396644
H	2.982849	-2.576422	0.428575
H	-0.826217	3.343648	-0.005705
H	-3.045638	0.128241	1.642316
H	-3.469070	-1.167080	-1.115120
N	1.332485	-1.439733	-0.132107
P	-1.325553	-1.547665	-0.100987
H	-1.020526	-2.346597	1.012926
H	-1.085995	-2.420285	-1.171025
H	-3.648852	-2.005689	0.427668
H	-4.460286	0.337975	0.614571
H	3.160184	-1.772152	-1.121584
H	3.254073	-0.444489	1.629487
H	3.559347	0.821582	-1.135854
H	-3.027622	1.338598	-1.167103

M9CH₂L1-TS1

SCF energy in gas phase: -863.837448

SCF energy in solution: -864.013164

Free energy in solution: -863.780048

C	3.652408	-0.400441	0.427154
C	3.187074	0.914947	-0.194735
C	1.684744	1.021978	-0.104942
C	0.925624	-0.196061	-0.093324
C	2.908183	-1.552713	-0.245555
C	1.036177	2.229034	-0.022157
C	-0.504977	-0.075578	0.057075
C	-1.146252	1.191408	0.086005
C	-0.363585	2.329824	0.055159
C	-2.653339	1.400324	0.023682
H	-2.924738	2.190416	0.731182
C	-3.548987	0.184226	0.248462
C	-3.087882	-1.009078	-0.594966
H	1.632160	3.139907	-0.027830
H	4.733469	-0.527522	0.313998
H	3.650329	1.776784	0.296892
H	3.167175	-2.504532	0.233102
H	-0.838904	3.306092	0.063195
H	-3.548412	-0.099406	1.310397
H	-2.945354	-0.722166	-1.642000
N	1.463053	-1.412887	-0.202044
P	-1.492358	-1.539338	0.145360
H	-2.033646	-2.030474	1.344923
H	0.064952	-2.393984	1.278160
H	-3.801358	-1.837857	-0.550163
H	-4.582089	0.448500	0.004254
H	3.243301	-1.630021	-1.291599
H	3.425190	-0.399917	1.499553
H	3.504680	0.940819	-1.246363
H	-2.875304	1.800661	-0.974595
H	0.738402	-2.130733	0.688634
H	-1.000978	-2.573502	-0.648982

M9CH₂L1-Pr

SCF energy in gas phase: -863.874528

SCF energy in solution: -864.045142

Free energy in solution: -863.806182

C	3.651233	-0.498239	0.595710
C	3.218064	0.870625	0.074414
C	1.711709	0.972229	-0.032343

C	0.918200	-0.191145	-0.102604
C	2.941012	-1.585883	-0.200145
C	1.082886	2.211641	-0.060226
C	-0.478025	-0.064358	-0.211927
C	-1.093686	1.193536	-0.242326
C	-0.297718	2.335403	-0.159909
C	-2.603717	1.314701	-0.281320
H	-2.870665	2.355929	-0.079332
C	-3.296249	0.401385	0.748293
C	-3.310848	-1.081499	0.341346
H	1.699374	3.105493	0.004998
H	4.734820	-0.619766	0.511998
H	3.593274	1.666922	0.725626
H	3.235041	-2.578797	0.151714
H	-0.761785	3.317186	-0.162590
H	-2.781582	0.509885	1.709500
H	-4.003262	-1.242497	-0.489273
N	1.507140	-1.448173	-0.019824
P	-1.602208	-1.506500	-0.245615
H	-1.190970	-1.916036	1.123468
H	-1.165258	-2.782531	-0.731790
H	-3.585313	-1.713245	1.189569
H	-4.329152	0.731076	0.899141
H	3.232896	-1.506405	-1.260682
H	3.378960	-0.603239	1.651180
H	3.669009	1.037900	-0.912728
H	-2.980021	1.078585	-1.285656
H	0.959081	-2.207813	-0.396704
H	-2.008458	-1.168317	-1.639238

M9NHL1

SCF energy in gas phase: -878.739612

SCF energy in solution: -878.928447

Free energy in solution: -878.720401

C	3.497083	-0.500872	0.575275
C	3.161031	0.850400	-0.067893
C	1.665432	1.033764	-0.082969
C	0.880911	-0.179572	-0.139939
C	2.736854	-1.632662	-0.128970
C	1.013337	2.237831	-0.034666
C	-0.535883	-0.002169	-0.144030
C	-1.192308	1.242581	-0.111237
C	-0.405532	2.371308	-0.051354

C	-2.702162	1.279457	-0.157249
H	-3.064040	2.208145	0.294484
C	-3.345934	0.092754	0.561067
H	1.613439	3.145104	0.022542
H	4.574668	-0.690771	0.537456
H	3.647479	1.676703	0.461778
H	2.939344	-2.581781	0.382221
H	-0.859656	3.355869	-0.011252
H	-3.081765	0.120081	1.627921
N	1.300250	-1.423888	-0.178047
P	-1.308117	-1.541842	-0.098958
H	-0.919683	-2.326799	1.001458
H	-1.150619	-2.413212	-1.181666
H	-4.433835	0.162514	0.483669
H	3.140573	-1.747133	-1.149221
H	3.201800	-0.479264	1.631209
H	3.550414	0.858488	-1.095574
H	-3.040725	1.267955	-1.200726
N	-2.949693	-1.181384	-0.069137
H	-3.586500	-1.948275	0.102152

M9NHL1-TS1

SCF energy in gas phase: -879.879869

SCF energy in solution: -880.065328

Free energy in solution: -879.843212

C	3.560944	-0.384879	0.694757
C	3.151196	0.945334	0.062540
C	1.647701	1.028081	-0.054499
C	0.914808	-0.208797	-0.133214
C	2.902886	-1.533783	-0.068771
C	0.975968	2.226552	-0.066025
C	-0.505938	-0.084876	-0.268701
C	-1.168886	1.163913	-0.291175
C	-0.426906	2.320695	-0.185416
C	-2.677992	1.178420	-0.358306
H	-3.046125	2.204308	-0.278634
C	-3.296799	0.340048	0.766647
H	1.557080	3.142791	0.024310
H	4.649472	-0.498915	0.690148
H	3.528203	1.794535	0.642878
H	3.171828	-2.492298	0.388939
H	-0.917617	3.288307	-0.178701
H	-2.958107	0.752009	1.725578

N	1.454680	-1.426325	-0.086699
P	-1.553656	-1.492974	-0.302509
H	-0.086103	-2.334148	-1.517052
H	0.627505	-2.127596	-0.989662
H	-1.087725	-2.612943	0.378005
H	-2.163163	-1.855000	-1.504494
H	-4.388517	0.420833	0.728031
H	3.306950	-1.553152	-1.094598
H	3.226821	-0.414649	1.738341
H	3.606064	1.019381	-0.934693
H	-3.032540	0.791297	-1.324624
N	-2.912102	-1.074615	0.647554
H	-2.949114	-1.567810	1.530844

M9NHL1-Pr

SCF energy in gas phase: -879.927027

SCF energy in solution: -880.106530

Free energy in solution: -879.877992

C	3.603998	-0.393136	0.628556
C	3.134502	0.970231	0.125283
C	1.628525	1.015208	-0.019888
C	0.886004	-0.177014	-0.156077
C	2.965283	-1.483573	-0.220570
C	0.952877	2.229195	-0.015293
C	-0.517790	-0.104397	-0.280426
C	-1.175008	1.137522	-0.279736
C	-0.429269	2.305563	-0.151274
C	-2.672316	1.173156	-0.440170
H	-3.034476	2.203755	-0.382014
C	-3.414205	0.301020	0.605155
H	1.532584	3.142731	0.098211
H	4.693731	-0.470304	0.581211
H	3.460807	1.766498	0.802201
H	3.289125	-2.474552	0.109849
H	-0.930263	3.268694	-0.151010
H	-3.490966	0.864731	1.540595
N	1.519129	-1.414233	-0.085942
P	-1.567224	-1.596892	-0.304449
H	-0.673346	-2.282828	-1.269520
H	1.021172	-2.149643	-0.571588
H	-1.287394	-2.621795	0.641012
H	-2.578125	-1.623831	-1.296040
H	-4.441365	0.147287	0.249510

H	3.286678	-1.359343	-1.267782
H	3.299777	-0.535586	1.671002
H	3.604701	1.174961	-0.845713
H	-2.927747	0.814520	-1.444568
N	-2.768331	-0.982018	0.875442
H	-2.347725	-0.980795	1.801518

M9OL1

SCF energy in gas phase: -898.608311

SCF energy in solution: -898.799436

Free energy in solution: -898.604408

C	3.426622	-0.529224	0.575279
C	3.139982	0.841018	-0.063414
C	1.650227	1.067491	-0.090223
C	0.853117	-0.123547	-0.152963
C	2.643937	-1.654600	-0.123552
C	0.987205	2.271650	-0.037416
C	-0.546891	0.047686	-0.161420
C	-1.221965	1.271705	-0.110943
C	-0.434013	2.404377	-0.049648
C	-2.731983	1.224841	-0.120874
H	-3.150194	2.102210	0.383074
C	-3.266223	-0.031948	0.569960
H	1.581037	3.182444	0.026538
H	4.498471	-0.749240	0.542941
H	3.650602	1.642636	0.480801
H	2.815362	-2.598350	0.407642
H	-0.884386	3.389945	0.003502
H	-2.946337	-0.049397	1.619971
N	1.215773	-1.390869	-0.185817
P	-1.233942	-1.529804	-0.105659
H	-0.937207	-2.293484	1.029943
H	-1.144956	-2.399140	-1.191271
H	-4.356664	-0.060718	0.539890
H	3.053150	-1.796014	-1.137654
H	3.128592	-0.498040	1.630085
H	3.539463	0.846582	-1.086918
H	-3.102709	1.236832	-1.153138
O	-2.843200	-1.251227	-0.077314

M9OL1-TS1

SCF energy in gas phase: -899.754485

SCF energy in solution: -899.944509

Free energy in solution: -899.733946

C	3.551551	-0.377117	0.693008
C	3.148629	0.928947	0.009293
C	1.644935	1.024411	-0.081933
C	0.900643	-0.213353	-0.126770
C	2.881394	-1.548485	-0.023349
C	0.984673	2.224901	-0.102363
C	-0.526522	-0.080522	-0.250797
C	-1.175012	1.181088	-0.275506
C	-0.423263	2.328512	-0.193826
C	-2.684113	1.208381	-0.275623
H	-3.042412	2.226190	-0.098150
C	-3.227503	0.287056	0.813326
H	1.573830	3.138004	-0.037175
H	4.638870	-0.501277	0.688347
H	3.547328	1.799175	0.541528
H	3.131004	-2.489518	0.479213
H	-0.906099	3.299841	-0.176238
H	-2.819521	0.581484	1.786431
N	1.434112	-1.426322	-0.065103
P	-1.556872	-1.488600	-0.280901
H	-0.121133	-2.344661	-1.504568
H	0.570850	-2.154697	-0.999773
H	-1.059479	-2.574865	0.428500
H	-2.181310	-1.921815	-1.453644
H	-4.318348	0.325517	0.859421
H	3.292157	-1.622142	-1.043466
H	3.221976	-0.361926	1.738279
H	3.583682	0.949181	-0.999416
H	-3.093189	0.888668	-1.244639
O	-2.894550	-1.088352	0.573977

M9OL1-Pr

SCF energy in gas phase: -899.809382

SCF energy in solution: -899.997162

Free energy in solution: -899.780387

C	3.601891	-0.394493	0.628781
C	3.134059	0.958067	0.096189
C	1.627023	1.008095	-0.036249
C	0.876587	-0.183634	-0.138628
C	2.951105	-1.502135	-0.188055
C	0.959872	2.226069	-0.051278

C	-0.528045	-0.100632	-0.250500
C	-1.175122	1.144868	-0.266116
C	-0.423396	2.310917	-0.172078
C	-2.675132	1.171631	-0.388031
H	-3.049696	2.195122	-0.297573
C	-3.337818	0.288654	0.684107
H	1.547789	3.137186	0.036005
H	4.690762	-0.477850	0.573938
H	3.469838	1.768849	0.750710
H	3.268752	-2.486232	0.167700
H	-0.918628	3.276703	-0.182790
H	-3.293386	0.811456	1.648168
N	1.506820	-1.418132	-0.047235
P	-1.582614	-1.578501	-0.317470
H	-1.452275	-2.642867	0.594468
H	-2.564437	-1.614323	-1.329807
H	-4.399798	0.155536	0.430738
H	3.266957	-1.409274	-1.240054
H	3.305549	-0.510014	1.676675
H	3.596174	1.136915	-0.883711
H	-2.966636	0.819760	-1.385414
O	-2.712990	-0.961018	0.845079
H	0.997935	-2.174954	-0.483683
H	-0.669652	-2.257871	-1.252166

M10CH₂L1

SCF energy in gas phase: -709.118976

SCF energy in solution: -709.261049

Free energy in solution: -709.086337

C	0.075646	0.333123	-0.185088
C	-2.397234	0.357539	0.174550
C	-1.077624	-1.809703	0.251151
C	-2.327431	-1.103441	-0.287313
C	0.170210	-1.166221	-0.352267
C	-1.093582	1.125199	-0.012860
H	-3.232466	-1.631520	0.029634
H	-3.204189	0.889095	-0.341100
H	-1.041953	-1.704597	1.344470
N	-0.984521	2.412615	0.065951
H	-1.889259	2.840713	0.265677
P	1.601943	1.046009	-0.027232
C	1.498903	-1.584619	0.303844
H	1.828820	-2.579299	-0.013008

C	2.565438	-0.522777	-0.042568
H	1.849285	1.826529	1.121734
H	2.187372	1.883215	-1.006414
H	-2.635129	0.385652	1.246221
H	-2.307139	-1.141324	-1.384106
H	-1.110456	-2.880698	0.020193
H	1.356676	-1.604550	1.390577
H	0.208009	-1.461835	-1.416776
H	3.410313	-0.509947	0.648318
H	2.956673	-0.664464	-1.055293

M10CH₂L1-TS1

SCF energy in gas phase: -710.259200

SCF energy in solution: -710.395341

Free energy in solution: -710.206721

C	0.086099	0.321173	-0.137707
C	-2.419699	0.341100	0.076474
C	-1.165731	-1.821731	0.220303
C	-2.359842	-1.105905	-0.408404
C	0.124384	-1.193155	-0.291012
C	-1.080561	1.064487	0.082476
H	-3.298056	-1.615071	-0.167539
H	-3.118092	0.930277	-0.528896
H	-1.210311	-1.717894	1.313349
N	-1.055006	2.354818	0.352871
H	-1.967284	2.799362	0.362492
P	1.711235	0.948584	-0.152073
C	1.386193	-1.665811	0.445084
H	1.620085	-2.713285	0.227270
C	2.522207	-0.729133	0.021415
H	2.162707	1.700286	0.938656
H	2.409504	1.430616	-1.271219
H	-2.800638	0.369967	1.105410
H	-2.254095	-1.129083	-1.500009
H	-1.180125	-2.892645	-0.010622
H	1.210718	-1.575359	1.523785
H	0.230553	-1.482789	-1.352060
H	3.360785	-0.707087	0.721597
H	2.914635	-1.016299	-0.960499
H	0.102118	2.811859	-0.127198
H	0.975702	2.828498	-0.515287

M10CH₂L1-Pr

SCF energy in gas phase: -710.294472

SCF energy in solution: -710.425484

Free energy in solution: -710.230800

C	0.092770	0.327603	-0.136316
C	-2.416338	0.342923	0.009292
C	-1.176964	-1.807954	0.291711
C	-2.375570	-1.134572	-0.370268
C	0.101540	-1.186605	-0.250575
C	-1.062281	1.028536	0.018831
H	-3.316917	-1.612673	-0.083250
H	-3.080218	0.897540	-0.667360
H	-1.221227	-1.658309	1.379281
N	-1.177230	2.369391	0.308859
H	-2.045882	2.806772	0.042234
P	1.790770	1.026058	-0.099879
C	1.386788	-1.660851	0.439284
H	1.547065	-2.734160	0.283260
C	2.486985	-0.780335	-0.127064
H	2.441291	1.316624	1.132691
H	2.608079	1.385168	-1.216841
H	-2.837955	0.463541	1.015798
H	-2.282524	-1.235510	-1.458342
H	-1.179098	-2.887989	0.107662
H	1.283991	-1.497101	1.521669
H	0.185285	-1.471123	-1.313727
H	3.427487	-0.826348	0.432086
H	2.697777	-1.061787	-1.167693
H	-0.353445	2.941186	0.194295
H	1.283777	2.425103	-0.114965

M10NHL1

SCF energy in gas phase: -725.154347

SCF energy in solution: -725.306030

Free energy in solution: -725.142133

C	-0.084898	0.336254	-0.218623
C	2.369755	0.374924	0.230435
C	1.078901	-1.806891	0.205308
C	2.329989	-1.069014	-0.284468
C	-0.171260	-1.163730	-0.395179
C	1.072558	1.138263	-0.008737
H	2.334668	-1.067534	-1.381989

H	2.549367	0.366151	1.313749
H	1.130260	-2.869667	-0.056842
N	0.957807	2.425589	0.041711
H	1.850049	2.855227	0.290360
P	-1.631792	0.982596	-0.051299
H	-2.390727	1.635850	-1.056541
H	-1.781809	1.894197	1.007609
C	-1.488345	-1.565241	0.301911
H	-1.920996	-2.489793	-0.089707
H	-1.299036	-1.702374	1.372588
H	3.199192	0.926184	-0.225054
H	3.233240	-1.598462	0.034873
H	1.025376	-1.737174	1.300627
H	-0.226620	-1.457774	-1.458321
N	-2.483290	-0.470790	0.143642
H	-3.187906	-0.644753	-0.563224

M10NHL1-TS1

SCF energy in gas phase: -726.302386

SCF energy in solution: -726.448902

Free energy in solution: -726.270569

C	0.095030	0.300698	0.151521
C	-2.395876	0.414192	-0.098632
C	-1.205024	-1.799752	-0.207785
C	-2.385804	-1.034075	0.393071
C	0.095065	-1.207273	0.321076
C	-1.033846	1.090054	-0.085942
H	-2.300048	-1.053121	1.486538
H	-2.761083	0.450480	-1.133023
H	-1.266421	-2.866645	0.033703
N	-0.930486	2.379883	-0.343599
H	-1.822583	2.865571	-0.355863
P	1.734044	0.860589	0.138684
H	0.244082	2.756227	0.274958
H	1.058433	2.686983	0.710287
H	2.548211	1.235635	1.224362
H	2.097090	1.703035	-0.914904
C	1.364792	-1.675697	-0.409548
H	1.698715	-2.666224	-0.087518
H	1.163761	-1.719150	-1.487226
H	-3.086510	1.023890	0.495238
H	-3.334843	-1.516215	0.139543
H	-1.226851	-1.705368	-1.302176

H	0.189424	-1.492319	1.383707
N	2.427840	-0.688005	-0.152751
H	3.100459	-0.983630	0.544000

M10NHL1-Pr

SCF energy in gas phase: -726.345785

SCF energy in solution: -726.490369

Free energy in solution: -726.305479

C	-0.100551	0.316034	-0.163701
C	2.400337	0.386696	0.010142
C	1.194235	-1.790944	0.301431
C	2.391785	-1.098433	-0.347263
C	-0.082454	-1.193553	-0.268281
C	1.033161	1.043527	0.001250
H	2.320969	-1.216953	-1.435169
H	2.811493	0.530334	1.017914
H	1.224004	-2.872007	0.125985
N	1.107248	2.388327	0.294626
H	1.962830	2.850176	0.025833
P	-1.816826	0.953717	-0.083020
H	0.270146	2.936254	0.161472
H	-1.374296	2.358449	-0.209615
H	-2.747223	1.213081	-1.129608
H	-2.336675	1.231723	1.197029
C	-1.390827	-1.634858	0.412658
H	-1.622564	-2.687056	0.214195
H	-1.275439	-1.524444	1.501190
H	3.060175	0.942415	-0.669580
H	3.336771	-1.553886	-0.036421
H	1.217369	-1.631257	1.388177
H	-0.156572	-1.491653	-1.328453
N	-2.448768	-0.751249	-0.046623
H	-2.722065	-1.021297	-0.991097

M10OL1

SCF energy in gas phase: -745.022966

SCF energy in solution: -745.179532

Free energy in solution: -745.027800

C	0.090331	0.331438	0.262807
C	-2.349928	0.407260	-0.238076
C	-1.086294	-1.792466	-0.210700
C	-2.332135	-1.039731	0.271133

C	0.165808	-1.170206	0.411697
C	-1.044560	1.150853	0.013613
H	-2.347373	-1.043555	1.368337
H	-2.523675	0.406672	-1.322311
H	-1.155942	-2.855872	0.042713
N	-0.896939	2.433823	-0.058342
H	-1.771230	2.882170	-0.335308
P	1.647018	0.931658	0.070825
H	2.454704	1.534865	1.055440
H	1.817436	1.816489	-1.008799
O	2.442828	-0.481809	-0.095279
C	1.475786	-1.552031	-0.297894
H	1.947481	-2.455649	0.092265
H	1.304927	-1.658721	-1.375709
H	-3.174668	0.966935	0.215411
H	-3.237887	-1.557130	-0.059940
H	-1.020712	-1.714337	-1.304575
H	0.223577	-1.489732	1.465235

M10OL1-TS1

SCF energy in gas phase: -746.176766

SCF energy in solution: -746.328755

Free energy in solution: -746.161734

C	0.101060	0.300971	0.176146
C	-2.381116	0.444394	-0.105416
C	-1.210222	-1.784150	-0.218874
C	-2.388370	-1.008197	0.375712
C	0.087446	-1.206880	0.333783
C	-1.014211	1.111516	-0.076554
H	-2.313779	-1.036822	1.469676
H	-2.735476	0.490789	-1.143091
H	-1.287621	-2.851477	0.014510
N	-0.888608	2.393319	-0.336915
H	-1.775799	2.886454	-0.380249
P	1.746184	0.800330	0.144762
H	0.377439	2.746257	0.269846
H	1.169659	2.660449	0.662548
H	2.558483	1.148654	1.231965
H	2.168060	1.593429	-0.927637
O	2.387772	-0.705317	-0.087882
C	1.357610	-1.661449	-0.391729
H	1.723527	-2.637171	-0.063660
H	1.185757	-1.681194	-1.476205

H	-3.073107	1.054396	0.486167
H	-3.339152	-1.479227	0.108790
H	-1.218743	-1.680046	-1.312380
H	0.172893	-1.507367	1.391344

M10OL1-Pr

SCF energy in gas phase: -746.229293

SCF energy in solution: -746.381787

Free energy in solution: -746.208600

C	0.109840	0.319277	-0.163731
C	-2.385077	0.377362	0.051125
C	-1.158901	-1.800303	0.316467
C	-2.382309	-1.112529	-0.288421
C	0.089336	-1.188048	-0.296077
C	-1.025685	1.048733	-0.016352
H	-2.355056	-1.239324	-1.377039
H	-3.071922	0.924252	-0.605497
H	-1.145991	-1.648611	1.404529
N	-1.122006	2.415210	0.082582
H	-1.969672	2.783488	0.483899
P	1.812848	0.928075	-0.028752
H	-0.285614	2.947859	0.259191
H	1.420243	2.338085	0.046454
H	2.395144	1.035493	1.254665
H	2.695742	1.231404	-1.082000
O	2.378475	-0.722444	-0.180164
C	1.424882	-1.616096	0.318525
H	1.349162	-1.564350	1.422381
H	1.699420	-2.641477	0.047835
H	-1.189939	-2.879952	0.133485
H	-3.313266	-1.566955	0.063335
H	-2.756079	0.522544	1.076120
H	0.128833	-1.460873	-1.362069

M11CH₂L1

SCF energy in gas phase: -786.504251

SCF energy in solution: -786.662321

Free energy in solution: -786.453543

C	0.507114	-0.293155	-0.527086
C	-1.760037	0.779964	-0.240372
C	0.276197	2.232294	-0.373652
C	-0.968574	1.888537	0.452496

C	-0.893490	-0.462400	-0.375128
H	-1.582644	2.785788	0.587625
H	0.826798	3.062493	0.084529
N	-1.501304	-1.591218	-0.204723
P	1.550953	-1.520960	-0.006780
C	2.353085	0.951580	0.481814
H	2.058451	-2.551306	-0.834025
H	1.093970	-2.291003	1.083307
C	-2.969311	0.187119	0.491610
C	1.236917	1.039406	-0.581587
C	-2.909057	-1.300410	0.079968
H	-3.289526	-1.965996	0.862125
H	-3.915620	0.674895	0.244283
C	2.996175	-0.446193	0.387733
H	3.513399	-0.759791	1.296226
H	3.110751	1.731518	0.351214
H	-3.519492	-1.486656	-0.816536
H	3.703544	-0.505528	-0.446005
H	1.901163	1.078356	1.472788
H	1.733301	1.190116	-1.553585
H	-0.059644	2.587581	-1.354692
H	-0.679696	1.541542	1.454095
H	-2.049729	1.124011	-1.245071
H	-2.814307	0.276450	1.573708

M11CH₂L1-TS1

SCF energy in gas phase: -787.644136

SCF energy in solution: -787.794952

Free energy in solution: -787.571632

C	0.512373	-0.264715	-0.402406
C	-1.778217	0.782529	-0.279093
C	0.212826	2.284427	-0.364959
C	-1.067912	1.947803	0.404454
C	-0.862152	-0.425103	-0.263128
H	-1.715836	2.829520	0.452912
H	0.740244	3.115229	0.117889
N	-1.509891	-1.543164	-0.009889
P	1.673533	-1.495098	-0.014445
C	2.338800	1.073955	0.490181
H	2.284292	-2.368050	-0.927329
H	1.567960	-2.201923	1.190743
C	-3.036713	0.212149	0.389817
C	1.187588	1.094786	-0.529428

C	-2.945201	-1.293664	0.071802
H	-3.406169	-1.916699	0.843629
H	-3.962277	0.673319	0.037783
C	3.055529	-0.270854	0.307692
H	3.670473	-0.563774	1.162084
H	3.023402	1.918403	0.352515
H	-3.441881	-1.527328	-0.881278
H	3.702763	-0.239233	-0.576214
H	1.915528	1.143054	1.500395
H	1.653431	1.199770	-1.522175
H	-0.080673	2.641116	-1.358981
H	-0.833413	1.657645	1.436976
H	-1.990823	1.052013	-1.324328
H	-2.969428	0.360700	1.473582
H	-0.639167	-2.496663	-0.225483
H	0.246295	-2.896362	-0.416417

M11CH₂L1-Pr

SCF energy in gas phase: -787.679215

SCF energy in solution: -787.825376

Free energy in solution: -787.597286

C	0.520404	-0.270239	-0.359016
C	-1.776305	0.745307	-0.270692
C	0.164676	2.293509	-0.343568
C	-1.114411	1.935460	0.411637
C	-0.822714	-0.437081	-0.253061
H	-1.793090	2.794701	0.440184
H	0.683001	3.120609	0.154799
N	-1.568488	-1.557679	-0.021439
P	1.742639	-1.565453	0.011347
C	2.323096	1.119777	0.478048
H	2.533951	-2.263850	-0.944749
H	2.002941	-2.051530	1.328811
C	-3.042350	0.181099	0.387912
C	1.142252	1.108575	-0.505745
C	-2.998764	-1.303339	0.009892
H	-3.494874	-1.944256	0.743813
H	-3.956508	0.678506	0.058597
C	3.083585	-0.170063	0.201916
H	3.799962	-0.437316	0.986049
H	2.930515	2.025189	0.355594
H	-3.469950	-1.476464	-0.969041
H	3.636743	-0.076808	-0.742663

H	1.926643	1.125195	1.503793
H	1.583463	1.186987	-1.511275
H	-0.124920	2.661800	-1.334901
H	-0.886575	1.660359	1.449265
H	-1.991956	1.001966	-1.318544
H	-2.962923	0.282857	1.475661
H	-1.170105	-2.479147	-0.106388
H	0.716709	-2.641280	-0.133070

M11NHL1

SCF energy in gas phase: -802.536327

SCF energy in solution: -802.703700

Free energy in solution: -802.505939

C	-0.534652	-0.281774	-0.382850
C	1.837072	0.598719	-0.491629
C	-0.107453	2.024657	0.399115
C	1.284764	2.018786	-0.246402
C	0.854326	-0.537596	-0.226349
H	1.978081	2.585462	0.385213
H	-0.483030	3.053647	0.458205
N	1.398031	-1.655790	0.121690
P	-1.756068	-1.398129	-0.080441
C	-2.452373	1.023384	0.389596
H	-3.182985	1.764687	0.055930
H	-1.534676	-2.313462	0.967220
H	-2.313087	-2.273217	-1.048166
C	-1.099774	1.130514	-0.355410
H	-2.280730	1.177457	1.460922
C	2.842404	-1.426519	0.232088
C	3.021130	0.101206	0.340681
H	3.252274	-1.967538	1.090997
H	2.891344	0.419477	1.382921
H	3.356197	-1.811279	-0.662907
H	3.991533	0.459664	-0.012528
H	1.227558	2.558136	-1.198362
H	-0.033915	1.641429	1.425686
H	2.105171	0.506986	-1.554748
H	-1.264517	1.554085	-1.360651
N	-3.035534	-0.331678	0.212449
H	-3.778345	-0.379592	-0.475148

M11NHL1-TS1

SCF energy in gas phase: -803.685339

SCF energy in solution: -803.845692

Free energy in solution: -803.633164

C	-0.529947	-0.245778	-0.203292
C	1.803600	0.655892	-0.472123
C	-0.134584	2.116659	0.406020
C	1.306639	2.079432	-0.136991
C	0.840884	-0.457277	-0.104001
H	1.976409	2.541132	0.596727
H	-0.511350	3.145685	0.365619
N	1.452417	-1.567259	0.240935
P	-1.793164	-1.399936	-0.009369
C	-2.483036	1.093127	0.285042
H	-3.152479	1.874398	-0.084933
H	0.468309	-2.498675	0.040408
H	-0.399646	-2.814468	-0.162450
H	-1.913781	-2.106718	1.191083
H	-2.333694	-2.251028	-0.990652
C	-1.072844	1.162311	-0.339136
H	-2.390406	1.221978	1.371010
C	2.898325	-1.389238	0.107212
C	3.090033	0.138219	0.183172
H	3.430786	-1.926303	0.896751
H	3.114843	0.454584	1.232471
H	3.255730	-1.777904	-0.858104
H	4.003539	0.485260	-0.305436
H	1.363045	2.699879	-1.036866
H	-0.133769	1.809398	1.459394
H	1.916416	0.574082	-1.563496
H	-1.156925	1.487533	-1.390834
N	-3.071645	-0.231931	0.024005
H	-3.619377	-0.245530	-0.830160

M11NHL1-Pr

SCF energy in gas phase: -803.730778

SCF energy in solution: -803.890598

Free energy in solution: -803.671418

C	-0.537202	-0.254620	-0.187115
C	1.789586	0.642389	-0.463368
C	-0.113786	2.108267	0.451377
C	1.316888	2.068236	-0.105747
C	0.800295	-0.467723	-0.142665
H	2.009386	2.513133	0.617376

H	-0.490180	3.137606	0.423514
N	1.529416	-1.583492	0.142184
P	-1.851386	-1.469793	0.070707
C	-2.480152	1.100541	0.252669
H	-3.076100	1.969514	-0.045759
H	1.098252	-2.488659	0.238463
H	-0.875197	-2.577015	0.204158
H	-2.318796	-1.722467	1.378387
H	-2.541556	-2.231090	-0.911271
C	-1.041137	1.163744	-0.309986
H	-2.417479	1.114476	1.351773
C	2.965487	-1.381710	0.043929
C	3.077660	0.138789	0.201326
H	3.493992	-1.931347	0.827426
H	3.062788	0.401284	1.264989
H	3.361010	-1.707867	-0.929471
H	3.985123	0.548605	-0.246442
H	1.365548	2.692440	-1.003366
H	-0.110805	1.790191	1.501453
H	1.930012	0.582229	-1.552620
H	-1.095750	1.482661	-1.365304
N	-3.093244	-0.150920	-0.157504
H	-3.328511	-0.093394	-1.149186

M11OL1

SCF energy in gas phase: -822.404826

SCF energy in solution: -822.577242

Free energy in solution: -822.391718

C	-0.539553	-0.275791	-0.442125
C	1.834385	0.599887	-0.489599
C	-0.115991	2.012950	0.400303
C	1.270578	2.016966	-0.255815
C	0.844523	-0.535937	-0.255475
H	1.962011	2.597356	0.364978
H	-0.491809	3.040128	0.479661
N	1.375333	-1.656289	0.103919
P	-1.763481	-1.371368	-0.104900
C	-2.441682	0.987862	0.401613
H	-3.217010	1.681091	0.071635
H	-1.532822	-2.279108	0.949199
H	-2.380705	-2.214388	-1.050322
O	-2.986530	-0.345418	0.191444
C	-1.112374	1.131868	-0.367138

H	-2.272222	1.114209	1.477449
C	2.816743	-1.428544	0.255686
C	2.992271	0.098902	0.376837
H	3.201123	-1.974033	1.123301
H	2.831243	0.412419	1.416245
H	3.355159	-1.809023	-0.626281
H	3.972819	0.458466	0.054401
H	1.199304	2.545656	-1.212720
H	-0.033572	1.611636	1.419218
H	2.134356	0.512424	-1.544283
H	-1.304159	1.582080	-1.353675

M11OL1-TS1

SCF energy in gas phase: -823.559765

SCF energy in solution: -823.725874

Free energy in solution: -823.524834

C	-0.532529	-0.244465	-0.253239
C	1.805647	0.655878	-0.468915
C	-0.145745	2.104875	0.406718
C	1.292016	2.076812	-0.144941
C	0.837530	-0.463357	-0.134311
H	1.960178	2.554939	0.579531
H	-0.521558	3.134653	0.385309
N	1.435900	-1.575081	0.214846
P	-1.801990	-1.369629	-0.029592
C	-2.478843	1.062038	0.276738
H	-3.189374	1.790314	-0.119700
H	0.380822	-2.516210	0.014431
H	-0.461113	-2.802689	-0.174711
H	-1.934448	-2.066318	1.179322
H	-2.369424	-2.202923	-1.001640
O	-3.012013	-0.241280	-0.002333
C	-1.081783	1.162341	-0.357123
H	-2.400823	1.195076	1.365194
C	2.885281	-1.389308	0.133827
C	3.070625	0.138412	0.226963
H	3.391747	-1.930613	0.937478
H	3.058076	0.447630	1.278730
H	3.277403	-1.770692	-0.820730
H	3.999126	0.492094	-0.227362
H	1.333607	2.688884	-1.051265
H	-0.139504	1.778511	1.454221
H	1.955300	0.578732	-1.555941

H -1.178549 1.509509 -1.398560

M11OL1-Pr

SCF energy in gas phase: -823.614447

SCF energy in solution: -823.782226

Free energy in solution: -823.574831

C -0.542368 -0.253959 -0.215768
C 1.784260 0.643817 -0.456857
C -0.132334 2.105291 0.440780
C 1.300934 2.068950 -0.109680
C 0.793149 -0.469579 -0.156867
H 1.987371 2.521982 0.614045
H -0.508858 3.134411 0.414457
N 1.519346 -1.586575 0.127625
P -1.852891 -1.450493 0.048111
C -2.477678 1.062657 0.237961
H -3.116550 1.887626 -0.094956
H -2.337232 -1.692006 1.352590
H -2.573413 -2.156476 -0.934203
O -3.011633 -0.154138 -0.195790
C -1.050907 1.161887 -0.331124
H -2.417691 1.108859 1.343344
C 2.957217 -1.378228 0.064881
C 3.059626 0.141901 0.233186
H 3.469079 -1.930340 0.857540
H 3.021215 0.398995 1.297618
H 3.375790 -1.697768 -0.900801
H 3.974610 0.557466 -0.193330
H 1.349994 2.687852 -1.010756
H -0.133100 1.783974 1.489805
H 1.946877 0.583585 -1.542893
H -1.115519 1.482643 -1.382582
H 1.092481 -2.494567 0.213185
H -0.915449 -2.576139 0.189151

M12CH₂L1

SCF energy in gas phase: -825.802388

SCF energy in solution: -825.966353

Free energy in solution: -825.729457

C 0.729227 -0.248000 -0.438360
C -1.403436 1.017576 -0.221441
C 0.786453 2.277187 -0.320973

C -0.490329 2.029225 0.482688
C -0.688555 -0.330058 -0.304005
H -1.027808 2.974559 0.623667
H 1.421955 3.016552 0.181084
P 1.647868 -1.588649 0.036342
C 2.774164 0.779285 0.393870
H 1.949195 -2.694627 -0.794905
H 1.224810 -2.272843 1.194454
C 1.595100 0.985786 -0.581076
C -2.656271 -1.604469 0.122489
C -2.763173 0.861062 0.452624
C -3.478972 -0.344142 -0.147213
H -3.058706 -2.443601 -0.458724
H -2.616533 0.699717 1.530065
H -3.584008 -0.196897 -1.229837
N -1.236740 -1.494557 -0.161983
C 3.238134 -0.686332 0.273887
H 3.800220 -1.045140 1.138095
H 3.853465 -0.836026 -0.619730
H 3.603528 1.466036 0.192691
H 2.417643 0.965454 1.414350
H 2.028930 1.067335 -1.591226
H -2.781977 -1.888389 1.179827
H -4.487027 -0.459106 0.264637
H -3.347852 1.781068 0.342295
H -1.565079 1.370923 -1.252423
H -0.245590 1.646222 1.482368
H 0.499921 2.717665 -1.282874

M12CH₂L1-TS1

SCF energy in gas phase: -826.941486

SCF energy in solution: -827.101885

Free energy in solution: -826.850530

C 0.729675 -0.242480 -0.366482
C -1.422821 1.016348 -0.245692
C 0.712730 2.316767 -0.401468
C -0.569273 2.110511 0.397933
C -0.662571 -0.305319 -0.194154
H -1.140035 3.045215 0.441992
H 1.329103 3.104775 0.046768
P 1.808679 -1.571629 -0.070108
C 2.684505 0.922555 0.501610
H 2.393902 -2.405108 -1.036811

H	1.587089	-2.367148	1.059756	H	-3.187111	-2.451303	-0.355530
C	1.548509	1.029947	-0.532998	H	-2.509542	0.652162	1.597611
C	-2.700279	-1.588964	0.229509	H	-3.779924	-0.177008	-1.062288
C	-2.806415	0.882727	0.384451	N	-1.401681	-1.412321	-0.499092
C	-3.497531	-0.353465	-0.179242	C	3.309995	-0.436586	0.153157
H	-3.027748	-2.464967	-0.343096	H	4.042837	-0.765163	0.897752
H	-2.705576	0.783891	1.474325	H	3.795952	-0.446470	-0.832066
H	-3.535856	-0.277897	-1.273155	H	3.425876	1.763270	0.245152
N	-1.267892	-1.447198	0.061443	H	2.373446	1.019661	1.460264
C	3.274154	-0.487141	0.364992	H	1.932890	1.006075	-1.542266
H	3.788035	-0.839698	1.262689	H	-2.593698	-1.849565	1.200284
H	3.989133	-0.525418	-0.464403	H	-4.485513	-0.466953	0.535158
H	3.447220	1.694370	0.349913	H	-3.321804	1.763036	0.496473
H	2.257209	1.060342	1.502308	H	-1.689348	1.336362	-1.257329
H	2.030373	1.055333	-1.524033	H	-0.328140	1.801909	1.435903
H	-2.912632	-1.813993	1.285763	H	0.415601	2.686563	-1.389145
H	-4.527633	-0.440454	0.179987	H	-0.849205	-2.257202	-0.556908
H	-3.384944	1.793013	0.194891	H	0.675601	-2.612424	0.188129
H	-1.557272	1.273094	-1.308288				
H	-0.341094	1.821748	1.432233				
H	0.433557	2.669429	-1.400923				
H	-0.450113	-2.397185	-0.331098				
H	0.328261	-2.873436	-0.678047				

M12NHL1

SCF energy in gas phase: -841.838570

SCF energy in solution: -842.012660

Free energy in solution: -841.786890

M12CH₂L1-Pr

SCF energy in gas phase: -826.973681

SCF energy in solution: -827.128988

Free energy in solution: -826.871736

C	0.723361	-0.252329	-0.333942	C	0.735549	-0.267831	-0.502415
C	-1.432922	1.026203	-0.231973	C	-1.379795	1.021320	-0.211523
C	0.697034	2.325668	-0.392886	C	0.817709	2.255260	-0.380148
C	-0.574836	2.111597	0.412038	C	-0.438112	2.026329	0.461610
C	-0.642945	-0.274917	-0.334494	C	-0.683219	-0.333618	-0.339129
H	-1.151258	3.040721	0.483124	H	-0.962430	2.977589	0.610731
H	1.318942	3.106938	0.058969	H	1.464195	3.010850	0.083013
P	1.811827	-1.657471	0.141739	P	1.671630	-1.568342	0.025451
C	2.723512	0.939409	0.420493	C	2.732533	0.733073	0.430967
H	2.472375	-2.546753	-0.754016	H	2.217115	-2.606380	-0.770820
H	2.078673	-2.016333	1.503195	H	1.084235	-2.315135	1.059397
C	1.517319	1.030840	-0.522543	C	1.619331	0.959695	-0.615992
C	-2.701814	-1.601080	0.131881	C	-2.658840	-1.588863	0.102086
C	-2.743489	0.834256	0.539196	C	-2.715155	0.867774	0.510071
C	-3.542264	-0.342930	-0.005076	C	-3.472430	-0.309387	-0.094267
				H	-3.094862	-2.402279	-0.490879
				H	-2.530314	0.675914	1.576474
				H	-3.620786	-0.127681	-1.166416
				N	-1.247958	-1.492266	-0.230604
				H	3.643596	1.299363	0.216505

H	2.365016	1.036085	1.418930
H	2.101653	1.031979	-1.603890
H	-2.747886	-1.907046	1.153089
H	-4.464183	-0.423285	0.355638
H	-3.289043	1.798857	0.445731
H	-1.579265	1.382688	-1.233171
H	-0.168882	1.649051	1.457318
H	0.509036	2.663213	-1.349235
N	3.069139	-0.713543	0.477583
H	3.904656	-0.960501	-0.040580

M12NHL1-TS1

SCF energy in gas phase: -842.984798

SCF energy in solution: -843.155229

Free energy in solution: -842.914637

C	0.732458	-0.233372	-0.362096
C	-1.410983	1.023375	-0.248651
C	0.740676	2.323180	-0.350388
C	-0.557102	2.102680	0.423901
C	-0.657574	-0.300736	-0.188658
H	-1.122327	3.040255	0.478312
H	1.363878	3.074871	0.149519
P	1.810088	-1.543159	-0.033528
C	2.715075	0.863663	0.448624
H	2.478022	-2.384280	-0.940976
H	1.489073	-2.340990	1.068909
C	1.553667	1.029472	-0.549715
C	-2.684741	-1.586971	0.220484
C	-2.804557	0.888904	0.358470
C	-3.478501	-0.355484	-0.209603
H	-3.004867	-2.466946	-0.349886
H	-2.721317	0.796233	1.450337
H	-3.497277	-0.286669	-1.304588
N	-1.248196	-1.447954	0.073962
H	3.565719	1.511511	0.214913
H	0.380515	-2.814353	-0.735065
H	-0.388162	-2.397179	-0.380438
H	2.361481	1.117925	1.456595
H	2.000272	1.062214	-1.556393
H	-2.911717	-1.804694	1.275054
H	-4.514809	-0.444678	0.130861
H	-3.385546	1.794405	0.154428
H	-1.524043	1.291684	-1.310874

H	-0.345379	1.792053	1.455082
H	0.483426	2.737805	-1.331355
N	3.143400	-0.546484	0.418695
H	3.984815	-0.698975	-0.124306

M12NHL1-Pr

SCF energy in gas phase: -843.025283

SCF energy in solution: -843.194308

Free energy in solution: -842.948907

C	0.736067	-0.237635	-0.020994
C	-1.384704	0.956626	-0.309217
C	0.740309	2.264205	0.358949
C	-0.786640	2.111707	0.512274
C	-0.625759	-0.332807	-0.015611
H	-1.305261	3.036107	0.235503
H	1.195325	2.334138	1.353103
P	1.959726	-1.554403	0.217202
C	2.880272	0.897109	-0.093740
H	2.376929	-2.536974	-0.722794
H	2.628245	-1.633757	1.458327
C	1.374366	1.081406	-0.383219
C	-2.785278	-1.571993	0.270266
C	-2.895415	0.866783	-0.076977
C	-3.455778	-0.472580	-0.537720
H	-3.094590	-2.560272	-0.082950
H	-3.101845	0.982522	0.996135
H	-3.251005	-0.625798	-1.603852
N	-1.343122	-1.483448	0.140419
H	3.493650	1.643467	-0.609606
H	0.950079	-2.509710	0.728714
H	-0.806890	-2.299865	0.395303
H	3.040248	1.039508	0.986191
H	1.259680	1.253780	-1.467737
H	-3.101522	-1.487543	1.322490
H	-4.539097	-0.518299	-0.393788
H	-3.387236	1.703490	-0.583040
H	-1.211008	1.166722	-1.376301
H	-1.035681	1.920363	1.561926
H	0.987176	3.194287	-0.163842
N	3.262425	-0.460910	-0.435255
H	3.287145	-0.552556	-1.452022

M12OL1

SCF energy in gas phase: -861.707893
 SCF energy in solution: -861.887417
 Free energy in solution: -861.673140

C	0.741550	-0.271864	-0.565380
C	-1.356921	1.032660	-0.216821
C	0.856671	2.244359	-0.383394
C	-0.400268	2.022511	0.458546
C	-0.673204	-0.325734	-0.366338
H	-0.912994	2.978540	0.615683
H	1.509460	2.994515	0.079506
P	1.660168	-1.558638	0.011802
C	2.706010	0.675594	0.459148
H	2.264820	-2.586611	-0.737045
H	1.048517	-2.278207	1.053225
C	1.646186	0.943524	-0.624167
C	-2.645174	-1.574056	0.109640
C	-2.684114	0.882260	0.520907
C	-3.454765	-0.290492	-0.074902
H	-3.094014	-2.385632	-0.475836
H	-2.486445	0.687227	1.584452
H	-3.616366	-0.107504	-1.144823
N	-1.239651	-1.482343	-0.247812
H	3.655831	1.184547	0.282086
H	2.317128	0.950774	1.448080
H	2.168304	1.027424	-1.588409
H	-2.717835	-1.891119	1.162051
H	-4.440864	-0.399802	0.388089
H	-3.254635	1.815879	0.466333
H	-1.564386	1.406534	-1.232065
H	-0.133759	1.636573	1.451921
H	0.552677	2.653991	-1.352895
O	3.007971	-0.745467	0.456734

M12OL1-TS1

SCF energy in gas phase: -862.859545
 SCF energy in solution: -863.035330
 Free energy in solution: -862.806255

C	0.733691	-0.238767	-0.393541
C	-1.399626	1.025143	-0.252807
C	0.763286	2.316171	-0.330881
C	-0.537556	2.088792	0.436573
C	-0.657985	-0.306705	-0.202722

H	-1.096655	3.028993	0.505218
H	1.391400	3.053384	0.184243
P	1.821437	-1.517728	-0.035756
C	2.710521	0.819411	0.440744
H	2.502074	-2.345472	-0.935533
H	1.549610	-2.295880	1.095328
C	1.563769	1.019559	-0.559263
C	-2.681446	-1.578130	0.225303
C	-2.794681	0.898137	0.352520
C	-3.472316	-0.346535	-0.209846
H	-3.009139	-2.460356	-0.337242
H	-2.712793	0.809572	1.444845
H	-3.491354	-0.283027	-1.305163
N	-1.244460	-1.448308	0.071485
H	3.592261	1.424367	0.213576
H	0.438010	-2.830632	-0.680487
H	-0.310894	-2.436730	-0.368111
H	2.365188	1.045534	1.459546
H	2.017925	1.069009	-1.560233
H	-2.903946	-1.788686	1.282272
H	-4.508747	-0.431005	0.131314
H	-3.372164	1.804962	0.144749
H	-1.505983	1.306326	-1.312139
H	-0.330168	1.760745	1.463301
H	0.512047	2.752047	-1.303768
O	3.112132	-0.557692	0.359719

M12OL1-Pr

SCF energy in gas phase: -862.909172
 SCF energy in solution: -863.086060
 Free energy in solution: -862.851346

C	0.737979	-0.240385	-0.048196
C	-1.379632	0.963164	-0.297761
C	0.761026	2.279211	0.288379
C	-0.749532	2.095798	0.529517
C	-0.622597	-0.334680	-0.040091
H	-1.294195	3.023688	0.323656
H	1.259437	2.431490	1.252174
P	1.953096	-1.545677	0.194923
C	2.875573	0.849221	-0.086444
H	2.421202	-2.478746	-0.752708
H	2.619601	-1.626538	1.437398
C	1.390422	1.069413	-0.415577

C	-2.780107	-1.570845	0.263325
C	-2.883589	0.877423	-0.023447
C	-3.466804	-0.447676	-0.496932
H	-3.105564	-2.547941	-0.105565
H	-3.057859	0.972533	1.057446
H	-3.295838	-0.576883	-1.572099
N	-1.341210	-1.487229	0.091404
H	3.531745	1.541876	-0.624271
H	3.022924	1.019267	0.998671
H	1.308231	1.213233	-1.504297
H	-3.062817	-1.511382	1.326535
H	-4.545437	-0.489985	-0.320730
H	-3.383345	1.727686	-0.498031
H	-1.233832	1.188718	-1.365930
H	-0.930084	1.857606	1.583653
H	0.949071	3.179242	-0.305770
O	3.178651	-0.467145	-0.441271
H	-0.806247	-2.314034	0.311728
H	0.969403	-2.520784	0.688000

M13CH₂L1

SCF energy in gas phase: -748.422179

SCF energy in solution: -748.572386

Free energy in solution: -748.369151

C	-1.377860	1.051685	-0.007014
C	-2.539654	-1.198252	-0.263329
C	-0.025895	-1.159571	-0.308667
C	-1.262996	-1.857699	0.260144
C	-0.146390	0.326632	-0.049104
C	-2.650806	0.251103	0.216722
C	2.697641	0.361365	0.262328
C	2.523397	-1.059058	-0.296782
C	1.270248	-1.755141	0.245807
N	-1.338952	2.346877	-0.079084
P	1.196932	1.370482	-0.028575
H	-2.524255	-1.220288	-1.360682
H	-1.237950	-1.793106	1.356899
H	-2.853722	0.258145	1.296005
H	2.849627	0.315190	1.345170
H	2.470255	-1.022724	-1.392938
H	1.260037	-1.683093	1.342466
H	1.311078	-2.820626	-0.010043
H	-2.263266	2.754314	0.058734

H	1.152398	2.347011	0.976025
H	1.520879	2.180310	-1.148566
H	-3.488206	0.762406	-0.269625
H	-3.423148	-1.762516	0.052186
H	-1.242578	-2.920685	-0.009342
H	3.417659	-1.638479	-0.045806
H	3.566938	0.861603	-0.173554
H	-0.023173	-1.369216	-1.395342

M13CH₂L1-TS1

SCF energy in gas phase: -749.556195

SCF energy in solution: -749.703544

Free energy in solution: -749.485656

C	1.374537	0.951588	-0.197847
C	2.524604	-1.225023	0.391127
C	-0.004705	-1.157483	0.366843
C	1.249284	-1.931418	-0.049851
C	0.157417	0.332627	0.079448
C	2.633704	0.115715	-0.326629
C	-2.617871	0.316483	-0.482384
C	-2.559129	-1.118679	0.046398
C	-1.231933	-1.789144	-0.308386
N	1.445566	2.275608	-0.342652
P	-1.271995	1.329094	0.286581
H	2.497918	-1.061294	1.475368
H	1.256691	-2.029460	-1.144484
H	2.831261	-0.051206	-1.393529
H	-2.470905	0.323818	-1.568414
H	-2.688959	-1.117107	1.138891
H	-1.091366	-1.747874	-1.397138
H	-1.270830	-2.849441	-0.029895
H	2.397821	2.621782	-0.400309
H	-1.306836	2.484731	-0.494617
H	-0.069850	2.670818	1.260275
H	3.473534	0.703716	0.059779
H	3.404241	-1.840301	0.177728
H	1.195575	-2.945265	0.362371
H	-3.393261	-1.699921	-0.360307
H	-3.584199	0.786358	-0.266851
H	-0.131390	-1.304699	1.454481
H	0.651976	2.707062	0.575911
H	-1.895918	1.514621	1.538276

M13CH₂L1-Pr

SCF energy in gas phase: -749.588182

SCF energy in solution: -749.730385

Free energy in solution: -749.506303

C	-1.365542	0.948961	0.143176
C	-2.559520	-1.192475	-0.417452
C	-0.032649	-1.151097	-0.342250
C	-1.302786	-1.899955	0.073859
C	-0.194736	0.349393	-0.159052
C	-2.662132	0.179407	0.240612
C	2.706648	0.332561	0.403216
C	2.542300	-1.152899	0.066201
C	1.166480	-1.707421	0.454929
N	-1.513394	2.322625	0.302504
P	1.332838	1.285755	-0.408337
H	-2.509572	-1.069572	-1.505868
H	-1.336076	-1.963453	1.170797
H	-2.933233	0.071076	1.300557
H	2.633077	0.512579	1.480573
H	2.708088	-1.308061	-1.005590
H	0.987403	-1.510039	1.521589
H	1.175424	-2.797654	0.332586
H	-2.325623	2.591670	0.840120
H	1.154709	2.131465	0.821415
H	1.319485	2.495840	-1.177401
H	-3.451711	0.779562	-0.226897
H	-3.453944	-1.782655	-0.196527
H	-1.256036	-2.927613	-0.302572
H	3.320751	-1.718437	0.589963
H	3.672638	0.711954	0.054498
H	0.158190	-1.355084	-1.407437
H	-0.675816	2.802923	0.611381
H	1.625067	0.551947	-1.673088

M13NHL1

SCF energy in gas phase: -764.458411

SCF energy in solution: -764.617954

Free energy in solution: -764.425987

C	1.334810	1.061063	0.024082
C	2.544156	-1.167236	0.258637
C	0.035912	-1.188888	0.295547
C	1.285813	-1.840310	-0.298237

C	0.134049	0.303200	0.088129
C	2.636849	0.302599	-0.166978
C	-2.491360	-1.019632	0.296306
C	-1.269880	-1.756369	-0.265983
N	1.225220	2.357146	0.036727
P	-1.220091	1.326879	0.017019
H	2.517625	-1.229112	1.354237
H	1.261720	-1.734251	-1.391622
H	2.886348	0.355846	-1.235074
H	-2.441590	-1.013868	1.392390
H	-1.270638	-1.670896	-1.361445
H	-1.347125	-2.821636	-0.016059
H	2.122561	2.819412	-0.099386
H	-1.274848	2.216341	-1.067178
H	3.440120	0.816966	0.371350
H	3.442256	-1.702481	-0.065736
H	1.293540	-2.912529	-0.067653
H	-3.419543	-1.531178	0.027073
H	0.039384	-1.435854	1.374185
H	-1.490992	2.199013	1.091819
N	-2.616635	0.378049	-0.157890
H	-2.979632	0.428119	-1.103061

M13NHL1-TS1

SCF energy in gas phase: -765.600222

SCF energy in solution: -765.756846

Free energy in solution: -765.549491

C	1.365354	0.965293	-0.183695
C	2.518770	-1.219078	0.386533
C	-0.005682	-1.162757	0.365551
C	1.247466	-1.925638	-0.069879
C	0.152126	0.330574	0.091324
C	2.629644	0.135048	-0.307524
C	-2.549018	-1.045062	0.030418
C	-1.246399	-1.774046	-0.307204
N	1.414343	2.284679	-0.333724
P	-1.299605	1.278377	0.270308
H	2.486374	-1.074471	1.473414
H	1.254069	-1.999398	-1.166403
H	2.840692	-0.013497	-1.374570
H	-2.696064	-1.030777	1.120127
H	-1.103985	-1.752756	-1.396500
H	-1.329663	-2.827779	-0.012082

H	2.362623	2.642572	-0.396618
H	-1.384805	2.422106	-0.519023
H	-0.166067	2.657295	1.230950
H	3.462976	0.719213	0.098396
H	3.401593	-1.827783	0.167652
H	1.200469	-2.948161	0.321396
H	-3.411714	-1.570882	-0.389986
H	-0.124466	-1.324801	1.452213
H	-1.922242	1.415983	1.522287
H	0.540359	2.708210	0.611240
N	-2.570227	0.348305	-0.434784
H	-2.498457	0.372374	-1.450697

M13NHL1-Pr

SCF energy in gas phase: -765.639141

SCF energy in solution: -765.792481

Free energy in solution: -765.579413

C	1.321542	0.943820	-0.144669
C	2.543762	-1.184280	0.412080
C	0.015026	-1.165518	0.349852
C	1.290355	-1.908193	-0.058055
C	0.143032	0.344667	0.150853
C	2.618772	0.176089	-0.268572
C	-2.514445	-1.108456	-0.045571
C	-1.186960	-1.786525	-0.380406
N	1.458173	2.292216	-0.441628
P	-1.364786	1.336418	0.384453
H	2.505546	-1.048412	1.499641
H	1.317157	-1.988803	-1.153739
H	2.860093	0.059189	-1.333103
H	-2.678614	-1.148277	1.042610
H	-1.018430	-1.714941	-1.464186
H	-1.226983	-2.855226	-0.131634
H	2.373295	2.675132	-0.251370
H	-1.663009	2.308181	-0.623118
H	-0.635465	2.388287	1.125925
H	3.424935	0.781273	0.165663
H	3.442369	-1.766871	0.188144
H	1.251670	-2.929782	0.335543
H	-3.350872	-1.653266	-0.498833
H	-0.147357	-1.344431	1.426683
H	-2.023197	1.003390	1.602923
H	0.716678	2.892189	-0.103017

N	-2.546045	0.287079	-0.448093
H	-2.447432	0.371417	-1.459938

M13OL1

SCF energy in gas phase: -784.328731

SCF energy in solution: -784.492272

Free energy in solution: -784.313021

C	1.286818	1.069815	0.037166
C	2.561543	-1.110883	0.264387
C	0.052134	-1.218085	0.310481
C	1.321958	-1.821378	-0.293930
C	0.123993	0.273973	0.143284
C	2.615739	0.366341	-0.151780
C	-2.465144	-1.023000	0.249694
C	-1.243984	-1.754124	-0.299932
N	1.087655	2.358406	0.022644
P	-1.226498	1.290696	-0.011737
H	2.539788	-1.179417	1.359627
H	1.289699	-1.703574	-1.385735
H	2.871610	0.437129	-1.217198
H	-2.463376	-1.056946	1.347927
H	-1.221651	-1.634566	-1.390340
H	-1.359060	-2.822451	-0.080221
H	1.930230	2.897449	-0.163881
H	-1.276275	2.111711	-1.143378
H	3.398298	0.900328	0.397664
H	3.473367	-1.618725	-0.064977
H	1.369330	-2.895039	-0.076147
H	-3.392474	-1.477554	-0.104474
H	0.041901	-1.500143	1.379560
H	-1.582963	2.180110	1.020620
O	-2.544109	0.349555	-0.177214

M13OL1-TS1

SCF energy in gas phase: -785.474634

SCF energy in solution: -785.637095

Free energy in solution: -785.441519

C	1.348940	0.979601	-0.178554
C	2.518296	-1.199549	0.402494
C	-0.002296	-1.171005	0.361205
C	1.260194	-1.916236	-0.074677
C	0.141614	0.324596	0.099366

C	2.623321	0.160244	-0.281506
C	-2.522926	-1.029902	0.003528
C	-1.233975	-1.763221	-0.340277
N	1.380350	2.291956	-0.347611
P	-1.315140	1.246829	0.243862
H	2.471432	-1.063910	1.490074
H	1.276133	-1.974696	-1.171750
H	2.851837	0.020084	-1.345956
H	-2.692931	-1.043916	1.093759
H	-1.088797	-1.710233	-1.425588
H	-1.341863	-2.819888	-0.065160
H	2.325527	2.656664	-0.423589
H	-1.439113	2.372064	-0.559586
H	-0.245822	2.655543	1.197629
H	3.443198	0.751868	0.140426
H	3.410403	-1.796635	0.189739
H	1.220863	-2.943888	0.303547
H	-3.388108	-1.496905	-0.472118
H	-0.131028	-1.349929	1.443935
H	-1.953583	1.411143	1.488578
H	0.442150	2.720923	0.616535
O	-2.486833	0.319803	-0.459325

M13OL1-Pr

SCF energy in gas phase: -785.522407

SCF energy in solution: -785.684046

Free energy in solution: -785.482255

C	1.302651	0.953501	-0.137764
C	2.539920	-1.171338	0.422347
C	0.017941	-1.172559	0.336686
C	1.299375	-1.898780	-0.075458
C	0.125364	0.339433	0.135842
C	2.610669	0.199946	-0.235860
C	-2.483283	-1.075532	-0.049741
C	-1.185199	-1.792701	-0.384694
N	1.436874	2.298084	-0.442142
P	-1.385887	1.318551	0.357801
H	2.485870	-1.054185	1.511497
H	1.335337	-1.958183	-1.171919
H	2.877861	0.102955	-1.296068
H	-2.649507	-1.103625	1.046197
H	-1.031482	-1.727906	-1.468526
H	-1.250501	-2.854762	-0.116479

H	2.342509	2.694483	-0.236520
H	-1.822542	2.268081	-0.594206
H	-0.665652	2.370459	1.085729
H	3.397896	0.809923	0.225711
H	3.447652	-1.740561	0.201254
H	1.265109	-2.927179	0.300273
H	-3.340742	-1.574603	-0.513893
H	-0.135744	-1.351965	1.414926
H	-2.095896	1.029546	1.550977
H	0.676373	2.900860	-0.158703
O	-2.433873	0.244998	-0.515051

M14CH₂L1

SCF energy in gas phase: -825.802323

SCF energy in solution: -825.968396

Free energy in solution: -825.732130

C	-3.179607	-1.276417	-0.017955
C	-3.314236	0.246998	0.227556
C	-1.975747	0.809041	-0.276761
C	-1.123195	-0.446449	-0.271620
C	-1.307915	1.861958	0.616508
C	0.286426	-0.270229	-0.344065
C	0.814329	1.103783	-0.691279
C	0.153329	2.176360	0.211793
C	2.348462	1.200536	-0.637987
H	2.632757	2.258219	-0.605361
C	2.975283	0.458066	0.546670
C	2.944561	-1.062266	0.334805
H	-1.902173	2.781500	0.638544
H	-3.678344	-1.574966	-0.951449
H	-4.184927	0.686624	-0.264722
H	0.206923	3.137996	-0.313060
H	4.017783	0.765852	0.674985
H	3.356424	-1.603221	1.190967
N	-1.747596	-1.566412	-0.114524
P	1.221209	-1.620158	0.046730
H	0.751678	-2.301834	1.187456
H	1.366519	-2.731465	-0.825456
H	3.539924	-1.333939	-0.542407
H	-3.640642	-1.864807	0.782905
H	-3.405145	0.444293	1.301948
H	2.775734	0.792184	-1.563635
H	2.449477	0.714991	1.473559

H	-1.318591	1.459788	1.636334
H	0.751652	2.290076	1.124533
H	-2.060015	1.190590	-1.304762
H	0.525867	1.347086	-1.725652

M14CH₂L1-Pr

SCF energy in gas phase: -826.964610

SCF energy in solution: -827.121986

Free energy in solution: -826.864244

M14CH₂L1-TS1

SCF energy in gas phase: -826.934833

SCF energy in solution: -827.095989

Free energy in solution: -826.845135

C	-3.204926	-1.231568	0.018183
C	-3.318916	0.293352	0.213726
C	-1.962310	0.815991	-0.281996
C	-1.085369	-0.404803	-0.121224
C	-1.349118	1.978573	0.499909
C	0.292056	-0.275747	-0.252629
C	0.791838	1.091715	-0.704183
C	0.128122	2.225290	0.118223
C	2.320149	1.241382	-0.643274
H	2.569186	2.306312	-0.711058
C	2.910059	0.622641	0.624674
C	2.967610	-0.900287	0.492081
H	-1.941883	2.888292	0.361060
H	-3.564034	-1.530180	-0.977010
H	-4.172271	0.731103	-0.308736
H	0.221354	3.148534	-0.465209
H	3.916807	1.009629	0.812412
H	3.254484	-1.372355	1.437409
N	-1.774296	-1.502604	0.151436
P	1.344452	-1.657555	-0.072824
H	1.023608	-2.482163	1.007642
H	-0.197908	-2.803174	-0.743884
H	3.731099	-1.173983	-0.245399
H	-3.780268	-1.794425	0.758520
H	-3.422134	0.517718	1.281224
H	2.782543	0.759736	-1.515970
H	2.297230	0.899279	1.490426
H	-1.415099	1.719532	1.562591
H	0.709081	2.380579	1.034446
H	-2.007730	1.072261	-1.351319
H	0.493653	1.249868	-1.752235
H	-1.049427	-2.417796	-0.325760
H	1.869806	-2.466457	-1.097784

C	-2.968417	-1.483798	0.474239
C	-3.069122	0.035163	0.686709
C	-2.131714	0.575076	-0.402037
C	-1.024757	-0.454572	-0.351955
C	-1.648224	2.027351	-0.289420
C	0.281117	-0.177484	-0.530629
C	0.760169	1.270282	-0.600495
C	-0.211946	2.131660	0.220831
C	2.205870	1.449652	-0.061589
H	2.304915	2.484727	0.284163
C	2.582899	0.496835	1.085775
C	2.957410	-0.914385	0.597185
H	-1.696022	2.498459	-1.277350
H	-3.737540	-1.833833	-0.225684
H	-4.091203	0.412118	0.605589
H	0.108690	3.179434	0.191057
H	3.427333	0.910474	1.646611
H	3.070928	-1.606139	1.434728
N	-1.629913	-1.674400	-0.099170
P	1.568927	-1.442325	-0.505202
H	0.901894	-2.174847	0.637825
H	1.564276	-2.663210	-1.243020
H	3.878963	-0.880297	0.009289
H	-3.082524	-2.048027	1.404160
H	-2.673470	0.308194	1.672352
H	2.929403	1.325462	-0.873704
H	1.743825	0.420338	1.789330
H	-2.325369	2.595588	0.358285
H	-0.159948	1.806896	1.268985
H	-2.638404	0.436238	-1.367476
H	0.749680	1.638673	-1.637402
H	-1.039992	-2.397055	0.291668
H	2.240341	-0.792193	-1.668881

M14NHL1

SCF energy in gas phase: -841.841760

SCF energy in solution: -842.016411

Free energy in solution: -841.790593

C	3.180920	-1.248864	0.013735	C	-2.332867	1.280638	0.584149
C	3.284919	0.267516	-0.277882	H	-2.573319	2.349452	0.532962
C	1.955648	0.819798	0.257221	C	-2.903645	0.530782	-0.619047
C	1.116013	-0.444741	0.278585	H	1.946802	2.907361	-0.205610
C	1.253243	1.866010	-0.611037	H	3.507735	-1.587221	0.978678
C	-0.299514	-0.282311	0.361276	H	4.159961	0.683331	0.401744
C	-0.845940	1.080319	0.736480	H	-0.298660	3.169620	0.323841
C	-0.181798	2.184143	-0.132406	H	-3.944509	0.810569	-0.805200
C	-2.379875	1.153651	0.619386	N	1.739301	-1.502173	-0.177286
H	-2.690081	2.204510	0.579873	P	-1.358028	-1.640275	0.024409
C	-2.904632	0.402946	-0.607756	H	-0.970957	-2.426721	-1.064622
H	1.844717	2.785845	-0.669217	H	-1.925566	-2.520409	0.969715
H	3.703533	-1.513390	0.944173	H	3.751737	-1.801323	-0.759179
H	4.164728	0.733859	0.171693	H	3.452316	0.532013	-1.214299
H	-0.193264	3.115198	0.446798	H	-2.819090	0.887895	1.485839
H	-3.962622	0.616894	-0.779408	H	-2.341472	0.782292	-1.525469
N	1.755789	-1.558479	0.153683	H	1.539526	1.811661	-1.514775
P	-1.245391	-1.615713	-0.030283	H	-0.656042	2.268817	-1.138753
H	-0.609972	-2.370540	-1.032015	H	0.137843	-2.773858	0.716982
H	-1.628044	-2.667860	0.849592	H	0.957772	-2.428202	0.321475
H	3.631046	-1.854870	-0.779851	H	1.973344	1.031944	1.392018
H	3.333711	0.436069	-1.360005	H	-0.513256	1.291665	1.719362
H	-2.850173	0.715633	1.509162	N	-2.850367	-0.915798	-0.412939
H	-2.363134	0.715404	-1.506791	H	-3.628226	-1.254127	0.141041
H	1.210277	1.456338	-1.627225				
H	-0.806777	2.367177	-1.015409				
H	2.063591	1.198895	1.284465				
H	-0.594054	1.304819	1.783681				
N	-2.772135	-1.057730	-0.470205				
H	-3.532092	-1.485619	0.044773				

M14NHL1-TS1

SCF energy in gas phase: -842.981234

SCF energy in solution: -843.151435

Free energy in solution: -842.910917

C	3.171623	-1.251727	-0.012628
C	3.314699	0.276706	-0.157822
C	1.952585	0.805167	0.315499
C	1.065937	-0.400802	0.106266
C	1.381101	2.002415	-0.447837
C	-0.315378	-0.266600	0.238704
C	-0.806501	1.111664	0.673754
C	-0.128896	2.210951	-0.179424

M14NHL1-Pr

SCF energy in gas phase: -843.016579

SCF energy in solution: -843.185134

Free energy in solution: -842.937806

C	3.270440	-1.207692	0.244585
C	3.347852	0.300567	-0.009238
C	1.928957	0.795581	0.312659
C	1.053741	-0.432363	0.141615
C	1.410157	1.909179	-0.606485
C	-0.306737	-0.307468	0.190646
C	-0.755453	1.123504	0.537832
C	-0.107889	2.128782	-0.439873
C	-2.269243	1.385616	0.619035
H	-2.452695	2.448152	0.415641
C	-3.085572	0.492783	-0.309123
H	1.966344	2.832511	-0.415269
H	3.501562	-1.446464	1.293289
H	4.121018	0.789946	0.585562

H	-0.309199	3.141170	-0.072178
H	-4.133856	0.816138	-0.334085
N	1.882396	-1.496342	-0.081110
P	-1.407177	-1.679761	-0.253709
H	-1.786281	-1.749665	-1.619290
H	-1.826286	-2.702004	0.648117
H	3.948038	-1.782384	-0.392118
H	3.564024	0.480631	-1.067235
H	-2.626779	1.201347	1.639894
H	-2.715365	0.575211	-1.343429
H	1.638030	1.611872	-1.635547
H	-0.610514	2.039938	-1.409990
H	-0.242535	-2.517636	-0.582781
H	1.522032	-2.436708	-0.076236
H	1.867975	1.125519	1.359059
H	-0.345262	1.362380	1.530714
N	-2.978842	-0.894836	0.096447
H	-3.214991	-0.986221	1.084252

M14OL1

SCF energy in gas phase: -861.710127

SCF energy in solution: -861.889968

Free energy in solution: -861.676447

C	3.167082	-1.242415	-0.010123
C	3.262614	0.273286	-0.307965
C	1.944096	0.826047	0.253058
C	1.107803	-0.439657	0.294434
C	1.222427	1.868018	-0.603564
C	-0.306305	-0.276297	0.395462
C	-0.870979	1.080582	0.759429
C	-0.197050	2.196390	-0.089412
C	-2.400979	1.108668	0.582997
H	-2.750966	2.145323	0.523317
C	-2.849950	0.346854	-0.658329
H	1.813938	2.786107	-0.684074
H	3.710425	-1.504752	0.908632
H	4.150709	0.741972	0.122212
H	-0.179479	3.110049	0.516032
H	-3.909771	0.501509	-0.866899
N	1.745474	-1.553336	0.163099
P	-1.257457	-1.601875	0.008708
H	-0.621837	-2.379040	-0.974290
H	-1.709371	-2.604808	0.896773

H	3.598884	-1.850025	-0.812462
H	3.288837	0.439131	-1.391269
H	-2.898906	0.651025	1.446309
H	-2.269034	0.644738	-1.539263
H	1.150412	1.451359	-1.615414
H	-0.831131	2.419858	-0.956427
O	-2.722709	-1.076827	-0.454168
H	2.072031	1.207750	1.276992
H	-0.662078	1.307035	1.814938

M14OL1-TS1

SCF energy in gas phase: -862.856216

SCF energy in solution: -863.032050

Free energy in solution: -862.803648

C	3.160631	-1.255599	-0.034664
C	3.307089	0.274822	-0.164217
C	1.948585	0.802331	0.321416
C	1.062310	-0.404945	0.114600
C	1.375325	2.005721	-0.432756
C	-0.319579	-0.260934	0.258308
C	-0.817447	1.116597	0.678484
C	-0.138736	2.210677	-0.178124
C	-2.345200	1.248743	0.561534
H	-2.619112	2.307320	0.486137
C	-2.878549	0.475694	-0.635316
H	1.936758	2.909140	-0.175931
H	3.513373	-1.604847	0.945913
H	4.156395	0.673049	0.395215
H	-0.317716	3.174426	0.312034
H	-3.931298	0.698734	-0.822904
N	1.725557	-1.504953	-0.176955
P	-1.377590	-1.610285	0.046779
H	-1.050599	-2.411693	-1.051119
H	-1.949415	-2.440020	1.021258
H	3.726816	-1.797523	-0.797411
H	3.440522	0.541428	-1.218438
H	-2.842618	0.849567	1.452964
H	-2.308614	0.712771	-1.543702
H	1.542979	1.828500	-1.500557
H	-0.657088	2.254495	-1.143089
H	0.085472	-2.771142	0.698072
H	0.878116	-2.452754	0.331561
O	-2.822144	-0.924233	-0.364307

H	1.976137	1.023742	1.398696
H	-0.544580	1.308975	1.727160

M14OL1-Pr

SCF energy in gas phase: -862.898550

SCF energy in solution: -863.075448

Free energy in solution: -862.840745

C	3.290926	-1.081407	0.095593
C	3.261227	0.416519	-0.230042
C	1.884834	0.871267	0.286752
C	1.066103	-0.399458	0.249771
C	1.206618	2.007363	-0.514435
C	-0.268617	-0.336716	0.436835
C	-0.827595	1.054283	0.689943
C	-0.341252	1.992715	-0.424743
C	-2.342099	1.017746	0.889064
H	-2.725733	2.023763	1.093029
C	-3.091415	0.420775	-0.308082
H	1.601834	2.964978	-0.161651
H	3.637986	-1.251629	1.125763
H	4.095872	0.959727	0.216814
H	-0.721063	3.007556	-0.259483
H	-4.093786	0.100173	0.020436
N	1.890044	-1.454823	-0.077970
P	-1.340770	-1.694185	-0.023289
H	-1.240487	-2.373572	-1.253964
H	-2.372283	-2.089555	0.855507
H	3.933313	-1.650541	-0.580964
H	3.303716	0.550813	-1.315602
H	-2.543451	0.421039	1.787512
H	-3.243963	1.194723	-1.071625
H	1.511428	1.912969	-1.561596
H	-0.766670	1.630967	-1.366508
O	-2.403770	-0.638652	-0.924437
H	1.967138	1.180765	1.338202
H	-0.396918	1.421104	1.635231
H	1.584209	-2.388606	0.159797
H	-0.452122	-2.687443	0.605783

M15CH₂L1

SCF energy in gas phase: -865.102644

SCF energy in solution: -865.275318

Free energy in solution: -865.010314

C	-3.637471	-0.527705	0.482368
C	-3.140544	0.726979	-0.229832
C	-1.706172	0.993694	0.213884
C	-0.870536	-0.272197	0.071248
C	-2.772930	-1.726469	0.080814
C	-1.026360	2.160176	-0.507678
C	0.546737	-0.116145	-0.007737
C	1.295261	1.162040	-0.315758
C	0.396763	2.361053	0.013707
C	2.653110	1.277213	0.417711
H	2.489499	1.751717	1.391944
C	3.398574	-0.052794	0.662707
H	-1.002096	1.957280	-1.587385
H	-3.570722	-0.367896	1.566143
H	-3.165969	0.572571	-1.317522
H	-3.103006	-2.084791	-0.907047
H	0.840910	3.276159	-0.395250
H	3.125625	-0.447792	1.647655
N	-1.344703	-1.479519	0.014109
P	1.342784	-1.601987	-0.232942
H	4.476888	0.131794	0.695748
H	1.051724	-2.430977	-1.343065
H	3.296178	1.956140	-0.155328
H	1.508904	1.231891	-1.398044
H	1.255272	-2.540945	0.812189
H	-2.953298	-2.560125	0.771658
H	-4.687608	-0.734493	0.250954
H	-1.725219	1.239627	1.287340
H	-1.619322	3.071480	-0.366597
H	0.356847	2.481582	1.105114
H	-3.773169	1.594155	-0.009815
C	3.105767	-1.140809	-0.383108
H	3.744874	-2.016571	-0.244503
H	3.271659	-0.764574	-1.398790

M15CH₂L1-TS1

SCF energy in gas phase: -866.234169

SCF energy in solution: -866.404312

Free energy in solution: -866.125142

C	-3.763744	-0.391167	0.272179
C	-3.123786	0.801711	-0.429942
C	-1.724895	1.002223	0.144358

C	-0.901214	-0.278384	0.035922
C	-2.939232	-1.647188	-0.009120
C	-0.986269	2.215267	-0.406569
C	0.501724	-0.185078	0.030761
C	1.259148	1.135305	-0.135119
C	0.383604	2.324809	0.252243
C	2.583566	1.142080	0.641700
H	2.366657	0.837784	1.673836
C	3.648613	0.214215	0.018819
H	-0.869079	2.119330	-1.494768
H	-3.790837	-0.192656	1.350543
H	-3.061672	0.617683	-1.511151
H	-3.219127	-2.036375	-0.999534
H	0.889669	3.252492	-0.039140
H	4.302305	-0.174997	0.806399
N	-1.500510	-1.457009	0.007136
P	1.525047	-1.603193	0.075304
H	4.290589	0.789276	-0.656274
H	1.166599	-2.683915	-0.738071
H	2.977940	2.163385	0.693616
H	1.512962	1.280354	-1.201040
H	2.165651	-2.105219	1.226372
H	-3.190414	-2.435936	0.710467
H	-4.796134	-0.549432	-0.055315
H	-1.845779	1.168637	1.227379
H	-1.584350	3.115535	-0.225143
H	0.262361	2.348641	1.344219
H	-3.714616	1.713217	-0.287345
C	3.040818	-0.960338	-0.770204
H	3.768907	-1.768602	-0.891820
H	2.734694	-0.638546	-1.771124
H	-0.691546	-2.248365	0.643083
H	0.083083	-2.566055	1.145131

M15CH₂L1-Pr

SCF energy in gas phase: -866.267427

SCF energy in solution: -866.434433

Free energy in solution: -866.147456

C	-3.696995	-0.607707	0.325500
C	-3.125920	0.685555	-0.246421
C	-1.724408	0.958632	0.311930
C	-0.810635	-0.240217	0.109334
C	-2.754384	-1.755606	-0.004331

C	-1.123603	2.235726	-0.264475
C	0.476395	-0.111966	-0.292091
C	1.159102	1.231875	-0.529387
C	0.344512	2.355048	0.114080
C	2.637935	1.281615	-0.034105
H	2.809783	2.265229	0.417356
C	3.029452	0.197244	0.979564
H	-1.213908	2.216416	-1.359311
H	-3.792639	-0.521698	1.414030
H	-3.063125	0.604106	-1.340665
H	-2.777933	-1.935861	-1.092768
H	0.754554	3.322874	-0.195551
H	2.266215	0.132556	1.765978
N	-1.405535	-1.450757	0.460746
P	1.608006	-1.512468	-0.552461
H	3.967700	0.477724	1.469520
H	2.133303	-0.840382	-1.777939
H	3.317726	1.213178	-0.890378
H	1.178608	1.413324	-1.613528
H	1.091161	-2.256839	0.643075
H	-3.078259	-2.676687	0.488576
H	-4.690551	-0.814984	-0.083922
H	-1.824005	1.076585	1.402571
H	-1.699654	3.098245	0.088376
H	0.449920	2.293967	1.206810
H	-3.775918	1.539151	-0.024420
C	3.202214	-1.185309	0.329053
H	3.386749	-1.957390	1.078928
H	4.016602	-1.162846	-0.400697
H	-0.773106	-2.238740	0.419876
H	1.353456	-2.674964	-1.346131

M15NHL1

SCF energy in gas phase: -881.142982

SCF energy in solution: -881.323884

Free energy in solution: -881.069300

C	-3.589746	-0.515472	0.550946
C	-3.103467	0.834232	0.032489
C	-1.613833	0.948909	0.333598
C	-0.870322	-0.289718	-0.162295
C	-2.841978	-1.641750	-0.168066
C	-0.967471	2.233712	-0.186527
C	0.560916	-0.166689	-0.284748

C	1.258431	1.140307	-0.612807	H	-1.083307	2.152103	-1.496118
C	0.530154	2.273748	0.119378	H	-3.497640	-0.304335	1.667909
C	2.774452	1.121736	-0.297858	H	-3.182224	0.669753	-1.216958
H	3.100310	2.132415	-0.022900	H	-3.196765	-1.968517	-0.865271
C	3.155300	0.130183	0.802006	H	0.892235	3.287167	-0.350425
H	-1.114539	2.301723	-1.273834	H	2.300577	0.179362	1.832699
H	-3.397206	-0.568796	1.630007	N	-1.389241	-1.448738	0.020479
H	-3.266094	0.899723	-1.052196	P	1.502101	-1.609940	-0.372461
H	-3.301523	-1.803240	-1.154662	H	4.018361	0.287693	1.462061
H	0.956267	3.237575	-0.185595	H	2.096252	-2.210631	-1.498756
H	2.561047	0.309168	1.703573	H	3.451971	1.159309	-0.815438
N	-1.418450	-1.438787	-0.388078	H	1.330236	1.334387	-1.638795
P	1.384929	-1.630413	-0.138812	H	0.954462	-2.613076	0.427704
H	4.207329	0.238548	1.079989	H	-3.004938	-2.504184	0.797129
H	1.699861	-2.570678	-1.162704	H	-4.682812	-0.602040	0.395571
H	3.339960	0.846516	-1.196912	H	-0.709088	-2.152446	-0.845359
H	1.160823	1.367984	-1.687066	H	-0.012624	-2.413165	-1.469301
H	0.698300	-2.464814	0.753996	H	-3.676488	1.690345	0.137469
H	-2.974117	-2.585560	0.375255	H	-1.598736	1.166468	1.338627
H	-4.668554	-0.639131	0.409808	H	-1.569414	3.130645	-0.109952
H	-3.648942	1.664814	0.494377	H	0.527921	2.349166	1.100317
H	-1.491279	0.949069	1.428796	N	2.977393	-1.163878	0.382227
H	-1.477096	3.097420	0.256455	H	3.795853	-1.347190	-0.187287
H	0.689687	2.170342	1.202149				
N	2.948414	-1.263993	0.379514				
H	3.687472	-1.622599	-0.213111				

M15NHL1-TS1

SCF energy in gas phase: -882.279895

SCF energy in solution: -882.459764

Free energy in solution: -882.190475

C	-3.617253	-0.439892	0.585929
C	-3.096875	0.799917	-0.129375
C	-1.633824	1.010068	0.248582
C	-0.818197	-0.253252	-0.017731
C	-2.824436	-1.658694	0.122818
C	-1.008102	2.236018	-0.403226
C	0.564125	-0.146259	-0.269123
C	1.274617	1.179711	-0.550389
C	0.453533	2.347072	0.003146
C	2.728090	1.255116	0.002802
H	2.895418	2.242866	0.449825
C	3.028685	0.154150	1.015288

M15NHL1-Pr

SCF energy in gas phase: -882.319378

SCF energy in solution: -882.497450

Free energy in solution: -882.220776

C	-3.709617	-0.484069	0.302007
C	-3.062712	0.675243	-0.446078
C	-1.697979	1.024655	0.158125
C	-0.804338	-0.207990	0.211823
C	-2.792325	-1.693428	0.223964
C	-1.019597	2.159581	-0.598533
C	0.522456	-0.155191	-0.098535
C	1.268705	1.170282	-0.232740
C	0.365624	2.388627	-0.018111
C	2.472749	1.254350	0.727421
H	2.104992	1.480656	1.735555
C	3.311557	-0.040442	0.753221
H	-0.944384	1.893701	-1.661454
H	-3.861209	-0.209693	1.352401
H	-2.925325	0.397862	-1.500644

H	-2.772174	-2.068476	-0.812048
H	0.844201	3.275319	-0.447502
H	3.004353	-0.652780	1.613322
N	-1.447629	-1.342977	0.678251
P	1.515276	-1.644358	-0.503862
H	4.371334	0.187006	0.914922
H	1.822186	-1.942452	-1.865515
H	3.089458	2.108576	0.419881
H	1.663191	1.231497	-1.258274
H	1.921940	-2.473655	0.576461
H	-3.158541	-2.502963	0.861542
H	-4.686522	-0.734605	-0.122393
H	-0.840142	-2.149136	0.731117
H	0.303448	-2.466078	-0.659994
H	-3.700683	1.565361	-0.428980
H	-1.869755	1.345878	1.197321
H	-1.635428	3.063118	-0.532371
H	0.262721	2.576509	1.059193
N	3.132509	-0.865076	-0.425705
H	3.355912	-0.353603	-1.277811

M15OL1

SCF energy in gas phase: -901.012296

SCF energy in solution: -901.198587

Free energy in solution: -900.956171

C	-3.571352	-0.511012	0.556127
C	-3.090147	0.835276	0.022395
C	-1.601471	0.956832	0.325468
C	-0.858388	-0.281274	-0.168051
C	-2.820472	-1.646010	-0.147091
C	-0.950544	2.240089	-0.194739
C	0.567369	-0.152964	-0.308417
C	1.279162	1.150181	-0.609550
C	0.545648	2.279158	0.123598
C	2.784777	1.087237	-0.254917
H	3.134325	2.074658	0.069448
C	3.108803	0.058298	0.818557
H	-1.089641	2.305706	-1.283114
H	-3.380564	-0.549519	1.636096
H	-3.251238	0.888567	-1.063059
H	-3.285084	-1.829360	-1.127270
H	0.975364	3.244701	-0.170147
H	2.491633	0.205795	1.712689

N	-1.399966	-1.436266	-0.382061
P	1.388343	-1.613614	-0.166670
O	2.911045	-1.272992	0.299778
H	4.161173	0.095892	1.105719
H	1.730735	-2.529467	-1.188013
H	3.371906	0.818631	-1.140074
H	1.212223	1.391766	-1.682585
H	0.735298	-2.450070	0.749584
H	-2.942217	-2.580012	0.415166
H	-4.649468	-0.640028	0.415350
H	-3.639774	1.667971	0.475222
H	-1.481615	0.958768	1.420978
H	-1.461869	3.105303	0.242842
H	0.694774	2.167847	1.207132

M15OL1-TS1

SCF energy in gas phase: -902.155404

SCF energy in solution: -902.340356

Free energy in solution: -902.082952

C	-3.608887	-0.435025	0.576325
C	-3.085077	0.810384	-0.127749
C	-1.621018	1.008172	0.252142
C	-0.815097	-0.257238	-0.034187
C	-2.816961	-1.654172	0.109402
C	-0.987165	2.246492	-0.369591
C	0.567424	-0.140537	-0.293443
C	1.281131	1.182889	-0.562587
C	0.478442	2.340806	0.033174
C	2.740886	1.199944	-0.032323
H	2.969097	2.184471	0.392996
C	2.994383	0.115591	1.001827
H	-1.065716	2.192571	-1.464144
H	-3.493366	-0.306362	1.659576
H	-3.172007	0.692607	-1.216553
H	-3.191329	-1.961252	-0.878700
H	0.919462	3.287862	-0.298302
H	2.262361	0.171801	1.817708
N	-1.380748	-1.450627	0.003883
P	1.517014	-1.583674	-0.369019
O	2.937699	-1.162360	0.364742
H	3.997048	0.194082	1.428099
H	2.137822	-2.139604	-1.494123
H	3.451405	1.035296	-0.849480

H	1.324419	1.364681	-1.647342
H	1.004865	-2.601743	0.435383
H	-2.999527	-2.501006	0.781364
H	-4.674075	-0.594008	0.381309
H	-0.644569	-2.177606	-0.886737
H	0.042824	-2.424331	-1.461953
H	-3.661304	1.699770	0.149691
H	-1.584403	1.139926	1.345448
H	-1.542472	3.136226	-0.051434
H	0.559533	2.311157	1.129437

M15OL1-Pr

SCF energy in gas phase: -902.204457

SCF energy in solution: -902.389931

Free energy in solution: -902.125040

C	-3.699727	-0.479838	0.291264
C	-3.045795	0.675918	-0.456384
C	-1.685652	1.025313	0.157995
C	-0.793414	-0.208076	0.214503
C	-2.784263	-1.691435	0.225981
C	-1.002994	2.165650	-0.586669
C	0.534072	-0.151003	-0.095574
C	1.281570	1.174123	-0.228406
C	0.380104	2.389355	0.001828
C	2.485595	1.231572	0.728839
H	2.130078	1.431734	1.746767
C	3.281863	-0.084499	0.695867
H	-0.921840	1.908392	-1.651208
H	-3.859391	-0.200513	1.339109
H	-2.900677	0.395934	-1.509165
H	-2.761394	-2.075073	-0.806703
H	0.859134	3.280437	-0.417401
H	2.999544	-0.709501	1.564073
N	-1.439496	-1.340293	0.680699
P	1.517549	-1.630329	-0.504592
O	3.033437	-0.772106	-0.499577
H	4.358239	0.096475	0.780571
H	0.331623	-2.474512	-0.628544
H	1.859480	-1.938787	-1.839840
H	3.116391	2.078629	0.435392
H	1.683092	1.231245	-1.248197
H	-0.834674	-2.146219	0.754064
H	1.998552	-2.461368	0.540057

H	-3.153641	-2.494838	0.869352
H	-4.673526	-0.731354	-0.139561
H	-1.864608	1.340269	1.197877
H	-1.620024	3.067994	-0.516370
H	0.273967	2.565661	1.081032
H	-3.682751	1.566742	-0.446159

M4CH₂L2

SCF energy in gas phase: -1168.651053

SCF energy in solution: -1168.912768

Free energy in solution: -1168.632909

C	-1.597743	-0.431075	0.012899
C	-3.441854	-0.912472	-1.458811
C	-3.796211	-0.746733	0.963095
C	-4.256505	-0.980762	-0.360564
C	-2.461540	-0.463063	1.130944
C	-2.030082	-0.598136	-1.352095
H	-5.307779	-1.216465	-0.509660
H	-3.847781	-1.088581	-2.451749
H	-4.478352	-0.773539	1.805267
N	-1.168248	-0.443034	-2.327234
P	0.032941	-0.070354	0.502143
C	-1.815495	-0.068020	2.443787
H	-2.185038	-0.673805	3.275618
C	0.610283	1.596591	0.077951
C	1.774553	2.113818	0.653579
C	-0.131648	2.356801	-0.828171
C	2.186307	3.403497	0.338490
C	0.292659	3.644886	-1.144235
C	1.442795	4.167939	-0.559754
C	1.381813	-1.208594	0.086172
C	2.337920	-1.523199	1.058866
C	1.487193	-1.738066	-1.205612
C	3.398030	-2.367082	0.744645
C	2.547597	-2.590177	-1.503285
C	3.499984	-2.902702	-0.536836
H	-1.007909	1.919899	-1.297913
H	-0.275527	4.238634	-1.852525
H	1.766971	5.173379	-0.809073
H	3.086953	3.810193	0.786477
H	2.364955	1.508152	1.337706
H	2.261599	-1.115532	2.063706
H	4.138980	-2.608010	1.499929

H	4.324777	-3.564735	-0.781168
H	2.630057	-3.010622	-2.500312
H	0.732941	-1.468192	-1.944181
H	-1.629358	-0.587795	-3.225153
H	-2.072799	0.973800	2.663994
C	-0.284178	-0.203525	2.306464
H	0.272841	0.540647	2.880126
H	0.044800	-1.200441	2.612243

M4CH₂L2-TS1

SCF energy in gas phase: -1169.791927

SCF energy in solution: -1170.047999

Free energy in solution: -1169.751972

C	-1.455766	-0.800777	-0.003739
C	-3.311667	-1.899295	-1.097418
C	-3.605487	-0.940868	1.120675
C	-4.099718	-1.628082	-0.003805
C	-2.290607	-0.522238	1.102279
C	-1.932903	-1.525203	-1.147901
H	-5.135350	-1.957956	-0.009831
H	-3.723028	-2.432221	-1.950331
H	-4.236197	-0.748998	1.982181
N	-1.106719	-1.813252	-2.155057
P	0.121506	-0.009636	0.220568
C	-1.645811	0.269472	2.221422
H	-1.990090	-0.082313	3.198086
H	-0.229660	-0.762097	-2.137045
H	0.270205	-0.035552	-1.840498
C	0.276872	1.754246	-0.220545
C	1.523220	2.356514	-0.399989
C	-0.889631	2.514227	-0.332373
C	1.599436	3.717837	-0.678379
C	-0.804964	3.875509	-0.610330
C	0.438001	4.479735	-0.779442
C	1.679460	-0.935136	0.108579
C	2.718709	-0.585259	0.977589
C	1.829400	-2.016736	-0.763900
C	3.917437	-1.292831	0.951360
C	3.022268	-2.732833	-0.764199
C	4.067808	-2.368277	0.081058
H	-1.860790	2.035896	-0.228427
H	-1.713586	4.461973	-0.701750
H	0.501080	5.540519	-0.999211

H	2.569534	4.182372	-0.823440
H	2.431201	1.763021	-0.346973
H	2.599240	0.241109	1.673309
H	4.727025	-1.007461	1.615006
H	4.998743	-2.926084	0.065320
H	3.135765	-3.578086	-1.435033
H	1.010406	-2.293720	-1.422998
H	-1.592000	-2.176518	-2.969824
H	-1.936370	1.324651	2.140931
C	-0.127764	0.133349	2.064545
H	0.425253	0.968816	2.499767
H	0.223308	-0.800155	2.514704

M4CH₂L2-Pr

SCF energy in gas phase: -1169.832925

SCF energy in solution: -1170.086926

Free energy in solution: -1169.783997

C	-1.778397	0.042270	-0.095431
C	-3.960104	-0.204198	-1.108227
C	-3.775487	0.738321	1.108509
C	-4.550521	0.336164	0.024413
C	-2.396141	0.584376	1.036108
C	-2.567632	-0.359588	-1.198248
H	-5.630938	0.440917	0.059742
H	-4.577229	-0.524474	-1.943708
H	-4.233180	1.157337	1.999463
N	-2.042174	-0.972429	-2.330545
P	0.072557	0.004231	0.013577
C	-1.462320	0.987524	2.155963
H	-1.922615	0.769235	3.125909
H	-1.092249	-0.713404	-2.558930
H	0.153973	-0.177779	-1.454284
C	1.177374	1.487379	-0.242881
C	2.006549	1.477664	-1.368081
C	1.237718	2.582919	0.622884
C	2.889795	2.522991	-1.615409
C	2.095800	3.648303	0.359659
C	2.929366	3.616774	-0.754268
C	1.012702	-1.580393	0.178340
C	2.040554	-1.722519	1.112773
C	0.707506	-2.641960	-0.675281
C	2.762511	-2.910592	1.185277
C	1.404576	-3.843049	-0.576773

C	2.438574	-3.974692	0.347006	C	-2.672332	3.016609	0.461229
H	0.611095	2.619479	1.506003	C	-0.672313	3.773728	-0.668851
H	2.115866	4.501514	1.030262	C	-1.959914	4.017692	-0.196952
H	3.606406	4.441989	-0.951657	H	-1.350840	-2.111437	2.057443
H	3.540772	2.488414	-2.483264	H	-3.062335	-3.807386	1.424330
H	1.958481	0.632969	-2.050897	H	-3.827784	-3.965629	-0.926362
H	2.286650	-0.897477	1.775176	H	-2.896089	-2.444694	-2.645335
H	3.574900	-3.007162	1.898619	H	-1.178746	-0.740716	-2.007096
H	2.993343	-4.905477	0.412096	H	-2.653716	0.971499	1.134924
H	1.146422	-4.673523	-1.226277	H	-3.680263	3.206152	0.815335
H	-0.087212	-2.528450	-1.409477	H	-2.416534	4.990145	-0.352264
H	-2.659658	-0.957047	-3.129501	H	-0.131878	4.551146	-1.198528
H	-1.317894	2.075311	2.121656	H	0.912663	2.309407	-0.857554
C	-0.158730	0.229524	1.938160	H	1.482490	-0.021710	-3.274143
H	0.694192	0.682802	2.448795	H	2.070692	-1.196530	2.985425
H	-0.276423	-0.784961	2.333482	N	0.381441	-0.227158	2.151123
				H	-0.132888	0.348484	2.804586

M4NHL2

SCF energy in gas phase: -1184.692715

SCF energy in solution: -1184.963480

Free energy in solution: -1184.694411

M4NHL2-TS1

SCF energy in gas phase: -1185.834338

SCF energy in solution: -1186.100039

Free energy in solution: -1185.815119

C	1.634425	-0.212912	-0.050925	C	1.690997	0.118474	-0.087462
C	3.426028	-0.429057	-1.625397	C	3.783575	0.368116	-1.279189
C	3.856631	-0.588362	0.794102	C	3.791693	-0.418847	1.022461
C	4.276449	-0.606478	-0.563900	C	4.458388	-0.084129	-0.172144
C	2.515696	-0.385985	1.028995	C	2.416799	-0.328086	1.036738
C	2.004541	-0.207064	-1.439732	C	2.362961	0.559030	-1.284146
H	5.331383	-0.770034	-0.772025	H	5.540315	-0.176597	-0.218763
H	3.811308	-0.456427	-2.641408	H	4.328390	0.631261	-2.181630
H	4.567360	-0.724909	1.600939	H	4.340545	-0.729486	1.905066
N	1.075892	0.003015	-2.339301	N	1.683591	1.112989	-2.281740
P	0.010126	-0.056043	0.517039	P	-0.045265	-0.036518	0.230662
C	1.841918	-0.311093	2.383446	C	1.578414	-0.640365	2.252118
H	2.188488	0.571398	2.933006	H	1.910013	-0.031660	3.101920
C	-1.201631	-1.315148	0.065344	H	0.390013	0.506140	-2.153077
C	-1.626477	-1.400197	-1.267043	H	-0.302133	0.081501	-1.807399
C	-1.709676	-2.182295	1.035352	C	-1.061712	-1.503139	-0.191806
C	-2.568052	-2.362409	-1.614292	C	-2.257515	-1.397465	-0.904732
C	-2.660789	-3.132932	0.675073	C	-0.622134	-2.754140	0.245597
C	-3.089037	-3.220732	-0.646717	C	-3.015583	-2.534459	-1.159248
C	-0.789727	1.532958	0.198860	C	-1.368188	-3.895302	-0.038005
C	-2.091830	1.766938	0.650069	C	-2.569392	-3.784508	-0.731959
C	-0.078330	2.530220	-0.471928				

C	-1.069190	1.457923	0.180541
C	-2.221402	1.495539	0.969074
C	-0.682094	2.577323	-0.559897
C	-2.999791	2.648250	1.005916
C	-1.459282	3.730450	-0.505135
C	-2.616301	3.766593	0.270210
H	0.312322	-2.839069	0.795319
H	-1.012939	-4.867380	0.287958
H	-3.156563	-4.671769	-0.945854
H	-3.951140	-2.447552	-1.702137
H	-2.582981	-0.425528	-1.265807
H	-2.515643	0.626629	1.552572
H	-3.899618	2.673456	1.611735
H	-3.220295	4.667887	0.301165
H	-1.162056	4.603173	-1.077418
H	0.209629	2.530303	-1.182027
H	2.251369	1.238169	-3.115011
H	1.697327	-1.695467	2.537252
N	0.197393	-0.332487	1.896935
H	-0.505909	-0.877305	2.376246

M4NHL2-Pr

SCF energy in gas phase: -1185.886400

SCF energy in solution: -1186.150285

Free energy in solution: -1185.859133

C	1.481234	-0.899980	-0.130645
C	3.438294	-1.826797	-1.188463
C	3.506930	-1.269505	1.166077
C	4.122773	-1.759630	0.016255
C	2.186911	-0.852356	1.071995
C	2.105276	-1.394009	-1.294630
H	5.151649	-2.104725	0.057837
H	3.933087	-2.216780	-2.074050
H	4.037783	-1.224632	2.111986
N	1.484030	-1.443805	-2.532657
P	-0.178798	-0.119782	-0.001100
C	1.377170	-0.305102	2.223157
H	1.734873	0.715405	2.453683
H	0.476768	-1.424122	-2.536557
H	-0.307044	-0.074083	-1.457976
C	-1.878835	-0.865863	0.028798
C	-2.779584	-0.424270	-0.944795
C	-2.285352	-1.842802	0.940108

C	-4.075799	-0.924237	-0.991093
C	-3.573285	-2.371805	0.870772
C	-4.471152	-1.907961	-0.086377
C	-0.127573	1.739776	-0.039987
C	-0.209280	2.532274	1.109866
C	0.032423	2.376193	-1.275518
C	-0.154899	3.920710	1.024507
C	0.100538	3.763229	-1.363755
C	-0.000069	4.539593	-0.212758
H	-1.581259	-2.182332	1.691158
H	-3.876341	-3.146430	1.568523
H	-5.476921	-2.314249	-0.131381
H	-4.774030	-0.556041	-1.736154
H	-2.457300	0.324191	-1.666211
H	-0.314137	2.065153	2.082259
H	-0.228064	4.519104	1.927276
H	0.046843	5.622135	-0.278516
H	0.231490	4.237033	-2.331532
H	0.114510	1.772365	-2.175215
H	1.881751	-2.105720	-3.181508
H	1.534058	-0.915933	3.121837
N	0.009668	-0.358102	1.767307
H	-0.675955	0.054984	2.387401

M4OL2

SCF energy in gas phase: -1204.561599

SCF energy in solution: -1204.831766

Free energy in solution: -1204.576019

C	-1.636093	0.000963	-0.038434
C	-3.578679	0.001607	-1.435587
C	-3.808763	0.001294	1.012624
C	-4.348937	0.001648	-0.300403
C	-2.436593	0.000936	1.116069
C	-2.130894	0.001194	-1.386820
H	-5.430489	0.001952	-0.412282
H	-4.053376	0.001865	-2.413311
H	-4.451819	0.001301	1.884823
N	-1.283975	0.001029	-2.389028
P	0.021720	0.000088	0.455539
C	-1.633936	0.000419	2.396077
H	-1.821326	-0.890826	3.001045
C	1.003645	1.463633	0.088920
C	1.029635	1.967271	-1.216652

C	1.731829	2.075465	1.113565
C	1.798716	3.095855	-1.484113
C	2.496527	3.201713	0.828405
C	2.530395	3.708487	-0.468922
C	1.002110	-1.464399	0.088546
C	1.728708	-2.077850	1.113357
C	1.028544	-1.967181	-1.217347
C	2.492266	-3.204837	0.828040
C	1.796413	-3.096554	-1.484956
C	2.526535	-3.710780	-0.469598
H	1.685389	1.679022	2.123353
H	3.060885	3.685811	1.618652
H	3.126243	4.588767	-0.688854
H	1.822627	3.501264	-2.490301
H	0.434997	1.478669	-1.988052
H	1.681916	-1.682043	2.123375
H	3.055459	-3.690124	1.618386
H	3.121493	-4.591627	-0.689660
H	1.820636	-3.501307	-2.491400
H	0.435133	-1.477348	-1.988893
H	-1.789530	0.001218	-3.273786
H	-1.820678	0.891552	3.001410
O	-0.220512	0.000001	2.057373

M4OL2-TS1

SCF energy in gas phase: -1205.707935

SCF energy in solution: -1205.977639

Free energy in solution: -1205.704465

C	-1.669617	-0.135282	-0.102598
C	-3.798749	-0.341064	-1.231446
C	-3.729502	0.356056	1.103383
C	-4.433202	0.070610	-0.087315
C	-2.358182	0.255678	1.064829
C	-2.375220	-0.537041	-1.295926
H	-5.515602	0.168549	-0.096095
H	-4.375574	-0.568483	-2.123665
H	-4.251523	0.627370	2.014309
N	-1.728786	-1.058107	-2.324064
P	0.056484	0.031083	0.200174
C	-1.453901	0.467358	2.252352
H	-1.653547	-0.273428	3.033609
H	-0.357932	-0.447807	-2.182490
H	0.323513	-0.061261	-1.849881

C	1.026909	1.524713	-0.187840
C	2.210057	1.469572	-0.925134
C	0.567584	2.745109	0.309423
C	2.935983	2.633087	-1.154011
C	1.282895	3.911099	0.055309
C	2.469896	3.854241	-0.670145
C	1.089248	-1.446907	0.152135
C	2.219991	-1.487533	0.971499
C	0.722126	-2.552831	-0.619203
C	2.999324	-2.640050	1.007066
C	1.504409	-3.701796	-0.567693
C	2.640636	-3.744758	0.238639
H	-0.348826	2.784450	0.891704
H	0.917221	4.861191	0.430520
H	3.031976	4.762666	-0.861579
H	3.861145	2.588705	-1.719069
H	2.554300	0.518013	-1.321647
H	2.484372	-0.626723	1.579473
H	3.882160	-2.675278	1.636743
H	3.248263	-4.643685	0.268582
H	1.227682	-4.565746	-1.162841
H	-0.158063	-2.497770	-1.257810
H	-2.328979	-1.177095	-3.135617
H	-1.567622	1.467378	2.687199
O	-0.102852	0.312237	1.819307

M4OL2-Pr

SCF energy in gas phase: -1205.772949

SCF energy in solution: -1206.042748

Free energy in solution: -1205.763946

C	-1.327674	1.036269	-0.093832
C	-3.136206	2.341971	-0.996576
C	-3.222766	1.615616	1.314769
C	-3.785005	2.285717	0.229462
C	-1.991034	1.004628	1.128900
C	-1.893471	1.715671	-1.191015
H	-4.744168	2.783091	0.339525
H	-3.590293	2.876370	-1.826733
H	-3.727224	1.579527	2.275211
N	-1.297931	1.762434	-2.440958
P	0.183449	0.006822	-0.072656
C	-1.218227	0.228231	2.169598
H	-1.714889	-0.740149	2.352869

H	-0.300994	1.617365	-2.472407	C	-1.813483	0.361622	1.897219
H	0.271022	0.008529	-1.521807	C	-2.898980	-0.549087	-2.560854
C	1.905196	0.662781	0.005196	H	-4.629525	-1.499842	-1.564184
C	2.692296	0.546051	-1.144689	C	0.588890	0.216989	2.538439
C	2.451119	1.273063	1.140146	H	0.752393	-0.791127	2.930156
C	4.001381	1.017584	-1.163882	H	-1.076953	0.378437	3.942408
C	3.753540	1.762778	1.113635	H	1.414426	0.855417	2.860408
C	4.531821	1.633205	-0.033974	H	-0.757369	1.846332	3.021366
C	-0.076946	-1.817024	-0.130558	H	-4.883394	0.209040	-1.909893
C	0.142448	-2.643391	0.976689	C	1.308774	1.458801	-0.105212
C	-0.521548	-2.384843	-1.327746	C	2.565270	1.902533	0.316439
C	-0.067915	-4.015883	0.877612	C	0.662300	2.072227	-1.182386
C	-0.756434	-3.753314	-1.418124	C	3.169496	2.977441	-0.325482
C	-0.521953	-4.571643	-0.316076	H	3.075096	1.410559	1.141513
H	1.847605	1.351235	2.034716	C	1.280405	3.142223	-1.824848
H	4.164261	2.242661	1.996418	H	-0.298273	1.688826	-1.520577
H	5.549632	2.010669	-0.047470	C	2.524512	3.596904	-1.394816
H	4.603096	0.908945	-2.060692	H	4.140646	3.330449	0.005343
H	2.278193	0.071514	-2.030657	H	0.787097	3.621795	-2.663710
H	0.481708	-2.197860	1.904602	H	2.997658	4.435018	-1.896500
H	0.119774	-4.652671	1.736568	C	1.377428	-1.423811	0.190557
H	-0.693191	-5.641348	-0.387245	C	2.469763	-1.876600	0.937332
H	-1.116362	-4.180555	-2.348703	C	0.989314	-2.090009	-0.978267
H	-0.694733	-1.745144	-2.189662	C	3.174585	-3.001361	0.522868
H	-1.615782	2.511899	-3.036518	H	2.774583	-1.357483	1.842783
H	-1.184656	0.770860	3.122513	C	1.701768	-3.217681	-1.379196
O	0.081131	0.045112	1.687350	H	0.137976	-1.717814	-1.549909

M5CH₂L2

SCF energy in gas phase: -1246.036367

SCF energy in solution: -1246.312444

Free energy in solution: -1245.999397

C	-1.241893	0.058515	0.624833
C	-3.496328	-0.183458	-0.276589
C	-3.170827	0.368184	2.073542
C	-4.016854	0.075723	0.951960
C	-2.064739	-0.182277	-0.518423
H	-5.094947	0.067024	1.098092
H	-3.604256	0.602850	3.039794
N	-1.683421	-0.392282	-1.751251
P	0.487062	0.063537	0.714139
C	-0.799169	0.753525	2.953839
C	-4.131738	-0.524584	-1.602946

C	-1.813483	0.361622	1.897219
C	-2.898980	-0.549087	-2.560854
H	-4.629525	-1.499842	-1.564184
C	0.588890	0.216989	2.538439
H	0.752393	-0.791127	2.930156
H	-1.076953	0.378437	3.942408
H	1.414426	0.855417	2.860408
H	-0.757369	1.846332	3.021366
H	-4.883394	0.209040	-1.909893
C	1.308774	1.458801	-0.105212
C	2.565270	1.902533	0.316439
C	0.662300	2.072227	-1.182386
C	3.169496	2.977441	-0.325482
H	3.075096	1.410559	1.141513
C	1.280405	3.142223	-1.824848
H	-0.298273	1.688826	-1.520577
C	2.524512	3.596904	-1.394816
H	4.140646	3.330449	0.005343
H	0.787097	3.621795	-2.663710
H	2.997658	4.435018	-1.896500
C	1.377428	-1.423811	0.190557
C	2.469763	-1.876600	0.937332
C	0.989314	-2.090009	-0.978267
C	3.174585	-3.001361	0.522868
H	2.774583	-1.357483	1.842783
C	1.701768	-3.217681	-1.379196
H	0.137976	-1.717814	-1.549909
C	2.788149	-3.671961	-0.635038
H	4.021334	-3.353486	1.102914
H	1.403954	-3.744699	-2.279825
H	3.336456	-4.551670	-0.957189
H	-2.960865	0.262705	-3.298836
H	-2.857905	-1.482561	-3.135317

M5CH₂L2-TS1

SCF energy in gas phase: -1247.176994

SCF energy in solution: -1247.448376

Free energy in solution: -1247.119740

C	-1.257741	0.043810	0.514731
C	-3.581462	-0.141052	-0.203069
C	-3.043756	0.939950	1.899255
C	-3.989793	0.500488	0.935637
C	-2.199908	-0.411473	-0.435548

H	-5.047689	0.682223	1.109911	SCF energy in solution: -1247.491148			
H	-3.377303	1.439423	2.803139	Free energy in solution: -1247.154614			
N	-1.942367	-1.057039	-1.577930				
P	0.502610	0.056186	0.388709	C	-1.271636	-0.025150	0.519212
C	-0.586605	1.192316	2.594896	C	-3.643067	-0.360665	0.124809
C	-4.327053	-0.740437	-1.372941	C	-2.917063	0.769835	2.124485
C	-1.700734	0.722255	1.679648	C	-3.946408	0.262641	1.320739
C	-3.174733	-1.029797	-2.376859	C	-2.307023	-0.500910	-0.289252
H	-4.816670	-1.674840	-1.073522	H	-4.982294	0.365130	1.633545
C	0.688774	0.423274	2.214886	H	-3.146110	1.275150	3.057953
H	0.719896	-0.541512	2.730309	N	-2.246533	-1.185313	-1.501968
H	-0.850454	1.038804	3.645427	P	0.523396	-0.023790	0.126376
H	1.604218	0.973222	2.444136	C	-0.394461	1.140641	2.476242
H	-0.427145	2.269582	2.463282	C	-4.526255	-1.029544	-0.902840
H	-5.095288	-0.081896	-1.786423	C	-1.596620	0.619967	1.721098
H	-0.701183	-0.607453	-1.827227	C	-3.580033	-1.127635	-2.115245
H	0.155410	-0.211639	-1.639007	H	-4.815067	-2.030947	-0.561940
C	1.350486	1.495580	-0.340402	C	0.797400	0.296984	2.034382
C	2.627349	1.392774	-0.894400	H	0.758139	-0.677237	2.536565
C	0.702107	2.731907	-0.300786	H	-0.567009	1.109280	3.557194
C	3.257045	2.528669	-1.393724	H	1.743181	0.776648	2.297776
H	3.118587	0.426087	-0.956581	H	-0.230364	2.193938	2.208452
C	1.337006	3.863025	-0.805519	H	-5.438884	-0.474630	-1.131091
H	-0.307986	2.804441	0.095555	H	-1.456016	-0.965491	-2.093892
C	2.616213	3.764359	-1.346688	H	0.191700	-0.280668	-1.302234
H	4.248210	2.445335	-1.827951	C	1.218098	1.606795	-0.404443
H	0.827634	4.821048	-0.781017	C	2.459566	2.076262	0.025443
H	3.108756	4.647475	-1.740497	C	0.461446	2.382808	-1.284307
C	1.409115	-1.501061	0.197704	C	2.939851	3.304805	-0.423323
C	2.668602	-1.625394	0.792401	H	3.066509	1.475045	0.696133
C	0.826893	-2.592161	-0.453345	C	0.922206	3.626011	-1.704569
C	3.359550	-2.831458	0.710161	H	-0.495606	2.003830	-1.637661
H	3.114995	-0.782758	1.315012	C	2.166841	4.085387	-1.278046
C	1.514004	-3.800114	-0.507221	H	3.915971	3.653154	-0.100962
H	-0.154354	-2.487356	-0.910656	H	0.316904	4.232595	-2.370767
C	2.780246	-3.918955	0.063086	H	2.535427	5.048547	-1.616448
H	4.343727	-2.921990	1.158065	C	1.646220	-1.501167	0.046292
H	1.060109	-4.651058	-1.004286	C	2.763404	-1.638114	0.875523
H	3.314756	-4.861908	0.006103	C	1.373663	-2.500611	-0.889943
H	-3.117898	-0.232759	-3.132267	C	3.603206	-2.741061	0.753580
H	-3.316547	-1.975011	-2.908036	H	2.987203	-0.880872	1.619114
				C	2.190788	-3.623343	-0.987873
M5CH₂L2-Pr				H	0.506940	-2.398992	-1.537810
SCF energy in gas phase: -1247.220856				C	3.313251	-3.739491	-0.172619

H	4.480405	-2.823672	1.387518
H	1.955753	-4.403284	-1.705282
H	3.960642	-4.606720	-0.257437
H	-3.687022	-0.232889	-2.746066
H	-3.765850	-2.010539	-2.730575

M5NHL2

SCF energy in gas phase: -1262.076521

SCF energy in solution: -1262.362691

Free energy in solution: -1262.062097

C	2.114843	-2.645289	-1.823610
H	0.726919	-0.981765	-1.914700
C	2.904248	-3.443840	-0.996524
H	3.560695	-3.835554	1.016198
H	2.068161	-2.847453	-2.888618
H	3.477307	-4.261354	-1.422965
H	-2.731413	0.697665	-3.403642
H	-2.590715	-1.052737	-3.404629
N	0.482480	-0.061833	2.440530
H	1.160112	0.522232	2.912451

C	-1.245595	-0.080633	0.584614
C	-3.428756	-0.257245	-0.468432
C	-3.228827	-0.265189	1.967167
C	-4.008626	-0.319375	0.760719
C	-1.990804	-0.139313	-0.630346
H	-5.089373	-0.412734	0.845558
H	-3.715177	-0.311399	2.935424
N	-1.533258	-0.087465	-1.850125
P	0.460127	0.001734	0.758873
C	-0.888084	-0.036590	3.009781
C	-3.987000	-0.287681	-1.871575
C	-1.869328	-0.142000	1.858477
C	-2.693531	-0.180473	-2.745755
H	-4.539656	-1.211083	-2.072662
H	-1.008598	-0.869262	3.709943
H	-1.045306	0.897089	3.561483
H	-4.674546	0.544571	-2.054808
C	1.230571	1.514351	0.132177
C	2.621890	1.641729	0.072245
C	0.403653	2.565671	-0.270426
C	3.185575	2.837546	-0.358681
H	3.258570	0.804584	0.348397
C	0.975521	3.754053	-0.714545
H	-0.674323	2.432700	-0.249609
C	2.361155	3.891111	-0.750836
H	4.264437	2.944602	-0.401454
H	0.339523	4.570549	-1.039710
H	2.802335	4.820122	-1.098130
C	1.438553	-1.355262	0.089220
C	2.213402	-2.162275	0.924332
C	1.379032	-1.592416	-1.290663
C	2.953021	-3.205841	0.374523
H	2.219110	-1.977917	1.994360

M5NHL2-TS1

SCF energy in gas phase: -1263.220001

SCF energy in solution: -1263.500257

Free energy in solution: -1263.182732

C	-1.307507	0.238769	0.466154
C	-3.615223	0.312817	-0.321109
C	-3.058781	1.175613	1.874534
C	-4.003139	0.909992	0.846971
C	-2.257829	-0.085060	-0.533156
H	-5.044987	1.180222	1.001880
H	-3.380030	1.615233	2.813251
N	-2.033693	-0.713240	-1.686851
P	0.446891	0.097833	0.417561
C	-0.630321	1.050942	2.675901
C	-4.380097	-0.147011	-1.540825
C	-1.737752	0.850994	1.667194
C	-3.232886	-0.539752	-2.515997
H	-4.992693	-1.022797	-1.296092
H	-0.867599	0.520339	3.606042
H	-0.521848	2.116510	2.922520
H	-5.045587	0.615585	-1.953765
H	-0.672140	-0.416019	-1.843301
H	0.164355	-0.156061	-1.588120
C	1.632540	1.294510	-0.308431
C	2.538166	0.909486	-1.299263
C	1.630312	2.611222	0.155126
C	3.446264	1.830931	-1.806437
H	2.517730	-0.109998	-1.674811
C	2.521749	3.540886	-0.376684
H	0.923896	2.914960	0.923557
C	3.434781	3.148903	-1.350225
H	4.157012	1.523998	-2.566833

H	2.504006	4.567680	-0.026123	C	1.453895	2.668077	0.597709
H	4.136283	3.869827	-1.757625	C	3.049751	2.631788	-1.681966
C	1.130864	-1.575509	0.285430	H	2.278616	0.648001	-1.996005
C	2.378952	-1.832866	0.855352	C	2.201501	3.792347	0.252607
C	0.398581	-2.607417	-0.306264	H	0.836098	2.683071	1.490287
C	2.906266	-3.120239	0.820972	C	3.009593	3.771055	-0.880298
H	2.942343	-1.030352	1.325122	H	3.679495	2.610184	-2.565799
C	0.926763	-3.894280	-0.323737	H	2.157471	4.682351	0.872555
H	-0.567154	-2.395183	-0.761168	H	3.603634	4.641162	-1.141602
C	2.178131	-4.150998	0.233338	C	1.395178	-1.581738	0.117781
H	3.880269	-3.316989	1.257054	C	1.839588	-2.240026	1.269419
H	0.361201	-4.699096	-0.781884	C	1.670345	-2.156594	-1.127827
H	2.586506	-5.156378	0.208740	C	2.552223	-3.431863	1.173413
H	-3.070243	0.258319	-3.254649	H	1.604935	-1.809480	2.235007
H	-3.457085	-1.454914	-3.071297	C	2.387266	-3.345307	-1.225985
N	0.589342	0.518872	2.069445	H	1.307866	-1.675005	-2.031439
H	1.453858	0.936603	2.382868	C	2.832700	-3.984878	-0.073064

M5NHL2-Pr

SCF energy in gas phase: -1263.273476

SCF energy in solution: -1263.551709

Free energy in solution: -1263.226344

C	-1.353595	0.063816	0.417137
C	-3.695072	-0.036855	-0.219222
C	-3.106670	0.499077	2.053525
C	-4.079158	0.282226	1.069684
C	-2.335112	-0.156021	-0.556436
H	-5.133984	0.367628	1.317206
H	-3.395057	0.751462	3.069616
N	-2.205236	-0.535398	-1.885729
P	0.454893	0.017919	0.171587
C	-0.620359	0.596711	2.673013
C	-4.514983	-0.375562	-1.443104
C	-1.765938	0.386855	1.713128
C	-3.470775	-0.249592	-2.569312
H	-4.884296	-1.406024	-1.377979
H	-0.782323	-0.014006	3.574327
H	-0.616475	1.649596	3.004478
H	-5.373523	0.281911	-1.596332
H	-1.344778	-0.289039	-2.353572
H	0.269748	-0.108548	-1.282191
C	1.479329	1.525319	-0.204441
C	2.270700	1.526901	-1.355729

C	1.453895	2.668077	0.597709
C	3.049751	2.631788	-1.681966
H	2.278616	0.648001	-1.996005
C	2.201501	3.792347	0.252607
H	0.836098	2.683071	1.490287
C	3.009593	3.771055	-0.880298
H	3.679495	2.610184	-2.565799
H	2.157471	4.682351	0.872555
H	3.603634	4.641162	-1.141602
C	1.395178	-1.581738	0.117781
C	1.839588	-2.240026	1.269419
C	1.670345	-2.156594	-1.127827
C	2.552223	-3.431863	1.173413
H	1.604935	-1.809480	2.235007
C	2.387266	-3.345307	-1.225985
H	1.307866	-1.675005	-2.031439
C	2.832700	-3.984878	-0.073064
H	2.886601	-3.932034	2.077129
H	2.589920	-3.774850	-2.202089
H	3.388633	-4.914682	-0.145091
H	-3.480048	0.771610	-2.978075
H	-3.639704	-0.953269	-3.387327
N	0.575596	0.218539	1.960213
H	1.428821	0.624782	2.321499

M5OL2

SCF energy in gas phase: -1281.945713

SCF energy in solution: -1282.231120

Free energy in solution: -1281.941851

C	1.195701	0.000188	0.614460
C	3.478277	0.000543	-0.211636
C	3.044023	-0.000285	2.191330
C	3.938418	0.000113	1.069412
C	2.061203	0.000515	-0.518083
H	5.009550	0.000110	1.258836
H	3.432641	-0.000623	3.203472
N	1.732620	0.000735	-1.783307
P	-0.522109	-0.000034	0.693247
C	0.596696	-0.000541	2.980922
C	4.180175	0.001068	-1.549362
C	1.696814	-0.000229	1.942253
C	2.982794	0.001029	-2.554423
H	4.818199	0.881901	-1.674185

H	0.620600	0.890466	3.613411	C	4.433159	0.030087	-1.470812
H	0.620559	-0.891935	3.612868	C	1.680119	-0.744249	1.704107
H	4.818720	-0.879315	-1.674674	C	3.324033	0.401221	-2.499537
C	-1.348645	-1.457243	0.044099	H	5.063445	0.899951	-1.252244
C	-2.363711	-2.092413	0.763582	H	0.661113	-0.124585	3.505307
C	-0.939840	-1.932092	-1.207993	H	0.386039	-1.827735	3.078898
C	-2.978735	-3.216755	0.222221	H	5.088306	-0.769812	-1.825672
H	-2.655325	-1.717428	1.740298	H	0.661483	0.339145	-1.873110
C	-1.567592	-3.055554	-1.736299	H	-0.152962	0.133697	-1.614227
H	-0.130975	-1.430839	-1.742045	C	-1.615419	-1.310503	-0.297906
C	-2.582459	-3.693686	-1.025681	C	-2.442664	-1.007970	-1.381171
H	-3.764439	-3.722283	0.773962	C	-1.689236	-2.566056	0.307022
H	-1.256892	-3.438111	-2.702838	C	-3.343252	-1.955663	-1.852149
H	-3.064119	-4.571843	-1.444080	H	-2.371432	-0.032383	-1.854343
C	-1.349169	1.457004	0.044454	C	-2.573103	-3.522716	-0.185731
C	-2.363421	2.092703	0.764627	H	-1.063747	-2.791747	1.164860
C	-0.941581	1.931101	-1.208319	C	-3.402541	-3.216357	-1.260378
C	-2.978849	3.216805	0.223240	H	-3.991884	-1.714004	-2.687622
H	-2.654043	1.718336	1.741877	H	-2.620334	-4.502821	0.277497
C	-1.569747	3.054330	-1.736642	H	-4.097590	-3.959480	-1.638012
H	-0.133194	1.429572	-1.742858	C	-1.140904	1.582742	0.227286
C	-2.583817	3.692967	-1.025352	C	-2.379968	1.839965	0.817250
H	-3.763919	3.722770	0.775485	C	-0.421534	2.603869	-0.399229
H	-1.259986	3.436280	-2.703722	C	-2.910847	3.125708	0.767114
H	-3.065842	4.570923	-1.443753	H	-2.920464	1.040891	1.317235
H	3.018860	-0.876929	-3.212288	C	-0.957830	3.886213	-0.436372
H	3.018597	0.879160	-3.212067	H	0.539271	2.385605	-0.862291
O	-0.693115	-0.000283	2.299483	C	-2.200085	4.146025	0.140869
M5OL2-TS1				H	-3.875835	3.329232	1.219540
SCF energy in gas phase: -1283.093418				H	-0.407348	4.684645	-0.922878
SCF energy in solution: -1283.377393				H	-2.614882	5.148350	0.101797
Free energy in solution: -1283.071178				H	3.183520	-0.414672	-3.222556
C	1.293398	-0.211655	0.452510	H	3.575403	1.299076	-3.071436
C	3.623661	-0.349988	-0.252131	O	-0.672003	-0.452553	1.974050
C	2.985560	-1.073139	1.977222	M5OL2-Pr			
C	3.964982	-0.878339	0.960904	SCF energy in gas phase: -1283.159668			
C	2.275064	0.045686	-0.538374	SCF energy in solution: -1283.444822			
H	4.998503	-1.147184	1.166035	Free energy in solution: -1283.131284			
H	3.275534	-1.452247	2.951403	C	1.292337	0.017434	0.427194
N	2.092665	0.605720	-1.726185	C	3.674711	-0.090148	0.006594
P	-0.449438	-0.078293	0.375145	C	2.879474	0.592808	2.179924
C	0.522874	-0.819735	2.670426	C	3.936990	0.327288	1.298534

C	2.351515	-0.235395	-0.445356	Free energy in solution: -1285.282909			
H	4.964536	0.437750	1.634863				
H	3.077948	0.910687	3.198968	C	-1.008211	-0.357453	0.821325
N	2.335836	-0.619465	-1.780597	C	-3.294724	-0.322091	0.015978
P	-0.487401	-0.025588	0.058149	C	-2.775690	-0.955169	2.344173
C	0.309934	0.671934	2.516244	C	-3.679302	-0.720313	1.268949
C	4.600133	-0.403397	-1.147098	C	-1.881133	-0.152774	-0.303331
C	1.578107	0.429225	1.729276	H	-4.744410	-0.860028	1.451258
C	3.662309	-1.155412	-2.112267	H	-3.138733	-1.272562	3.315309
H	4.959192	0.524801	-1.607502	P	0.700469	-0.062797	0.790900
H	0.165053	1.756651	2.657703	C	-0.312607	-1.002962	3.091011
H	0.366757	0.212778	3.511419	H	-0.083526	-2.074005	3.125517
H	5.471095	-0.999721	-0.867053	C	-1.437827	-0.764599	2.104938
H	1.529545	-1.135585	-2.102940	C	-2.294624	0.398082	-2.558356
H	-0.225177	-0.181478	-1.365810	C	-4.272880	-0.069252	-1.104064
C	-1.529470	-1.546132	0.009965	C	-3.606500	-0.383736	-2.444439
C	-1.983202	-1.976131	-1.240924	H	-2.531831	1.473612	-2.630682
C	-1.878065	-2.283446	1.147165	H	-5.182389	-0.662320	-0.957199
C	-2.777834	-3.112012	-1.359258	H	-4.270763	-0.139031	-3.279883
H	-1.717899	-1.409120	-2.129387	N	-1.365838	0.162215	-1.466231
C	-2.655888	-3.431147	1.025931	H	-1.792830	0.141535	-3.499751
H	-1.536921	-1.943423	2.115870	H	-3.387333	-1.457019	-2.497520
C	-3.110155	-3.845511	-0.223648	H	-4.580791	0.986134	-1.105431
H	-3.132028	-3.426476	-2.335752	H	-0.589993	-0.698611	4.103930
H	-2.913044	-4.001506	1.912982	C	1.186283	1.598965	0.256114
H	-3.722031	-4.738106	-0.311223	C	2.512050	1.892400	-0.068520
C	-1.313119	1.583768	-0.289553	C	0.209540	2.596425	0.211239
C	-2.158793	2.201765	0.638161	C	2.865314	3.192926	-0.416408
C	-1.086038	2.202643	-1.522332	H	3.263469	1.107194	-0.063491
C	-2.774249	3.410704	0.327883	C	0.568803	3.891892	-0.144136
H	-2.327689	1.719762	1.593707	H	-0.822519	2.343796	0.436428
C	-1.684162	3.422806	-1.822414	C	1.894477	4.190312	-0.453201
H	-0.428492	1.727603	-2.245818	H	3.895469	3.424375	-0.666606
C	-2.535174	4.024735	-0.899230	H	-0.188643	4.667331	-0.191595
H	-3.440519	3.875880	1.047657	H	2.169966	5.202437	-0.732201
H	-1.491575	3.899758	-2.778217	C	1.747782	-1.235611	-0.111151
H	-3.012065	4.970970	-1.135766	C	2.968993	-1.684574	0.401433
H	3.712106	-2.236457	-1.916986	C	1.293846	-1.689765	-1.356642
H	3.902196	-0.979642	-3.162997	C	3.737428	-2.587354	-0.328154
O	-0.754624	0.112085	1.801186	H	3.329706	-1.332752	1.363907
				C	2.068875	-2.595273	-2.074054
M6CH₂L2				H	0.346959	-1.310170	-1.739734
SCF energy in gas phase: -1285.340219				C	3.285606	-3.043301	-1.563970
SCF energy in solution: -1285.625869				H	4.684824	-2.936055	0.069682

H	1.720060	-2.952341	-3.037458
H	3.884256	-3.749684	-2.130397
C	0.933816	-0.227103	2.607919
H	0.941762	0.792483	3.004021
H	1.875243	-0.705899	2.882079

M6CH₂L2-TS1

SCF energy in gas phase: -1286.481011

SCF energy in solution: -1286.764839

Free energy in solution: -1286.408137

C	-1.001869	-0.456380	0.628577
C	-3.374062	-0.615572	0.109651
C	-2.430118	-1.825383	2.022436
C	-3.505661	-1.471043	1.177926
C	-2.093719	-0.031435	-0.198890
H	-4.492827	-1.881981	1.384225
H	-2.586957	-2.469887	2.880893
P	0.702244	-0.034111	0.469948
C	0.076300	-1.598031	2.530142
H	0.526797	-2.541066	2.194208
C	-1.183407	-1.317850	1.735111
C	-2.947162	1.163504	-2.098640
C	-4.531874	-0.238089	-0.781828
C	-4.017825	0.075509	-2.187630
H	-3.426258	2.111199	-1.806759
H	-5.272115	-1.045044	-0.797592
H	-4.833964	0.399427	-2.840950
N	-1.877328	0.849482	-1.168988
H	0.258615	0.208368	-1.596104
H	-0.594820	0.573332	-1.555658
H	-2.499902	1.336474	-3.084914
H	-3.579504	-0.829526	-2.624760
H	-5.040122	0.652295	-0.385991
H	-0.143045	-1.705302	3.596188
C	1.139702	1.711653	0.276247
C	2.144268	2.123723	-0.599120
C	0.441144	2.648032	1.039277
C	2.467515	3.473138	-0.688612
H	2.652058	1.392497	-1.221552
C	0.759099	3.998816	0.933974
H	-0.365167	2.322848	1.691782
C	1.776954	4.409758	0.077979
H	3.250441	3.795954	-1.366975

H	0.207292	4.729279	1.516289
H	2.025839	5.463220	-0.000706
C	1.881853	-1.171392	-0.336461
C	3.246074	-1.091111	-0.045588
C	1.405511	-2.177412	-1.177341
C	4.132636	-2.000732	-0.617370
H	3.621664	-0.312953	0.614989
C	2.289990	-3.102370	-1.721314
H	0.344248	-2.215163	-1.407532
C	3.653674	-3.009422	-1.448553
H	5.194470	-1.924743	-0.406850
H	1.916809	-3.889282	-2.368432
H	4.344322	-3.723957	-1.884802
C	1.044307	-0.437216	2.254196
H	0.770542	0.439004	2.849825
H	2.089228	-0.683867	2.449858

M6CH₂L2-Pr

SCF energy in gas phase: -1286.519640

SCF energy in solution: -1286.799943

Free energy in solution: -1286.436571

C	-1.122900	-0.289825	0.602973
C	-3.526082	-0.282201	0.249264
C	-2.554233	-1.565396	2.082948
C	-3.651093	-1.136983	1.337111
C	-2.239089	0.157294	-0.143237
H	-4.650049	-1.468841	1.613070
H	-2.682141	-2.220284	2.939239
P	0.647663	0.005946	0.223773
C	-0.005350	-1.493317	2.421098
H	0.367701	-2.452232	2.034943
C	-1.290414	-1.128732	1.709001
C	-3.214005	1.480626	-2.008432
C	-4.733873	0.180854	-0.532128
C	-4.352358	0.467008	-1.983754
H	-3.589321	2.450748	-1.649524
H	-5.520301	-0.578726	-0.478470
H	-5.205603	0.858201	-2.544961
N	-2.102817	1.029723	-1.192633
H	0.311579	0.206765	-1.221218
H	-1.166425	1.223550	-1.510045
H	-2.853859	1.631765	-3.030478
H	-4.024043	-0.459202	-2.468161

H	-5.148633	1.095500	-0.086741	C	-2.212431	-0.054358	-2.661479
H	-0.182590	-1.627342	3.493319	C	-4.212151	0.506832	-1.262391
C	1.471823	1.659391	0.193258	C	-3.653333	-0.447981	-2.320291
C	2.298655	1.940940	-0.898229	H	-2.229725	0.920221	-3.179511
C	1.287924	2.630996	1.178243	H	-5.220582	0.214008	-0.949463
C	2.964667	3.158505	-0.984259	H	-4.274753	-0.441212	-3.221829
H	2.418293	1.194040	-1.680471	N	-1.323157	0.001965	-1.513699
C	1.924825	3.866163	1.072764	H	-1.800022	-0.769811	-3.384072
H	0.631204	2.438028	2.019890	H	-3.657619	-1.470628	-1.922949
C	2.773437	4.125847	0.001047	H	-4.295892	1.509903	-1.703887
H	3.623835	3.358504	-1.823186	H	-0.376968	1.436430	3.757668
H	1.760164	4.623864	1.832246	N	0.879572	0.344632	2.448245
H	3.280144	5.083059	-0.071789	H	1.573380	-0.219737	2.920110
C	1.708508	-1.399744	-0.360974	C	1.709263	1.250925	-0.105893
C	3.036667	-1.554212	0.039947	C	1.686984	1.240875	-1.506649
C	1.155447	-2.310051	-1.263922	C	2.523277	2.148427	0.588091
C	3.802254	-2.605880	-0.458560	C	2.491509	2.136600	-2.202051
H	3.483919	-0.839735	0.725511	H	1.008961	0.563197	-2.019904
C	1.906219	-3.384540	-1.729940	C	3.331049	3.033664	-0.120872
H	0.130810	-2.166395	-1.601627	H	2.511203	2.151999	1.673432
C	3.233643	-3.529626	-1.331402	C	3.315241	3.025717	-1.512749
H	4.841331	-2.706082	-0.160832	H	2.473001	2.143946	-3.286921
H	1.462323	-4.101538	-2.413516	H	3.967460	3.730962	0.414209
H	3.826223	-4.358132	-1.706582	H	3.942158	3.719333	-2.064492
C	0.982294	-0.376243	2.100186	C	1.203225	-1.558442	0.295036
H	0.731063	0.499441	2.706346	C	2.560655	-1.850486	0.135973
H	2.017366	-0.647461	2.316851	C	0.236582	-2.547331	0.095058

M6NHL2

SCF energy in gas phase: -1301.381831

SCF energy in solution: -1301.675592

Free energy in solution: -1301.345008

C	-1.048065	0.331307	0.812860
C	-3.279988	0.538067	-0.077646
C	-2.840261	0.806490	2.340867
C	-3.700240	0.773252	1.207019
C	-1.873055	0.282246	-0.357303
H	-4.764365	0.944240	1.366601
H	-3.235680	0.991087	3.333313
P	0.660825	0.091768	0.797846
C	-0.406637	0.517194	3.163481
H	-0.574267	-0.322874	3.847011
C	-1.503129	0.575050	2.120230

C	-2.212431	-0.054358	-2.661479
C	-4.212151	0.506832	-1.262391
C	-3.653333	-0.447981	-2.320291
H	-2.229725	0.920221	-3.179511
H	-5.220582	0.214008	-0.949463
H	-4.274753	-0.441212	-3.221829
N	-1.323157	0.001965	-1.513699
H	-1.800022	-0.769811	-3.384072
H	-3.657619	-1.470628	-1.922949
H	-4.295892	1.509903	-1.703887
H	-0.376968	1.436430	3.757668
N	0.879572	0.344632	2.448245
H	1.573380	-0.219737	2.920110
C	1.709263	1.250925	-0.105893
C	1.686984	1.240875	-1.506649
C	2.523277	2.148427	0.588091
C	2.491509	2.136600	-2.202051
H	1.008961	0.563197	-2.019904
C	3.331049	3.033664	-0.120872
H	2.511203	2.151999	1.673432
C	3.315241	3.025717	-1.512749
H	2.473001	2.143946	-3.286921
H	3.967460	3.730962	0.414209
H	3.942158	3.719333	-2.064492
C	1.203225	-1.558442	0.295036
C	2.560655	-1.850486	0.135973
C	0.236582	-2.547331	0.095058
C	2.953581	-3.143724	-0.194056
H	3.306087	-1.067964	0.255909
C	0.636917	-3.835256	-0.245443
H	-0.814878	-2.289260	0.183128
C	1.991002	-4.133358	-0.383508
H	4.006555	-3.376083	-0.314561
H	-0.109133	-4.605019	-0.412335
H	2.297814	-5.139676	-0.650669

M6NHL2-TS1

SCF energy in gas phase: -1302.523636

SCF energy in solution: -1302.815757

Free energy in solution: -1302.469198

C	-1.078506	-0.218579	0.643205
C	-3.463007	-0.154391	0.161324
C	-2.639531	-1.201557	2.219359

C	-3.677325	-0.842234	1.330752	H	3.632752	-4.415182	-1.691676
C	-2.128385	0.243528	-0.226465				
H	-4.702675	-1.103444	1.588164	M6NHL2-Pr			
H	-2.854720	-1.692016	3.162458	SCF energy in gas phase: -1302.574428			
P	0.662684	-0.065320	0.460797	SCF energy in solution: -1302.862803			
C	-0.124844	-1.186437	2.685584	Free energy in solution: -1302.507965			
H	0.119278	-2.258027	2.625857				
C	-1.351296	-0.887538	1.856114	C	-1.094962	0.030426	0.667027
C	-2.891359	1.307960	-2.232035	C	-3.497479	0.175973	0.355699
C	-4.590692	0.239550	-0.761426	C	-2.581066	-0.833320	2.378889
C	-4.073846	0.339804	-2.196441	C	-3.659281	-0.455094	1.585772
H	-3.260110	2.326999	-2.034498	C	-2.193585	0.426373	-0.130621
H	-5.410342	-0.482340	-0.680100	H	-4.673336	-0.641083	1.934019
H	-4.862591	0.677423	-2.875988	H	-2.732778	-1.308424	3.343192
N	-1.839951	0.977096	-1.288218	P	0.684940	0.043128	0.203156
H	0.257943	0.100333	-1.607992	C	-0.026201	-0.910795	2.637366
H	-0.515600	0.524733	-1.626210	H	0.133136	-2.004274	2.595811
H	-2.452395	1.332176	-3.237062	C	-1.302990	-0.574756	1.904395
H	-3.742025	-0.648945	-2.534973	C	-3.136516	1.698473	-2.011463
H	-4.997307	1.216532	-0.464814	C	-4.713912	0.597096	-0.444043
H	-0.296210	-0.938218	3.738141	C	-4.375608	0.817846	-1.916475
N	0.946038	-0.350731	2.130462	H	-3.350793	2.676432	-1.549229
H	1.879665	-0.672605	2.361346	H	-5.498768	-0.159230	-0.338886
C	1.459699	1.540859	0.195897	H	-5.213500	1.285894	-2.440683
C	2.163108	1.844559	-0.972067	N	-2.026272	1.027533	-1.365270
C	1.365432	2.480088	1.225197	H	0.358312	0.304917	-1.198666
C	2.776728	3.084968	-1.103722	H	-1.106648	1.390265	-1.557999
H	2.217749	1.112895	-1.772456	H	-2.864309	1.878741	-3.055266
C	1.964440	3.728106	1.077574	H	-4.162589	-0.139671	-2.403324
H	0.828348	2.222927	2.131986	H	-5.122404	1.527875	-0.028406
C	2.672002	4.028089	-0.082643	H	-0.111765	-0.633226	3.695981
H	3.327682	3.320306	-2.008199	N	0.994188	-0.146046	1.961078
H	1.878817	4.463711	1.870420	H	1.943111	-0.323133	2.266961
H	3.142219	5.000053	-0.194562	C	1.895656	1.444575	0.087031
C	1.621183	-1.405781	-0.319885	C	2.520925	1.641798	-1.147717
C	3.018021	-1.376138	-0.307130	C	2.194755	2.304796	1.146454
C	0.950492	-2.522979	-0.821759	C	3.453912	2.658688	-1.316940
C	3.739114	-2.457322	-0.808488	H	2.275127	0.984048	-1.979081
H	3.545062	-0.506707	0.079858	C	3.103956	3.345888	0.967502
C	1.675859	-3.605306	-1.306639	H	1.703953	2.149489	2.100278
H	-0.136553	-2.526231	-0.844096	C	3.741141	3.518100	-0.258000
C	3.069506	-3.572351	-1.304106	H	3.949063	2.787651	-2.274249
H	4.823970	-2.427398	-0.810287	H	3.317093	4.021900	1.789827
H	1.153418	-4.473111	-1.696170	H	4.458286	4.322245	-0.390592

C	1.309982	-1.617785	-0.358013
C	2.118730	-2.442053	0.431030
C	0.922091	-2.078560	-1.620477
C	2.547919	-3.680576	-0.038214
H	2.418330	-2.119234	1.421388
C	1.330748	-3.324989	-2.084705
H	0.283545	-1.452290	-2.238091
C	2.153120	-4.125787	-1.296432
H	3.186653	-4.300548	0.583060
H	1.009973	-3.669445	-3.062784
H	2.482795	-5.094121	-1.659648

M6OL2

SCF energy in gas phase: -1321.250140

SCF energy in solution: -1321.546267

Free energy in solution: -1321.227671

C	-1.009872	0.371459	0.781835
C	-3.300159	0.560912	0.053319
C	-2.675029	0.978201	2.409385
C	-3.619718	0.881278	1.348024
C	-1.920154	0.276023	-0.320094
H	-4.667116	1.075670	1.575616
H	-2.989821	1.237956	3.413403
P	0.686767	0.085818	0.717000
C	-0.176565	0.732771	3.034427
H	-0.284611	0.017748	3.854094
C	-1.363112	0.716509	2.098271
C	-2.440050	-0.172201	-2.572101
C	-4.321925	0.471290	-1.051835
C	-3.849426	-0.540133	-2.098987
H	-2.496187	0.774330	-3.136763
H	-5.302979	0.201043	-0.645838
H	-4.539284	-0.575751	-2.948431
N	-1.462726	-0.059105	-1.501750
H	-2.083799	-0.925444	-3.285820
H	-3.824497	-1.541199	-1.650468
H	-4.437973	1.450642	-1.536897
H	0.010401	1.727442	3.449156
C	1.739474	1.222197	-0.197373
C	1.525688	1.383129	-1.572016
C	2.741951	1.936090	0.464300
C	2.332284	2.269020	-2.278204
H	0.713675	0.837083	-2.049380

C	3.546133	2.812796	-0.258486
H	2.880748	1.806749	1.533226
C	3.340767	2.977227	-1.625950
H	2.170570	2.410995	-3.341711
H	4.329135	3.368575	0.246846
H	3.966513	3.664427	-2.186814
C	1.195722	-1.582972	0.286828
C	2.552005	-1.918189	0.242184
C	0.213057	-2.538934	0.019473
C	2.925409	-3.226238	-0.043069
H	3.308587	-1.159359	0.424766
C	0.597148	-3.842703	-0.278429
H	-0.832369	-2.245509	0.021386
C	1.947068	-4.184946	-0.303053
H	3.975655	-3.496795	-0.070730
H	-0.157863	-4.590877	-0.495331
H	2.240372	-5.204131	-0.534565
O	1.009281	0.349672	2.286352

M6OL2-TS1

SCF energy in gas phase: -1322.395278

SCF energy in solution: -1322.692497

Free energy in solution: -1322.359714

C	-1.056835	-0.139391	0.642670
C	-3.457892	-0.141968	0.243216
C	-2.545492	-1.032190	2.342176
C	-3.619028	-0.747284	1.463306
C	-2.140786	0.246176	-0.227824
H	-4.630789	-1.002240	1.775034
H	-2.722791	-1.457899	3.323687
P	0.674993	-0.031225	0.426586
C	-0.006511	-0.940496	2.693499
H	0.260678	-2.003891	2.743506
C	-1.279885	-0.724694	1.909725
C	-2.996102	1.162626	-2.260159
C	-4.625240	0.174903	-0.660132
C	-4.164205	0.186835	-2.117081
H	-3.369017	2.188130	-2.108533
H	-5.430424	-0.550046	-0.499928
H	-4.982840	0.470413	-2.785887
N	-1.901571	0.900442	-1.344378
H	0.281671	0.091967	-1.670970
H	-0.479601	0.461088	-1.693343

H	-2.600953	1.131163	-3.282870	C	-3.289188	1.409885	-1.992767
H	-3.832644	-0.818480	-2.403625	C	-4.731862	0.281644	-0.315250
H	-5.034632	1.164560	-0.413382	C	-4.470270	0.466146	-1.808453
H	-0.075792	-0.546475	3.710567	H	-3.538418	2.392191	-1.558784
C	1.500576	1.538789	0.100901	H	-5.474351	-0.505952	-0.150076
C	2.338508	1.732463	-0.997469	H	-5.355138	0.867451	-2.310187
C	1.291485	2.565192	1.023619	N	-2.114478	0.829115	-1.371827
C	2.971066	2.958553	-1.169169	H	0.335980	0.232038	-1.286949
H	2.483275	0.930231	-1.715299	H	-1.229202	1.250608	-1.603549
C	1.915158	3.794748	0.837119	H	-3.073112	1.562029	-3.054015
H	0.645252	2.396123	1.879425	H	-4.225853	-0.496112	-2.270806
C	2.755109	3.989116	-0.255695	H	-5.164645	1.206449	0.088774
H	3.625603	3.113493	-2.020411	H	0.195188	-0.559409	3.571093
H	1.747028	4.597820	1.546683	C	1.693327	1.576451	0.042734
H	3.242712	4.948232	-0.398589	C	2.080349	2.047189	-1.215503
C	1.583679	-1.437056	-0.280242	C	2.048834	2.308287	1.180879
C	2.948578	-1.565533	-0.010931	C	2.819747	3.219227	-1.340598
C	0.907585	-2.431737	-0.987295	H	1.807359	1.483233	-2.104001
C	3.639318	-2.682024	-0.472983	C	2.766704	3.493839	1.053393
H	3.465756	-0.797153	0.557524	H	1.758775	1.936063	2.154841
C	1.598822	-3.554656	-1.428729	C	3.157223	3.948656	-0.203819
H	-0.152733	-2.311665	-1.194049	H	3.126642	3.564680	-2.322614
C	2.964211	-3.676131	-1.177395	H	3.027149	4.062343	1.940634
H	4.701836	-2.779856	-0.275683	H	3.723353	4.870379	-0.296983
H	1.074137	-4.332306	-1.973734	C	1.493139	-1.567144	-0.400086
H	3.503702	-4.549544	-1.529904	C	2.433137	-2.230299	0.396473
O	1.041746	-0.229479	2.021859	C	1.116901	-2.132881	-1.621346

M6OL2-Pr

SCF energy in gas phase: -1322.461045

SCF energy in solution: -1322.755145

Free energy in solution: -1322.413624

C	-1.044941	-0.074595	0.631920
C	-3.460651	-0.054973	0.436697
C	-2.396369	-0.962093	2.438861
C	-3.529019	-0.659282	1.689360
C	-2.197208	0.249356	-0.119824
H	-4.514516	-0.885771	2.091505
H	-2.479237	-1.419023	3.420042
P	0.703372	0.023435	0.103175
C	0.184975	-0.904306	2.529687
H	0.401942	-1.986440	2.533186
C	-1.160171	-0.654347	1.889640

C	-3.289188	1.409885	-1.992767
C	-4.731862	0.281644	-0.315250
C	-4.470270	0.466146	-1.808453
H	-3.538418	2.392191	-1.558784
H	-5.474351	-0.505952	-0.150076
H	-5.355138	0.867451	-2.310187
N	-2.114478	0.829115	-1.371827
H	0.335980	0.232038	-1.286949
H	-1.229202	1.250608	-1.603549
H	-3.073112	1.562029	-3.054015
H	-4.225853	-0.496112	-2.270806
H	-5.164645	1.206449	0.088774
H	0.195188	-0.559409	3.571093
C	1.693327	1.576451	0.042734
C	2.080349	2.047189	-1.215503
C	2.048834	2.308287	1.180879
C	2.819747	3.219227	-1.340598
H	1.807359	1.483233	-2.104001
C	2.766704	3.493839	1.053393
H	1.758775	1.936063	2.154841
C	3.157223	3.948656	-0.203819
H	3.126642	3.564680	-2.322614
H	3.027149	4.062343	1.940634
H	3.723353	4.870379	-0.296983
C	1.493139	-1.567144	-0.400086
C	2.433137	-2.230299	0.396473
C	1.116901	-2.132881	-1.621346
C	2.990228	-3.432244	-0.032208
H	2.720892	-1.790271	1.344327
C	1.656570	-3.345653	-2.038368
H	0.386626	-1.620958	-2.242947
C	2.599920	-3.993685	-1.245497
H	3.728566	-3.934030	0.585470
H	1.345006	-3.781123	-2.982580
H	3.030052	-4.935307	-1.572844
O	1.143680	-0.200433	1.793260

M7NHL2

SCF energy in gas phase: -1223.991783

SCF energy in solution: -1224.270271

Free energy in solution: -1223.972058

C	-1.616790	-0.771253	-1.512741
C	-3.844902	-1.626815	-0.967688

C	-2.340874	-1.170281	0.867620	Free energy in solution: -1225.091573			
C	-3.574799	-1.596700	0.424009				
C	-1.366590	-0.785527	-0.088402	C	-1.186019	2.085154	-1.100016
C	-2.930068	-1.230336	-1.903295	C	-3.503466	2.555556	-0.466175
C	-1.119411	0.047061	2.725513	C	-2.359066	0.757759	0.653841
C	-2.061108	-1.097612	2.355099	C	-3.497630	1.522025	0.490175
N	-0.650570	-0.335736	-2.286090	C	-1.203596	1.031377	-0.124123
P	0.152545	-0.068759	0.394937	C	-2.403074	2.823063	-1.240628
H	-4.823689	-1.964563	-1.300060	C	-1.133304	-0.212912	2.633042
H	-4.337742	-1.891691	1.136601	C	-2.321396	-0.353772	1.676791
H	-3.173283	-1.251419	-2.962402	N	-0.074882	2.302416	-1.805899
H	-0.970797	0.105360	3.807307	P	0.169043	-0.042790	0.203560
H	-3.009520	-0.991646	2.890959	H	-4.402290	3.152337	-0.597363
H	-1.609147	-2.039145	2.698497	H	-4.375859	1.324298	1.095872
H	-0.937929	-0.327719	-3.263331	H	-2.430567	3.617097	-1.982243
H	-1.536135	1.007476	2.401228	H	-1.154438	-1.032050	3.361839
N	0.199752	-0.106609	2.092349	H	-3.245390	-0.348027	2.260719
H	0.655173	-0.959114	2.410693	H	-2.264922	-1.332141	1.181426
C	0.254412	1.691570	-0.033660	H	-0.223460	2.964928	-2.561893
C	1.428635	2.405477	0.209672	H	0.357799	1.001983	-2.016053
C	-0.872406	2.342611	-0.538729	H	0.440018	0.095191	-1.887770
C	1.474240	3.772371	-0.045459	H	-1.245049	0.729874	3.182958
H	2.309333	1.897023	0.590405	N	0.145945	-0.225270	1.913108
C	-0.821824	3.709962	-0.789439	H	0.856155	0.343542	2.357016
H	-1.773841	1.772431	-0.741644	C	1.857869	0.591370	0.068509
C	0.348803	4.423660	-0.543771	C	2.916024	-0.273083	-0.210547
H	2.387920	4.326390	0.143023	C	2.091441	1.941005	0.336015
H	-1.695796	4.216730	-1.185258	C	4.218247	0.216268	-0.210582
H	0.385175	5.489823	-0.744284	H	2.721375	-1.317233	-0.438698
C	1.710897	-0.909076	-0.006935	C	3.397632	2.421687	0.329409
C	2.799618	-0.773848	0.866185	H	1.255236	2.610158	0.514956
C	1.819840	-1.719702	-1.140885	C	4.458847	1.561480	0.060216
C	3.991328	-1.440826	0.599844	H	5.044564	-0.452668	-0.427676
H	2.716880	-0.153515	1.754404	H	3.584216	3.472396	0.525425
C	3.014057	-2.389306	-1.390904	H	5.475652	1.940935	0.054874
H	0.976145	-1.780059	-1.820749	C	-0.052873	-1.790127	-0.288822
C	4.098168	-2.249419	-0.528487	C	0.461373	-2.802414	0.526748
H	4.832746	-1.329937	1.276010	C	-0.795951	-2.122842	-1.424714
H	3.096900	-3.020168	-2.269883	C	0.266573	-4.138359	0.183734
H	5.027806	-2.770530	-0.734693	H	0.996585	-2.534888	1.431951
				C	-1.015201	-3.457846	-1.744169
M7NHL2-TS1				H	-1.194179	-1.328920	-2.048448
SCF energy in gas phase: -1225.129382				C	-0.474631	-4.466032	-0.947818
SCF energy in solution: -1225.404617				H	0.681855	-4.921297	0.810052

H	-1.602980	-3.712221	-2.619939
H	-0.638214	-5.507592	-1.206176

M7NHL2-Pr

SCF energy in gas phase: -1225.166420

SCF energy in solution: -1225.439805

Free energy in solution: -1225.121275

C	-2.232726	0.747805	-1.288094
C	-4.452320	-0.007310	-0.672610
C	-2.599910	-0.383050	0.830825
C	-3.957449	-0.476284	0.540786
C	-1.689297	0.159100	-0.110323
C	-3.605850	0.616743	-1.565472
C	-0.959231	0.070694	2.634389
C	-2.158001	-0.774837	2.222349
N	-1.497344	1.528582	-2.155416
P	0.162060	-0.053438	0.032427
H	-5.509795	-0.095431	-0.903029
H	-4.630481	-0.896488	1.281832
H	-3.993917	1.043529	-2.486573
H	-0.711997	-0.077505	3.692667
H	-3.004475	-0.644021	2.905384
H	-1.869158	-1.833810	2.268630
H	-1.883714	1.651046	-3.078397
H	-0.492965	1.470032	-2.126898
H	0.182874	-0.036098	-1.433919
H	-1.204686	1.132905	2.508068
N	0.191270	-0.267548	1.817368
H	0.480131	-1.211821	2.045687
C	1.209307	1.473222	0.023780
C	1.829550	1.862721	-1.167403
C	1.404410	2.253002	1.167113
C	2.616283	3.009811	-1.223422
H	1.713568	1.246375	-2.057045
C	2.167670	3.415568	1.107104
H	0.972975	1.927896	2.106087
C	2.775453	3.796295	-0.086486
H	3.102667	3.287977	-2.153037
H	2.297613	4.019972	1.999478
H	3.378163	4.698190	-0.127491
C	1.117918	-1.644184	-0.165270
C	2.263025	-1.951517	0.577229
C	0.689446	-2.530297	-1.154445

C	2.963415	-3.130002	0.328636
H	2.614070	-1.257504	1.336092
C	1.364561	-3.726803	-1.374820
H	-0.179036	-2.271968	-1.757098
C	2.508445	-4.024136	-0.637353
H	3.865542	-3.350206	0.890966
H	1.007506	-4.420386	-2.129670
H	3.048540	-4.947593	-0.820898

M7OL2

SCF energy in gas phase: -1243.865077

SCF energy in solution: -1244.148178

Free energy in solution: -1243.862186

C	-1.632185	-0.383752	-1.623796
C	-3.975116	-1.015435	-1.305016
C	-2.594433	-0.828590	0.663742
C	-3.826272	-1.089950	0.105378
C	-1.522748	-0.481391	-0.188666
C	-2.947711	-0.679854	-2.143893
C	-1.286391	0.044277	2.629875
C	-2.369612	-0.911070	2.156880
N	-0.549800	-0.033905	-2.275495
P	0.063324	-0.099165	0.409116
H	-4.951675	-1.227740	-1.733958
H	-4.671729	-1.345995	0.734897
H	-3.102007	-0.632675	-3.218566
H	-1.116571	-0.033108	3.705113
H	-3.301966	-0.689788	2.685994
H	-2.072121	-1.929625	2.436362
H	-0.720723	0.017321	-3.277885
H	-1.542214	1.083766	2.387221
C	0.565136	1.615402	0.140149
C	1.838673	2.027749	0.538655
C	-0.343746	2.534898	-0.387206
C	2.203320	3.364331	0.408294
H	2.543236	1.305828	0.943198
C	0.026670	3.868963	-0.514062
H	-1.321362	2.191250	-0.711134
C	1.297550	4.282202	-0.117965
H	3.192480	3.687783	0.714980
H	-0.673153	4.585864	-0.930500
H	1.584322	5.323886	-0.222870
C	1.469684	-1.157780	0.012911

C	1.856985	-2.151284	0.916808
C	2.166561	-0.978137	-1.186864
C	2.943971	-2.967499	0.617058
H	1.317089	-2.273221	1.849349
C	3.251883	-1.798195	-1.473493
H	1.824728	-0.221299	-1.883883
C	3.639660	-2.790750	-0.575721
H	3.247995	-3.738587	1.317325
H	3.793277	-1.664920	-2.404256
H	4.486986	-3.428690	-0.807246
O	-0.023643	-0.288757	2.021146

M7OL2-TS1

SCF energy in gas phase: -1245.003134

SCF energy in solution: -1245.285751

Free energy in solution: -1244.985560

C	3.820210	2.706297	0.086502
H	4.679235	1.274292	-1.273348
H	2.713135	3.959439	1.443208
H	4.695062	3.348650	0.083826
C	0.467892	-1.738572	-0.247533
C	1.387980	-2.447417	0.529628
C	-0.219634	-2.378895	-1.280042
C	1.639122	-3.788470	0.251357
H	1.898338	-1.949109	1.348557
C	0.012328	-3.726427	-1.532967
H	-0.926427	-1.811229	-1.878964
C	0.948395	-4.427951	-0.774749
H	2.366173	-4.335766	0.842451
H	-0.528546	-4.226969	-2.329284
H	1.138690	-5.475843	-0.984068
O	0.116118	-0.136242	1.825488

C	-1.688661	1.683137	-1.148432
C	-4.064156	1.562600	-0.554932
C	-2.536370	0.098616	0.589222
C	-3.823105	0.557527	0.407516
C	-1.471818	0.648516	-0.171607
C	-3.053215	2.096536	-1.309470
C	-1.076602	-0.490420	2.534147
C	-2.213093	-0.950482	1.624673
N	-0.654710	2.159837	-1.830124
P	0.126086	0.000296	0.179582
H	-5.079441	1.921839	-0.700993
H	-4.635431	0.155798	1.003960
H	-3.263187	2.863587	-2.050128
H	-0.802937	-1.281219	3.239377
H	-3.092756	-1.157038	2.240830
H	-1.928300	-1.895717	1.143955
H	-0.947265	2.793261	-2.569519
H	0.082198	0.928335	-2.045651
H	0.338933	0.097544	-1.905161
H	-1.392894	0.392554	3.100250
C	1.581510	1.067370	0.085249
C	2.688900	0.722369	-0.686606
C	1.589294	2.224566	0.863151
C	3.812829	1.541426	-0.677474
H	2.663400	-0.174401	-1.299090
C	2.708704	3.049734	0.852200
H	0.721697	2.478262	1.464021

M7OL2-Pr

SCF energy in gas phase: -1245.061360

SCF energy in solution: -1245.340938

Free energy in solution: -1245.033375

C	-0.062274	2.531517	-0.987613
C	-1.853048	4.015932	-0.301358
C	-1.755633	1.787665	0.600986
C	-2.380090	3.028470	0.528197
C	-0.602667	1.523393	-0.159878
C	-0.711239	3.776133	-1.045496
C	-1.184371	0.091829	2.352058
C	-2.293328	0.692253	1.480356
N	1.126173	2.367522	-1.678717
P	0.143592	-0.142403	-0.082070
H	-2.336433	4.986149	-0.365870
H	-3.272657	3.218364	1.115960
H	-0.295081	4.555147	-1.678623
H	-1.570659	-0.815514	2.840197
H	-3.085725	1.077493	2.128969
H	-2.740119	-0.095565	0.861802
H	1.274582	3.011988	-2.440081
H	1.414409	1.422931	-1.887854
H	0.323259	-0.116092	-1.537146
H	-0.926471	0.810818	3.141362
C	1.966790	-0.359825	0.092929
C	2.679268	0.001300	1.240791

C	2.659268	-0.890875	-0.998915	P	0.470056	-0.087741	0.654896
C	4.061919	-0.153680	1.280778	H	-2.035322	-0.008503	-3.759201
H	2.140019	0.397720	2.091421	H	-4.070456	-0.745513	-2.801618
C	4.038143	-1.071815	-0.947227	H	-1.472655	-0.042407	3.582597
H	2.109471	-1.172009	-1.894300	H	0.157808	-2.328552	2.373323
C	4.742489	-0.693801	0.192299	C	1.044965	1.595853	0.336712
H	4.610143	0.144130	2.169008	C	2.414363	1.874224	0.357443
H	4.560338	-1.501239	-1.796306	C	0.113678	2.613785	0.125004
H	5.820002	-0.820072	0.232203	C	2.850780	3.184255	0.189271
C	-0.936118	-1.616190	-0.328759	H	3.132015	1.069918	0.498800
C	-1.064109	-2.613011	0.643873	C	0.559364	3.919700	-0.051670
C	-1.637667	-1.737267	-1.530462	H	-0.943181	2.369110	0.085635
C	-1.881099	-3.715953	0.409242	C	1.922860	4.203739	-0.015047
H	-0.513262	-2.515029	1.573340	H	3.912159	3.408477	0.209500
C	-2.482722	-2.820408	-1.748689	H	-0.158054	4.715004	-0.223963
H	-1.521965	-0.971286	-2.293197	H	2.266178	5.224217	-0.153139
C	-2.599035	-3.815223	-0.780287	C	1.520165	-1.210777	-0.311579
H	-1.963257	-4.496076	1.159554	C	2.459366	-2.007974	0.351271
H	-3.040405	-2.894873	-2.676852	C	1.389058	-1.281846	-1.705297
H	-3.246324	-4.669105	-0.954843	C	3.260117	-2.884223	-0.376002
O	-0.000477	-0.219644	1.654546	H	2.564005	-1.929792	1.428757

M8NHL2

SCF energy in gas phase: -1301.379911

SCF energy in solution: -1301.672790

Free energy in solution: -1301.342085

C	-2.289112	0.568541	-2.860809
C	-3.663802	0.120994	-2.269483
C	-3.300026	-0.226155	-0.846550
C	-1.865669	-0.043972	-0.748075
C	-4.025857	-0.652065	0.217414
C	-1.246169	-0.305594	0.520235
C	-2.039417	-0.743807	1.631073
C	-3.390733	-0.920484	1.473805
C	-1.411911	-0.968631	2.993086
H	-1.989518	-1.723323	3.536178
C	0.053437	-1.389659	2.929427
H	-5.100289	-0.798092	0.128935
H	-2.316836	1.621898	-3.171638
H	-4.416308	0.913904	-2.324070
H	-3.988221	-1.254446	2.316179
H	0.460749	-1.557420	3.930351
N	-1.264322	0.380442	-1.828838

P	0.470056	-0.087741	0.654896
H	-2.035322	-0.008503	-3.759201
H	-4.070456	-0.745513	-2.801618
H	-1.472655	-0.042407	3.582597
H	0.157808	-2.328552	2.373323
C	1.044965	1.595853	0.336712
C	2.414363	1.874224	0.357443
C	0.113678	2.613785	0.125004
C	2.850780	3.184255	0.189271
H	3.132015	1.069918	0.498800
C	0.559364	3.919700	-0.051670
H	-0.943181	2.369110	0.085635
C	1.922860	4.203739	-0.015047
H	3.912159	3.408477	0.209500
H	-0.158054	4.715004	-0.223963
H	2.266178	5.224217	-0.153139
C	1.520165	-1.210777	-0.311579
C	2.459366	-2.007974	0.351271
C	1.389058	-1.281846	-1.705297
C	3.260117	-2.884223	-0.376002
H	2.564005	-1.929792	1.428757
C	2.196512	-2.162467	-2.418372
H	0.649462	-0.653844	-2.197510
C	3.127583	-2.962458	-1.759381
H	3.988681	-3.502048	0.139049
H	2.097038	-2.222720	-3.497421
H	3.752875	-3.645472	-2.326093
N	0.897203	-0.381305	2.262799
H	0.951539	0.485886	2.789334

M8NHL2-TS1

SCF energy in gas phase: -1302.514748

SCF energy in solution: -1302.802622

Free energy in solution: -1302.454504

C	-3.173887	1.104153	-2.275564
C	-4.316795	0.630439	-1.342635
C	-3.547108	-0.024548	-0.223434
C	-2.174249	0.361671	-0.379289
C	-3.948189	-0.795190	0.824521
C	-1.197017	-0.105605	0.556511
C	-1.661991	-0.891443	1.670570
C	-2.995539	-1.224179	1.779999
C	-0.778097	-1.291456	2.841480

H	-1.181195	-2.202869	3.293974			
C	0.694395	-1.481701	2.512003	C	-3.234771	0.216758 -2.584540
H	-4.992192	-1.075994	0.940202	C	-4.304012	-0.354412 -1.636281
H	-3.370640	2.086875	-2.713370	C	-3.461100	-0.893026 -0.504786
H	-4.881302	1.489213	-0.959665	C	-2.170457	-0.338952 -0.595784
H	-3.323201	-1.799978	2.640068	C	-3.790194	-1.719926 0.545643
H	1.271222	-1.687969	3.419258	C	-1.175422	-0.614741 0.367033
N	-1.963707	1.134493	-1.449697	C	-1.555583	-1.428320 1.468456
P	0.567383	0.026245	0.307063	C	-2.833458	-1.980962 1.528594
H	-3.044646	0.396933	-3.108877	C	-0.657211	-1.697860 2.661178
H	-5.027184	-0.039090	-1.834609	H	-0.798067	-2.733685 2.990672
H	-0.855953	-0.505239	3.606353	C	0.816651	-1.403434 2.426109
H	0.832646	-2.337751	1.842498	H	-4.782882	-2.156673 0.616082
H	-0.641585	0.741763	-1.763003	H	-3.566736	1.111931 -3.115105
H	0.162687	0.376839	-1.652498	H	-4.958265	0.446019 -1.270367
C	1.281620	1.686429	0.102648	H	-3.088540	-2.615259 2.372642
C	2.640601	1.863019	0.374522	H	1.376812	-1.509751 3.363717
C	0.483976	2.779765	-0.248584	N	-2.125201	0.526183 -1.681939
C	3.207899	3.131013	0.276569	P	0.523989	0.068714 0.140315
H	3.252195	1.016734	0.668398	H	-2.944374	-0.541217 -3.327436
C	1.057870	4.044332	-0.323243	H	-4.931122	-1.108694 -2.116603
H	-0.566101	2.629626	-0.487329	H	-1.011740	-1.065157 3.488113
C	2.416444	4.221957	-0.067751	H	1.233436	-2.144182 1.733124
H	4.266423	3.263960	0.475019	H	-1.222581	0.735290 -2.083925
H	0.440224	4.895165	-0.591701	H	0.247844	0.175273 -1.304409
H	2.857312	5.211301	-0.138944	C	0.639005	1.902213 0.207358
C	1.380727	-1.376105	-0.562094	C	1.532073	2.558293 -0.641007
C	2.677850	-1.764255	-0.216013	C	-0.187827	2.649972 1.047154
C	0.679432	-2.098968	-1.529829	C	1.625131	3.946206 -0.622364
C	3.279908	-2.840741	-0.863535	H	2.156514	1.975401 -1.314770
H	3.200528	-1.242537	0.578073	C	-0.112567	4.040976 1.047031
C	1.272672	-3.190396	-2.153070	H	-0.909856	2.146775 1.686747
H	-0.330599	-1.797501	-1.792100	C	0.800833	4.689141 0.221198
C	2.578805	-3.554518	-1.830269	H	2.335504	4.449543 -1.270734
H	4.293772	-3.126426	-0.602256	H	-0.768326	4.618045 1.691402
H	0.717670	-3.752729	-2.896723	H	0.866140	5.772501 0.227898
H	3.046317	-4.398326	-2.327740	C	1.995375	-0.937583 -0.405174
N	1.252453	-0.300029	1.851001	C	3.221771	-0.919628 0.266855
H	1.185691	0.521037	2.448816	C	1.873800	-1.689677 -1.575821
				C	4.306525	-1.633785 -0.236383
				H	3.303290	-0.345276 1.182916
				C	2.943949	-2.438485 -2.054870
				H	0.928097	-1.684581 -2.113621
				C	4.167248	-2.401773 -1.389496
M8NHL2-Pr						
SCF energy in gas phase: -1302.559485						
SCF energy in solution: -1302.849104						
Free energy in solution: -1302.496137						

H	5.261445	-1.595634	0.278808
H	2.828834	-3.038242	-2.952384
H	5.010941	-2.968681	-1.771164
N	1.025881	-0.082996	1.854813
H	0.630494	0.637265	2.452932

M8OL2

SCF energy in gas phase: -1321.248431

SCF energy in solution: -1321.546013

Free energy in solution: -1321.226936

C	-2.277454	0.461942	-2.890091
C	-3.650072	0.011429	-2.295646
C	-3.294330	-0.284110	-0.858899
C	-1.861439	-0.087714	-0.760507
C	-4.023287	-0.679171	0.214883
C	-1.250957	-0.314484	0.517142
C	-2.045470	-0.717826	1.637102
C	-3.394667	-0.904097	1.484719
C	-1.390468	-0.889876	2.990025
H	-1.954298	-1.613611	3.586892
C	0.052924	-1.347476	2.885831
H	-5.096342	-0.833563	0.125094
H	-2.315719	1.508486	-3.221676
H	-4.415458	0.788494	-2.383948
H	-3.994219	-1.211369	2.335546
H	0.518941	-1.453301	3.866958
N	-1.255854	0.307229	-1.848809
P	0.455106	-0.073872	0.653187
H	-2.012636	-0.130447	-3.774920
H	-4.035884	-0.879827	-2.801780
H	-1.399863	0.061441	3.537092
H	0.129090	-2.302096	2.349546
C	1.013011	1.608225	0.344123
C	0.066556	2.615065	0.147159
C	2.379349	1.900423	0.334932
C	0.493940	3.924521	-0.045320
H	-0.988739	2.360598	0.133231
C	2.797727	3.213747	0.153246
H	3.109064	1.105971	0.467173
C	1.854716	4.222342	-0.037293
H	-0.235106	4.711466	-0.206252
H	3.856626	3.449921	0.152961
H	2.184320	5.245732	-0.187071

C	1.539279	-1.183265	-0.283270
C	2.456251	-1.978286	0.413368
C	1.466220	-1.244897	-1.681161
C	3.292703	-2.843724	-0.285468
H	2.521461	-1.909427	1.494720
C	2.306517	-2.117179	-2.365618
H	0.740298	-0.621475	-2.198387
C	3.215617	-2.914711	-1.673584
H	4.004774	-3.458792	0.255102
H	2.250459	-2.173189	-3.447914
H	3.867382	-3.590983	-2.218010
O	0.843782	-0.350227	2.200681

M8OL2-TS1

SCF energy in gas phase: -1322.386426

SCF energy in solution: -1322.684157

Free energy in solution: -1322.349209

C	-3.091432	1.052493	-2.389130
C	-4.246695	0.307531	-1.663545
C	-3.512146	-0.413353	-0.560518
C	-2.169680	0.103843	-0.556408
C	-3.913144	-1.337018	0.352912
C	-1.232886	-0.410657	0.397736
C	-1.707413	-1.335875	1.391334
C	-3.003139	-1.792743	1.347603
C	-0.871206	-1.703769	2.603550
H	-1.110147	-2.723044	2.923732
C	0.627128	-1.576206	2.409715
H	-4.931609	-1.717784	0.345132
H	-3.353832	2.087786	-2.627272
H	-4.963043	1.021238	-1.240940
H	-3.351384	-2.471167	2.120532
H	1.159594	-1.684953	3.357208
N	-1.932197	1.009694	-1.492716
P	0.478033	-0.008737	0.354024
H	-2.848209	0.556860	-3.340102
H	-4.804411	-0.364439	-2.321732
H	-1.160799	-1.034755	3.423810
H	1.006411	-2.338945	1.716178
H	-0.543575	0.648749	-1.792029
H	0.216680	0.253442	-1.683818
C	0.924819	1.737493	0.255730
C	1.781469	2.230083	-0.728065

C	0.413868	2.583682	1.240368	P	0.516163	0.056136	0.099419
C	2.129991	3.575669	-0.723509	H	-3.185288	-0.688978	-3.128496
H	2.157985	1.562665	-1.498004	H	-5.168962	-0.682998	-1.785190
C	0.753445	3.933131	1.229124	H	-0.861534	-0.282406	3.562806
H	-0.248727	2.186720	2.003224	H	0.811748	-2.132504	1.811484
C	1.612178	4.426734	0.251154	H	-1.235699	0.535841	-2.215729
H	2.797555	3.962672	-1.486131	H	0.184131	0.158442	-1.306914
H	0.347192	4.598118	1.983863	C	1.035072	1.824061	0.068415
H	1.877043	5.479353	0.245232	C	1.217744	2.591905	1.224614
C	1.695000	-1.116774	-0.441914	C	1.225264	2.425724	-1.178322
C	3.040191	-1.008070	-0.080931	C	1.574191	3.933135	1.125136
C	1.286468	-2.102605	-1.339988	H	1.079845	2.127393	2.192092
C	3.977722	-1.868952	-0.646475	C	1.602816	3.761342	-1.277219
H	3.349043	-0.256058	0.640074	H	1.085977	1.839248	-2.082700
C	2.222055	-2.979312	-1.878205	C	1.771441	4.519574	-0.122866
H	0.237265	-2.166817	-1.617046	H	1.702092	4.522108	2.028058
C	3.568512	-2.855993	-1.539300	H	1.757426	4.209491	-2.253526
H	5.025865	-1.774352	-0.381559	H	2.055456	5.565004	-0.194313
H	1.902263	-3.752676	-2.568840	C	1.717230	-1.259458	-0.428640
H	4.299510	-3.532523	-1.970479	C	2.924296	-1.492448	0.237515
O	0.947946	-0.271609	1.915025	C	1.416122	-2.009194	-1.567229

M8OL2-Pr

SCF energy in gas phase: -1322.447111

SCF energy in solution: -1322.741828

Free energy in solution: -1322.399397

C	-3.319170	0.236197	-2.547678
C	-4.406325	0.036659	-1.479848
C	-3.591403	-0.408106	-0.289507
C	-2.236960	-0.085475	-0.511498
C	-3.992764	-0.972805	0.898345
C	-1.249888	-0.335053	0.468554
C	-1.699294	-0.890689	1.698332
C	-3.039071	-1.213438	1.889330
C	-0.771660	-1.128076	2.869040
H	-1.086612	-2.026068	3.411302
C	0.673511	-1.238590	2.439426
H	-5.036413	-1.225929	1.064830
H	-3.541624	1.051135	-3.240049
H	-4.905355	0.987884	-1.259487
H	-3.342008	-1.652935	2.835046
H	1.341310	-1.339770	3.302648
N	-2.130038	0.539549	-1.750821

H	-3.185288	-0.688978	-3.128496
H	-5.168962	-0.682998	-1.785190
H	-0.861534	-0.282406	3.562806
H	0.811748	-2.132504	1.811484
H	-1.235699	0.535841	-2.215729
H	0.184131	0.158442	-1.306914
C	1.035072	1.824061	0.068415
C	1.217744	2.591905	1.224614
C	1.225264	2.425724	-1.178322
C	1.574191	3.933135	1.125136
H	1.079845	2.127393	2.192092
C	1.602816	3.761342	-1.277219
H	1.085977	1.839248	-2.082700
C	1.771441	4.519574	-0.122866
H	1.702092	4.522108	2.028058
H	1.757426	4.209491	-2.253526
H	2.055456	5.565004	-0.194313
C	1.717230	-1.259458	-0.428640
C	2.924296	-1.492448	0.237515
C	1.416122	-2.009194	-1.567229
C	3.814055	-2.452159	-0.237699
H	3.156137	-0.914500	1.125827
C	2.287048	-2.994107	-2.022915
H	0.485847	-1.818837	-2.098386
C	3.493239	-3.210162	-1.361670
H	4.758183	-2.612612	0.273429
H	2.030493	-3.583638	-2.897376
H	4.183910	-3.965421	-1.723581
O	1.028225	-0.065231	1.747625

M9NHL2

SCF energy in gas phase: -1340.685113

SCF energy in solution: -1340.986988

Free energy in solution: -1340.626924

C	-3.012689	0.863994	-2.677990
C	-3.735435	-0.332771	-2.054193
C	-3.077297	-0.683592	-0.744422
C	-1.661143	-0.386068	-0.634866
C	-1.516628	0.557127	-2.798676
C	-3.732335	-1.238139	0.320814
C	-1.051910	-0.704303	0.630255
C	-1.752112	-1.296859	1.706919

C	-3.094327	-1.558737	1.549944	SCF energy in solution: -1342.116957			
C	-1.030936	-1.626620	2.992861	Free energy in solution: -1341.742814			
H	-1.750496	-1.659418	3.816469				
C	0.068569	-0.622633	3.318596	C	-4.488145	0.536843	-1.131478
H	-4.798276	-1.439850	0.221423	C	-4.417217	-0.974829	-0.920557
H	-3.432677	1.108108	-3.659281	C	-3.140469	-1.349033	-0.204123
H	-4.800840	-0.126373	-1.903936	C	-2.014866	-0.461543	-0.323747
H	-0.992505	1.442378	-3.182949	C	-3.198763	1.009871	-1.800256
H	-3.663306	-1.998418	2.362510	C	-3.039556	-2.490042	0.554377
H	-0.363952	0.382306	3.434891	C	-0.811776	-0.852849	0.356918
N	-0.896185	0.163194	-1.548078	C	-0.736232	-2.057951	1.103127
P	0.615103	-0.216780	0.709364	C	-1.849852	-2.866392	1.206145
H	0.556649	-0.890385	4.259472	C	0.553234	-2.426334	1.798618
H	-1.378250	-0.229971	-3.559568	H	0.400652	-3.322542	2.405979
H	-3.143517	1.741876	-2.032711	C	1.064294	-1.300667	2.704227
H	-3.670714	-1.182651	-2.748188	H	-3.917490	-3.127506	0.646952
H	-0.569591	-2.619622	2.918276	H	-5.357356	0.805699	-1.739958
C	0.835664	1.579713	0.536717	H	-5.282160	-1.338567	-0.354906
C	2.114843	2.128156	0.422329	H	-3.221721	2.096273	-1.942849
C	-0.278806	2.416994	0.633163	H	-1.808605	-3.778416	1.792649
C	2.279421	3.511458	0.405679	H	0.328454	-1.140821	3.501518
H	2.982633	1.479053	0.329837	N	-2.024479	0.680195	-1.015461
C	-0.109049	3.796300	0.614739	P	0.686467	0.095384	0.351622
H	-1.269257	1.975927	0.704072	H	0.145637	0.475017	-1.656907
C	1.168443	4.343912	0.501922	H	-0.738773	0.688304	-1.535929
H	3.273479	3.936369	0.311169	H	2.005558	-1.611841	3.173331
H	-0.975286	4.446697	0.678910	H	-3.140140	0.563531	-2.807523
H	1.296680	5.421550	0.484158	H	-4.590767	1.039597	-0.162499
C	1.849036	-1.016330	-0.350404	H	-4.452832	-1.469724	-1.900905
C	2.522069	-2.145845	0.123607	H	1.331008	-2.671809	1.063395
C	2.104124	-0.534659	-1.639495	C	0.592400	1.902776	0.308662
C	3.453224	-2.788706	-0.687569	C	1.643724	2.651890	-0.217990
H	2.311380	-2.514645	1.121991	C	-0.513594	2.532861	0.881397
C	3.040531	-1.179375	-2.439261	C	1.591264	4.040968	-0.162562
H	1.543770	0.320250	-2.002063	H	2.489917	2.152756	-0.681502
C	3.713068	-2.305169	-1.966253	C	-0.559013	3.923321	0.928011
H	3.973024	-3.667400	-0.319728	H	-1.341854	1.938244	1.255280
H	3.238551	-0.807990	-3.439422	C	0.491527	4.675999	0.409991
H	4.438196	-2.808274	-2.598419	H	2.407192	4.627159	-0.572569
N	1.097988	-0.661273	2.266633	H	-1.421620	4.417733	1.362554
H	1.977165	-0.238360	2.546231	H	0.450959	5.759936	0.447157
				C	2.102336	-0.635672	-0.544930
				C	3.394329	-0.463844	-0.039710
				C	1.898796	-1.421218	-1.682097
M9NHL2-TS1							
SCF energy in gas phase: -1341.817972							

C	4.479892	-1.039704	-0.696140
H	3.536355	0.106321	0.872785
C	2.981808	-2.022684	-2.312443
H	0.890444	-1.550656	-2.062645
C	4.273830	-1.821613	-1.828519
H	5.483480	-0.889412	-0.311515
H	2.818045	-2.642385	-3.188019
H	5.118471	-2.282023	-2.331383
N	1.271787	-0.050186	1.961696
H	1.051293	0.773387	2.508014

M9NHL2-Pr

SCF energy in gas phase: -1341.862487

SCF energy in solution: -1342.160824

Free energy in solution: -1341.778967

C	-4.628441	-0.009025	-1.064697
C	-4.370983	-1.482095	-0.756753
C	-3.001619	-1.692882	-0.145076
C	-1.974130	-0.740715	-0.334305
C	-3.438743	0.551191	-1.831488
C	-2.738681	-2.828472	0.608956
C	-0.703124	-0.969989	0.247993
C	-0.469959	-2.133214	1.003297
C	-1.491877	-3.061535	1.178025
C	0.889891	-2.361986	1.606629
H	0.878992	-3.265185	2.223901
C	1.352434	-1.169634	2.463164
H	-3.539657	-3.550546	0.752463
H	-5.545073	0.111020	-1.649071
H	-5.137143	-1.875850	-0.080863
H	-3.588000	1.609386	-2.063988
H	-1.310133	-3.959820	1.760019
H	0.774453	-1.174835	3.395534
N	-2.245157	0.437592	-1.014174
P	0.677498	0.221467	0.072074
H	0.336458	0.396820	-1.367540
H	-1.432111	0.917977	-1.374575
H	2.404907	-1.342235	2.738555
H	-3.337231	0.011048	-2.787438
H	-4.743918	0.556789	-0.134033
H	-4.450108	-2.060446	-1.686959
H	1.622713	-2.534361	0.810026
C	0.312420	2.017331	0.289434

C	1.001589	2.938568	-0.500396
C	-0.683988	2.464317	1.159071
C	0.732336	4.298926	-0.386986
H	1.751018	2.584495	-1.205188
C	-0.973424	3.823961	1.250679
H	-1.252982	1.746493	1.745996
C	-0.257741	4.742475	0.487905
H	1.288368	5.012526	-0.986857
H	-1.759910	4.164795	1.916653
H	-0.476699	5.802555	0.567569
C	2.315509	-0.397333	-0.530218
C	3.494717	-0.250956	0.206416
C	2.360380	-1.034929	-1.773273
C	4.699990	-0.731622	-0.301421
H	3.445807	0.243861	1.170271
C	3.556605	-1.550092	-2.260843
H	1.445494	-1.128564	-2.353413
C	4.730734	-1.390883	-1.527128
H	5.615853	-0.597237	0.265803
H	3.576589	-2.064759	-3.216297
H	5.668790	-1.777937	-1.913108
N	1.189037	0.116541	1.796084
H	0.710523	0.784613	2.384162

M9OL2

SCF energy in gas phase: -1360.554776

SCF energy in solution: -1360.860737

Free energy in solution: -1360.513839

C	-3.157622	0.674526	-2.619508
C	-3.845612	-0.480521	-1.885215
C	-3.122684	-0.746488	-0.589917
C	-1.707291	-0.431680	-0.567085
C	-1.666087	0.367340	-2.790142
C	-3.716422	-1.240682	0.540169
C	-1.036565	-0.666112	0.680665
C	-1.672010	-1.193014	1.827743
C	-3.016574	-1.478071	1.755941
C	-0.865880	-1.411790	3.087018
H	-1.520360	-1.366807	3.963241
C	0.243785	-0.381714	3.236816
H	-4.783326	-1.458152	0.507472
H	-3.623809	0.851280	-3.594211
H	-4.902853	-0.263840	-1.696970

H	-1.168036	1.225642	-3.259747	C	-3.033966	-2.523801	0.496829
H	-3.541932	-1.867866	2.621560	C	-0.808354	-0.880722	0.333030
H	-0.165023	0.636611	3.262724	C	-0.733617	-2.099891	1.058118
N	-0.985243	0.063649	-1.544775	C	-1.842873	-2.910657	1.147292
P	0.622093	-0.162337	0.661290	C	0.556434	-2.453206	1.756495
H	0.830906	-0.547035	4.142018	H	0.408126	-3.324081	2.401413
H	-1.557940	-0.470937	-3.499602	C	1.057097	-1.293061	2.613266
H	-3.264898	1.593438	-2.029293	H	-3.910288	-3.165157	0.576471
H	-3.813037	-1.373297	-2.525221	H	-5.359894	0.814980	-1.717976
H	-0.405935	-2.408436	3.075752	H	-5.277779	-1.371379	-0.402789
C	0.843395	1.616134	0.425826	H	-3.228113	2.120325	-1.877822
C	2.130821	2.148079	0.330506	H	-1.803092	-3.829752	1.722512
C	-0.270605	2.458891	0.434235	H	0.346295	-1.100344	3.423965
C	2.302911	3.526821	0.242012	N	-2.020355	0.674555	-1.011633
H	2.994414	1.488392	0.320836	P	0.668668	0.077991	0.331479
C	-0.091979	3.834268	0.345016	H	0.161676	0.428408	-1.670707
H	-1.264588	2.024998	0.495053	H	-0.686534	0.657444	-1.562626
C	1.192834	4.367171	0.248628	H	2.033006	-1.528708	3.050020
H	3.301891	3.943327	0.165631	H	-3.147643	0.620286	-2.796794
H	-0.955318	4.491307	0.344011	H	-4.593652	1.005000	-0.134622
H	1.328667	5.441720	0.176249	H	-4.437628	-1.450596	-1.946916
C	1.839972	-1.030318	-0.349026	H	1.331861	-2.722243	1.026962
C	2.589788	-2.058320	0.229521	C	0.554536	1.877959	0.326278
C	2.021983	-0.691849	-1.694243	C	1.501348	2.656748	-0.334566
C	3.521599	-2.749074	-0.539358	C	-0.478375	2.471860	1.050807
H	2.447372	-2.305493	1.275611	C	1.421814	4.043983	-0.256952
C	2.959571	-1.385548	-2.451421	H	2.287332	2.183109	-0.916208
H	1.407624	0.089190	-2.128718	C	-0.556810	3.858483	1.115431
C	3.705888	-2.412953	-1.877413	H	-1.221846	1.849844	1.540375
H	4.103514	-3.547603	-0.090979	C	0.394016	4.643164	0.466562
H	3.103400	-1.127643	-3.495489	H	2.158234	4.655315	-0.768010
H	4.432482	-2.953839	-2.475708	H	-1.364387	4.327455	1.667759
O	1.185349	-0.489503	2.151907	H	0.329780	5.725365	0.520153

M9OL2-TS1

SCF energy in gas phase: -1361.691699

SCF energy in solution: -1361.996929

Free energy in solution: -1361.635012

C	-4.489412	0.531659	-1.117968	H	1.008508	-1.595719	-2.062014
C	-4.411991	-0.985139	-0.951812	C	4.392436	-1.692984	-1.724182
C	-3.137123	-1.371269	-0.239557	H	5.511496	-0.666889	-0.197927
C	-2.012750	-0.473584	-0.342025	H	3.022653	-2.612044	-3.108383
C	-3.202882	1.029669	-1.774098	H	5.273545	-2.121052	-2.191648

O 1.209907 -0.070242 1.884756

M9OL2-Pr

SCF energy in gas phase: -1361.749527

SCF energy in solution: -1362.053243

Free energy in solution: -1361.682914

C	-4.700334	0.247827	-0.899712
C	-4.492258	-1.248813	-0.679364
C	-3.126953	-1.538998	-0.092797
C	-2.063232	-0.622955	-0.265587
C	-3.508249	0.805560	-1.665439
C	-2.903946	-2.704174	0.627067
C	-0.794384	-0.929148	0.284435
C	-0.607828	-2.113966	1.014887
C	-1.664258	-3.002973	1.181571
C	0.746445	-2.391170	1.607530
H	0.697183	-3.253304	2.279508
C	1.259310	-1.177886	2.390296
H	-3.733696	-3.395019	0.760422
H	-5.624609	0.434882	-1.453517
H	-5.266310	-1.653677	-0.019405
H	-3.614670	1.882972	-1.820563
H	-1.516883	-3.918383	1.745995
H	0.687708	-1.092978	3.324468
N	-2.298416	0.582122	-0.899313
P	0.643432	0.172185	0.035597
H	0.255758	0.351451	-1.367139
H	-1.487739	1.107461	-1.188487
H	2.313361	-1.346284	2.658007
H	-3.459566	0.329543	-2.658734
H	-4.771659	0.763502	0.063658
H	-4.599227	-1.769071	-1.640691
H	1.459813	-2.644529	0.814326
C	0.501682	2.000337	0.259987
C	0.589852	2.800522	-0.883308
C	0.289886	2.610748	1.500736
C	0.480992	4.185375	-0.793846
H	0.752935	2.332608	-1.851592
C	0.154910	3.993228	1.585480
H	0.239068	1.993290	2.387845
C	0.255112	4.783012	0.442590
H	0.566582	4.794081	-1.688414
H	-0.022752	4.456589	2.550913

H 0.157756 5.861827 0.515808

C 2.224775 -0.548677 -0.579039

C 3.416048 -0.432432 0.143657

C 2.228053 -1.220528 -1.803394

C 4.593752 -0.979110 -0.359217

H 3.406761 0.094081 1.091976

C 3.397108 -1.800323 -2.286354

H 1.303830 -1.293354 -2.371582

C 4.583372 -1.672718 -1.566858

H 5.520158 -0.869503 0.195881

H 3.386030 -2.341150 -3.227296

H 5.500174 -2.110341 -1.949564

O 1.141038 0.046408 1.703684

M10NHL2

SCF energy in gas phase: -1187.101151

SCF energy in solution: -1187.365863

Free energy in solution: -1187.050314

C	1.541750	-0.311217	-0.037502
C	3.457127	-0.077839	-1.623833
C	3.828958	-0.007512	0.885260
C	4.318622	-0.568770	-0.454620
C	2.428870	-0.542655	1.169927
C	1.954782	-0.205585	-1.390959
H	4.285389	-1.665100	-0.408599
H	3.660340	0.987484	-1.796545
H	4.522019	-0.277793	1.690660
N	1.078611	-0.154489	-2.347847
H	1.541300	-0.007341	-3.245792
P	-0.062363	-0.058242	0.470123
C	1.691822	0.137823	2.335388
H	1.974570	-0.250520	3.318022
H	1.902642	1.213826	2.315789
H	3.723178	-0.604120	-2.547051
H	5.363748	-0.292423	-0.627665
H	3.789299	1.089081	0.829659
H	2.526052	-1.618439	1.408323
N	0.226500	-0.039917	2.151968
H	-0.124718	-0.882908	2.596896
C	-1.307287	-1.347782	0.175548
C	-2.598841	-1.240281	0.700615
C	-0.942575	-2.457820	-0.587433
C	-3.515445	-2.264052	0.488980

H	-2.884106	-0.355453	1.265071
C	-1.870372	-3.472863	-0.808509
H	0.056549	-2.497383	-1.013437
C	-3.149300	-3.378634	-0.265734
H	-4.516451	-2.190454	0.901600
H	-1.596975	-4.334687	-1.408505
H	-3.869976	-4.172027	-0.437709
C	-0.895622	1.493124	0.038139
C	-1.148759	2.433858	1.040233
C	-1.273002	1.749331	-1.286032
C	-1.779240	3.632985	0.719166
H	-0.854514	2.213100	2.062052
C	-1.896606	2.953884	-1.595044
H	-1.046722	1.016602	-2.054818
C	-2.152151	3.892516	-0.596805
H	-1.979073	4.363180	1.496977
H	-2.185510	3.160827	-2.620617
H	-2.643762	4.827950	-0.845708

M10NHL2-TS1

SCF energy in gas phase: -1188.237806

SCF energy in solution: -1188.499257

Free energy in solution: -1188.168699

C	1.611340	-0.127626	-0.135886
C	3.798791	0.148543	-1.348015
C	3.775860	-0.229296	1.132691
C	4.432032	-0.621345	-0.190429
C	2.318667	-0.664138	1.100517
C	2.282123	0.275093	-1.293294
H	4.299016	-1.699488	-0.343342
H	4.194680	1.172075	-1.369501
H	4.294504	-0.691908	1.980054
N	1.660683	0.817769	-2.329711
H	2.244480	0.895765	-3.157278
P	-0.115343	-0.085418	0.171849
H	0.380296	0.345319	-2.199657
H	-0.374552	-0.017739	-1.813563
C	1.461093	-0.173901	2.271220
H	1.654729	-0.718270	3.200625
H	1.665755	0.889500	2.450640
H	4.066031	-0.304476	-2.309964
H	5.509894	-0.433359	-0.169360
H	3.826943	0.860207	1.264256

H	2.304033	-1.769462	1.121670
N	0.056599	-0.339015	1.879845
H	-0.356101	-1.200663	2.214008
C	-1.304194	-1.451477	-0.139741
C	-2.544767	-1.209512	-0.731769
C	-0.948114	-2.755279	0.210738
C	-3.428554	-2.260335	-0.949883
H	-2.807785	-0.198057	-1.029258
C	-1.826948	-3.809642	-0.027320
H	0.023740	-2.950941	0.658482
C	-3.070329	-3.561520	-0.600451
H	-4.396222	-2.066242	-1.401373
H	-1.539857	-4.822556	0.236327
H	-3.759139	-4.380731	-0.780048
C	-1.001941	1.509883	0.115610
C	-1.940856	1.753511	1.122636
C	-0.753570	2.487213	-0.853372
C	-2.648555	2.951838	1.144776
H	-2.101716	1.007643	1.894127
C	-1.447962	3.692384	-0.809697
H	-0.010691	2.307840	-1.624275
C	-2.402076	3.923008	0.179187
H	-3.385692	3.127583	1.921672
H	-1.246849	4.452736	-1.557630
H	-2.948561	4.860809	0.199586

M10NHL2-Pr

SCF energy in gas phase: -1188.283261

SCF energy in solution: -1188.544682

Free energy in solution: -1188.205716

C	1.332919	-0.893054	-0.034370
C	3.513722	-1.717584	-0.966077
C	3.344376	-1.120654	1.463688
C	3.892631	-2.128646	0.455377
C	1.826831	-1.128987	1.377336
C	2.112906	-1.150947	-1.113993
H	3.469859	-3.115342	0.679459
H	4.200869	-0.942941	-1.331471
H	3.674297	-1.365024	2.479680
N	1.832652	-0.844861	-2.434705
H	2.312237	-1.411453	-3.118351
P	-0.296699	-0.040445	-0.051078
H	0.870796	-0.641911	-2.662769

H	-0.352590	-0.087238	-1.518987
C	1.096902	-0.069510	2.217265
H	1.174201	-0.273292	3.291195
H	1.548166	0.916120	2.033528
H	3.622697	-2.568035	-1.652503
H	4.980163	-2.222814	0.530462
H	3.716817	-0.114835	1.226489
H	1.471305	-2.112051	1.731780
N	-0.290497	-0.045348	1.779423
H	-0.745335	-0.895691	2.107666
C	-1.965355	-0.856981	-0.075770
C	-2.965536	-0.586751	0.864379
C	-2.227867	-1.768169	-1.099940
C	-4.203141	-1.219231	0.773805
H	-2.771667	0.125607	1.659738
C	-3.451433	-2.426729	-1.171976
H	-1.461635	-1.959729	-1.848005
C	-4.444572	-2.146376	-0.237159
H	-4.980321	-0.988854	1.495974
H	-3.633785	-3.149086	-1.961439
H	-5.406744	-2.645157	-0.299791
C	-0.220080	1.803987	-0.156653
C	-0.619625	2.642102	0.888184
C	0.272898	2.375198	-1.333724
C	-0.545219	4.025778	0.745552
H	-0.975650	2.191811	1.807846
C	0.370537	3.756385	-1.466343
H	0.594407	1.730487	-2.147174
C	-0.048247	4.585220	-0.428318
H	-0.871450	4.668402	1.557505
H	0.767683	4.184880	-2.381181
H	0.015218	5.663971	-0.534073

M10OL2

SCF energy in gas phase: -1206.970822

SCF energy in solution: -1207.238632

Free energy in solution: -1206.935290

C	1.505985	-0.442317	-0.061891
C	3.496336	-0.289637	-1.549407
C	3.762586	-0.405112	0.972661
C	4.256107	-0.928883	-0.381094
C	2.306529	-0.820718	1.167298
C	1.980069	-0.309859	-1.388560

H	4.120491	-2.017598	-0.407744
H	3.793484	0.763855	-1.639180
H	4.391033	-0.789963	1.784006
N	1.155604	-0.146782	-2.380501
H	1.669141	0.015608	-3.247093
P	-0.078256	-0.086584	0.431873
C	1.587818	-0.116127	2.321955
H	1.715695	-0.601797	3.291302
H	1.904570	0.932563	2.385462
H	3.762936	-0.776457	-2.493683
H	5.328479	-0.740792	-0.494000
H	3.829704	0.691194	0.985858
H	2.285484	-1.907226	1.359974
C	-1.421496	-1.260204	0.142336
C	-2.424946	-1.453152	1.095546
C	-1.438186	-1.959690	-1.067545
C	-3.448423	-2.358483	0.838681
H	-2.391797	-0.907349	2.034177
C	-2.473734	-2.857032	-1.317987
H	-0.648868	-1.783025	-1.796568
C	-3.472578	-3.056598	-0.367984
H	-4.225996	-2.521263	1.577949
H	-2.497787	-3.405290	-2.254179
H	-4.273723	-3.761854	-0.566234
C	-0.748457	1.550669	0.053637
C	-0.947928	2.452933	1.102482
C	-1.056320	1.913507	-1.263093
C	-1.454176	3.721360	0.834427
H	-0.709686	2.157094	2.119741
C	-1.555396	3.186613	-1.518261
H	-0.868984	1.209074	-2.067787
C	-1.757214	4.087461	-0.474210
H	-1.613049	4.422657	1.647259
H	-1.789204	3.476273	-2.537680
H	-2.152245	5.077316	-0.680793
O	0.159433	-0.141898	2.043835

M10OL2-TS1

SCF energy in gas phase: -1208.115122

SCF energy in solution: -1208.381328

Free energy in solution: -1208.061149

C	1.577631	-0.278320	-0.162094
C	3.814377	-0.195263	-1.301997

C	3.669496	-0.697106	1.155687	SCF energy in gas phase: -1208.168843			
C	4.309925	-1.098904	-0.173409	SCF energy in solution: -1208.436845			
C	2.172243	-0.950101	1.063695	Free energy in solution: -1208.110834			
C	2.322049	0.109946	-1.280723				
H	4.047581	-2.141719	-0.389674	C	1.399433	-0.783914	-0.171339
H	4.331247	0.771813	-1.253571	C	3.620592	-1.373801	-1.170365
H	4.105693	-1.261314	1.987403	C	3.412265	-1.095637	1.313217
N	1.793464	0.787276	-2.284841	C	4.004322	-1.947116	0.192052
H	2.408889	0.851326	-3.091159	C	1.897392	-1.150427	1.209106
P	-0.129123	-0.078163	0.129592	C	2.191474	-0.873106	-1.267954
H	0.413812	0.422490	-2.192455	H	3.617185	-2.968907	0.283976
H	-0.335780	0.091431	-1.850644	H	4.267025	-0.521773	-1.419297
C	1.340123	-0.389968	2.212604	H	3.746444	-1.453264	2.293263
H	1.383020	-0.994482	3.122871	N	1.889398	-0.437319	-2.545574
H	1.651226	0.638764	2.441406	H	2.407095	-0.889037	-3.284909
H	4.057404	-0.625568	-2.280517	P	-0.264548	-0.042792	-0.101006
H	5.401520	-1.050267	-0.114894	C	1.129212	-0.194038	2.119990
H	3.848961	0.369872	1.344974	H	1.142273	-0.512701	3.168454
H	2.016262	-2.042785	1.041093	H	1.574133	0.815376	2.058920
C	-1.447581	-1.312469	-0.180383	H	3.784612	-2.121219	-1.957823
C	-2.476385	-1.071155	-1.094181	H	5.093883	-2.009755	0.268082
C	-1.415390	-2.521270	0.518656	H	3.748573	-0.055440	1.207139
C	-3.465335	-2.026096	-1.300769	H	1.563248	-2.169593	1.461250
H	-2.497193	-0.133907	-1.643080	C	-1.841929	-1.003093	-0.113643
C	-2.391820	-3.487194	0.289114	C	-2.232225	-1.851638	0.928217
H	-0.637055	-2.693808	1.253693	C	-2.671721	-0.882072	-1.231879
C	-3.418908	-3.239281	-0.616179	C	-3.420796	-2.570360	0.840229
H	-4.268087	-1.826975	-2.003272	H	-1.599838	-1.932258	1.802561
H	-2.354846	-4.428559	0.827781	C	-3.872789	-1.580491	-1.308569
H	-4.185295	-3.988767	-0.786700	H	-2.375188	-0.228192	-2.047934
C	-0.844942	1.586666	0.119573	C	-4.245292	-2.433500	-0.273444
C	-2.030733	1.799557	0.826312	H	-3.707633	-3.234496	1.649625
C	-0.184009	2.654945	-0.491825	H	-4.512684	-1.464382	-2.177705
C	-2.565740	3.081889	0.907697	H	-5.176046	-2.989217	-0.334105
H	-2.529017	0.966403	1.314507	C	-0.373628	1.799283	-0.005943
C	-0.723734	3.933926	-0.399689	C	-0.814392	2.462076	1.144172
H	0.729572	2.470951	-1.051433	C	0.001955	2.552096	-1.121893
C	-1.912160	4.148303	0.295715	C	-0.890952	3.851815	1.166510
H	-3.489774	3.248157	1.451929	H	-1.091306	1.874762	2.011664
H	-0.215796	4.766145	-0.876366	C	-0.047244	3.942547	-1.089407
H	-2.329148	5.148338	0.362438	H	0.350934	2.044749	-2.017604
O	-0.018154	-0.398084	1.763607	C	-0.503230	4.594077	0.053525
				H	-1.249047	4.357049	2.058247
M10OL2-Pr				H	0.262520	4.516221	-1.957291

H	-0.555350	5.678250	0.077361
O	-0.193901	-0.196885	1.653149
H	0.913637	-0.293573	-2.757961
H	-0.365520	0.059397	-1.552487

M11NHL2

SCF energy in gas phase: -1264.482646

SCF energy in solution: -1264.763262

Free energy in solution: -1264.412941

C	-1.075830	-0.554148	0.570349
C	-3.312059	-1.122486	-0.446269
C	-3.104641	0.061462	1.844900
C	-4.010327	-0.712450	0.870904
C	-1.860894	-0.671329	-0.597234
H	-4.895745	-0.106791	0.646762
H	-3.591875	0.120027	2.826486
N	-1.487426	-0.455143	-1.822216
P	0.537557	-0.034541	0.693319
C	-0.751096	0.228039	2.852283
H	-0.818884	-0.039104	3.910147
C	-1.714573	-0.572102	1.950577
H	-0.975229	1.297422	2.757004
C	-2.648085	-0.677352	-2.688147
C	-3.881928	-0.600953	-1.768524
H	-2.675314	0.059521	-3.497868
H	-4.187105	0.445551	-1.640231
H	-2.585384	-1.669385	-3.163791
H	-4.742607	-1.167315	-2.134245
H	-4.376983	-1.610616	1.379230
H	-2.965986	1.089520	1.483763
H	-3.278083	-2.221093	-0.493952
H	-1.822864	-1.593744	2.357231
N	0.651942	0.031531	2.394784
H	1.015819	-0.855473	2.739298
C	0.934128	1.604826	0.018487
C	2.223321	2.136533	0.121320
C	-0.084855	2.340847	-0.588240
C	2.486086	3.411175	-0.365713
H	3.018076	1.554670	0.580814
C	0.188065	3.611851	-1.087446
H	-1.071359	1.898415	-0.686594
C	1.467874	4.146651	-0.972013
H	3.483100	3.830477	-0.278131

H	-0.598587	4.181915	-1.570728
H	1.676678	5.138799	-1.360191
C	1.862089	-1.122657	0.114796
C	3.029621	-1.346242	0.849153
C	1.667053	-1.752333	-1.120526
C	4.002569	-2.209501	0.350962
H	3.181886	-0.848620	1.804159
C	2.648919	-2.606461	-1.611320
H	0.751510	-1.560763	-1.680340
C	3.811173	-2.837151	-0.877379
H	4.908408	-2.391203	0.920367
H	2.505218	-3.096758	-2.568611
H	4.570694	-3.509372	-1.263857

M11NHL2-TS1

SCF energy in gas phase: -1265.622659

SCF energy in solution: -1265.897988

Free energy in solution: -1265.533177

C	-1.105363	-0.474063	0.478808
C	-3.485539	-1.026314	-0.135199
C	-2.887246	0.076400	2.113479
C	-3.959084	-0.654540	1.286575
C	-2.094062	-0.531295	-0.494636
H	-4.856815	-0.029474	1.225934
H	-3.185955	0.086020	3.168704
N	-1.982874	-0.241557	-1.777738
P	0.570581	-0.057258	0.283438
C	-0.390838	0.240270	2.674204
H	-0.310545	-0.018315	3.734069
H	-0.630132	-0.267532	-1.929374
H	0.269282	-0.281445	-1.649889
C	-1.498530	-0.544390	1.943601
H	-0.614301	1.313203	2.606641
C	-3.234738	-0.554309	-2.464115
C	-4.286509	-0.517267	-1.339633
H	-3.434433	0.168224	-3.260313
H	-4.594773	0.518975	-1.157499
H	-3.196750	-1.553312	-2.925315
H	-5.177326	-1.111009	-1.558385
H	-4.254489	-1.565566	1.816696
H	-2.818328	1.120260	1.781911
H	-3.418663	-2.122122	-0.206513
H	-1.518449	-1.578603	2.330177

N	0.895008	-0.000791	2.001639	H	-0.431036	1.775825	2.162175
H	1.297031	-0.885103	2.301723	C	-3.442832	-1.315601	-2.222746
C	0.997964	1.660852	-0.184075	C	-4.400873	-0.855769	-1.119456
C	1.930011	2.358610	0.590780	H	-3.670580	-0.876384	-3.197726
C	0.353630	2.314674	-1.240608	H	-4.659045	0.197614	-1.273427
C	2.249143	3.679248	0.282224	H	-3.461602	-2.411064	-2.327224
H	2.375977	1.871762	1.451371	H	-5.322520	-1.439994	-1.085182
C	0.660145	3.639856	-1.527960	H	-4.374499	-0.865894	2.138931
H	-0.397719	1.791859	-1.822708	H	-2.721130	1.586683	1.440136
C	1.618130	4.320071	-0.778699	H	-3.517830	-2.054998	0.423669
H	2.984248	4.208612	0.880105	H	-1.579820	-1.020697	2.523065
H	0.150593	4.142169	-2.343908	N	0.915902	0.210895	1.876005
H	1.862683	5.350970	-1.015365	H	1.125108	-0.693335	2.297091
C	1.884424	-1.262436	-0.133077	C	1.048397	1.687196	-0.363071
C	3.200523	-1.036442	0.275036	C	1.846353	2.499130	0.449333
C	1.554274	-2.443676	-0.797401	C	0.564026	2.203877	-1.568059
C	4.183263	-1.987041	0.007419	C	2.166211	3.794348	0.049133
H	3.459638	-0.119651	0.796419	H	2.198246	2.100540	1.394510
C	2.533724	-3.398674	-1.045725	C	0.865334	3.504759	-1.958039
H	0.529068	-2.597942	-1.123656	H	-0.058874	1.577827	-2.201495
C	3.849871	-3.168476	-0.648248	C	1.676066	4.300342	-1.151909
H	5.208286	-1.803738	0.313542	H	2.797332	4.412278	0.680514
H	2.273308	-4.318990	-1.558449	H	0.474009	3.894967	-2.892405
H	4.615751	-3.910289	-0.851307	H	1.923464	5.312214	-1.458108

M11NHL2-Pr

SCF energy in gas phase: -1265.668710

SCF energy in solution: -1265.945427

Free energy in solution: -1265.572822

C	-1.147304	-0.367352	0.498289
C	-3.545708	-0.990459	0.147745
C	-2.841529	0.651428	2.000406
C	-3.982019	-0.175908	1.385615
C	-2.144196	-0.687978	-0.360069
H	-4.811325	0.486203	1.113104
H	-3.096754	0.920212	3.032200
N	-2.164904	-0.836670	-1.720632
P	0.588562	-0.046954	0.087495
C	-0.307885	0.727170	2.470502
H	-0.257740	0.713910	3.564594
H	-1.310759	-0.890906	-2.252289
H	0.319811	-0.314836	-1.338802
C	-1.506177	-0.087537	1.937968

C	1.048397	1.687196	-0.363071
C	1.846353	2.499130	0.449333
C	0.564026	2.203877	-1.568059
C	2.166211	3.794348	0.049133
H	2.198246	2.100540	1.394510
C	0.865334	3.504759	-1.958039
H	-0.058874	1.577827	-2.201495
C	1.676066	4.300342	-1.151909
H	2.797332	4.412278	0.680514
H	0.474009	3.894967	-2.892405
H	1.923464	5.312214	-1.458108
C	1.930646	-1.324178	-0.013924
C	3.117972	-1.245907	0.721856
C	1.744247	-2.397446	-0.885974
C	4.097977	-2.225522	0.577902
H	3.269392	-0.412699	1.400557
C	2.707781	-3.393905	-1.007059
H	0.831864	-2.447773	-1.476056
C	3.891597	-3.303490	-0.279258
H	5.025038	-2.146779	1.137385
H	2.541273	-4.232290	-1.676248
H	4.654044	-4.069074	-0.384106

M11OL2

SCF energy in gas phase: -1284.354308

SCF energy in solution: -1284.639167

Free energy in solution: -1284.302637

C	-1.145932	-0.507144	0.505010
C	-3.424958	-0.797446	-0.533143
C	-3.115709	0.264663	1.800708

C	-4.076172	-0.425555	0.818878	M11OL2-TS1			
C	-1.941099	-0.458940	-0.663664	SCF energy in gas phase: -1285.497187			
H	-4.940296	0.225644	0.645922	SCF energy in solution: -1285.777822			
H	-3.593260	0.340900	2.785686	Free energy in solution: -1285.424308			
N	-1.558496	-0.170332	-1.867956				
P	0.490787	-0.092744	0.641568	C	-1.110654	-0.514907	0.435666
C	-0.757416	0.239826	2.781239	C	-3.465059	-1.158760	-0.171073
H	-0.755756	-0.103451	3.817283	C	-2.871859	-0.197250	2.145393
C	-1.779530	-0.478908	1.887753	C	-3.918463	-0.930210	1.287593
H	-0.929666	1.324180	2.754371	C	-2.115477	-0.554870	-0.522084
C	-2.734761	-0.233068	-2.738811	H	-4.854114	-0.360520	1.298950
C	-3.954376	-0.127657	-1.803736	H	-3.144660	-0.283510	3.203941
H	-2.704283	0.564665	-3.488541	N	-2.050781	-0.149525	-1.774660
H	-4.169443	0.927015	-1.591236	P	0.546558	-0.060757	0.256935
H	-2.752891	-1.187130	-3.289376	C	-0.377018	0.081644	2.632276
H	-4.860370	-0.590483	-2.203914	H	-0.186040	-0.269417	3.649382
H	-4.466600	-1.331051	1.295780	H	-0.643196	-0.110771	-1.936401
H	-2.903740	1.284538	1.454278	H	0.223516	-0.128326	-1.669074
H	-3.489233	-1.888011	-0.662662	C	-1.455555	-0.721517	1.896660
H	-1.960792	-1.489201	2.291094	H	-0.662782	1.143230	2.664508
C	1.092307	1.505346	0.037464	C	-3.299257	-0.488905	-2.456572
C	1.736526	2.379674	0.918260	C	-4.325105	-0.604771	-1.312948
C	0.896271	1.860116	-1.302951	H	-3.562012	0.276298	-3.192335
C	2.194528	3.610395	0.455493	H	-4.689481	0.393112	-1.041587
H	1.873150	2.092485	1.956883	H	-3.211557	-1.446635	-2.992255
C	1.356303	3.094794	-1.750829	H	-5.184330	-1.232107	-1.561987
H	0.355432	1.183424	-1.962016	H	-4.140879	-1.896692	1.750857
C	2.006475	3.965311	-0.877968	H	-2.873690	0.869951	1.890143
H	2.696673	4.290920	1.135762	H	-3.335700	-2.239393	-0.331376
H	1.202416	3.380179	-2.786556	H	-1.395533	-1.776831	2.208993
H	2.363701	4.925464	-1.236992	C	0.939057	1.671405	-0.145718
C	1.721252	-1.303441	0.106876	C	2.133361	2.225957	0.315879
C	3.070388	-0.963330	-0.030004	C	0.010548	2.466390	-0.821705
C	1.289366	-2.602236	-0.168935	C	2.409151	3.571155	0.084318
C	3.988288	-1.932358	-0.418301	H	2.845983	1.610681	0.857312
H	3.396836	0.055407	0.160161	C	0.287125	3.811704	-1.039659
C	2.211256	-3.565727	-0.565743	H	-0.916076	2.024516	-1.181467
H	0.231274	-2.833085	-0.080454	C	1.486415	4.363588	-0.591850
C	3.557689	-3.230819	-0.686323	H	3.342060	3.998832	0.437271
H	5.037286	-1.674895	-0.521172	H	-0.433185	4.430845	-1.564667
H	1.879268	-4.574417	-0.788502	H	1.700183	5.412800	-0.769877
H	4.275314	-3.982770	-0.999710	C	1.929708	-1.188822	-0.171930
O	0.577310	-0.014726	2.267307	C	3.017682	-1.282126	0.706477
				C	1.911035	-1.985983	-1.319299

C	4.078406	-2.136110	0.421060
H	3.020390	-0.702872	1.622395
C	2.964970	-2.853493	-1.589661
H	1.069292	-1.928799	-1.999687
C	4.054449	-2.923497	-0.726489
H	4.920103	-2.192529	1.103817
H	2.934486	-3.472988	-2.480057
H	4.879519	-3.594410	-0.944174
O	0.844255	-0.058769	1.900997

M11OL2-Pr

SCF energy in gas phase: -1285.553537

SCF energy in solution: -1285.837171

Free energy in solution: -1285.477452

C	-1.166461	-0.439321	0.396280
C	-3.555201	-1.026416	-0.060812
C	-2.885192	0.331064	2.017598
C	-4.000762	-0.442290	1.297326
C	-2.153955	-0.641300	-0.506245
H	-4.865577	0.213661	1.148690
H	-3.145850	0.452813	3.075410
N	-2.163613	-0.587307	-1.873558
P	0.559118	-0.061829	0.050191
C	-0.356853	0.430287	2.458730
H	-0.242944	0.253478	3.533844
H	-1.304516	-0.607201	-2.399603
H	0.350689	-0.171700	-1.395107
C	-1.530704	-0.355769	1.857449
H	-0.531708	1.511040	2.306428
C	-3.442285	-0.978246	-2.447950
C	-4.403272	-0.683605	-1.292330
H	-3.662632	-0.396689	-3.347002
H	-4.649744	0.383723	-1.279521
H	-3.466181	-2.045579	-2.714253
H	-5.330674	-1.256476	-1.352749
H	-4.341205	-1.261175	1.938462
H	-2.795523	1.335011	1.585318
H	-3.521633	-2.122517	0.026197
H	-1.563296	-1.353696	2.323494
C	1.059550	1.701449	-0.187318
C	1.803517	2.402698	0.767669
C	0.673070	2.357461	-1.358832
C	2.157913	3.730306	0.545879

H	2.094523	1.892871	1.678831
C	1.007885	3.691587	-1.571429
H	0.096009	1.818547	-2.105988
C	1.757408	4.378304	-0.620321
H	2.744742	4.262208	1.288363
H	0.689587	4.192630	-2.480402
H	2.028318	5.416295	-0.787634
C	1.908888	-1.312181	-0.083092
C	2.309832	-2.123295	0.983305
C	2.540117	-1.460693	-1.321021
C	3.312872	-3.072106	0.803900
H	1.833214	-1.995578	1.946773
C	3.561994	-2.389329	-1.493022
H	2.231064	-0.837071	-2.156257
C	3.944024	-3.203815	-0.430347
H	3.607321	-3.705740	1.634776
H	4.052710	-2.482925	-2.456763
H	4.731209	-3.939395	-0.564104
O	0.808290	0.014165	1.797792

M12NHL2

SCF energy in gas phase: -1303.785719

SCF energy in solution: -1304.073667

Free energy in solution: -1303.696002

C	-0.828555	-1.068586	-0.338584
C	-3.138915	-0.922706	0.552145
C	-2.721891	-2.142315	-1.630275
C	-3.492702	-1.017163	-0.937489
C	-1.652401	-0.592204	0.713503
H	-4.570700	-1.186458	-1.047538
H	-2.983654	-2.187876	-2.694683
P	0.683865	-0.363106	-0.649788
C	-0.473273	-1.433574	-2.695480
C	-1.191340	-2.011066	-1.464640
C	-1.995836	0.819429	2.606516
C	-3.991226	0.095093	1.304001
C	-3.423454	0.280747	2.706684
H	-1.515318	0.778728	3.592381
H	-3.961716	1.056189	0.769275
H	-3.416183	-0.688795	3.221192
N	-1.137217	0.145052	1.650993
H	-0.349476	-2.175501	-3.490716
H	-1.053847	-0.583170	-3.086316

H	-0.776020	-3.018058	-1.303894	P	0.704616	-0.174099	-0.337520
H	-2.039672	1.889704	2.341752	C	-0.244261	-1.223027	-2.568490
H	-4.040765	0.960313	3.303787	C	-0.999651	-1.892908	-1.409086
H	-5.038322	-0.227242	1.325458	C	-2.767621	1.036620	2.289262
H	-3.307610	-1.914388	1.001561	C	-4.408935	-0.111269	0.823809
H	-3.272324	-0.053572	-1.416538	C	-4.058661	0.221450	2.270180
H	-3.045040	-3.093695	-1.193337	H	-2.368253	1.097785	3.308790
C	2.183039	-0.821282	0.262784	H	-4.484069	0.817388	0.240935
C	3.185966	-1.600483	-0.315363	H	-3.920057	-0.711571	2.831146
C	2.287878	-0.407327	1.596878	N	-1.727838	0.517783	1.423564
C	4.307431	-1.949552	0.434552	H	0.052337	-1.938147	-3.342957
H	3.076883	-1.935596	-1.341970	H	0.471558	0.101968	1.690386
C	3.408818	-0.763355	2.337802	H	-0.429769	0.401143	1.718084
H	1.473938	0.164524	2.038637	H	-0.900840	-0.474261	-3.035491
C	4.419880	-1.528656	1.756369	H	-0.457151	-2.822728	-1.173362
H	5.090972	-2.552043	-0.014007	H	-2.995702	2.069803	1.986102
H	3.493402	-0.448155	3.372841	H	-4.860004	0.782441	2.761251
H	5.293848	-1.803026	2.338878	H	-5.375861	-0.619851	0.747003
C	0.720518	1.459017	-0.672579	H	-3.366450	-1.977585	0.729277
C	-0.481619	2.159523	-0.810610	H	-3.304369	-0.264402	-1.789477
C	1.930619	2.156122	-0.649152	H	-2.703389	-3.218181	-1.272085
C	-0.470740	3.544781	-0.920897	C	2.218192	-0.932510	0.345002
H	-1.415843	1.605611	-0.813120	C	3.474470	-0.449194	-0.025379
C	1.938581	3.544036	-0.772856	C	2.114474	-2.049923	1.174147
H	2.866619	1.618705	-0.523317	C	4.625283	-1.083446	0.440361
C	0.739568	4.237275	-0.905455	H	3.553847	0.427313	-0.664591
H	-1.406525	4.086461	-1.014178	C	3.264073	-2.688152	1.623616
H	2.880743	4.082362	-0.756785	H	1.127167	-2.392567	1.474468
H	0.746107	5.319212	-0.993071	C	4.520373	-2.203331	1.259578
N	0.861034	-1.007798	-2.215038	H	5.602357	-0.700639	0.163016
H	1.383749	-0.434960	-2.868265	H	3.184213	-3.557914	2.267978
M12NHL2-TS1				H	5.417354	-2.696495	1.620510
SCF energy in gas phase: -1304.920990				C	0.874187	1.643017	-0.332057
SCF energy in solution: -1305.209187				C	0.416174	2.335979	-1.454090
Free energy in solution: -1304.817698				C	1.477469	2.340264	0.715542
				C	0.533987	3.721469	-1.513875
				H	-0.021209	1.785256	-2.281053
C	-0.873269	-0.892982	-0.272136	C	1.615920	3.722524	0.641935
C	-3.313342	-0.994898	0.234012	H	1.825516	1.794957	1.587557
C	-2.454134	-2.264325	-1.750572	C	1.136465	4.414882	-0.467750
C	-3.459626	-1.220317	-1.272483	H	0.164422	4.257543	-2.382203
C	-1.931296	-0.416288	0.517212	H	2.092299	4.259618	1.455803
H	-4.480126	-1.549629	-1.500118	H	1.236347	5.494713	-0.518654
H	-2.546743	-2.426080	-2.831738	N	0.949084	-0.566227	-2.014912

H 1.806974 -1.071108 -2.200764

M12NHL2-Pr

SCF energy in gas phase: -1304.962303

SCF energy in solution: -1305.247305

Free energy in solution: -1304.848946

C	-0.773742	-1.010109	-0.076443
C	-3.219228	-1.369612	0.324899
C	-2.075715	-2.728109	-1.455601
C	-3.254967	-1.822431	-1.134088
C	-1.881416	-0.713149	0.652949
H	-4.203995	-2.333020	-1.332421
H	-2.115172	-3.070508	-2.496697
P	0.761274	-0.031205	-0.078100
C	-0.192732	-1.236481	-2.391495
C	-0.743972	-2.021541	-1.198406
C	-3.019631	0.965995	2.095219
C	-4.406703	-0.447231	0.624602
C	-4.308842	0.166020	2.015208
H	-2.858845	1.348975	3.107024
H	-4.425981	0.360941	-0.120530
H	-4.294230	-0.623288	2.775958
N	-1.884038	0.121065	1.756277
H	0.150119	-1.922311	-3.180393
H	0.642193	0.320270	1.350510
H	-0.984297	0.538183	1.951532
H	-1.008026	-0.621034	-2.819713
H	0.013499	-2.782100	-0.956357
H	-3.092205	1.835560	1.420793
H	-5.164417	0.816419	2.220908
H	-5.336082	-1.013601	0.501679
H	-3.309802	-2.253513	0.975686
H	-3.229264	-0.931150	-1.774872
H	-2.139614	-3.623779	-0.826598
C	2.408655	-0.771523	0.375327
C	3.194563	-1.489289	-0.533695
C	2.880338	-0.616892	1.684198
C	4.416550	-2.030624	-0.143690
H	2.823761	-1.616086	-1.543407
C	4.105040	-1.150563	2.073981
H	2.275300	-0.080886	2.409603
C	4.877146	-1.860180	1.158842
H	5.010569	-2.588551	-0.861105

H 4.452996 -1.016814 3.093516

H 5.831235 -2.281191 1.461353

C 0.722852 1.796552 -0.419856

C 0.005210 2.329084 -1.492657

C 1.371370 2.664659 0.460027

C -0.063388 3.707543 -1.680905

H -0.511525 1.657966 -2.173343

C 1.339818 4.040044 0.251265

H 1.910307 2.253822 1.311451

C 0.614403 4.563616 -0.816896

H -0.640868 4.113139 -2.506037

H 1.871757 4.703958 0.925666

H 0.574385 5.637139 -0.972764

N 0.892868 -0.461144 -1.835146

H 1.303625 0.225404 -2.454581

M12OL2

SCF energy in gas phase: -1323.653810

SCF energy in solution: -1323.945384

Free energy in solution: -1323.579870

C 0.775405 -1.036855 0.491855

C 3.152008 -0.998238 -0.231520

C 2.581325 -1.792409 2.101341

C 3.386310 -0.791846 1.270260

C 1.680990 -0.737856 -0.558187

H 4.454041 -0.900430 1.494937

H 2.767337 -1.642902 3.172313

P -0.702559 -0.219778 0.633486

C 0.287388 -0.892701 2.843002

C 1.064742 -1.723159 1.811129

C 2.152985 0.286001 -2.661904

C 4.053753 -0.131860 -1.105952

C 3.587059 -0.232336 -2.554225

H 1.747360 0.048425 -3.653503

H 3.986553 0.912892 -0.771150

H 3.623073 -1.282789 -2.870462

N 1.229380 -0.216547 -1.659315

H 0.005830 -1.451185 3.738506

H 0.865630 -0.002989 3.127303

H 0.658906 -2.745738 1.843014

H 2.169361 1.387347 -2.602035

H 4.241172 0.332487 -3.226790

H 5.099373 -0.439478 -0.993021

H	3.359395	-2.055244	-0.463785	C	4.093214	-0.131153	-2.227339
H	3.103393	0.236277	1.531737	H	2.502242	0.869516	-3.309334
H	2.939161	-2.800580	1.865932	H	4.566712	0.500217	-0.221146
C	-2.191906	-0.861428	-0.161862	H	3.868781	-1.066969	-2.754643
C	-3.438124	-0.828221	0.467867	N	1.792437	0.407240	-1.415271
C	-2.054810	-1.387737	-1.449545	H	-0.323706	-1.714457	3.349435
C	-4.552645	-1.331411	-0.194801	H	-0.459973	0.213055	-1.679142
H	-3.527053	-0.424774	1.472357	H	0.429623	0.404500	-1.718193
C	-3.178906	-1.877464	-2.108967	H	0.700287	-0.293068	2.984554
H	-1.070556	-1.399193	-1.915321	H	0.257468	-2.761580	1.268015
C	-4.422212	-1.851478	-1.482041	H	3.204557	1.816556	-2.007683
H	-5.523020	-1.319242	0.291088	H	4.945379	0.333739	-2.732894
H	-3.082574	-2.287570	-3.109038	H	5.320490	-1.032875	-0.663557
H	-5.295308	-2.241254	-1.996198	H	3.209717	-2.208607	-0.573935
C	-0.713985	1.572808	0.367707	H	3.235847	-0.322135	1.819778
C	-0.732767	2.401691	1.492879	H	2.461213	-3.265264	1.531292
C	-0.680112	2.129747	-0.915539	C	-2.286425	-0.843424	-0.357963
C	-0.706951	3.784552	1.336521	C	-3.467274	-0.697180	0.378038
H	-0.776940	1.960682	2.484127	C	-2.290668	-1.595783	-1.532794
C	-0.646535	3.512547	-1.061284	C	-4.648183	-1.272027	-0.082316
H	-0.652260	1.478316	-1.782399	H	-3.454502	-0.144623	1.312413
C	-0.659775	4.339355	0.060787	C	-3.467697	-2.191678	-1.974727
H	-0.724489	4.426938	2.210936	H	-1.368665	-1.705948	-2.094703
H	-0.610528	3.946267	-2.055522	C	-4.648602	-2.020740	-1.256873
H	-0.635927	5.417753	-0.060953	H	-5.566090	-1.144567	0.482546
O	-0.956081	-0.456467	2.229466	H	-3.463864	-2.783696	-2.884074

M12OL2-TS1

SCF energy in gas phase: -1324.796497

SCF energy in solution: -1325.088643

Free energy in solution: -1324.707573

C	0.799104	-0.901455	0.287684
C	3.230537	-1.192967	-0.148461
C	2.252402	-2.258334	1.908522
C	3.333061	-1.321332	1.374647
C	1.904216	-0.523693	-0.493197
H	4.324519	-1.699987	1.648827
H	2.301792	-2.322222	3.002587
P	-0.742700	-0.123186	0.301959
C	0.059349	-1.074083	2.549086
C	0.832989	-1.846837	1.475321
C	2.884696	0.799955	-2.283943
C	4.405405	-0.440222	-0.767176

C	4.093214	-0.131153	-2.227339
H	2.502242	0.869516	-3.309334
H	4.566712	0.500217	-0.221146
H	3.868781	-1.066969	-2.754643
N	1.792437	0.407240	-1.415271
H	-0.323706	-1.714457	3.349435
H	-0.459973	0.213055	-1.679142
H	0.429623	0.404500	-1.718193
H	0.700287	-0.293068	2.984554
H	0.257468	-2.761580	1.268015
H	3.204557	1.816556	-2.007683
H	4.945379	0.333739	-2.732894
H	5.320490	-1.032875	-0.663557
H	3.209717	-2.208607	-0.573935
H	3.235847	-0.322135	1.819778
H	2.461213	-3.265264	1.531292
C	-2.286425	-0.843424	-0.357963
C	-3.467274	-0.697180	0.378038
C	-2.290668	-1.595783	-1.532794
C	-4.648183	-1.272027	-0.082316
H	-3.454502	-0.144623	1.312413
C	-3.467697	-2.191678	-1.974727
H	-1.368665	-1.705948	-2.094703
C	-4.648602	-2.020740	-1.256873
H	-5.566090	-1.144567	0.482546
H	-3.463864	-2.783696	-2.884074
H	-5.569224	-2.474795	-1.609966
C	-0.780250	1.687407	0.289900
C	0.356806	2.367025	0.729959
C	-1.912356	2.398276	-0.109868
C	0.354534	3.757760	0.778015
H	1.238511	1.801778	1.018899
C	-1.910608	3.788232	-0.053186
H	-2.787353	1.867812	-0.474354
C	-0.778646	4.468090	0.390719
H	1.240467	4.287292	1.113665
H	-2.792535	4.341363	-0.359783
H	-0.778411	5.552795	0.429567
O	-1.067933	-0.473216	1.906882

M12OL2-Pr

SCF energy in gas phase: -1324.848255

SCF energy in solution: -1325.140698

Free energy in solution: -1324.752767

C	0.803281	-0.885546	0.430918
C	3.270997	-1.209928	0.203749
C	2.245783	-1.520583	2.474579
C	3.306558	-0.783417	1.671017
C	1.891624	-0.934201	-0.387712
H	4.304264	-0.971207	2.083164
H	2.253110	-1.192682	3.521296
P	-0.771900	-0.043594	0.059117
C	-0.015543	-0.275188	2.579783
C	0.845891	-1.321642	1.878734
C	2.918892	-0.225844	-2.548187
C	4.384796	-0.508513	-0.582748
C	4.263486	-0.756896	-2.080225
H	2.740340	-0.479459	-3.596975
H	4.325202	0.572597	-0.393452
H	4.323010	-1.830964	-2.291023
N	1.846734	-0.817688	-1.761127
H	-0.325176	-0.595474	3.582215
H	-0.504710	0.022270	-1.370999
H	0.919309	-0.661214	-2.128896
H	0.548175	0.671018	2.677475
H	0.292050	-2.268904	1.958380
H	2.917578	0.874158	-2.467996
H	5.069897	-0.261124	-2.628783
H	5.354249	-0.844464	-0.200395
H	3.444968	-2.295691	0.140850
H	3.132694	0.299217	1.720422
H	2.493576	-2.587871	2.481670
C	-2.355690	-0.906171	-0.333162
C	-3.046475	-1.695719	0.592331
C	-2.869900	-0.776960	-1.626626
C	-4.216414	-2.351843	0.221028
H	-2.659517	-1.781716	1.599364
C	-4.053316	-1.411583	-1.990778
H	-2.339668	-0.166989	-2.353439
C	-4.724609	-2.208231	-1.067527
H	-4.736787	-2.972629	0.943722
H	-4.447018	-1.289645	-2.994893
H	-5.641810	-2.715342	-1.350965
C	-0.767988	1.812267	0.075200
C	-1.285055	2.565663	1.135362
C	-0.207574	2.484421	-1.014818
C	-1.244042	3.956587	1.097231

H	-1.720296	2.047059	1.980870
C	-0.148344	3.874676	-1.045832
H	0.191171	1.911710	-1.848617
C	-0.672003	4.613949	0.010745
H	-1.659118	4.529282	1.920971
H	0.301051	4.379194	-1.895538
H	-0.635714	5.698763	-0.012810
O	-1.154450	-0.115494	1.775891

M13NHL2

SCF energy in gas phase: -1226.403080

SCF energy in solution: -1226.675816

Free energy in solution: -1226.331867

C	1.722014	-0.112470	-1.471733
C	4.081478	0.806736	-1.176158
C	2.440688	1.100483	0.709350
C	3.873614	0.719537	0.333505
C	1.458546	0.286108	-0.122924
C	3.181048	-0.193277	-1.900536
C	0.779646	1.248988	2.627334
C	2.222537	0.959388	2.218180
N	0.752480	-0.484560	-2.252039
P	-0.152375	0.055695	0.424974
H	3.843416	1.824673	-1.510978
H	4.068118	-0.308419	0.671027
H	3.529493	-1.212533	-1.682572
H	0.469927	2.231066	2.246139
H	2.480185	-0.062370	2.531598
H	2.897010	1.644832	2.746116
H	1.115743	-0.853120	-3.130915
H	3.240707	-0.059493	-2.985798
H	5.129308	0.622899	-1.435224
H	4.576986	1.377432	0.858621
H	0.672903	1.282826	3.715724
H	2.334366	2.178308	0.483089
C	-0.785693	-1.631369	0.208636
C	-2.154207	-1.892211	0.276295
C	0.124539	-2.680680	0.064899
C	-2.611192	-3.206498	0.207802
H	-2.859492	-1.071885	0.375311
C	-0.336839	-3.989291	-0.007660
H	1.184864	-2.450437	0.003855
C	-1.704421	-4.252423	0.065070

H	-3.675580	-3.411064	0.260804
H	0.368581	-4.805167	-0.127841
H	-2.063208	-5.275297	0.006909
C	-1.477806	1.187951	-0.122940
C	-2.312182	1.809138	0.812554
C	-1.632944	1.461274	-1.488751
C	-3.294772	2.699761	0.386288
H	-2.185623	1.585968	1.867093
C	-2.620320	2.348993	-1.903336
H	-0.978477	0.962515	-2.198917
C	-3.449161	2.969632	-0.970309
H	-3.940202	3.180083	1.115084
H	-2.743563	2.558254	-2.961300
H	-4.216217	3.662855	-1.301944
N	-0.174088	0.252385	2.115489
H	-0.039800	-0.650749	2.561963

M13NHL2-TS1

SCF energy in gas phase: -1227.536262

SCF energy in solution: -1227.807941

Free energy in solution: -1227.448125

C	1.701888	-1.481938	-1.080419
C	4.134818	-0.817501	-0.810030
C	2.428462	0.146137	0.785515
C	3.807477	-0.502599	0.642661
C	1.376559	-0.574179	-0.067101
C	3.152072	-1.862167	-1.323229
C	0.733065	0.923008	2.529441
C	2.062740	0.217970	2.275602
N	0.758344	-2.024697	-1.844507
P	-0.263392	0.012978	0.178913
H	4.051612	0.096509	-1.411474
H	3.820892	-1.437181	1.221231
H	3.346312	-2.823354	-0.829288
H	0.775641	1.947315	2.136457
H	2.009836	-0.804287	2.675370
H	2.864420	0.739323	2.814385
H	1.135521	-2.539993	-2.634345
H	-0.467444	-0.150766	-1.850152
H	3.280859	-2.032399	-2.397921
H	5.162799	-1.179616	-0.911434
H	4.559425	0.159862	1.086026
H	0.531282	1.005807	3.602470

H	2.523182	1.190414	0.435070
H	-0.081121	-1.000368	-2.009566
C	-1.642917	-1.155734	0.035204
C	-2.933426	-0.695833	-0.227558
C	-1.409148	-2.510743	0.268534
C	-3.993408	-1.595254	-0.247937
H	-3.105729	0.357760	-0.428451
C	-2.476458	-3.405345	0.244969
H	-0.394829	-2.859186	0.439876
C	-3.766315	-2.949688	-0.010157
H	-4.997735	-1.238968	-0.453387
H	-2.295827	-4.461402	0.417803
H	-4.595596	-3.649633	-0.029843
C	-0.619008	1.754167	-0.278347
C	-1.520866	2.514709	0.472204
C	0.060034	2.341975	-1.347684
C	-1.763617	3.843232	0.129792
H	-2.011597	2.060556	1.327081
C	-0.160774	3.677089	-1.666343
H	0.750867	1.736504	-1.928179
C	-1.082033	4.425287	-0.934933
H	-2.477688	4.425836	0.703149
H	0.376949	4.132591	-2.491633
H	-1.265415	5.463553	-1.193609
N	-0.400797	0.247392	1.893725
H	-0.583431	-0.647969	2.341050

M13NHL2-Pr

SCF energy in gas phase: -1227.572303

SCF energy in solution: -1227.845115

Free energy in solution: -1227.479477

C	0.853707	-2.108131	-1.042115
C	3.304765	-2.640276	-0.824779
C	2.231050	-0.978742	0.749979
C	3.169844	-2.181481	0.619328
C	0.994462	-1.102193	-0.139480
C	1.944866	-3.121936	-1.310547
C	1.016225	0.466006	2.453466
C	1.879176	-0.771540	2.229091
N	-0.300024	-2.379276	-1.754928
P	-0.274123	0.208513	-0.022239
H	3.643294	-1.803610	-1.448097
H	2.767576	-3.011465	1.217585

H	1.679135	-4.069536	-0.824314	C	-2.394739	-1.219730	0.703207
H	1.557522	1.350157	2.089887	C	-3.838598	-0.861121	0.350720
H	1.341710	-1.659457	2.592250	C	-1.444990	-0.381134	-0.135674
H	2.810892	-0.696574	2.805777	C	-3.191425	0.080519	-1.890063
H	-0.160164	-2.825515	-2.649739	C	-0.677846	-1.307647	2.553610
H	-0.426880	0.182429	-1.499377	C	-2.134640	-1.059932	2.201919
H	1.967309	-3.326141	-2.389026	N	-0.767904	0.436270	-2.249884
H	4.046159	-3.439265	-0.919969	P	0.146180	-0.062087	0.401968
H	4.143917	-1.923041	1.048886	H	-3.808216	-1.952850	-1.502261
H	0.849559	0.626620	3.525915	H	-4.045254	0.160976	0.698003
H	2.787894	-0.081571	0.428613	H	-3.560617	1.091214	-1.666895
H	-1.013374	-1.663280	-1.775146	H	-0.343945	-2.284634	2.174417
C	-2.061922	-0.277211	0.056753	H	-2.397106	-0.042927	2.519252
C	-2.992919	0.491704	-0.644903	H	-2.759571	-1.762653	2.766260
C	-2.486028	-1.436138	0.710207	H	-1.137326	0.820337	-3.119490
C	-4.338209	0.137182	-0.649142	H	-3.258587	-0.053386	-2.974844
H	-2.657025	1.370598	-1.191697	H	-5.116146	-0.777389	-1.403117
C	-3.828265	-1.809932	0.678428	H	-4.524327	-1.534714	0.879175
H	-1.760279	-2.064672	1.222315	H	-0.510129	-1.281181	3.632490
C	-4.756985	-1.016884	0.011065	H	-2.270940	-2.294870	0.474836
H	-5.059274	0.754008	-1.176425	C	0.682961	1.654573	0.224104
H	-4.146394	-2.722314	1.173304	C	2.037257	1.986841	0.228364
H	-5.804011	-1.302652	-0.004886	C	-0.287826	2.656323	0.160327
C	0.326268	1.948703	-0.255734	C	2.419509	3.325269	0.176852
C	0.007289	2.992801	0.615647	H	2.790089	1.204910	0.267387
C	1.096439	2.216031	-1.390474	C	0.098516	3.989003	0.102396
C	0.447492	4.287313	0.345699	H	-1.336534	2.371981	0.149384
H	-0.578128	2.768293	1.500945	C	1.452393	4.323445	0.113005
C	1.571272	3.499283	-1.637577	H	3.472814	3.586199	0.182130
H	1.317215	1.404321	-2.080894	H	-0.653863	4.768972	0.044478
C	1.236954	4.540080	-0.772508	H	1.752882	5.365683	0.068708
H	0.179363	5.098819	1.015206	C	1.541799	-1.109560	-0.129630
H	2.187833	3.693308	-2.509796	C	2.388747	-1.684904	0.824299
H	1.589630	5.547181	-0.973066	C	1.745251	-1.365382	-1.491882
N	-0.266803	0.397620	1.770827	C	3.431372	-2.514524	0.419407
H	-0.876735	-0.270593	2.229630	H	2.230947	-1.475835	1.877700
M13OL2 SCF energy in gas phase: -1246.273031 SCF energy in solution: -1246.551364 Free energy in solution: -1246.219187				C	2.791487	-2.193606	-1.885415
				H	1.078209	-0.903421	-2.215042
				C	3.632192	-2.769164	-0.934354
				H	4.087424	-2.958817	1.161283
				H	2.951530	-2.391778	-2.940506
C	-1.728190	0.033459	-1.473817	H	4.446074	-3.415239	-1.248695
C	-4.061911	-0.941874	-1.158061	O	0.165915	-0.276034	2.017393

M13OL2-TS1

SCF energy in gas phase: -1247.410556

SCF energy in solution: -1247.688831

Free energy in solution: -1247.340841

C	-1.777295	1.406862	-1.083129
C	-4.173621	0.610826	-0.816149
C	-2.425241	-0.274146	0.772769
C	-3.832519	0.310510	0.637170
C	-1.414639	0.494436	-0.082929
C	-3.246610	1.706982	-1.326930
C	-0.656381	-0.928497	2.470171
C	-2.025124	-0.306976	2.253446
N	-0.857904	2.003849	-1.828591
P	0.243675	0.006307	0.161370
H	-4.041300	-0.296944	-1.418536
H	-3.886524	1.243130	1.216074
H	-3.492153	2.655494	-0.831534
H	-0.643225	-1.966804	2.104396
H	-2.011553	0.718455	2.641953
H	-2.770301	-0.876138	2.823715
H	-1.259245	2.520627	-2.606173
H	0.434385	0.159953	-1.848188
H	-3.382783	1.871540	-2.401556
H	-5.219080	0.918216	-0.919026
H	-4.552595	-0.386122	1.080837
H	-0.386377	-0.941282	3.529342
H	-2.473675	-1.324353	0.430752
H	0.041132	0.968776	-2.008548
C	1.572663	1.225257	0.042440
C	2.855668	0.856169	-0.357515
C	1.295246	2.539339	0.414718
C	3.870601	1.807288	-0.369692
H	3.057727	-0.164754	-0.669825
C	2.313220	3.487325	0.390681
H	0.284697	2.812785	0.702730
C	3.599734	3.121708	0.003566
H	4.871783	1.522992	-0.676874
H	2.099337	4.514065	0.669362
H	4.392252	3.863334	-0.013687
C	0.713385	-1.709553	-0.274741
C	1.678640	-2.381759	0.481104
C	0.056333	-2.375194	-1.310779
C	2.007708	-3.699911	0.174355

H	2.160576	-1.870134	1.309160
C	0.364563	-3.701256	-1.594351
H	-0.688804	-1.838033	-1.891794
C	1.348142	-4.360373	-0.859345
H	2.771489	-4.213981	0.749008
H	-0.154644	-4.217994	-2.394934
H	1.598374	-5.391010	-1.090671
O	0.356734	-0.172197	1.813055

M13OL2-Pr

SCF energy in gas phase: -1247.459648

SCF energy in solution: -1247.737437

Free energy in solution: -1247.382623

C	-1.517873	1.800696	-1.009404
C	-4.011620	1.555504	-0.734074
C	-2.445648	0.298920	0.793331
C	-3.700167	1.170481	0.704837
C	-1.327073	0.790423	-0.121004
C	-2.875309	2.419731	-1.262144
C	-0.782046	-0.719330	2.382629
C	-1.981001	0.200841	2.248709
N	-0.517887	2.433453	-1.719004
P	0.279596	-0.073182	-0.071652
H	-4.103396	0.649944	-1.346259
H	-3.537671	2.086447	1.290237
H	-2.901425	3.413079	-0.796092
H	-1.056116	-1.728894	2.033471
H	-1.706388	1.200430	2.608410
H	-2.806663	-0.167334	2.871243
H	-0.777874	2.814894	-2.615963
H	0.373656	0.038772	-1.525918
H	-2.981270	2.584844	-2.342657
H	-4.961009	2.094634	-0.804804
H	-4.538966	0.639769	1.168123
H	-0.476111	-0.811742	3.431812
H	-2.720505	-0.721882	0.476300
H	0.414858	2.047992	-1.688633
C	1.897245	0.827101	0.036885
C	2.717596	0.820225	-1.095912
C	2.311848	1.541143	1.166837
C	3.934047	1.497811	-1.101200
H	2.399512	0.270923	-1.979394
C	3.514148	2.241365	1.151506

H	1.684672	1.536095	2.048559
C	4.329807	2.217676	0.022199
H	4.566585	1.468884	-1.982799
H	3.817760	2.805834	2.027690
H	5.270048	2.760332	0.017867
C	0.260964	-1.905599	-0.298855
C	0.903281	-2.771623	0.589576
C	-0.380064	-2.430131	-1.422633
C	0.910787	-4.142957	0.347591
H	1.389135	-2.356254	1.466703
C	-0.405931	-3.803519	-1.644912
H	-0.858296	-1.750499	-2.124976
C	0.248767	-4.660647	-0.762989
H	1.427938	-4.809129	1.031213
H	-0.922697	-4.204546	-2.511274
H	0.245193	-5.731159	-0.943286
O	0.322468	-0.219567	1.669050

M14NHL2

SCF energy in gas phase: -1303.786933

SCF energy in solution: -1304.075634

Free energy in solution: -1303.697758

C	1.884942	0.665277	-3.060294
C	3.295922	0.325338	-2.526421
C	3.013505	-0.669511	-1.391924
C	1.550756	-0.367061	-1.101927
C	3.839908	-0.478447	-0.114555
C	1.034329	-0.854159	0.131418
C	1.886033	-1.863275	0.876917
C	3.309139	-1.298239	1.087303
C	1.266121	-2.318914	2.207645
H	2.052207	-2.728796	2.852225
C	0.537954	-1.199008	2.943842
H	4.892963	-0.712403	-0.303383
H	1.639542	0.062667	-3.947324
H	3.966909	-0.065834	-3.294888
H	3.981164	-2.136809	1.308411
H	0.237743	-1.537510	3.939320
N	0.942572	0.361803	-1.983296
P	-0.490949	-0.302264	0.629748
H	1.801478	1.714880	-3.363643
H	3.758960	1.226068	-2.106109
H	0.536316	-3.116591	2.031125

H	1.197370	-0.326669	3.069095
H	3.803722	0.590291	0.130105
H	3.303922	-0.659418	1.979515
H	3.103937	-1.708862	-1.740309
H	1.995796	-2.768023	0.259482
C	-1.999672	-0.837096	-0.237646
C	-2.223458	-0.362716	-1.537288
C	-2.886135	-1.749094	0.339924
C	-3.341787	-0.795473	-2.241030
H	-1.499607	0.314172	-1.985889
C	-4.007088	-2.171129	-0.371458
H	-2.689853	-2.124363	1.339419
C	-4.235839	-1.693113	-1.658535
H	-3.515967	-0.432613	-3.248981
H	-4.700266	-2.874408	0.079281
H	-5.109597	-2.023555	-2.211803
C	-0.625712	1.519115	0.634513
C	-1.874854	2.141573	0.699341
C	0.537787	2.290382	0.693489
C	-1.959373	3.525296	0.831349
H	-2.782832	1.547614	0.635254
C	0.449964	3.672610	0.815334
H	1.501520	1.792585	0.628230
C	-0.797569	4.290082	0.886681
H	-2.931444	4.005213	0.882774
H	1.354803	4.270957	0.847500
H	-0.863700	5.369515	0.981261
N	-0.693496	-0.859259	2.212219
H	-1.343630	-0.296589	2.750572

M14NHL2-TS1

SCF energy in gas phase: -1304.913186

SCF energy in solution: -1305.198709

Free energy in solution: -1304.805414

C	2.836409	0.257535	-2.886381
C	4.060358	-0.056500	-2.007865
C	3.443105	-0.715982	-0.766932
C	2.005186	-0.231588	-0.815345
C	4.064068	-0.317889	0.573737
C	1.153432	-0.511069	0.265134
C	1.826917	-1.375702	1.348909
C	3.176821	-0.745359	1.761617
C	1.008400	-1.625339	2.626950

H	1.696422	-1.818340	3.458803	M14NHL2-Pr			
C	0.079254	-0.457255	2.931872	SCF energy in gas phase: -1304.950295			
H	5.069397	-0.741807	0.662242	SCF energy in solution: -1305.237375			
H	2.621107	-0.571809	-3.575437	Free energy in solution: -1304.837361			
H	4.800188	-0.683811	-2.509907				
H	3.705187	-1.472555	2.388908	C	2.744676	-1.838951	-2.577489
H	-0.370883	-0.549657	3.925320	C	3.939423	-1.457244	-1.700713
N	1.743904	0.426907	-1.932655	C	3.320029	-1.292692	-0.304278
P	-0.554438	-0.092518	0.295356	C	1.856335	-0.993060	-0.574181
H	2.969412	1.159213	-3.491007	C	3.908951	-0.150607	0.533503
H	4.551266	0.877961	-1.714839	C	1.038880	-0.619245	0.456777
H	0.384573	-2.522805	2.523351	C	1.750269	-0.692610	1.818832
H	0.626533	0.492963	2.915032	C	3.055090	0.133832	1.785433
H	4.182422	0.771028	0.568118	C	0.922352	-0.300336	3.049550
H	2.964999	0.122524	2.397267	H	1.607115	-0.019549	3.859920
H	-0.444736	0.157053	-1.648229	C	-0.070402	0.814458	2.744189
H	0.416810	0.334025	-1.982473	H	4.943926	-0.384346	0.803045
H	3.446938	-1.811225	-0.863022	H	2.580669	-2.926776	-2.572174
H	2.060762	-2.361847	0.918880	H	4.741978	-2.196140	-1.733510
C	-1.915547	-1.132340	-0.387354	H	3.623156	-0.089998	2.695391
C	-2.956291	-0.583043	-1.137186	H	-0.521097	1.201580	3.666977
C	-1.886591	-2.506684	-0.148537	N	1.655311	-1.125336	-1.925502
C	-3.970094	-1.401088	-1.622768	P	-0.632762	0.029671	0.141791
H	-2.959595	0.482950	-1.349219	H	2.855354	-1.515540	-3.615632
C	-2.891962	-3.328187	-0.654631	H	4.342939	-0.495989	-2.035373
H	-1.065236	-2.940557	0.419168	H	0.347317	-1.163043	3.410117
C	-3.938504	-2.774869	-1.385253	H	0.442391	1.665040	2.272390
H	-4.783169	-0.967315	-2.196321	H	3.941894	0.735567	-0.109371
H	-2.855783	-4.398437	-0.477509	H	2.794961	1.197645	1.827983
H	-4.725582	-3.412452	-1.774783	H	-0.421033	-0.173913	-1.298623
C	-0.973088	1.689033	0.210333	H	0.715704	-1.167507	-2.288487
C	-2.086164	2.138015	0.925562	H	3.389368	-2.234987	0.256912
C	-0.189279	2.606856	-0.495464	H	2.058645	-1.738284	1.969514
C	-2.432882	3.487000	0.908677	C	-2.113489	-1.073039	-0.068919
H	-2.667084	1.429265	1.506540	C	-2.978405	-0.806835	-1.132521
C	-0.523618	3.956802	-0.483436	C	-2.345504	-2.195585	0.727670
H	0.677185	2.263796	-1.052705	C	-4.081482	-1.619585	-1.369470
C	-1.649770	4.398759	0.208222	H	-2.777835	0.046033	-1.778439
H	-3.308304	3.824017	1.454906	C	-3.429349	-3.033743	0.469870
H	0.094710	4.665862	-1.024737	H	-1.664695	-2.432268	1.542660
H	-1.912429	5.452159	0.204512	C	-4.305549	-2.739565	-0.570306
N	-0.982292	-0.404509	1.937164	H	-4.760757	-1.388113	-2.184144
H	-1.630772	-1.175844	2.036060	H	-3.588914	-3.915553	1.082980
				H	-5.156264	-3.385231	-0.764554

C	-0.735301	1.839729	-0.285372	H	2.322788	-2.108481	1.393591
C	-1.542164	2.754409	0.394597	O	-0.741893	0.016969	2.248243
C	0.038596	2.286966	-1.361377	C	-1.815693	-1.126041	0.060360
C	-1.586956	4.088212	-0.009107	C	-3.148412	-0.787808	0.314121
H	-2.124790	2.403433	1.238873	C	-1.501461	-2.279227	-0.657726
C	0.022451	3.624219	-1.741844	C	-4.165994	-1.623433	-0.129391
H	0.659380	1.572276	-1.898697	H	-3.383511	0.123370	0.858302
C	-0.800813	4.526634	-1.070479	C	-2.526556	-3.104816	-1.113524
H	-2.233230	4.787448	0.512903	H	-0.459246	-2.504132	-0.865319
H	0.641926	3.961357	-2.567292	C	-3.852994	-2.780275	-0.843991
H	-0.829293	5.568235	-1.376026	H	-5.202133	-1.373850	0.075040
N	-1.100825	0.341340	1.840468	H	-2.289253	-3.999015	-1.680445
H	-1.644602	-0.400647	2.264843	H	-4.650077	-3.427424	-1.196757

M14OL2

SCF energy in gas phase: -1323.655064

SCF energy in solution: -1323.948683

Free energy in solution: -1323.583673

C	2.100539	-0.467228	-3.063176
C	3.480107	-0.303711	-2.383027
C	3.214873	-0.748704	-0.938240
C	1.703140	-0.598284	-0.864250
C	3.858403	0.106686	0.159546
C	1.124379	-0.613957	0.435272
C	2.030988	-1.061987	1.569861
C	3.336980	-0.235289	1.576361
C	1.337029	-1.031398	2.938934
H	2.088236	-1.017824	3.737270
C	0.413592	0.163932	3.097120
H	4.949434	0.021592	0.121449
H	2.033343	-1.423746	-3.602291
H	4.273881	-0.869619	-2.876453
H	4.092816	-0.795192	2.141255
H	0.010697	0.232804	4.109524
N	1.098094	-0.434068	-1.996971
P	-0.466230	-0.072879	0.650737
H	1.909460	0.319832	-3.801229
H	3.772098	0.752783	-2.385704
H	0.726773	-1.930868	3.078334
H	0.926702	1.104635	2.856855
H	3.618155	1.150604	-0.071831
H	3.164320	0.698280	2.126515
H	3.482526	-1.805618	-0.790991

H	2.322788	-2.108481	1.393591
O	-0.741893	0.016969	2.248243
C	-1.815693	-1.126041	0.060360
C	-3.148412	-0.787808	0.314121
C	-1.501461	-2.279227	-0.657726
C	-4.165994	-1.623433	-0.129391
H	-3.383511	0.123370	0.858302
C	-2.526556	-3.104816	-1.113524
H	-0.459246	-2.504132	-0.865319
C	-3.852994	-2.780275	-0.843991
H	-5.202133	-1.373850	0.075040
H	-2.289253	-3.999015	-1.680445
H	-4.650077	-3.427424	-1.196757
C	-0.883371	1.583956	0.029660
C	-1.132836	2.606822	0.950077
C	-0.958743	1.843657	-1.344653
C	-1.442648	3.887499	0.500952
H	-1.102432	2.395384	2.014357
C	-1.263957	3.128660	-1.782335
H	-0.752375	1.044730	-2.050220
C	-1.505057	4.149144	-0.864702
H	-1.639324	4.677740	1.218469
H	-1.317596	3.332838	-2.846920
H	-1.747197	5.147891	-1.214508

M14OL2-TS1

SCF energy in gas phase: -1324.790321

SCF energy in solution: -1325.081243

Free energy in solution: -1324.700115

C	2.914331	0.378840	-2.828838
C	4.109036	-0.085998	-1.975663
C	3.440300	-0.805578	-0.796398
C	2.032896	-0.236692	-0.821719
C	4.073054	-0.556544	0.574425
C	1.151302	-0.561113	0.224917
C	1.759365	-1.509812	1.272719
C	3.136559	-0.976415	1.726865
C	0.897927	-1.726022	2.529011
H	1.545505	-1.956012	3.382675
C	0.037430	-0.510781	2.812185
H	5.034146	-1.076081	0.641112
H	2.661165	-0.369649	-3.593363
H	4.811114	-0.715225	-2.527050

H	3.608308	-1.753333	2.339387	C	4.134826	-1.201692	-1.579940
H	-0.486206	-0.590508	3.768106	C	3.465599	-1.027941	-0.208716
N	1.815476	0.524429	-1.877181	C	1.997290	-0.819200	-0.530815
P	-0.536078	-0.102264	0.248419	C	3.975580	0.158160	0.617373
H	3.106768	1.322204	-3.347834	C	1.130793	-0.462556	0.464436
H	4.657412	0.786509	-1.603952	C	1.800341	-0.449229	1.848732
H	0.218149	-2.576402	2.405973	C	3.061131	0.441894	1.826628
H	0.631312	0.414153	2.817716	C	0.899815	-0.039094	3.020603
H	4.291738	0.514384	0.645258	H	1.516369	0.378425	3.825683
H	2.960389	-0.119959	2.388496	C	-0.160799	0.943397	2.567529
H	-0.395782	0.205791	-1.667269	H	5.006290	-0.029244	0.934981
H	0.424097	0.428353	-1.950358	H	2.893544	-2.786143	-2.420439
H	3.378251	-1.887951	-0.979557	H	4.982788	-1.888476	-1.562690
H	1.930649	-2.496042	0.815789	H	3.604774	0.284023	2.764789
O	-0.968480	-0.459187	1.809625	H	-0.732106	1.342991	3.414048
C	-1.957023	-1.058703	-0.427313	N	1.841392	-1.018757	-1.881537
C	-2.792061	-0.537228	-1.416953	P	-0.585749	-0.008293	0.077644
C	-2.195142	-2.340930	0.068320	H	3.114219	-1.407432	-3.519126
C	-3.862105	-1.286123	-1.894037	H	4.486962	-0.229394	-1.939650
H	-2.598103	0.455784	-1.814239	H	0.374678	-0.909605	3.427366
C	-3.247097	-3.102406	-0.433167	H	0.298475	1.803621	2.050433
H	-1.561430	-2.738472	0.854517	H	4.002839	1.028320	-0.046971
C	-4.085715	-2.573651	-1.409679	H	2.742830	1.490757	1.819204
H	-4.516854	-0.868365	-2.652071	H	-0.318033	-0.225471	-1.331765
H	-3.417018	-4.104235	-0.051810	H	0.918695	-1.169593	-2.258222
H	-4.913209	-3.162320	-1.793043	H	3.560844	-1.952058	0.379031
C	-0.915032	1.678585	0.239102	H	2.149285	-1.472064	2.054004
C	-2.147615	2.080963	0.759913	O	-1.051913	0.253487	1.727420
C	0.013222	2.632658	-0.183463	C	-1.947399	-1.252160	-0.061365
C	-2.460567	3.435042	0.835391	C	-2.502341	-1.472904	-1.324380
H	-2.854167	1.334501	1.112126	C	-2.416375	-2.002015	1.022031
C	-0.302040	3.984801	-0.091498	C	-3.517551	-2.407946	-1.505301
H	0.964672	2.312214	-0.597848	H	-2.142301	-0.895515	-2.173020
C	-1.537385	4.387176	0.411825	C	-3.408133	-2.961016	0.836754
H	-3.421763	3.746203	1.231870	H	-1.999453	-1.820987	2.004893
H	0.418932	4.726992	-0.419335	C	-3.965478	-3.161472	-0.424021
H	-1.779229	5.443501	0.476018	H	-3.952385	-2.552714	-2.489394
M14OL2-Pr				H	-3.752512	-3.548493	1.682349
SCF energy in gas phase: -1324.839473				H	-4.746325	-3.902799	-0.562977
SCF energy in solution: -1325.132322				C	-0.962674	1.750602	-0.374584
Free energy in solution: -1324.743721				C	-1.875860	2.533488	0.337452
				C	-0.323310	2.299123	-1.489550
				C	-2.151407	3.836622	-0.069035
C	2.992177	-1.691693	-2.470861	H	-2.366987	2.106789	1.205263

C	-0.574113	3.611513	-1.878181
H	0.379586	1.687783	-2.052187
C	-1.496911	4.379609	-1.171611
H	-2.875616	4.430961	0.479595
H	-0.059295	4.032153	-2.736510
H	-1.706570	5.399019	-1.481011

M15NHL2

SCF energy in gas phase: -1343.084855

SCF energy in solution: -1343.380516

Free energy in solution: -1342.974899

C	3.091659	1.775120	-2.211501
C	3.718189	0.403380	-1.984049
C	3.153379	-0.162231	-0.686819
C	1.626188	-0.109657	-0.697514
C	1.574095	1.625879	-2.353915
C	3.658996	-1.561621	-0.338975
C	0.947802	-0.908171	0.285040
C	1.515020	-2.217318	0.810522
C	3.033227	-2.066581	0.958902
C	0.863316	-2.708052	2.130698
H	1.642695	-3.073038	2.810474
C	0.035099	-1.647818	2.844644
H	3.407027	-2.253513	-1.155180
H	3.323233	2.414418	-1.349560
H	3.468353	-0.265857	-2.818709
H	1.340335	1.323345	-3.386349
H	3.468104	-3.032246	1.245305
H	0.660555	-0.782350	3.108955
N	0.934475	0.674456	-1.463406
P	-0.662223	-0.425323	0.575924
H	-0.379418	-2.058955	3.769357
H	0.195818	-3.550889	1.925108
H	1.365860	-3.018170	0.068346
H	1.090766	2.602391	-2.214061
H	3.501856	2.268819	-3.098578
H	4.811051	0.461253	-1.927726
H	3.470447	0.505698	0.131874
H	4.752804	-1.543533	-0.264123
H	3.244002	-1.356614	1.771989
C	-2.059767	-0.776751	-0.549033
C	-2.944985	-1.823625	-0.277109
C	-2.200276	-0.037922	-1.731390

C	-3.972892	-2.118894	-1.170023
H	-2.821149	-2.403912	0.631382
C	-3.228437	-0.338608	-2.617401
H	-1.482045	0.747699	-1.945910
C	-4.116642	-1.376495	-2.337825
H	-4.660034	-2.930433	-0.951970
H	-3.334444	0.234857	-3.532930
H	-4.917267	-1.608080	-3.033592
C	-0.797517	1.362513	0.929651
C	0.331082	2.061519	1.369844
C	-2.035813	2.006289	0.895472
C	0.221162	3.392364	1.754417
H	1.288041	1.547573	1.398020
C	-2.144356	3.339014	1.289765
H	-2.917311	1.473490	0.549496
C	-1.016981	4.032960	1.715542
H	1.102639	3.933482	2.083761
H	-3.109819	3.833844	1.257009
H	-1.100263	5.072252	2.017633
N	-1.093998	-1.271894	1.980373
H	-1.871128	-0.851362	2.478701

M15NHL2-TS1

SCF energy in gas phase: -1344.212627

SCF energy in solution: -1344.508955

Free energy in solution: -1344.087150

C	4.347511	0.889172	-1.369827
C	4.256141	-0.623398	-1.204508
C	3.296482	-0.938677	-0.060482
C	1.955641	-0.236590	-0.269997
C	2.973076	1.444645	-1.734624
C	3.135651	-2.431667	0.204082
C	0.806482	-0.776282	0.320202
C	0.723051	-2.211585	0.843131
C	2.104206	-2.680989	1.299048
C	-0.333838	-2.390798	1.959437
H	-0.031864	-3.219572	2.609150
C	-0.530426	-1.126177	2.783768
H	2.812728	-2.934045	-0.718483
H	4.690549	1.330276	-0.425427
H	3.885579	-1.079499	-2.133012
H	2.782440	1.239310	-2.799464
H	2.058717	-3.746195	1.554518

H	0.454615	-0.754360	3.109351	C	4.221298	1.553684	-1.451082
N	1.877086	0.898078	-0.954733	C	4.302685	0.040343	-1.278785
P	-0.724876	0.069585	0.332638	C	3.538370	-0.410208	-0.028536
H	-1.119536	-1.343347	3.681054	C	2.112027	0.114564	-0.050621
H	-1.304460	-2.662394	1.527702	C	2.759216	1.971315	-1.521090
H	0.424182	-2.879812	0.018068	C	3.588069	-1.923892	0.149087
H	2.966384	2.536456	-1.627945	C	1.042808	-0.641098	0.282561
H	5.073252	1.169493	-2.140063	C	1.165597	-2.082413	0.770081
H	0.679791	0.843719	-1.473867	C	2.599404	-2.377122	1.213521
H	-0.233976	0.546310	-1.645640	C	0.156719	-2.413863	1.890094
H	5.237523	-1.064099	-0.996203	H	0.592460	-3.172525	2.551529
H	3.722777	-0.491272	0.851947	C	-0.218712	-1.171124	2.691157
H	4.109243	-2.857156	0.474540	H	3.335080	-2.408267	-0.804289
H	2.392092	-2.137945	2.210524	H	4.695553	2.050171	-0.596540
C	-2.117751	-0.749211	-0.530869	H	3.863014	-0.450479	-2.158406
C	-3.397090	-0.735885	0.031451	H	2.316608	1.582247	-2.453154
C	-1.890151	-1.456943	-1.714014	H	2.703649	-3.449291	1.414764
C	-4.447618	-1.389100	-0.609403	H	0.700658	-0.732630	3.115704
H	-3.553971	-0.231478	0.978940	N	2.040494	1.481195	-0.345162
C	-2.933444	-2.137031	-2.332273	P	-0.649299	0.061857	0.131777
H	-0.891838	-1.455119	-2.141349	H	-0.849946	-1.457733	3.540367
C	-4.215774	-2.092521	-1.788008	H	-0.757189	-2.840342	1.465725
H	-5.443586	-1.359588	-0.178946	H	0.942779	-2.742807	-0.082165
H	-2.747895	-2.693790	-3.245147	H	2.666962	3.060839	-1.539823
H	-5.032466	-2.611533	-2.280144	H	4.742843	1.875749	-2.357855
C	-0.795510	1.884332	0.310919	H	1.107337	1.870334	-0.284570
C	0.195583	2.600273	0.984279	H	-0.332861	0.444394	-1.258311
C	-1.852983	2.551498	-0.305695	H	5.343386	-0.296175	-1.209413
C	0.126952	3.989837	1.034145	H	4.021947	0.064577	0.839555
H	1.023101	2.067901	1.445874	H	4.611494	-2.225525	0.398101
C	-1.923931	3.939380	-0.237569	H	2.800299	-1.848679	2.156387
H	-2.606975	1.987386	-0.847662	C	-1.876881	-1.146155	-0.556649
C	-0.934275	4.658653	0.429062	C	-2.885632	-1.715981	0.225083
H	0.904848	4.549176	1.543868	C	-1.796520	-1.499516	-1.907154
H	-2.748830	4.459825	-0.713294	C	-3.801303	-2.604443	-0.331756
H	-0.988268	5.741797	0.473146	H	-2.939485	-1.467761	1.279573
N	-1.251028	-0.132606	1.981841	C	-2.694432	-2.408044	-2.461769
H	-1.311320	0.761867	2.455108	H	-1.018389	-1.057042	-2.523259
				C	-3.704602	-2.955530	-1.675838
				H	-4.586634	-3.028467	0.286294
				H	-2.609272	-2.682485	-3.508622
				H	-4.412944	-3.655762	-2.107709
				C	-1.307947	1.809173	0.300222
				C	-1.105026	2.619314	1.419921
M15NHL2-Pr							
SCF energy in gas phase: -1344.251876							
SCF energy in solution: -1344.547395							
Free energy in solution: -1344.120032							

C	-1.984333	2.336892	-0.804007
C	-1.576438	3.931941	1.434685
H	-0.568597	2.214698	2.271776
C	-2.493586	3.629901	-0.773974
H	-2.110239	1.719031	-1.691328
C	-2.282160	4.433546	0.345990
H	-1.392703	4.560510	2.300709
H	-3.042760	4.017184	-1.626640
H	-2.660696	5.450829	0.364480
N	-0.928856	-0.204730	1.868516
H	-1.756069	0.194605	2.290118

M15OL2

SCF energy in gas phase: -1362.955206

SCF energy in solution: -1363.255415

Free energy in solution: -1362.861166

C	3.501209	1.686418	-1.753572
C	4.010378	0.267183	-1.525470
C	3.206674	-0.346185	-0.384453
C	1.707534	-0.170961	-0.624219
C	2.027013	1.636660	-2.161870
C	3.557146	-1.808646	-0.099158
C	0.843061	-0.974542	0.199289
C	1.222973	-2.384484	0.624290
C	2.701529	-2.391938	1.026051
C	0.303627	-2.930654	1.736009
H	0.846578	-3.663245	2.344821
C	-0.251315	-1.834011	2.627933
H	3.400717	-2.401807	-1.011570
H	3.609389	2.254232	-0.821001
H	3.871701	-0.330239	-2.437317
H	1.958272	1.398761	-3.234163
H	3.017205	-3.418483	1.251624
H	0.549808	-1.183831	3.000401
N	1.193182	0.682389	-1.449950
P	-0.697152	-0.345626	0.522447
H	-0.802838	-2.241675	3.477796
H	-0.555901	-3.450917	1.297307
H	1.136514	-3.079682	-0.226970
H	1.572834	2.630879	-2.047856
H	4.081190	2.209543	-2.520885
H	5.079674	0.253267	-1.286758
H	3.428204	0.225192	0.531175

H	4.623465	-1.881236	0.145539
H	2.835983	-1.795516	1.939674
C	-2.116742	-0.669629	-0.570825
C	-3.378385	-0.993544	-0.064499
C	-1.907303	-0.599554	-1.952085
C	-4.430142	-1.242723	-0.941029
H	-3.525199	-1.060562	1.008770
C	-2.967526	-0.840955	-2.821484
H	-0.914418	-0.349758	-2.322145
C	-4.225438	-1.163187	-2.317051
H	-5.409813	-1.500842	-0.551283
H	-2.810135	-0.785717	-3.893970
H	-5.048189	-1.357840	-2.998153
C	-0.742679	1.437299	0.865458
C	-0.595760	1.840604	2.193475
C	-0.938902	2.392494	-0.135957
C	-0.623075	3.194670	2.518586
H	-0.471625	1.095167	2.972892
C	-0.962666	3.743103	0.192806
H	-1.051923	2.071489	-1.166007
C	-0.802375	4.144801	1.518198
H	-0.507972	3.505118	3.551989
H	-1.107717	4.484427	-0.586374
H	-0.822466	5.200468	1.770492
O	-1.213919	-1.046606	1.902797

M15OL2-TS1

SCF energy in gas phase: -1364.089552

SCF energy in solution: -1364.392019

Free energy in solution: -1363.983308

C	4.321667	0.960842	-1.392468
C	4.283088	-0.552915	-1.216116
C	3.322264	-0.890669	-0.079851
C	1.961673	-0.233716	-0.309862
C	2.931986	1.464183	-1.776590
C	3.205419	-2.385484	0.198597
C	0.824075	-0.803519	0.293574
C	0.785499	-2.235152	0.831066
C	2.180387	-2.653049	1.295514
C	-0.265084	-2.414931	1.951712
H	0.069576	-3.187271	2.654159
C	-0.528437	-1.113848	2.690707
H	2.898952	-2.907113	-0.718854

H	4.637396	1.420980	-0.447847	SCF energy in solution: -1364.443885		
H	3.939126	-1.029806	-2.144392	Free energy in solution: -1364.024394		
H	2.763984	1.256108	-2.844273			
H	2.168214	-3.715282	1.566789	C	3.833408	1.841051 -1.912407
H	0.417889	-0.667011	3.026476	C	4.111465	0.460925 -1.324407
N	1.843026	0.873467	-1.019271	C	3.500166	0.322547 0.075097
P	-0.701208	0.026202	0.287947	C	2.018884	0.658198 0.024920
H	-1.165525	-1.270797	3.565136	C	2.329112	2.060558 -1.988320
H	-1.220035	-2.754048	1.533455	C	3.717263	-1.071669 0.652855
H	0.509794	-2.928070	0.018955	C	1.079960	-0.089701 0.660298
H	2.881001	2.554104	-1.666070	C	1.440632	-1.104083 1.737459
H	5.045594	1.262050	-2.156441	C	2.953767	-1.202484 1.962509
H	0.601319	0.756940	-1.543767	C	0.715143	-0.785869 3.063693
H	-0.268423	0.435543	-1.675973	H	1.343210	-0.144527 3.693787
H	5.277086	-0.956452	-0.993191	C	-0.608461	-0.080375 2.786133
H	3.721923	-0.421837	0.833735	H	3.357901	-1.820121 -0.065812
H	4.190543	-2.779220	0.474951	H	4.277975	2.612361 -1.272750
H	2.449679	-2.088068	2.199389	H	3.675110	-0.307622 -1.977659
C	-2.145248	-0.737477	-0.530844	H	1.902535	1.393950 -2.756023
C	-3.418534	-0.570345	0.021620	H	3.187546	-2.141602 2.475402
C	-1.975103	-1.550117	-1.652776	H	-0.423731	0.994073 2.622837
C	-4.517662	-1.188427	-0.568602	N	1.722876	1.812115 -0.683304
H	-3.538978	0.032839	0.916076	P	-0.669686	-0.102566 0.099805
C	-3.070933	-2.191873	-2.219996	H	-1.294931	-0.158608 3.638117
H	-0.981176	-1.660639	-2.077286	H	0.545105	-1.717614 3.614522
C	-4.343826	-2.002439	-1.684933	H	1.079932	-2.085375 1.396724
H	-5.507894	-1.044044	-0.148419	H	2.099822	3.090571 -2.276410
H	-2.934098	-2.831718	-3.085904	H	4.271277	1.940860 -2.910227
H	-5.200229	-2.492018	-2.137979	H	0.754187	2.095109 -0.620756
C	-0.766015	1.841191	0.322939	H	-0.249951	0.341497 -1.217328
C	-0.096588	2.497062	1.355546	H	5.187537	0.263609 -1.269797
C	-1.516233	2.564596	-0.601007	H	3.988187	1.062764 0.727877
C	-0.158160	3.883785	1.446914	H	4.789064	-1.246423 0.796879
H	0.474985	1.920498	2.076951	H	3.271909	-0.390081 2.629805
C	-1.598422	3.948957	-0.489678	C	-1.282515	-1.671213 -0.661022
H	-2.021839	2.042113	-1.408178	C	-1.578292	-2.826480 0.073479
C	-0.913981	4.608652	0.528782	C	-1.435386	-1.701214 -2.050296
H	0.376718	4.397585	2.239079	C	-2.004255	-3.982130 -0.575090
H	-2.190274	4.513694	-1.202660	H	-1.477994	-2.803253 1.150802
H	-0.970836	5.689853	0.607482	C	-1.884184	-2.849072 -2.696489
O	-1.227317	-0.191007	1.858602	H	-1.201475	-0.813023 -2.630633
				C	-2.163449	-3.995498 -1.958466
M15OL2-Pr				H	-2.221411	-4.874122 0.004347
SCF energy in gas phase: -1364.142204				H	-2.009041	-2.849560 -3.774717

H	-2.504432	-4.896477	-2.459384
C	-1.839394	1.353038	0.133195
C	-2.801038	1.549874	1.132497
C	-1.785513	2.269208	-0.922769
C	-3.660357	2.643672	1.083762
H	-2.882791	0.824678	1.932585
C	-2.637529	3.369341	-0.970371
H	-1.079199	2.108643	-1.735230
C	-3.575943	3.560589	0.038624
H	-4.403328	2.778073	1.863735
H	-2.574270	4.068577	-1.798134
H	-4.245458	4.414406	0.006274
O	-1.229880	-0.657795	1.663488

M4NHL3

SCF energy in gas phase: -1222.802792

SCF energy in solution: -1223.082781

Free energy in solution: -1222.805034

C	1.743135	-0.024956	0.217514
C	3.251894	-0.121774	2.066702
C	4.101877	-0.013270	-0.244169
C	4.284806	-0.084760	1.163393
C	2.802507	0.018333	-0.699904
C	1.864655	-0.088812	1.645212
H	5.302327	-0.111997	1.546695
H	3.463365	-0.176945	3.131473
H	4.950065	0.015129	-0.918386
N	0.776984	-0.108224	2.374661
P	0.217135	-0.001646	-0.595088
C	2.347981	0.108753	-2.143315
H	2.787396	-0.693383	-2.746175
C	-0.864344	1.412835	-0.336964
C	-1.958855	1.288234	0.531093
C	-0.591728	2.618025	-0.989148
C	-2.773630	2.405856	0.720887
C	-1.414358	3.717953	-0.788278
C	-2.507278	3.605372	0.069907
C	-0.903768	-1.388212	-0.375702
C	-1.994975	-1.256807	0.495137
C	-0.667801	-2.577788	-1.068864
C	-2.843378	-2.354128	0.651092
C	-1.523156	-3.658177	-0.899225
C	-2.611431	-3.540691	-0.035980

H	0.270048	2.686882	-1.648568
H	-1.207270	4.655480	-1.292891
H	-3.158390	4.458720	0.231659
H	-3.626539	2.330830	1.389472
H	-3.694639	-2.273668	1.321152
H	-3.287799	-4.378851	0.099544
H	-1.345271	-4.584865	-1.434149
H	0.185107	-2.641215	-1.738769
H	1.019459	-0.158247	3.363457
H	2.650801	1.067942	-2.581328
N	0.879547	-0.015575	-2.126695
H	0.352874	0.251025	-2.944809
C	-2.212967	0.007925	1.286741
H	-1.469517	-0.015818	2.103600
H	-3.219886	0.016806	1.711805

M4NHL3-TS1

SCF energy in gas phase: -1223.943004

SCF energy in solution: -1224.219210

Free energy in solution: -1223.926484

C	1.839676	0.021390	0.208361
C	3.819450	-0.267699	1.567819
C	4.016700	0.647653	-0.681117
C	4.578619	0.260524	0.554393
C	2.653232	0.528382	-0.827593
C	2.405924	-0.486389	1.432865
H	5.649868	0.368317	0.703948
H	4.287919	-0.574865	2.499046
H	4.639272	1.004501	-1.494459
N	1.647052	-1.114336	2.315184
P	0.146085	0.084242	-0.283490
C	1.912520	0.850320	-2.104258
H	2.394086	0.352862	-2.953905
H	0.375352	-0.490465	2.150809
H	-0.270119	0.016121	1.814112
C	-1.046127	1.418544	0.028862
C	-2.330001	1.129988	0.510897
C	-0.689627	2.726424	-0.312092
C	-3.242525	2.181291	0.625245
C	-1.600990	3.763744	-0.162973
C	-2.885416	3.484826	0.299534
C	-0.836205	-1.422639	-0.270379
C	-2.136129	-1.431917	0.248772

C	-0.290889	-2.556693	-0.875595
C	-2.876740	-2.611068	0.138687
C	-1.035003	-3.725710	-0.956174
C	-2.333617	-3.746829	-0.450633
H	0.311763	2.929456	-0.685046
H	-1.316356	4.780230	-0.413383
H	-3.611614	4.284219	0.405892
H	-4.245903	1.970559	0.985802
H	-3.890143	-2.636880	0.529953
H	-2.927712	-4.652830	-0.517556
H	-0.609804	-4.612420	-1.413760
H	0.716268	-2.507932	-1.280049
H	2.140245	-1.307746	3.182521
H	1.932867	1.932391	-2.300801
N	0.552284	0.355554	-1.915948
H	-0.157314	0.767429	-2.507422
C	-2.722751	-0.249559	0.981890
H	-2.392245	-0.330533	2.029224
H	-3.813669	-0.332079	0.983702

M4NHL3-Pr

SCF energy in gas phase: -1223.993791

SCF energy in solution: -1224.266516

Free energy in solution: -1223.966900

C	1.881678	0.565815	0.293831
C	3.996559	0.150341	1.381977
C	3.931663	1.517794	-0.614969
C	4.641994	0.926780	0.425995
C	2.555021	1.320659	-0.654850
C	2.610257	-0.055889	1.326655
H	5.716736	1.065639	0.496338
H	4.569157	-0.322595	2.176006
H	4.434528	2.114622	-1.370101
N	2.006068	-0.919365	2.231188
P	0.014387	0.530389	0.072656
C	1.638971	1.869234	-1.721142
H	1.890225	1.417994	-2.692309
H	1.008159	-0.825989	2.346994
H	-0.134395	0.504816	1.522774
C	-1.828683	1.040197	0.066603
C	-2.767710	0.126936	0.574989
C	-2.268185	2.325968	-0.262579
C	-4.109166	0.493656	0.682488

C	-3.605777	2.694811	-0.135184
C	-4.534295	1.770219	0.327799
C	-0.227785	-1.239918	-0.323590
C	-1.351643	-1.931824	0.144752
C	0.691854	-1.883676	-1.153190
C	-1.530473	-3.264595	-0.226633
C	0.502843	-3.211270	-1.520851
C	-0.611481	-3.902613	-1.053548
H	-1.549944	3.063230	-0.610354
H	-3.917793	3.700959	-0.397924
H	-5.581531	2.040164	0.420352
H	-4.828128	-0.231320	1.056608
H	-2.401310	-3.804451	0.136039
H	-0.767089	-4.939821	-1.333603
H	1.223450	-3.704643	-2.164814
H	1.566485	-1.339546	-1.500105
H	2.497922	-1.046989	3.102858
H	1.762466	2.956077	-1.821932
N	0.303235	1.520542	-1.301667
H	-0.469035	1.770542	-1.899935
C	-2.335182	-1.242546	1.055864
H	-1.869427	-1.126295	2.047213
H	-3.214164	-1.876930	1.202914

M4OL3

SCF energy in gas phase: -1242.669171

SCF energy in solution: -1242.952150

Free energy in solution: -1242.685889

C	-1.738195	-0.002984	0.222838
C	-3.309764	-0.003211	2.020016
C	-4.079778	-0.003898	-0.324387
C	-4.309603	-0.003822	1.080462
C	-2.765378	-0.003368	-0.729738
C	-1.906753	-0.002540	1.647364
H	-5.339724	-0.004272	1.429118
H	-3.559700	-0.003126	3.077814
H	-4.904698	-0.004173	-1.026955
N	-0.843423	-0.001429	2.409054
P	-0.211666	-0.000978	-0.572098
C	-2.231014	-0.002885	-2.144122
H	-2.534377	0.886696	-2.703382
C	0.883875	-1.397319	-0.356733
C	1.963199	-1.269995	0.529476

C	0.643123	-2.585802	-1.049685	H	0.292186	-0.022542	1.832703
C	2.795009	-2.376653	0.705392	C	0.963725	-1.444925	0.011218
C	1.485741	-3.672858	-0.863296	C	2.265674	-1.237800	0.482567
C	2.560123	-3.562935	0.018686	C	0.523141	-2.720481	-0.348298
C	0.879586	1.398743	-0.356871	C	3.113075	-2.343978	0.577057
C	1.959410	1.275141	0.529215	C	1.372644	-3.811099	-0.225774
C	0.634803	2.586313	-1.049995	C	2.674329	-3.617255	0.233179
C	2.787714	2.384476	0.704713	C	0.902035	1.412153	-0.231900
C	1.473902	3.676120	-0.863985	C	2.209587	1.339434	0.263634
C	2.548851	3.569841	0.017776	C	0.403230	2.587875	-0.796242
H	-0.197689	-2.646351	-1.734980	C	3.006893	2.482015	0.170687
H	1.309375	-4.598846	-1.399633	C	1.207322	3.717402	-0.864830
H	3.224628	-4.408066	0.168436	C	2.513441	3.657913	-0.382841
H	3.636907	-2.302969	1.387757	H	-0.490382	-2.856291	-0.717392
H	3.630023	2.313643	1.386873	H	1.027760	-4.803688	-0.494750
H	3.210640	4.417165	0.167202	H	3.351167	-4.461124	0.320037
H	1.294405	4.601435	-1.400446	H	4.129692	-2.200505	0.933116
H	-0.206382	2.644015	-1.735074	H	4.026066	2.446518	0.545514
H	-1.113888	-0.001069	3.391924	H	3.152339	4.533527	-0.438657
H	-2.533176	-0.892625	-2.703747	H	0.821364	4.636296	-1.292480
C	2.185876	0.002982	1.309666	H	-0.615756	2.609275	-1.172867
H	1.437825	0.002027	2.122264	H	-2.217769	1.187591	3.256695
H	3.188587	0.004496	1.744416	H	-1.863206	-1.648552	-2.466710
O	-0.778521	-0.001923	-2.091781	C	2.746471	0.111880	0.961076
M4OL3-TS1				H	2.455336	0.196971	2.019977
SCF energy in gas phase: -1243.813331				H	3.839802	0.133687	0.932558
SCF energy in solution: -1244.094805				O	-0.458258	-0.264362	-1.866042
Free energy in solution: -1243.813938							

C	-1.828280	0.053496	0.211291
C	-3.847550	0.275428	1.525586
C	-3.984710	-0.487117	-0.787345
C	-4.578720	-0.174010	0.457690
C	-2.618566	-0.370291	-0.878963
C	-2.423023	0.484412	1.455963
H	-5.655008	-0.278743	0.568408
H	-4.343419	0.522504	2.460344
H	-4.586177	-0.783052	-1.639753
N	-1.690331	1.033262	2.401582
P	-0.141400	-0.043743	-0.263114
C	-1.818472	-0.603447	-2.136223
H	-2.170801	0.031105	-2.955308
H	-0.347271	0.425604	2.187349

M4OL3-Pr			
SCF energy in gas phase: -1243.871336			
SCF energy in solution: -1224.266516			
Free energy in solution: -1223.966900			
C	-1.949808	0.187582	0.224773
C	-4.082643	0.292051	1.349896
C	-4.019117	0.035221	-1.055871
C	-4.734378	0.150899	0.134365
C	-2.634565	0.059681	-0.982081
C	-2.678530	0.319498	1.431830
H	-5.820186	0.136734	0.118301
H	-4.658365	0.396125	2.265588
H	-4.525330	-0.065661	-2.010780
N	-2.096825	0.532190	2.662169
P	-0.133399	0.082470	0.019052

C	-1.706277	-0.042345	-2.167120	P	-0.264867	0.000004	0.697190
H	-1.949541	0.736050	-2.904569	C	0.983979	0.001081	2.928785
H	-1.123385	0.297433	2.769000	C	4.277886	-0.000969	-1.818755
H	0.062398	0.092589	1.473199	C	2.023056	0.000483	1.829493
C	0.819474	-1.468011	-0.038463	C	3.012331	-0.001403	-2.738669
C	2.093582	-1.438610	0.544614	H	4.906297	0.879489	-1.987681
C	0.340710	-2.624776	-0.648223	H	1.048282	0.891936	3.559672
C	2.871823	-2.596111	0.499845	H	1.048332	-0.888980	3.560783
C	1.114996	-3.780791	-0.655680	H	4.906462	-0.881437	-1.987011
C	2.384247	-3.762002	-0.083281	C	-1.216608	-1.390189	0.089272
C	1.130900	1.387813	-0.115008	C	-2.613809	-1.271406	0.026959
C	2.366937	1.117089	0.488414	C	-0.562014	-2.540348	-0.351022
C	0.910860	2.586504	-0.788209	C	-3.344665	-2.354554	-0.453321
C	3.371837	2.081542	0.402619	C	-1.309078	-3.609632	-0.833378
C	1.911017	3.551932	-0.834586	H	0.523694	-2.575528	-0.327773
C	3.143557	3.294989	-0.239450	C	-2.697481	-3.514643	-0.875254
H	-0.638747	-2.615205	-1.119172	H	-4.427480	-2.286632	-0.509924
H	0.737271	-4.686825	-1.118342	H	-0.811580	-4.507788	-1.182747
H	3.001080	-4.654930	-0.099099	H	-3.284435	-4.345032	-1.255091
H	3.870303	-2.582187	0.929347	C	-1.216011	1.390277	0.088462
H	4.343383	1.878263	0.845782	C	-2.613264	1.272046	0.026344
H	3.935299	4.036116	-0.287147	C	-0.561009	2.540018	-0.352313
H	1.737006	4.492728	-1.346546	C	-3.343728	2.355319	-0.454275
H	-0.040944	2.746697	-1.285346	C	-1.307674	3.609425	-0.834997
H	-2.674832	0.336501	3.464029	H	0.524716	2.574796	-0.329155
H	-1.839760	-1.015462	-2.667307	C	-2.696122	3.514981	-0.876718
C	2.616826	-0.186623	1.223406	H	-4.426576	2.287814	-0.510739
H	2.144035	-0.114666	2.214716	H	-0.809850	4.507256	-1.184734
H	3.690816	-0.297254	1.398926	H	-3.282771	4.345471	-1.256809
O	-0.400054	0.115924	-1.714036	H	3.001204	-0.879273	-3.397256

M5OL3

SCF energy in gas phase: -1320.050351

SCF energy in solution: -1320.350946

Free energy in solution: -1320.053477

C	1.432455	-0.000552	0.533126
C	3.668474	-0.000477	-0.437085
C	3.379357	0.000872	1.990255
C	4.206690	0.000349	0.809408
C	2.227828	-0.000870	-0.656337
H	5.287327	0.000677	0.934458
H	3.832282	0.001657	2.975511
N	1.816199	-0.001366	-1.886884

C	0.983979	0.001081	2.928785
C	4.277886	-0.000969	-1.818755
C	2.023056	0.000483	1.829493
C	3.012331	-0.001403	-2.738669
H	4.906297	0.879489	-1.987681
H	1.048282	0.891936	3.559672
H	1.048332	-0.888980	3.560783
H	4.906462	-0.881437	-1.987011
C	-1.216608	-1.390189	0.089272
C	-2.613809	-1.271406	0.026959
C	-0.562014	-2.540348	-0.351022
C	-3.344665	-2.354554	-0.453321
C	-1.309078	-3.609632	-0.833378
H	0.523694	-2.575528	-0.327773
C	-2.697481	-3.514643	-0.875254
H	-4.427480	-2.286632	-0.509924
H	-0.811580	-4.507788	-1.182747
H	-3.284435	-4.345032	-1.255091
C	-1.216011	1.390277	0.088462
C	-2.613264	1.272046	0.026344
C	-0.561009	2.540018	-0.352313
C	-3.343728	2.355319	-0.454275
C	-1.307674	3.609425	-0.834997
H	0.524716	2.574796	-0.329155
C	-2.696122	3.514981	-0.876718
H	-4.426576	2.287814	-0.510739
H	-0.809850	4.507256	-1.184734
H	-3.282771	4.345471	-1.256809
H	3.001204	-0.879273	-3.397256
H	3.000947	0.876136	-3.397700
O	-0.335732	0.000637	2.323595
C	-3.300353	0.000571	0.482887
H	-4.337881	0.000717	0.138844
H	-3.334948	0.000864	1.581730

M5OL3-TS1

SCF energy in gas phase: -1321.199449

SCF energy in solution: -1321.494544

Free energy in solution: -1321.181078

C	1.494093	-0.054831	0.388656
C	3.757160	-0.019459	-0.532764
C	3.404487	-0.649130	1.786141

C	4.261767	-0.423898	0.668165	M5OL3-Pr		
C	2.349224	0.213477	-0.717306	SCF energy in gas phase: -1321.259065		
H	5.332592	-0.572581	0.786093	SCF energy in solution: -1321.554103		
H	3.818012	-0.941119	2.745597	Free energy in solution: -1321.232199		
N	2.009247	0.639096	-1.917819			
P	-0.249605	-0.072309	0.496108	C	1.582155	0.173268 0.360095
C	1.006310	-0.622968	2.699227	C	3.897978	0.205836 -0.363565
C	4.411228	0.348944	-1.844358	C	3.390959	0.046982 1.988883
C	2.054582	-0.464856	1.624285	C	4.326200	0.115431 0.947214
C	3.184309	0.525064	-2.787125	C	2.525131	0.239092 -0.672838
H	4.958517	1.293483	-1.744611	H	5.389925	0.092481 1.169167
H	1.179716	0.065774	3.532787	H	3.718419	-0.029855 3.021211
H	0.975931	-1.644120	3.097490	N	2.348484	0.372856 -2.039113
H	5.117419	-0.403560	-2.205136	P	-0.228818	0.099640 0.202731
H	0.596152	0.321777	-1.912765	C	0.898229	0.012690 2.662395
H	-0.179027	0.061875	-1.577111	C	4.673794	0.341218 -1.653710
C	-1.338755	-1.413949	-0.024020	C	2.040787	0.080658 1.675710
C	-2.479017	-1.137980	-0.788750	C	3.600737	0.008321 -2.709191
C	-1.064303	-2.709565	0.417613	H	5.025486	1.372312 -1.777870
C	-3.336028	-2.196920	-1.095539	H	0.994602	0.810837 3.412362
C	-1.916489	-3.753410	0.083330	H	0.926010	-0.946313 3.204945
H	-0.179087	-2.896225	1.020487	H	5.540038	-0.320543 -1.719238
C	-3.057915	-3.491474	-0.672069	H	1.476894	0.055744 -2.437506
H	-4.231151	-1.998795	-1.678962	H	-0.113197	0.125565 -1.262211
H	-1.699173	-4.762521	0.416770	C	-1.162572	-1.455635 0.079624
H	-3.736678	-4.298850	-0.927397	C	-2.294831	-1.445194 -0.746673
C	-1.216292	1.425607	0.300946	C	-0.806064	-2.600304 0.787907
C	-2.373355	1.423813	-0.488554	C	-3.057039	-2.609723 -0.843751
C	-0.837367	2.554851	1.029379	C	-1.558126	-3.762895 0.657312
C	-3.139540	2.590366	-0.527697	H	0.059874	-2.575094 1.444085
C	-1.604016	3.710458	0.964052	C	-2.687677	-3.763349 -0.157726
H	0.059153	2.519391	1.642352	H	-3.949228	-2.611338 -1.464573
C	-2.759522	3.722268	0.185046	H	-1.275680	-4.658878 1.200425
H	-4.043363	2.608603	-1.130368	H	-3.289521	-4.661868 -0.251046
H	-1.309300	4.592770	1.521719	C	-1.513456	1.388762 0.084716
H	-3.371084	4.617623	0.137037	C	-2.597602	1.103905 -0.757619
H	3.079074	-0.345808	-3.449784	C	-1.455515	2.585233 0.794190
H	3.278608	1.407443	-3.427133	C	-3.614139	2.052597 -0.874531
O	-0.268888	-0.318668	2.130837	C	-2.460759	3.534644 0.641363
C	-2.764369	0.239308	-1.340817	H	-0.630059	2.754325 1.478749
H	-2.206371	0.328278	-2.286196	C	-3.541396	3.264677 -0.194358
H	-3.826651	0.312568	-1.591512	H	-4.472234	1.836127 -1.505709
				H	-2.410958	4.472510 1.185017
				H	-4.337552	3.993849 -0.306449

H	3.624537	-1.065215	-2.946313
H	3.725521	0.571763	-3.636307
O	-0.297368	0.155063	1.959648
C	-2.676436	-0.201589	-1.527484
H	-2.004881	-0.126740	-2.396081
H	-3.688320	-0.322515	-1.924789

M6CH₂L3

SCF energy in gas phase: -1323.448438

SCF energy in solution: -1323.743324

Free energy in solution: -1323.391561

C	-1.281077	-0.217394	0.760178
C	-3.357864	0.142957	-0.422525
C	-3.337286	-0.625564	1.927799
C	-3.999965	-0.241065	0.726006
C	-1.901282	0.153700	-0.478939
H	-5.089504	-0.251531	0.715609
H	-3.905032	-0.926238	2.801437
P	0.432122	-0.206663	0.970845
C	-1.058140	-1.051196	3.064628
H	-1.094646	-2.143046	3.150871
C	-1.963797	-0.611596	1.928449
C	-1.829219	0.835850	-2.731104
C	-4.082099	0.547344	-1.681818
C	-3.215898	0.207165	-2.896792
H	-1.932352	1.933401	-2.784238
H	-5.060164	0.056433	-1.736223
H	-3.684135	0.558020	-3.822479
N	-1.146334	0.454839	-1.506160
H	-1.196914	0.553839	-3.583510
H	-3.105540	-0.881280	-2.971139
H	-4.270823	1.630271	-1.677674
H	-1.397835	-0.648650	4.023087
C	1.310041	1.339345	0.646994
C	2.058557	1.470859	-0.531879
C	1.216343	2.399403	1.552888
C	2.731305	2.673354	-0.756469
C	1.889476	3.589609	1.311122
H	0.599273	2.304190	2.442155
C	2.654356	3.720504	0.154255
H	3.315946	2.787271	-1.665057
H	1.814854	4.409669	2.017076
H	3.188225	4.644901	-0.041858

C	1.416526	-1.422514	0.067072
C	2.147467	-1.025320	-1.060407
C	1.420036	-2.754832	0.490206
C	2.898021	-1.991557	-1.733829
C	2.169279	-3.702937	-0.193037
H	0.824851	-3.051787	1.350637
C	2.913572	-3.313834	-1.305526
H	3.473327	-1.698824	-2.607596
H	2.173229	-4.736358	0.136359
H	3.506940	-4.046416	-1.843367
C	0.395232	-0.603511	2.766426
H	0.658074	0.303816	3.315675
H	1.145747	-1.357744	3.012770
C	2.072322	0.387528	-1.579816
H	1.103675	0.471377	-2.101121
H	2.879874	0.566965	-2.294260

M6CH₂L3-TS1

SCF energy in gas phase: -1324.588029

SCF energy in solution: -1324.878960

Free energy in solution: -1324.512796

C	-1.273691	-0.488299	0.542240
C	-3.597183	-0.322355	-0.183284
C	-2.983123	-1.742683	1.715703
C	-3.926345	-1.217668	0.806123
C	-2.235846	0.124629	-0.333385
H	-4.968616	-1.519720	0.897016
H	-3.293199	-2.403357	2.518426
P	0.477694	-0.257252	0.559121
C	-0.549692	-1.852513	2.483124
H	-0.256318	-2.877347	2.226752
C	-1.663541	-1.378510	1.570924
C	-2.784634	1.562875	-2.177359
C	-4.619615	0.240195	-1.141829
C	-3.943504	0.607931	-2.462620
H	-3.192508	2.525379	-1.831030
H	-5.425970	-0.485027	-1.293953
H	-4.655944	1.069224	-3.153485
N	-1.843234	1.050718	-1.198973
H	0.247543	0.256041	-1.552893
H	-0.576791	0.697610	-1.513587
H	-2.231232	1.776651	-3.099833
H	-3.554738	-0.299774	-2.938946

H	-5.080039	1.143320	-0.717392	C	-1.710834	-1.418940	1.504280
H	-0.892014	-1.878932	3.521860	C	-3.114617	1.609809	-2.121599
C	1.137871	1.417357	0.586961	C	-4.828448	0.223349	-0.977796
C	2.261893	1.751842	-0.177683	C	-4.270933	0.640725	-2.337233
C	0.543586	2.350541	1.439329	H	-3.505424	2.548719	-1.701056
C	2.794812	3.034794	-0.031941	H	-5.627239	-0.515733	-1.096668
C	1.074169	3.628923	1.552217	H	-5.041987	1.116507	-2.949612
H	-0.346625	2.073283	1.998655	N	-2.117613	1.031280	-1.242060
C	2.211950	3.964324	0.821603	H	0.218539	0.139763	-1.113177
H	3.672367	3.308984	-0.611157	H	-1.147808	1.238452	-1.416449
H	0.606850	4.357111	2.206345	H	-2.634393	1.856643	-3.073329
H	2.643544	4.955965	0.912976	H	-3.907697	-0.242057	-2.874692
C	1.705369	-1.271679	-0.308391	H	-5.280079	1.099815	-0.493330
C	2.774459	-0.661796	-0.978590	H	-0.855617	-2.000882	3.386826
C	1.621060	-2.663431	-0.221535	C	1.196311	1.389877	0.609620
C	3.762650	-1.482769	-1.525914	C	2.258208	1.773170	-0.223524
C	2.600647	-3.464047	-0.795462	C	0.731326	2.253031	1.601312
H	0.774102	-3.122517	0.281234	C	2.862832	3.012185	-0.005569
C	3.681765	-2.868100	-1.439861	C	1.323849	3.498611	1.785585
H	4.602080	-1.021763	-2.039786	H	-0.105246	1.951823	2.226065
H	2.523482	-4.544556	-0.735875	C	2.400812	3.871537	0.986706
H	4.460400	-3.482606	-1.880133	H	3.702444	3.308550	-0.628966
C	0.634113	-0.891903	2.302464	H	0.951686	4.170094	2.552399
H	0.527767	-0.028763	2.966565	H	2.880842	4.833886	1.133683
H	1.609211	-1.347514	2.483564	C	1.844759	-1.262200	-0.357623
C	2.839326	0.826665	-1.221568	C	2.824868	-0.583263	-1.095545
H	2.268601	1.013234	-2.144938	C	1.948020	-2.638356	-0.160068
H	3.876302	1.112891	-1.421983	C	3.906112	-1.306216	-1.601290

M6CH₂L3-Pr

SCF energy in gas phase: -1324.623863

SCF energy in solution: -1324.910931

Free energy in solution: -1324.538742

C	-1.379418	-0.506048	0.499831
C	-3.733060	-0.351294	-0.109353
C	-3.026515	-1.816590	1.705216
C	-4.014045	-1.284640	0.880609
C	-2.395617	0.064619	-0.310732
H	-5.049045	-1.593932	1.012796
H	-3.274558	-2.526259	2.488667
P	0.441173	-0.252091	0.315323
C	-0.550779	-1.924848	2.337040
H	-0.289666	-2.943308	2.021447

C	3.012112	-3.354397	-0.700644
H	1.190631	-3.156806	0.421448
C	3.997712	-2.682568	-1.417355
H	4.684052	-0.781884	-2.150835
H	3.077026	-4.427752	-0.553515
H	4.841242	-3.227434	-1.829432
C	0.604360	-0.955403	2.122231
H	0.495228	-0.113563	2.813184
H	1.587862	-1.398087	2.292499
C	2.716034	0.901455	-1.375023
H	1.997191	1.034985	-2.197580
H	3.679434	1.269225	-1.740238

M6NHL3

SCF energy in gas phase: -1339.491826

SCF energy in solution: -1339.794516

Free energy in solution: -1339.454256

C	-1.273929	0.318224	0.728773
C	-3.371617	0.123200	-0.433821
C	-3.288241	0.770992	1.952323
C	-3.981207	0.469762	0.746687
C	-1.921152	0.019197	-0.510039
H	-5.069576	0.518997	0.756008
H	-3.828436	1.047235	2.850744
P	0.438439	0.240020	0.941799
C	-0.954741	0.972031	3.058156
H	-1.205410	0.377368	3.943092
C	-1.915157	0.691293	1.920008
C	-1.912700	-0.614726	-2.775820
C	-4.132056	-0.182530	-1.700157
C	-3.325337	-1.164144	-2.553569
H	-1.982979	0.284876	-3.411845
H	-5.126038	-0.579217	-1.464843
H	-3.819068	-1.343586	-3.514435
N	-1.194057	-0.309852	-1.550434
H	-1.325625	-1.342528	-3.352065
H	-3.254062	-2.125728	-2.031270
H	-4.287551	0.739789	-2.277730
H	-0.990023	2.031626	3.340452
C	1.472409	1.387726	0.017673
C	2.164269	0.931022	-1.113581
C	1.563922	2.718777	0.432077
C	2.953773	1.846478	-1.811704
C	2.354511	3.614395	-0.275087
H	1.008486	3.046346	1.307587
C	3.050240	3.170950	-1.398744
H	3.498191	1.513344	-2.690848
H	2.428250	4.648465	0.043920
H	3.673949	3.862075	-1.956886
C	1.274127	-1.328409	0.674619
C	1.981249	-1.537909	-0.517866
C	1.202150	-2.317487	1.658211
C	2.614225	-2.769280	-0.696306
C	1.838317	-3.535899	1.461710
H	0.649950	-2.117731	2.572212
C	2.543880	-3.757242	0.280065
H	3.166844	-2.952233	-1.613550
H	1.785095	-4.308023	2.221770
H	3.046100	-4.706158	0.119940

C	2.009876	-0.488534	-1.600950
H	2.789729	-0.721345	-2.330461
H	1.023133	-0.534452	-2.093958
N	0.388514	0.609828	2.568549
H	1.200398	0.933431	3.072431

M6NHL3-TS1

SCF energy in gas phase: -1340.632489

SCF energy in solution: -1340.932413

Free energy in solution: -1340.577513

C	-1.287425	-0.431131	0.554261
C	-3.611346	-0.295729	-0.170232
C	-3.009965	-1.567213	1.834742
C	-3.947159	-1.112212	0.882114
C	-2.247273	0.143090	-0.354254
H	-4.991416	-1.400098	0.993264
H	-3.323597	-2.148614	2.695262
P	0.466629	-0.254901	0.570517
C	-0.579903	-1.582583	2.608296
H	-0.389230	-2.665894	2.594779
C	-1.691124	-1.224070	1.650548
C	-2.805474	1.467532	-2.271393
C	-4.635653	0.203311	-1.161513
C	-3.961763	0.494990	-2.501568
H	-3.216529	2.446235	-1.977004
H	-5.439584	-0.532571	-1.269838
H	-4.675827	0.913321	-3.217692
N	-1.857802	1.015628	-1.269594
H	0.247241	0.170600	-1.533635
H	-0.525212	0.607468	-1.551162
H	-2.258014	1.634598	-3.207161
H	-3.570646	-0.437766	-2.924766
H	-5.099282	1.128572	-0.791689
H	-0.861433	-1.311349	3.632233
C	1.178980	1.395897	0.571323
C	2.258240	1.719006	-0.259557
C	0.675067	2.317256	1.492219
C	2.821201	2.991810	-0.137993
C	1.234847	3.583942	1.584040
H	-0.154713	2.027956	2.130939
C	2.314661	3.916595	0.768050
H	3.664248	3.259086	-0.769277
H	0.838047	4.305326	2.290172

H	2.767223	4.900484	0.841505
C	1.695509	-1.287663	-0.279442
C	2.730764	-0.703564	-1.022161
C	1.642906	-2.672674	-0.097523
C	3.709995	-1.541664	-1.560344
C	2.609703	-3.492503	-0.664309
H	0.831929	-3.107747	0.482247
C	3.651649	-2.920444	-1.391499
H	4.525639	-1.100839	-2.127463
H	2.557082	-4.568208	-0.533576
H	4.421435	-3.550124	-1.825905
C	2.772564	0.775807	-1.320924
H	3.794615	1.059250	-1.589656
H	2.149077	0.934649	-2.214729
N	0.587677	-0.819831	2.173748
H	1.486398	-1.178101	2.469038

M6NHL3-Pr

SCF energy in gas phase: -1340.682144

SCF energy in solution: -1340.979135

Free energy in solution: -1340.616327

C	-1.294479	0.920003	0.189905
C	-3.635831	0.648942	-0.407256
C	-2.974792	2.347952	1.211224
C	-3.946282	1.690799	0.465559
C	-2.292806	0.235599	-0.536191
H	-4.988977	1.986802	0.559917
H	-3.238876	3.150695	1.893333
P	0.561122	0.638884	0.061967
C	-0.477079	2.530047	1.791279
H	-0.577739	2.329940	2.868009
C	-1.653421	1.942801	1.052025
C	-2.930139	-1.390982	-2.270794
C	-4.726549	-0.038744	-1.201132
C	-4.309268	-1.446499	-1.624383
H	-2.980729	-0.772734	-3.182340
H	-5.647315	-0.072785	-0.609424
H	-5.034586	-1.871737	-2.323844
N	-1.977019	-0.868040	-1.312117
H	0.395431	0.329762	-1.353552
H	-1.002043	-0.993930	-1.534464
H	-2.601806	-2.391117	-2.567944
H	-4.258177	-2.101847	-0.748573

H	-4.957144	0.550227	-2.099054
H	-0.437399	3.620328	1.661754
C	2.410700	0.854441	-0.384076
C	3.109036	-0.265696	-0.865002
C	3.055766	2.094306	-0.407527
C	4.431651	-0.134991	-1.288806
C	4.370863	2.224904	-0.849809
H	2.517369	2.983407	-0.091244
C	5.067552	1.102339	-1.280509
H	4.966982	-1.016262	-1.634466
H	4.846185	3.201047	-0.857430
H	6.096154	1.187487	-1.616512
C	0.686917	-1.048894	0.760065
C	1.597360	-1.975182	0.234521
C	-0.093001	-1.388190	1.866994
C	1.706336	-3.231726	0.830752
C	0.026461	-2.641859	2.457017
H	-0.802613	-0.663485	2.257752
C	0.928487	-3.565469	1.935007
H	2.411550	-3.952388	0.425338
H	-0.581919	-2.898165	3.318158
H	1.029062	-4.546358	2.389103
C	2.427797	-1.613804	-0.970922
H	3.174203	-2.391922	-1.155100
H	1.771861	-1.598206	-1.855613
N	0.688037	1.884696	1.237347
H	1.594900	2.130795	1.602458

M6OL3

SCF energy in gas phase: -1359.355458

SCF energy in solution: -1359.663300

Free energy in solution: -1359.336275

C	-1.255701	0.154911	0.788151
C	-3.522468	0.163387	-0.048752
C	-3.053699	0.363633	2.373861
C	-3.933747	0.287105	1.251275
C	-2.099025	0.075572	-0.370971
H	-5.005821	0.333786	1.439359
H	-3.444643	0.468385	3.379294
P	0.455074	0.084062	0.780377
C	-0.571356	0.351215	3.109744
H	-0.616034	-0.466793	3.834198
C	-1.708928	0.296396	2.114910

C	-2.450741	-0.161287	-2.681328	C	-3.937117	-0.890048	1.062245
C	-4.469800	0.098009	-1.219980	C	-2.261691	0.197263	-0.365216
C	-3.833115	-0.727521	-2.340826	H	-4.980210	-1.150935	1.234213
H	-2.580991	0.831167	-3.145046	H	-3.271663	-1.724429	2.965725
H	-5.435276	-0.317541	-0.910727	P	0.468088	-0.177840	0.562148
H	-4.471242	-0.736550	-3.230538	C	-0.515854	-1.175726	2.722039
N	-1.549035	-0.065079	-1.545586	H	-0.346597	-2.244071	2.904812
H	-1.975446	-0.787550	-3.446282	C	-1.666044	-0.933748	1.776819
H	-3.719224	-1.765579	-2.004833	C	-2.871744	1.280882	-2.409196
H	-4.667206	1.110621	-1.599746	C	-4.677382	0.193943	-1.091727
H	-0.538383	1.302582	3.648276	C	-4.048014	0.308455	-2.479135
C	1.403344	1.372070	-0.024503	H	-3.257869	2.297164	-2.231938
C	2.785151	1.182147	-0.174674	H	-5.499577	-0.529457	-1.081998
C	0.763567	2.506938	-0.521030	H	-4.780964	0.650332	-3.216514
C	3.521666	2.182670	-0.803862	N	-1.897784	0.945143	-1.386393
C	1.515219	3.492860	-1.150895	H	0.274582	0.135544	-1.567295
H	-0.315335	2.593196	-0.426122	H	-0.484573	0.526127	-1.627385
C	2.891846	3.329497	-1.283271	H	-2.352177	1.317109	-3.374624
H	4.593448	2.058342	-0.931144	H	-3.685455	-0.675389	-2.799330
H	1.030062	4.378781	-1.545861	H	-5.108067	1.168143	-0.820487
H	3.480517	4.094584	-1.779656	H	-0.681509	-0.684633	3.685932
C	1.289414	-1.397385	0.222457	C	1.283211	1.413373	0.457016
C	2.680473	-1.349335	0.047215	C	2.395410	1.593439	-0.373732
C	0.552894	-2.542514	-0.077937	C	0.830172	2.433432	1.296117
C	3.325663	-2.499570	-0.400073	C	3.045743	2.828571	-0.333853
C	1.214632	-3.679629	-0.528284	C	1.481399	3.659018	1.309753
H	-0.528697	-2.518846	0.022181	H	-0.035087	2.257318	1.929520
C	2.598814	-3.655077	-0.680351	C	2.594869	3.850400	0.494005
H	4.402522	-2.488142	-0.543027	H	3.913514	2.989691	-0.967695
H	0.654120	-4.575850	-0.770519	H	1.128357	4.457340	1.953389
H	3.118544	-4.538733	-1.037380	H	3.117266	4.801771	0.504219
C	3.450232	-0.077538	0.345470	C	1.596449	-1.358479	-0.209168
H	3.561450	0.013905	1.435462	C	2.676924	-0.908169	-0.977302
H	4.460010	-0.155541	-0.065835	C	1.419673	-2.718335	0.055910
O	0.681096	0.220136	2.389165	C	3.576205	-1.858859	-1.465988
M6OL3-TS1				C	2.311010	-3.650165	-0.458116
SCF energy in gas phase: -1360.502778				H	0.575034	-3.042969	0.658606
SCF energy in solution: -1360.807977				C	3.396024	-3.214320	-1.216615
Free energy in solution: -1360.465452				H	4.425793	-1.526895	-2.056715
				H	2.167054	-4.707394	-0.262766
				H	4.105923	-3.933171	-1.612820
C	-1.282538	-0.276913	0.586184	C	2.851369	0.543055	-1.358615
C	-3.626662	-0.204632	-0.084341	H	3.899970	0.722981	-1.613287
C	-2.976627	-1.246333	2.037997	H	2.270335	0.702205	-2.280894

O 0.662548 -0.618927 2.137421

M6OL3-Pr

SCF energy in gas phase: -1360.559246

SCF energy in solution: -1360.863419

Free energy in solution: -1360.514436

C -1.381087 0.045306 0.607257

C -3.758322 0.096050 0.095186

C -3.001996 -0.467058 2.345264

C -4.014547 -0.274250 1.410604

C -2.420040 0.266954 -0.336574

H -5.052788 -0.405662 1.708840

H -3.227438 -0.739419 3.371604

P 0.425327 0.046595 0.305840

C -0.471716 -0.450974 2.790569

H -0.397254 -1.487519 3.158743

C -1.693660 -0.296242 1.919418

C -3.225342 1.031520 -2.545185

C -4.906207 0.316999 -0.867961

C -4.457660 0.166503 -2.319112

H -3.493060 2.090564 -2.400362

H -5.713047 -0.387239 -0.640355

H -5.255605 0.462566 -3.005624

N -2.172124 0.620447 -1.639995

H 0.220302 0.228705 -1.132946

H -1.226728 0.870302 -1.875995

H -2.854431 0.922967 -3.568263

H -4.200320 -0.877290 -2.527713

H -5.321830 1.323346 -0.725240

H -0.550878 0.199648 3.672869

C 1.674907 1.377276 0.241003

C 2.684577 1.223104 -0.720907

C 1.663680 2.480950 1.090487

C 3.671574 2.204777 -0.812147

C 2.636592 3.467985 0.964048

H 0.900720 2.548237 1.859867

C 3.641937 3.326578 0.011030

H 4.471968 2.086446 -1.537950

H 2.621416 4.334269 1.617460

H 4.413484 4.084233 -0.083319

C 1.368904 -1.460342 -0.086846

C 2.426023 -1.317034 -0.995583

C 1.090981 -2.695433 0.493412

C 3.196438 -2.438786 -1.303440

C 1.848694 -3.811860 0.153544

H 0.279217 -2.780427 1.210891

C 2.905333 -3.679225 -0.743699

H 4.030911 -2.337961 -1.992687

H 1.625994 -4.777289 0.596280

H 3.510125 -4.542415 -1.003033

C 2.719792 0.020956 -1.646199

H 3.698102 -0.024609 -2.133514

H 1.979193 0.179219 -2.444465

O 0.646722 -0.101905 2.037783

M7OL3

SCF energy in gas phase: -1281.971444

SCF energy in solution: -1282.264132

Free energy in solution: -1281.969444

C 1.573204 -0.174326 -1.760315

C 4.021122 -0.128598 -1.782389

C 2.919889 0.184178 0.339189

C 4.089273 0.106969 -0.382334

C 1.689858 0.010691 -0.334771

C 2.838595 -0.270511 -2.453877

C 1.795102 -0.260051 2.540114

C 2.917647 0.468300 1.822425

N 0.363698 -0.224345 -2.261822

P 0.156796 0.038262 0.476141

H 4.951670 -0.196547 -2.340940

H 5.048380 0.225551 0.110275

H 2.827602 -0.439793 -3.527269

H 1.781871 -0.031660 3.607310

H 3.874741 0.172312 2.263467

H 2.799406 1.545450 2.000186

H 0.393215 -0.390017 -3.266166

H 1.903594 -1.343835 2.415694

C -0.911394 -1.395907 0.287052

C -2.125957 -1.289015 -0.403976

C -0.541935 -2.591673 0.906912

C -2.955428 -2.411111 -0.451052

C -1.376274 -3.699388 0.843390

H 0.405102 -2.658409 1.434537

C -2.588165 -3.603091 0.163037

H -3.901125 -2.345255 -0.981910

H -1.086591 -4.628604 1.322050

H	-3.251483	-4.460784	0.113088
C	-0.945912	1.429592	0.224452
C	-2.138404	1.270375	-0.492085
C	-0.593543	2.663364	0.778066
C	-2.968316	2.385043	-0.635113
C	-1.427747	3.760017	0.619149
H	0.332159	2.752147	1.339888
C	-2.619330	3.614686	-0.090266
H	-3.900878	2.281316	-1.182797
H	-1.156861	4.719001	1.047496
H	-3.283313	4.464403	-0.214443
O	0.503865	0.155366	2.058163
C	-2.508358	-0.035531	-1.146834
H	-3.579555	-0.047087	-1.365761
H	-1.950233	-0.068724	-2.094012

M7OL3-TS1

SCF energy in gas phase: -1283.105434

SCF energy in solution: -1283.395759

Free energy in solution: -1283.085946

C	2.169252	-0.766861	-1.409802
C	4.436882	0.123517	-1.143452
C	2.727579	0.857491	0.394647
C	4.041406	0.874353	-0.015172
C	1.757711	0.077702	-0.306767
C	3.543529	-0.662189	-1.812739
C	1.435169	0.671513	2.494625
C	2.361482	1.557376	1.682253
N	1.297886	-1.572844	-2.000902
P	0.065888	0.143088	0.224549
H	5.472394	0.157392	-1.470955
H	4.774414	1.438032	0.552364
H	3.855727	-1.248205	-2.672942
H	1.198957	1.107804	3.468122
H	3.271967	1.775932	2.247084
H	1.854154	2.514599	1.507824
H	1.695845	-2.015550	-2.825221
H	0.158146	-0.727454	-2.033204
H	-0.352105	-0.035714	-1.825480
H	1.891320	-0.314324	2.651357
C	-0.795344	-1.431260	0.286752
C	-2.110994	-1.539616	-0.173046
C	-0.156631	-2.504743	0.909946

C	-2.777414	-2.751379	0.026212
C	-0.829312	-3.705051	1.086162
H	0.875293	-2.397833	1.234367
C	-2.147279	-3.822603	0.647614
H	-3.801739	-2.853604	-0.321751
H	-0.331880	-4.544114	1.560491
H	-2.684560	-4.755091	0.788442
C	-1.194686	1.395193	-0.149007
C	-2.461515	0.992516	-0.592114
C	-0.918431	2.743025	0.086245
C	-3.436548	1.975529	-0.779139
C	-1.891054	3.708561	-0.135170
H	0.064587	3.037956	0.440452
C	-3.158654	3.319627	-0.561939
H	-4.427076	1.675174	-1.110233
H	-1.666609	4.755874	0.036941
H	-3.932132	4.063785	-0.721735
O	0.189102	0.541253	1.819774
C	-2.785450	-0.437770	-0.954256
H	-3.869508	-0.578423	-0.909859
H	-2.491734	-0.572253	-2.007302

M7OL3-Pr

SCF energy in gas phase: -1283.154533

SCF energy in solution: -1283.444094

Free energy in solution: -1283.127684

C	2.466863	-0.867456	-1.150202
C	4.654136	0.131497	-0.816997
C	2.730287	1.109879	0.243129
C	4.099018	1.112491	0.002113
C	1.895732	0.136348	-0.332412
C	3.853664	-0.844303	-1.380718
C	1.201020	1.487717	2.172608
C	2.097255	2.149257	1.124648
N	1.735990	-1.925165	-1.663752
P	0.081404	0.150798	-0.031583
H	5.721709	0.127130	-1.014461
H	4.723742	1.877465	0.452256
H	4.290471	-1.616381	-2.008578
H	0.647332	2.261108	2.724518
H	2.863364	2.746341	1.628141
H	1.513196	2.841822	0.505703
H	2.175055	-2.416554	-2.427590

H	0.745068	-1.782497	-1.792835
H	-0.084929	-0.146265	-1.465224
H	1.842199	0.961985	2.894139
C	-0.744050	-1.412434	0.382874
C	-1.959078	-1.668072	-0.266748
C	-0.209853	-2.324302	1.290271
C	-2.627466	-2.859257	0.019085
C	-0.874967	-3.519020	1.543767
H	0.718395	-2.081537	1.798023
C	-2.086152	-3.783042	0.908201
H	-3.581380	-3.062183	-0.460719
H	-0.457912	-4.235854	2.243488
H	-2.616547	-4.707793	1.112608
C	-1.319724	1.329228	-0.248925
C	-2.473594	0.776367	-0.832357
C	-1.328689	2.654779	0.180934
C	-3.597934	1.585831	-0.995461
C	-2.445959	3.459615	-0.020379
H	-0.465326	3.066240	0.691595
C	-3.583590	2.923380	-0.613590
H	-4.498914	1.156994	-1.426590
H	-2.432844	4.495434	0.303161
H	-4.465796	3.537989	-0.762078
O	0.284986	0.564196	1.638719
C	-2.534289	-0.677998	-1.261137
H	-3.575494	-0.943068	-1.466103
H	-1.990045	-0.782784	-2.211433

M8OL3

SCF energy in gas phase: -1359.354989

SCF energy in solution: -1359.664136

Free energy in solution: -1359.337739

C	-2.165475	0.244790	-3.045822
C	-3.626622	0.277182	-2.488577
C	-3.401949	0.194724	-0.998002
C	-1.959686	0.186801	-0.825550
C	-4.233483	0.138415	0.070727
C	-1.458901	0.129408	0.519670
C	-2.360309	0.071291	1.632654
C	-3.710267	0.067917	1.410525
C	-1.789865	0.028560	3.032873
H	-2.507284	-0.439277	3.714292
C	-0.470216	-0.725243	3.099885

H	-5.312217	0.139433	-0.069751
H	-1.961728	1.113759	-3.683730
H	-4.146173	1.200424	-2.765730
H	-4.394456	0.016195	2.251377
H	-0.067483	-0.751171	4.113743
N	-1.239352	0.226870	-1.908210
P	0.239878	0.026871	0.716470
H	-2.001725	-0.641820	-3.672951
H	-4.230190	-0.555911	-2.862200
H	-1.608467	1.047309	3.398956
H	-0.581930	-1.754996	2.736280
C	1.270625	1.381212	0.162846
C	2.649737	1.154965	0.051901
C	0.699410	2.602555	-0.187731
C	3.453817	2.205863	-0.383753
C	1.517454	3.638203	-0.624879
H	-0.378916	2.721034	-0.127964
C	2.892571	3.437207	-0.714492
H	4.525826	2.055435	-0.476602
H	1.085279	4.593073	-0.903952
H	3.534702	4.241089	-1.060507
C	1.050837	-1.396276	-0.023692
C	2.451275	-1.380558	-0.103066
C	0.307345	-2.474132	-0.501282
C	3.092237	-2.490361	-0.649433
C	0.964030	-3.572813	-1.044556
H	-0.777536	-2.429725	-0.456497
C	2.354985	-3.577901	-1.112356
H	4.176206	-2.499162	-0.723140
H	0.395287	-4.415795	-1.422022
H	2.871900	-4.429950	-1.542734
O	0.532308	-0.047167	2.312873
C	3.243584	-0.193170	0.408876
H	3.301410	-0.264644	1.504224
H	4.269510	-0.250945	0.035740

M8OL3-TS1

SCF energy in gas phase: -1360.494538

SCF energy in solution: -1360.796549

Free energy in solution: -1360.452372

C	-3.174907	1.578573	-2.247938
C	-4.409690	0.953753	-1.543548
C	-3.764353	0.087136	-0.490919

C	-2.373797	0.439536	-0.463045	H	4.310299	0.313751	0.159649
C	-4.270835	-0.835270	0.371815				
C	-1.495108	-0.235391	0.440388	M8OL3-Pr			
C	-2.072677	-1.164819	1.376694	SCF energy in gas phase:	-1360.546460		
C	-3.416287	-1.455380	1.321227	SCF energy in solution:	-1360.849069		
C	-1.280434	-1.743981	2.533025	Free energy in solution:	-1360.497224		
H	-1.683641	-2.725489	2.801707				
C	0.208461	-1.853129	2.277466	C	-3.566414	1.116782	-2.350540
H	-5.327132	-1.092095	0.352560	C	-4.669035	0.736275	-1.349438
H	-3.313739	2.642084	-2.462693	C	-3.895503	-0.061010	-0.327446
H	-5.020491	1.732359	-1.071984	C	-2.521430	0.197440	-0.487872
H	-3.836293	-2.142953	2.048901	C	-4.338488	-0.877465	0.688270
H	0.749283	-2.139862	3.182110	C	-1.558976	-0.364047	0.380030
N	-2.036772	1.378675	-1.344342	C	-2.045413	-1.167247	1.447359
P	0.263307	-0.097305	0.361930	C	-3.407318	-1.428625	1.570858
H	-2.983468	1.077328	-3.207481	C	-1.143798	-1.729877	2.523689
H	-5.056906	0.396694	-2.226242	H	-1.488808	-2.729263	2.810792
H	-1.421542	-1.086760	3.400221	C	0.314308	-1.752234	2.116167
H	0.426983	-2.598004	1.498708	H	-5.398461	-1.085687	0.806577
H	-0.734673	0.885086	-1.659952	H	-3.721626	2.094765	-2.810729
H	-0.020475	0.370625	-1.572989	H	-5.091686	1.635010	-0.884555
C	1.101653	1.486481	0.351038	H	-3.745047	-2.063059	2.384953
C	2.503416	1.441726	0.363870	H	0.952583	-2.037849	2.959876
C	0.404509	2.693442	0.335924	N	-2.355157	1.116859	-1.524852
C	3.192306	2.654334	0.361946	P	0.230014	-0.066588	0.047236
C	1.115453	3.888396	0.344536	H	-3.501536	0.361275	-3.147005
H	-0.680020	2.684904	0.279434	H	-5.486010	0.181306	-1.815442
C	2.507699	3.865982	0.357593	H	-1.240549	-1.087160	3.407755
H	4.278858	2.646324	0.364987	H	0.475802	-2.500042	1.321451
H	0.583546	4.833670	0.331826	H	-1.467201	1.120593	-2.006820
H	3.065924	4.796842	0.356573	H	-0.122661	0.215957	-1.339827
C	1.346354	-1.231335	-0.554222	C	1.048174	1.544009	0.236165
C	2.723244	-0.987718	-0.448890	C	2.433861	1.543962	0.453055
C	0.854481	-2.281310	-1.326705	C	0.345385	2.736965	0.077142
C	3.592639	-1.825723	-1.148778	C	3.088875	2.775184	0.510402
C	1.737889	-3.121596	-1.994113	C	1.012698	3.954852	0.162934
H	-0.220674	-2.422198	-1.411197	H	-0.725429	2.710042	-0.114414
C	3.108521	-2.887151	-1.907154	C	2.387832	3.970311	0.377833
H	4.662643	-1.643532	-1.094474	H	4.164654	2.795196	0.664536
H	1.360508	-3.945862	-2.590122	H	0.464785	4.885241	0.054815
H	3.803582	-3.528882	-2.439125	H	2.919416	4.915133	0.433972
O	0.711643	-0.575742	1.885473	C	1.522639	-1.192468	-0.604994
C	3.264810	0.129805	0.422011	C	2.855063	-0.885017	-0.287172
H	3.252004	-0.217401	1.463910	C	1.223077	-2.242208	-1.470567

C	3.864090	-1.666319	-0.853878
C	2.238908	-3.033917	-1.996783
H	0.185156	-2.439703	-1.731103
C	3.563964	-2.739799	-1.687406
H	4.902027	-1.428583	-0.634927
H	1.999661	-3.865254	-2.651993
H	4.366876	-3.338748	-2.105520
O	0.680295	-0.464257	1.689705
C	3.217255	0.257800	0.644579
H	3.048811	-0.079611	1.674175
H	4.284252	0.475229	0.536896

M9OL3

SCF energy in gas phase: -1398.660658

SCF energy in solution: -1398.976371

Free energy in solution: -1398.619683

C	-3.136412	0.589528	-2.842262
C	-4.033976	-0.205076	-1.889047
C	-3.380410	-0.271847	-0.533333
C	-1.926483	-0.238728	-0.520764
C	-1.731041	-0.020800	-2.863646
C	-4.060101	-0.339800	0.649861
C	-1.314978	-0.299629	0.782790
C	-2.049900	-0.380634	1.992894
C	-3.421630	-0.397448	1.923373
C	-1.312350	-0.441170	3.311135
H	-1.949241	-0.051925	4.111747
C	-0.009787	0.344306	3.277115
H	-5.148984	-0.344513	0.617896
H	-3.558502	0.609490	-3.852308
H	-5.033247	0.237330	-1.812015
H	-1.073337	0.593611	-3.490536
H	-4.016328	-0.445192	2.829573
H	-0.192040	1.400567	3.038520
N	-1.124853	-0.147374	-1.550959
P	0.401516	-0.134023	0.748625
H	0.522796	0.286529	4.228022
H	-1.780891	-1.007159	-3.355234
H	-3.068192	1.626969	-2.491627
H	-4.164821	-1.218475	-2.293994
H	-1.071172	-1.481733	3.561803
C	1.069867	1.412372	0.119036
C	2.456915	1.480213	-0.070534

C	0.243760	2.501186	-0.155276
C	3.001348	2.679988	-0.527662
C	0.804444	3.689712	-0.607831
H	-0.830774	2.395666	-0.029668
C	2.183271	3.775358	-0.790214
H	4.073751	2.753055	-0.686497
H	0.170650	4.541740	-0.829298
H	2.624319	4.698964	-1.151848
C	1.438053	-1.367488	-0.031243
C	2.788849	-1.047642	-0.220305
C	0.907683	-2.584447	-0.452809
C	3.609135	-2.000494	-0.823037
C	1.741451	-3.522138	-1.050137
H	-0.154390	-2.773223	-0.324275
C	3.091481	-3.227301	-1.229109
H	4.659970	-1.775803	-0.983254
H	1.340794	-4.472590	-1.385648
H	3.745670	-3.953311	-1.701639
O	0.888830	-0.220055	2.302618
C	3.344050	0.287948	0.234204
H	3.496298	0.242805	1.321843
H	4.328839	0.443785	-0.214364

M9OL3-TS1

SCF energy in gas phase: -1399.797182

SCF energy in solution: -1400.107573

Free energy in solution: -1399.735347

C	-4.421259	1.745457	-1.092073
C	-4.757377	0.268658	-0.895603
C	-3.629765	-0.446803	-0.186571
C	-2.307959	0.117597	-0.264363
C	-3.042338	1.856440	-1.738860
C	-3.845233	-1.598410	0.528163
C	-1.257339	-0.594384	0.414217
C	-1.518546	-1.807425	1.109757
C	-2.805844	-2.296121	1.172137
C	-0.395085	-2.521492	1.821022
H	-0.803447	-3.306750	2.463231
C	0.407060	-1.546057	2.669883
H	-4.860953	-1.984597	0.594344
H	-5.177665	2.237906	-1.711178
H	-5.688176	0.143902	-0.331659
H	-2.773734	2.908065	-1.888967

H	-3.015614	-3.202349	1.730533	C	-2.468709	-0.038594	-0.251662
H	-0.243293	-1.093358	3.427248	C	-3.520266	1.647540	-1.705145
N	-2.009519	1.236175	-0.928512	C	-3.831044	-1.738235	0.787730
P	0.448929	-0.123343	0.364941	C	-1.314825	-0.676562	0.265699
H	0.015271	0.396978	-1.555349	C	-1.440130	-1.861082	1.015068
H	-0.740696	0.863195	-1.452882	C	-2.702044	-2.388754	1.268656
H	1.233726	-2.053483	3.175689	C	-0.201754	-2.566498	1.496792
H	-3.084885	1.397593	-2.740612	H	-0.471226	-3.392620	2.161167
H	-4.400355	2.254589	-0.121510	C	0.759160	-1.611707	2.222650
H	-4.923752	-0.189437	-1.880052	H	-4.818440	-2.141298	1.002439
H	0.280969	-3.008923	1.105893	H	-5.622665	1.983115	-1.344021
C	1.114601	1.550963	0.365967	H	-5.790943	-0.002859	0.275513
C	2.516000	1.637231	0.328287	H	-3.317031	2.683068	-1.992724
C	0.319414	2.693040	0.458923	H	-2.796094	-3.301634	1.848576
C	3.093785	2.906573	0.350860	H	0.443973	-1.502573	3.267578
C	0.923111	3.945482	0.495261	N	-2.369161	1.158404	-0.962329
H	-0.760157	2.588414	0.463056	P	0.375179	-0.010491	-0.012596
C	2.308935	4.052022	0.434289	H	0.005694	0.338463	-1.391938
H	4.176083	2.993922	0.308715	H	-1.491561	1.260110	-1.456043
H	0.308496	4.836940	0.563196	H	1.767707	-2.057449	2.222650
H	2.782427	5.028640	0.451596	H	-3.689234	1.071142	-2.629340
C	1.611618	-1.117999	-0.602337	H	-4.587272	2.139088	0.084623
C	2.959538	-0.743267	-0.541229	H	-5.363446	-0.434602	-1.372677
C	1.194412	-2.191884	-1.387085	H	0.312388	-3.011023	0.637188
C	3.881601	-1.477778	-1.288683	C	1.098037	1.650678	0.245126
C	2.129797	-2.926467	-2.105525	C	2.485000	1.703520	0.462147
H	0.135118	-2.434260	-1.439048	C	0.352294	2.823710	0.138543
C	3.474744	-2.564021	-2.056743	C	3.093678	2.956365	0.545591
H	4.930119	-1.192970	-1.265721	C	0.974187	4.063448	0.256818
H	1.811848	-3.767918	-2.711939	H	-0.721989	2.768475	-0.015012
H	4.208833	-3.124119	-2.627102	C	2.349458	4.128630	0.451775
O	0.980260	-0.495082	1.893815	H	4.168836	3.011071	0.695918
C	3.410736	0.410280	0.329634	H	0.385996	4.973244	0.192968
H	3.471449	0.048255	1.365120	H	2.845556	5.090857	0.530790
H	4.421349	0.707544	0.036376	C	1.727470	-1.038968	-0.672217
M9OL3-Pr				C	3.036069	-0.689476	-0.310454
SCF energy in gas phase: -1399.845674				C	1.489843	-2.077398	-1.572018
SCF energy in solution: -1400.157380				C	4.089882	-1.423788	-0.860384
Free energy in solution: -1399.778177				C	2.548442	-2.816192	-2.087827
				H	0.466234	-2.307038	-1.862571
				C	3.852859	-2.484796	-1.728008
C	-4.758923	1.556515	-0.826753	H	5.111309	-1.156113	-0.602501
C	-5.002756	0.091063	-0.478495	H	2.359767	-3.634622	-2.774842
C	-3.742531	-0.578434	0.029246	H	4.688620	-3.045288	-2.134971

O	0.793909	-0.324529	1.664630	H	1.024913	2.361948	-0.677530
C	3.323855	0.452286	0.646082	C	-2.043571	3.810346	-0.451853
H	3.154016	0.093248	1.668582	H	-3.823973	2.827575	0.251069
H	4.381467	0.720382	0.563084	H	-0.130898	4.537765	-1.122815

M10OL3

SCF energy in gas phase: -1245.077796

SCF energy in solution: -1245.358692

Free energy in solution: -1245.046497

O	0.273604	-0.286919	2.017288
C	-2.897237	0.337957	0.874375
H	-3.970743	0.521769	0.777807
H	-2.683155	0.279585	1.951198

C	1.700788	-0.340978	-0.048134
C	3.728598	0.024804	-1.459265
C	3.915083	-0.160483	1.064109
C	4.496528	-0.595235	-0.286168
C	2.495637	-0.706441	1.189489
C	2.211044	-0.105213	-1.357211
H	4.448382	-1.689828	-0.352645
H	3.953938	1.099206	-1.504406
H	4.545741	-0.516241	1.886936
N	1.405396	0.074654	-2.353292
H	1.930326	0.304351	-3.198658
P	0.082682	-0.144234	0.394797
C	1.677390	-0.125659	2.345893
H	1.827711	-0.634443	3.300427
H	1.887824	0.945901	2.459876
H	4.061190	-0.406027	-2.409765
H	5.554189	-0.321330	-0.353844
H	3.885543	0.936903	1.113315
H	2.567149	-1.798887	1.332476
C	-1.210671	-1.333524	0.001576
C	-2.549033	-0.996468	0.249807
C	-0.869359	-2.547107	-0.591935
C	-3.536454	-1.921836	-0.079433
C	-1.866970	-3.461183	-0.914818
H	0.175966	-2.750848	-0.808807
C	-3.197520	-3.146095	-0.652226
H	-4.579581	-1.679901	0.105243
H	-1.610990	-4.408063	-1.378145
H	-3.981689	-3.851744	-0.908422
C	-0.752254	1.411593	0.042948
C	-2.126848	1.512428	0.303843
C	-0.032822	2.490993	-0.468172
C	-2.759931	2.728830	0.054376
C	-0.681163	3.695216	-0.717544

M10OL3-TS1

SCF energy in gas phase: -1246.221350

SCF energy in solution: -1246.496167

Free energy in solution: -1246.168062

C	1.787115	-0.194160	-0.089889
C	4.064618	0.096361	-1.102555
C	3.824965	-0.377543	1.354448
C	4.568228	-0.746822	0.069151
C	2.360828	-0.760610	1.197162
C	2.553495	0.262215	-1.166184
H	4.402790	-1.810625	-0.140370
H	4.490256	1.106093	-1.040112
H	4.265154	-0.883454	2.220574
N	2.008412	0.879918	-2.200052
H	2.644586	0.996767	-2.983853
P	0.063383	-0.106707	0.092587
H	0.706718	0.374458	-2.187200
H	-0.027931	-0.072084	-1.886375
C	1.423975	-0.216941	2.274776
H	1.457192	-0.785580	3.208025
H	1.660357	0.836735	2.481291
H	4.402363	-0.320928	-2.058353
H	5.647358	-0.608257	0.185240
H	3.903340	0.704913	1.525328
H	2.290309	-1.860895	1.217796
C	-1.176994	-1.389829	-0.222695
C	-2.481673	-1.129823	0.215550
C	-0.856503	-2.578205	-0.872452
C	-3.459279	-2.098247	-0.016981
C	-1.838206	-3.540834	-1.077968
H	0.159569	-2.732138	-1.227430
C	-3.141444	-3.295620	-0.650945
H	-4.480438	-1.909779	0.303877

H	-1.592957	-4.471039	-1.579668
H	-3.916322	-4.036604	-0.819810
C	-0.856502	1.435793	-0.051184
C	-2.191199	1.412527	0.378624
C	-0.267349	2.604175	-0.533056
C	-2.925119	2.596598	0.305384
C	-1.015930	3.775002	-0.589552
H	0.759249	2.575069	-0.887823
C	-2.344024	3.768303	-0.170390
H	-3.963364	2.598031	0.626514
H	-0.567286	4.688117	-0.966562
H	-2.933697	4.678445	-0.218473
O	0.096946	-0.325286	1.756494
C	-2.816440	0.153315	0.950531
H	-3.902308	0.276147	0.990300
H	-2.465507	0.046150	1.986054

M10OL3-Pr

SCF energy in gas phase: -1246.267879

SCF energy in solution: -1246.545237

Free energy in solution: -1246.210639

C	1.822456	-0.513660	-0.102448
C	4.198886	-0.444382	-0.894147
C	3.709120	-0.373015	1.560237
C	4.587828	-0.994653	0.476091
C	2.269268	-0.791233	1.313804
C	2.704417	-0.304710	-1.113096
H	4.451489	-2.082483	0.490607
H	4.634662	0.552809	-1.039103
H	4.036262	-0.685394	2.557742
N	2.412514	0.168359	-2.378167
H	3.073345	-0.082871	-3.098716
P	0.019950	-0.260162	-0.207456
H	1.446260	0.135604	-2.670546
H	0.054773	-0.326822	-1.672128
C	1.208868	-0.066944	2.145628
H	1.208911	-0.390343	3.192723
H	1.403211	1.021160	2.118345
H	4.610156	-1.075588	-1.693345
H	5.648985	-0.801710	0.658646
H	3.785853	0.721978	1.514023
H	2.169359	-1.865834	1.530829
C	-1.473340	-1.316247	-0.235974

C	-2.648235	-0.800723	0.330917
C	-1.481149	-2.541973	-0.895584
C	-3.817312	-1.556726	0.226668
C	-2.647155	-3.298153	-0.963207
H	-0.567718	-2.904963	-1.361663
C	-3.818111	-2.799548	-0.399914
H	-4.740870	-1.163120	0.643592
H	-2.645648	-4.261543	-1.462926
H	-4.738553	-3.371845	-0.459975
C	-0.633031	1.436576	-0.207390
C	-1.893878	1.655770	0.367650
C	0.075684	2.482150	-0.796338
C	-2.419443	2.948090	0.328923
C	-0.454171	3.768991	-0.806030
H	1.046425	2.283929	-1.247545
C	-1.706703	3.998030	-0.243889
H	-3.401316	3.132598	0.757400
H	0.101908	4.585139	-1.256027
H	-2.134735	4.995591	-0.256834
O	-0.022138	-0.386924	1.561286
C	-2.668866	0.538460	1.043018
H	-3.707582	0.856424	1.174897
H	-2.235737	0.390002	2.039202

M11OL3

SCF energy in gas phase: -1322.462702

SCF energy in solution: -1322.757673

Free energy in solution: -1322.411306

C	-1.306531	-0.591799	0.379859
C	-3.602296	-0.724713	-0.671935
C	-3.282390	-0.235368	1.836452
C	-4.231553	-0.737677	0.738945
C	-2.134963	-0.298196	-0.735293
H	-5.143705	-0.130610	0.744315
H	-3.736943	-0.402560	2.820888
N	-1.793046	0.298862	-1.830665
P	0.329234	-0.229717	0.581750
C	-0.909532	-0.356472	2.760827
H	-0.883486	-0.910363	3.701263
C	-1.912274	-0.912440	1.738878
H	-1.127424	0.700224	2.964662
C	-2.987945	0.402821	-2.672072
C	-4.187539	0.222223	-1.722982

H	-3.003700	1.359771	-3.203890	H	-3.484053	-0.162163	3.087198
H	-4.434270	1.180237	-1.247167	N	-2.158381	0.149853	-1.806704
H	-2.982864	-0.387671	-3.439230	P	0.320593	-0.206845	0.283828
H	-5.087156	-0.161226	-2.211690	C	-0.669099	-0.100791	2.641317
H	-4.541069	-1.757529	0.991994	H	-0.558326	-0.530115	3.640060
H	-3.126044	0.846020	1.722895	H	-0.803905	-0.016774	-1.937055
H	-3.627547	-1.747670	-1.076051	H	0.060840	-0.243378	-1.645945
H	-2.039162	-1.994511	1.909486	C	-1.802623	-0.737855	1.824835
C	0.964017	1.405519	0.174524	H	-0.847645	0.981402	2.734381
C	2.350408	1.621133	0.208578	C	-3.404439	0.036927	-2.564699
C	0.079535	2.428986	-0.167680	C	-4.490226	-0.030666	-1.472805
C	2.829217	2.895672	-0.085271	H	-3.527140	0.887469	-3.240514
C	0.576374	3.694256	-0.462686	H	-4.735882	0.982681	-1.133951
H	-0.981763	2.207881	-0.234600	H	-3.413554	-0.877412	-3.176732
C	1.948823	3.923783	-0.415620	H	-5.410063	-0.517689	-1.805094
H	3.899206	3.083426	-0.063935	H	-4.593277	-1.567901	1.494702
H	-0.101575	4.494922	-0.738143	H	-3.015715	1.015361	1.853320
H	2.341317	4.908372	-0.650747	H	-3.774111	-1.854415	-0.590947
C	1.628902	-1.285618	-0.082220	H	-1.883111	-1.805336	2.085577
C	2.957817	-0.837169	-0.042162	C	0.982078	1.438910	-0.053729
C	1.298066	-2.511209	-0.657144	C	2.353907	1.633277	0.155525
C	3.949879	-1.659778	-0.570123	C	0.158155	2.479120	-0.479995
C	2.300380	-3.320583	-1.182007	C	2.881265	2.903665	-0.078794
H	0.253226	-2.808034	-0.693099	C	0.700744	3.740566	-0.699004
C	3.624094	-2.892138	-1.133125	H	-0.896011	2.281476	-0.660475
H	4.985002	-1.330092	-0.549355	C	2.063538	3.949072	-0.497824
H	2.051346	-4.275034	-1.633465	H	3.944204	3.073853	0.070642
H	4.410080	-3.515511	-1.547884	H	0.066788	4.555706	-1.031911
O	0.423917	-0.443876	2.200254	H	2.494441	4.929861	-0.673247
C	3.297836	0.499448	0.582945	C	1.675967	-1.317711	-0.167945
H	3.274537	0.380964	1.675760	C	2.980182	-0.849977	0.039767
H	4.321536	0.779616	0.320245	C	1.438374	-2.577194	-0.710861

M11OL3-TS1

SCF energy in gas phase: -1323.605151

SCF energy in solution: -1323.895239

Free energy in solution: -1323.534285

C	-1.372556	-0.511509	0.389612	H	4.650855	-3.583198	-1.108932
C	-3.766048	-0.781617	-0.348106	O	0.555328	-0.324773	1.941985
C	-3.155876	-0.056082	2.046426	C	3.237893	0.509055	0.661789
C	-4.246472	-0.603964	1.109327	H	3.076985	0.416386	1.744480
C	-2.335479	-0.342025	-0.598426	H	4.287189	0.780592	0.515775
H	-5.112361	0.066610	1.134329				

M11OL3-Pr

SCF energy in gas phase: -1323.652786

SCF energy in solution: -1323.946583

Free energy in solution: -1323.578657

C	-1.432637	-0.419046	0.421104
C	-3.890184	-0.747168	0.047693
C	-3.007671	0.633290	2.026725
C	-4.220746	-0.059723	1.390153
C	-2.465611	-0.551450	-0.449782
H	-5.025905	0.668005	1.240589
H	-3.220342	0.852734	3.079412
N	-2.512058	-0.558619	-1.812574
P	0.303757	-0.236185	0.000556
C	-0.472269	0.480996	2.405826
H	-0.352055	0.359465	3.487905
H	-1.675398	-0.617858	-2.370795
H	0.018230	-0.464665	-1.423053
C	-1.742574	-0.208129	1.882307
H	-0.539761	1.564077	2.189246
C	-3.846051	-0.786850	-2.345607
C	-4.727704	-0.344747	-1.173486
H	-4.011373	-0.199421	-3.252618
H	-4.845351	0.744443	-1.190056
H	-4.015162	-1.846585	-2.587385
H	-5.718461	-0.803052	-1.188578
H	-4.608479	-0.810428	2.085377
H	-2.824530	1.591495	1.524284
H	-3.987876	-1.835036	0.177579
H	-1.869197	-1.165859	2.410734
C	1.023655	1.402885	-0.338216
C	2.367818	1.617101	-0.000574
C	0.277543	2.401359	-0.959839
C	2.936022	2.854311	-0.308290
C	0.850877	3.638852	-1.236670
H	-0.758796	2.200564	-1.226384
C	2.186150	3.860282	-0.911751
H	3.981177	3.032080	-0.067943
H	0.265244	4.420659	-1.709707
H	2.649146	4.816823	-1.133610
C	1.727261	-1.376792	-0.095420
C	2.997605	-0.866212	0.208676
C	1.578297	-2.683236	-0.553167
C	4.101278	-1.706414	0.052220

C	2.684662	-3.517715	-0.675502
H	0.587439	-3.047727	-0.815571
C	3.949801	-3.023392	-0.371850
H	5.094503	-1.320335	0.267330
H	2.562870	-4.540823	-1.016415
H	4.823187	-3.659494	-0.477304
O	0.616174	-0.099298	1.746841
C	3.191214	0.554726	0.703739
H	2.918305	0.573594	1.765414
H	4.250826	0.817279	0.626773

M12NHL3

SCF energy in gas phase: -1341.894865

SCF energy in solution: -1342.191053

Free energy in solution: -1341.803807

C	0.989127	-1.180182	-0.039750
C	3.223794	-0.527025	-0.905599
C	3.046321	-2.395514	0.787335
C	3.671458	-1.036342	0.469698
C	1.707703	-0.315406	-0.904920
H	4.764931	-1.115893	0.495075
H	3.391371	-2.763233	1.761650
P	-0.512582	-0.672544	0.575445
C	0.856211	-2.220283	2.143587
C	1.502803	-2.361634	0.752582
C	1.812551	1.643530	-2.266713
C	3.939482	0.751601	-1.332558
C	3.268598	1.303760	-2.584590
H	1.274267	1.868358	-3.196972
H	3.867126	1.492490	-0.523584
H	3.304401	0.543938	-3.375776
N	1.076065	0.619686	-1.548720
H	0.812056	-3.176213	2.675286
H	1.442840	-1.508108	2.746138
H	1.145981	-3.317746	0.338472
H	1.787553	2.574445	-1.675145
H	3.788152	2.191321	-2.961142
H	5.005067	0.553462	-1.494239
H	3.447832	-1.311949	-1.645779
H	3.383228	-0.296495	1.228787
H	3.402079	-3.116194	0.042484
C	-2.105248	-0.907231	-0.253744
C	-2.712808	-2.165431	-0.246888

C	-2.694064	0.169848	-0.934141	H	3.896027	0.030228	-3.087123
C	-3.916089	-2.363465	-0.912343	N	1.686616	0.768885	-1.392140
H	-2.234640	-2.976963	0.293612	H	0.497144	-2.676390	2.937250
C	-3.904341	-0.047094	-1.595139	H	-0.493770	0.248047	-1.644191
C	-4.510711	-1.298616	-1.586388	H	0.385701	0.608625	-1.642495
H	-4.390347	-3.339322	-0.903423	H	1.205018	-1.040739	2.848868
H	-4.376551	0.779227	-2.119527	H	0.923011	-3.092351	0.633742
H	-5.455042	-1.442051	-2.102218	H	2.763440	2.517328	-1.733185
C	-0.638605	1.065399	1.071439	H	4.691787	1.581465	-2.798896
C	0.003672	1.482927	2.238199	H	5.456284	-0.077908	-1.079278
C	-1.387236	1.967611	0.304043	H	3.598225	-1.624717	-1.212071
C	-0.092437	2.805481	2.654796	H	3.511728	-0.366629	1.561780
H	0.587203	0.769138	2.815545	H	3.197268	-3.239253	0.565264
C	-1.473118	3.292330	0.733134	C	-2.169235	-0.979133	-0.353716
C	-0.833861	3.709076	1.896908	C	-2.511933	-2.333675	-0.328523
H	0.406482	3.130226	3.561902	C	-3.080072	-0.025827	-0.830400
H	-2.047413	4.003592	0.145767	C	-3.746721	-2.756694	-0.803983
H	-0.916836	4.743447	2.215518	H	-1.807041	-3.047944	0.085741
N	-0.513621	-1.733818	1.892557	C	-4.330100	-0.465496	-1.272869
H	-1.080191	-1.504569	2.699195	C	-4.660848	-1.815581	-1.272148
C	-2.023238	1.523178	-0.989242	H	-4.001572	-3.811416	-0.794509
H	-2.735190	2.276136	-1.338159	H	-5.049267	0.266653	-1.630903
H	-1.202532	1.450932	-1.720250	H	-5.635749	-2.132897	-1.628530

M12NHL3-TS1

SCF energy in gas phase: -1343.031278

SCF energy in solution: -1343.325956

Free energy in solution: -1342.923982

C	1.069621	-1.005420	0.056836
C	3.474616	-0.748648	-0.555842
C	2.878634	-2.414867	1.212993
C	3.736963	-1.199448	0.882221
C	2.024942	-0.287479	-0.679706
H	4.798773	-1.441323	1.008098
H	3.050171	-2.746169	2.244543
P	-0.563844	-0.466136	0.335864
C	0.630035	-1.800725	2.291452
C	1.376900	-2.158790	0.999701
C	2.617096	1.531000	-2.199644
C	4.442133	0.332623	-1.028625
C	3.978672	0.864781	-2.379634
H	2.152009	1.719349	-3.175046
H	4.461271	1.153648	-0.297986

H	3.896027	0.030228	-3.087123
N	1.686616	0.768885	-1.392140
H	0.497144	-2.676390	2.937250
H	-0.493770	0.248047	-1.644191
H	0.385701	0.608625	-1.642495
H	1.205018	-1.040739	2.848868
H	0.923011	-3.092351	0.633742
H	2.763440	2.517328	-1.733185
H	4.691787	1.581465	-2.798896
H	5.456284	-0.077908	-1.079278
H	3.598225	-1.624717	-1.212071
H	3.511728	-0.366629	1.561780
H	3.197268	-3.239253	0.565264
C	-2.169235	-0.979133	-0.353716
C	-2.511933	-2.333675	-0.328523
C	-3.080072	-0.025827	-0.830400
C	-3.746721	-2.756694	-0.803983
H	-1.807041	-3.047944	0.085741
C	-4.330100	-0.465496	-1.272869
C	-4.660848	-1.815581	-1.272148
H	-4.001572	-3.811416	-0.794509
H	-5.049267	0.266653	-1.630903
H	-5.635749	-2.132897	-1.628530
C	-0.779327	1.297300	0.684410
C	0.101338	1.900320	1.585122
C	-1.842986	2.021217	0.133272
C	-0.072310	3.227555	1.955001
H	0.933950	1.320616	1.977274
C	-2.014665	3.349956	0.529314
C	-1.141787	3.949991	1.429863
H	0.619248	3.695657	2.647783
H	-2.840379	3.921582	0.113492
H	-1.293991	4.985221	1.718789
N	-0.661143	-1.316866	1.823508
H	-1.357940	-1.053691	2.506921
C	-2.734439	1.439631	-0.937248
H	-3.657552	2.024150	-0.997028
H	-2.203606	1.571219	-1.892914

M12NHL3-Pr

SCF energy in gas phase: -1343.068209

SCF energy in solution: -1343.361308

Free energy in solution: -1342.951968

C	1.077235	-1.207672	-0.336156	C	-0.474076	3.658314	1.685655
C	3.535029	-0.799209	-0.606148	H	1.235864	2.962816	2.798115
C	2.767086	-2.917322	0.524992	H	-2.191380	4.068526	0.457723
C	3.672933	-1.698108	0.623119	H	-0.445663	4.658059	2.107687
C	2.072434	-0.435322	-0.834935	N	-0.688456	-1.672508	1.280489
H	4.719897	-2.000414	0.738630	H	-1.455358	-1.622565	1.937073
H	2.888677	-3.567938	1.399740	C	-2.542241	1.712132	-0.855838
P	-0.651041	-0.589812	-0.110850	H	-3.295803	2.504354	-0.893915
C	0.527213	-2.336930	1.689519	H	-2.041061	1.706853	-1.836086
C	1.298306	-2.515346	0.377423				
C	2.693027	1.880115	-1.497368	M12OL3			
C	4.409816	0.450709	-0.444633	SCF energy in gas phase:	-1361.761500		
C	4.155736	1.470288	-1.547803	SCF energy in solution:	-1362.064731		
H	2.444414	2.543714	-2.330629	Free energy in solution:	-1361.690463		
H	4.181441	0.916825	0.525106				
H	4.375006	1.029361	-2.527306	C	-1.089187	-0.933239	-0.440205
N	1.845816	0.700390	-1.601132	C	-3.451719	-0.599492	0.264677
H	0.314949	-3.305879	2.160112	C	-2.974787	-1.526251	-2.041113
H	-0.684913	-0.059689	-1.496938	C	-3.658451	-0.414680	-1.244182
H	0.867114	0.915908	-1.728640	C	-1.962130	-0.479194	0.593722
H	1.138373	-1.746556	2.396860	H	-4.731228	-0.403799	-1.470884
H	0.773633	-3.308997	-0.174991	H	-3.123278	-1.375141	-3.117719
H	2.500674	2.433917	-0.562773	P	0.496620	-0.371025	-0.594245
H	4.794304	2.350290	-1.423464	C	-0.566724	-0.997451	-2.782420
H	5.462289	0.149139	-0.411976	C	-1.467011	-1.648213	-1.724908
H	3.886856	-1.346675	-1.494482	C	-2.326588	0.694710	2.634564
H	3.409951	-1.110088	1.513089	C	-4.262367	0.385980	1.101414
H	3.067338	-3.506168	-0.349585	C	-3.803058	0.307620	2.553120
C	-2.500831	-0.775651	-0.326803	H	-1.934434	0.467578	3.633419
C	-3.158626	-2.000278	-0.213979	H	-4.094645	1.404639	0.720990
C	-3.228434	0.373652	-0.675968	H	-3.935103	-0.719751	2.916129
C	-4.527996	-2.098363	-0.449705	N	-1.460722	0.066919	1.654091
H	-2.584551	-2.876876	0.069874	H	-0.383607	-1.626636	-3.656726
C	-4.604716	0.270062	-0.877121	H	-0.991967	-0.035543	-3.100624
C	-5.253729	-0.957447	-0.775480	H	-1.208107	-2.717773	-1.692048
H	-5.025884	-3.059704	-0.369177	H	-2.238924	1.788934	2.524208
H	-5.173492	1.163775	-1.121964	H	-4.400557	0.959544	3.198956
H	-6.323916	-1.019022	-0.946451	H	-5.333546	0.179620	0.998537
C	-0.561268	1.096775	0.593176	H	-3.769076	-1.621805	0.525857
C	0.417123	1.428822	1.531045	H	-3.259275	0.565693	-1.537777
C	-1.507644	2.049372	0.194820	H	-3.465586	-2.473940	-1.794427
C	0.468608	2.708505	2.073527	C	1.897271	-1.135996	0.240603
H	1.148689	0.677163	1.819072	C	3.149704	-0.508295	0.201915
C	-1.455543	3.326549	0.757421	C	1.704412	-2.318346	0.952650

SCF energy in gas phase: -1361.761500

Free energy in solution: -1361.690463

C	-1.089187	-0.933239	-0.440205
C	-3.451719	-0.599492	0.264677
C	-2.974787	-1.526251	-2.041113
C	-3.658451	-0.414680	-1.244182
C	-1.962130	-0.479194	0.593722
H	-4.731228	-0.403799	-1.470884
H	-3.123278	-1.375141	-3.117719
P	0.496620	-0.371025	-0.594245
C	-0.566724	-0.997451	-2.782420
C	-1.467011	-1.648213	-1.724908
C	-2.326588	0.694710	2.634564
C	-4.262367	0.385980	1.101414
C	-3.803058	0.307620	2.553120
H	-1.934434	0.467578	3.633419
H	-4.094645	1.404639	0.720990
H	-3.935103	-0.719751	2.916129
N	-1.460722	0.066919	1.654091
H	-0.383607	-1.626636	-3.656726
H	-0.991967	-0.035543	-3.100624
H	-1.208107	-2.717773	-1.692048
H	-2.238924	1.788934	2.524208
H	-4.400557	0.959544	3.198956
H	-5.333546	0.179620	0.998537
H	-3.769076	-1.621805	0.525857
H	-3.259275	0.565693	-1.537777
H	-3.465586	-2.473940	-1.794427
C	1.897271	-1.135996	0.240603
C	3.149704	-0.508295	0.201915
C	1.704412	-2.318346	0.952650

C	4.214031	-1.110236	0.869809	H	0.294679	-2.540555	2.935238
C	2.777141	-2.909597	1.611802	H	-0.452216	0.254007	-1.621858
H	0.707950	-2.750845	0.991398	H	0.400377	0.606573	-1.644144
C	4.029983	-2.304060	1.564338	H	1.094546	-0.943716	2.864457
H	5.192381	-0.637542	0.852484	H	0.910324	-3.038593	0.672048
H	2.636054	-3.831108	2.166576	H	2.864258	2.488847	-1.760583
H	4.869387	-2.756284	2.083332	H	4.781941	1.482663	-2.787256
C	0.866092	1.382520	-0.385401	H	5.495765	-0.148345	-1.019826
C	-0.163136	2.317327	-0.262174	H	3.608152	-1.661202	-1.111123
C	2.209510	1.786095	-0.393464	H	3.486516	-0.290695	1.607900
C	0.138873	3.668543	-0.144001	H	3.173400	-3.210111	0.755690
H	-1.191347	1.968497	-0.241089	C	-2.113820	-1.018041	-0.338521
C	2.494577	3.146803	-0.279142	C	-3.052070	-0.119299	-0.862432
C	1.469978	4.079796	-0.153841	C	-2.402261	-2.382117	-0.259577
H	-0.657363	4.397781	-0.038902	C	-4.275517	-0.624994	-1.308110
H	3.530038	3.476179	-0.283311	C	-3.613152	-2.871085	-0.731747
H	1.712504	5.133455	-0.056662	H	-1.678281	-3.055799	0.189233
O	0.725599	-0.759207	-2.173259	C	-4.553330	-1.985820	-1.255133
C	3.332424	0.781846	-0.567077	H	-5.016864	0.063394	-1.705169
H	4.282604	1.245751	-0.288418	H	-3.829970	-3.932776	-0.678286
H	3.405042	0.535965	-1.636310	H	-5.508996	-2.355250	-1.613197

M12OL3-TS1

SCF energy in gas phase: -1362.904319

SCF energy in solution: -1363.205552

Free energy in solution: -1362.815550

C	1.080261	-0.953577	0.084937
C	3.493662	-0.757110	-0.492383
C	2.835188	-2.345949	1.337544
C	3.715206	-1.154655	0.969917
C	2.058319	-0.267652	-0.656151
H	4.770082	-1.404744	1.131388
H	2.966197	-2.614245	2.393290
P	-0.543356	-0.410247	0.332998
C	0.537610	-1.695112	2.284471
C	1.343223	-2.097684	1.045866
C	2.701750	1.495866	-2.206427
C	4.491181	0.286573	-0.987242
C	4.049222	0.793739	-2.355560
H	2.252004	1.672380	-3.190865
H	4.524881	1.126308	-0.278844
H	3.952992	-0.056821	-3.041990
N	1.743268	0.775475	-1.391417

C	-0.828363	1.341434	0.648636
C	0.005896	1.996385	1.555122
C	-1.912372	2.003756	0.059428
C	-0.232979	3.322806	1.891121
H	0.849833	1.460022	1.982095
C	-2.146397	3.332312	0.419462
C	-1.318820	3.987080	1.324872
H	0.419026	3.834767	2.590990
H	-2.986410	3.859517	-0.024956
H	-1.520958	5.020835	1.587220
O	-0.696928	-1.141683	1.826579
C	-2.761600	1.355856	-1.008239
H	-2.226667	1.486317	-1.961817
H	-3.706756	1.899817	-1.096419

M12OL3-Pr

SCF energy in gas phase: -1362.947300

SCF energy in solution: -1363.250853

Free energy in solution: -1362.855021

C	1.180642	-0.963636	-0.024133
C	3.638924	-0.743052	-0.391365
C	2.836242	-2.411910	1.308153

C	3.755546	-1.226203	1.054986	H	-1.948822	4.905823	1.677903
C	2.195894	-0.346930	-0.693476	O	-0.636473	-1.053836	1.654453
H	4.797010	-1.492957	1.266422	C	-2.755217	1.284908	-1.169785
H	2.909296	-2.747760	2.349935	H	-2.141549	1.357317	-2.080413
P	-0.525346	-0.349755	0.045846	H	-3.679411	1.834468	-1.371413
C	0.543340	-1.606420	2.167909				
C	1.378885	-2.076141	0.975287	M13OL3			
C	2.990779	1.617112	-2.029487	SCF energy in gas phase:	-1284.379772		
C	4.631885	0.392134	-0.660671	SCF energy in solution:	-1284.668582		
C	4.392230	1.032407	-2.020774	Free energy in solution:	-1284.328163		
H	2.729224	1.994336	-3.022369				
H	4.519981	1.158020	0.119717	C	1.868557	-0.157352	-1.478587
H	4.481418	0.280058	-2.813092	C	4.364643	0.178687	-1.034470
N	2.014415	0.601275	-1.671381	C	2.774265	0.477020	0.877752
H	0.293724	-2.436415	2.841907	C	4.092452	-0.154244	0.433099
H	-0.466158	0.145654	-1.342820	C	1.671250	0.055321	-0.075032
H	1.051581	0.855982	-1.837283	C	3.292548	-0.423022	-1.946430
H	1.122700	-0.863030	2.746139	C	1.079097	0.736250	2.722740
H	0.893684	-2.985124	0.588321	C	2.427802	0.151913	2.330241
H	2.953194	2.470444	-1.332759	N	0.837824	-0.210890	-2.261668
H	5.123292	1.820922	-2.221826	P	0.042229	0.034013	0.409523
H	5.650268	-0.000727	-0.576171	H	4.375155	1.270289	-1.151214
H	3.891390	-1.577695	-1.063869	H	4.028313	-1.243708	0.560990
H	3.493836	-0.392875	1.720199	H	3.419673	-1.513966	-1.975124
H	3.170337	-3.249638	0.685775	H	1.042808	1.812540	2.499802
C	-2.151318	-1.064233	-0.393631	H	2.392267	-0.935086	2.474691
C	-3.088922	-0.177691	-0.944012	H	3.196133	0.558914	2.998669
C	-2.480788	-2.400910	-0.182785	H	1.107532	-0.460738	-3.212997
C	-4.350371	-0.667187	-1.283988	H	3.404830	-0.062537	-2.974547
C	-3.729877	-2.882555	-0.561043	H	5.353281	-0.180802	-1.337450
H	-1.760876	-3.053898	0.300785	H	4.911133	0.208258	1.066835
C	-4.666356	-2.011398	-1.111317	H	0.870527	0.598332	3.785723
H	-5.092560	0.015768	-1.689491	H	2.926904	1.572832	0.836352
H	-3.978961	-3.927693	-0.407738	C	-0.964877	-1.418526	0.069057
H	-5.649821	-2.374474	-1.392733	C	-2.347411	-1.326505	0.275318
C	-0.932537	1.336924	0.599726	C	-0.374950	-2.602735	-0.366622
C	-0.237952	1.977654	1.622946	C	-3.124847	-2.461844	0.045368
C	-2.006449	1.969766	-0.042377	C	-1.164106	-3.723687	-0.592579
C	-0.589566	3.268650	2.003920	H	0.699083	-2.622680	-0.529579
H	0.573940	1.455586	2.122609	C	-2.539642	-3.649314	-0.383456
C	-2.365350	3.253773	0.369288	H	-4.199396	-2.411703	0.198877
C	-1.658419	3.904359	1.376364	H	-0.713322	-4.648790	-0.936257
H	-0.044893	3.771128	2.796848	H	-3.162870	-4.519643	-0.564463
H	-3.208219	3.748340	-0.106641	C	-1.068061	1.369422	-0.091773

SCF energy in gas phase: -1284.379772

Free energy in solution: -1284.328163

C	-2.444640	1.217844	0.125569
C	-0.556760	2.512396	-0.701369
C	-3.294193	2.254362	-0.256382
C	-1.415973	3.541114	-1.073531
H	0.511274	2.569342	-0.896007
C	-2.783297	3.409098	-0.845188
H	-4.365025	2.153067	-0.100767
H	-1.025436	4.434591	-1.549176
H	-3.460771	4.203839	-1.141823
O	0.002999	0.073219	2.041770
C	-2.984293	-0.041942	0.770115
H	-2.812623	0.025636	1.853593
H	-4.067045	-0.093212	0.625519

M13OL3-TS1

SCF energy in gas phase: -1285.511318

SCF energy in solution: -1285.798841

Free energy in solution: -1285.442790

C	2.086220	-0.947612	-1.286400
C	4.353826	0.199849	-1.203518
C	2.649275	0.758124	0.572039
C	4.106963	0.389755	0.285646
C	1.677926	-0.112442	-0.233568
C	3.552902	-1.003978	-1.680453
C	0.986712	1.054113	2.470555
C	2.399884	0.663120	2.081830
N	1.219724	-1.696066	-1.952631
P	-0.012438	0.035087	0.193756
H	4.035770	1.097646	-1.747632
H	4.345206	-0.547467	0.808306
H	3.985189	-1.922513	-1.262450
H	0.784722	2.104780	2.216463
H	2.576903	-0.370986	2.402422
H	3.109987	1.307985	2.615081
H	1.629478	-2.136601	-2.771363
H	-0.395454	-0.142777	-1.823063
H	3.600753	-1.104369	-2.770340
H	5.418669	0.054551	-1.410316
H	4.757624	1.165173	0.705235
H	0.828677	0.942665	3.546729
H	2.531889	1.818980	0.286756
H	0.136863	-0.873289	-2.019374
C	-1.075863	-1.413082	0.206277

C	-2.408494	-1.306392	-0.198878
C	-0.572426	-2.598913	0.740295
C	-3.234207	-2.420838	-0.032256
C	-1.402274	-3.703533	0.875496
H	0.471706	-2.643837	1.036877
C	-2.739666	-3.607258	0.496302
H	-4.276294	-2.355405	-0.333809
H	-1.011951	-4.632306	1.277803
H	-3.400289	-4.461055	0.610010
C	-1.049913	1.474494	-0.189274
C	-2.391013	1.276185	-0.549809
C	-0.539836	2.770077	-0.063430
C	-3.205150	2.397735	-0.716482
C	-1.360883	3.875069	-0.256073
H	0.511372	2.920380	0.162932
C	-2.704066	3.686329	-0.566496
H	-4.248165	2.253264	-0.986442
H	-0.953376	4.876217	-0.162061
H	-3.358868	4.540456	-0.705865
O	0.031366	0.208560	1.845995
C	-2.947828	-0.084504	-0.903051
H	-4.036879	-0.063056	-0.798931
H	-2.738483	-0.228548	-1.975372

M13OL3-Pr

SCF energy in gas phase: -1285.552824

SCF energy in solution: -1285.841224

Free energy in solution: -1285.477921

C	2.252256	-1.006497	-1.217480
C	4.462660	0.201725	-1.152828
C	2.716292	0.668479	0.613012
C	4.194092	0.377952	0.334132
C	1.777314	-0.169582	-0.254911
C	3.706945	-1.028218	-1.633352
C	1.001100	0.839214	2.457674
C	2.428246	0.466874	2.103011
N	1.514107	-1.974628	-1.865462
P	-0.024000	-0.020597	-0.010916
H	4.116610	1.086861	-1.699930
H	4.477298	-0.546506	0.856828
H	4.172774	-1.941392	-1.241431
H	0.844813	1.918835	2.300292
H	2.593344	-0.589058	2.352265

H	3.130563	1.066151	2.696873	C	4.035513	-0.940491	0.144225
H	1.812039	-2.208382	-2.801006	C	1.201634	-0.753335	0.422249
H	-0.197591	-0.194748	-1.465741	C	1.939963	-1.797620	1.244149
H	3.746308	-1.108224	-2.727757	C	3.375370	-1.310943	1.473633
H	5.532347	0.090545	-1.353145	C	1.220553	-2.165802	2.567776
H	4.802397	1.183041	0.759988	H	1.955310	-2.281529	3.373863
H	0.812047	0.649454	3.521184	C	0.166560	-1.157792	2.993980
H	2.542362	1.734281	0.385625	H	4.007684	-1.810935	-0.526655
H	0.510959	-1.962419	-1.748648	H	3.088671	2.630009	-1.678101
C	-1.239323	-1.362722	0.232153	H	3.866570	-0.194236	-2.564726
C	-2.492024	-1.189559	-0.369168	H	1.530621	0.819271	-3.567206
C	-0.951487	-2.515535	0.960986	H	3.950901	-2.094606	1.981844
C	-3.451309	-2.191690	-0.209846	H	0.590960	-0.153039	3.114822
C	-1.903822	-3.522457	1.077167	N	1.072555	0.462057	-1.583394
H	0.014694	-2.604002	1.448521	P	-0.456703	-0.468548	0.583751
C	-3.158595	-3.354906	0.495374	H	-0.310755	-1.451938	3.931206
H	-4.436582	-2.058154	-0.649506	H	0.711506	-3.129263	2.461187
H	-1.675569	-4.425032	1.634845	H	2.034616	-2.734163	0.670258
H	-3.914224	-4.127268	0.598881	H	0.949010	2.214596	-2.683116
C	-0.985181	1.523732	-0.190203	H	3.456408	2.198035	-3.347400
C	-2.288285	1.372178	-0.695817	H	4.955260	0.941157	-1.758260
C	-0.508163	2.794285	0.133405	H	3.423101	1.096795	0.162818
C	-3.099324	2.501265	-0.807195	H	5.092215	-0.688298	0.291738
C	-1.319952	3.915550	-0.015285	H	3.357792	-0.432307	2.134659
H	0.509189	2.918833	0.487840	C	-1.723812	-1.152571	-0.505321
C	-2.625004	3.765675	-0.470528	C	-3.021837	-0.627466	-0.466884
H	-4.114253	2.387442	-1.179459	C	-1.379876	-2.157033	-1.406738
H	-0.934506	4.899670	0.231229	C	-3.977915	-1.157696	-1.331898
H	-3.271767	4.631242	-0.573076	C	-2.345282	-2.681965	-2.259095
O	0.076783	0.076493	1.728791	H	-0.350450	-2.504563	-1.440012
C	-2.798550	0.036498	-1.204813	C	-3.644086	-2.181273	-2.215524
H	-3.879944	0.103427	-1.356042	H	-4.989703	-0.761323	-1.318240
H	-2.353633	-0.118756	-2.199912	H	-2.085783	-3.467218	-2.961366
M15OL3				H	-4.400097	-2.579114	-2.885314
SCF energy in gas phase: -1401.062729				C	-0.958562	1.269480	0.674891
SCF energy in solution: -1401.373977				C	-0.011381	2.279103	0.847937
Free energy in solution: -1400.971033				C	-2.327017	1.570552	0.629829
				C	-0.415784	3.603071	0.963093
				H	1.040226	2.008262	0.887397
C	3.059158	1.807436	-2.404869	C	-2.717938	2.904984	0.749255
C	3.903262	0.654641	-1.868172	C	-1.773193	3.913492	0.910340
C	3.323593	0.237418	-0.521923	H	0.321101	4.389020	1.091013
C	1.824166	-0.017268	-0.646837	H	-3.775040	3.154362	0.712461
C	1.612184	1.343338	-2.603301	H	-2.098637	4.945720	0.993817

O	-0.888832	-1.127537	2.016492
C	-3.370702	0.476758	0.506891
H	-3.503369	0.025775	1.500458
H	-4.332229	0.919549	0.232294

M15OL3-TS1

SCF energy in gas phase: -1402.197852

SCF energy in solution: -1402.506439

Free energy in solution: -1402.087077

C	4.215940	1.457411	-1.956791
C	4.422353	0.046357	-1.425307
C	3.659122	-0.118535	-0.113178
C	2.200598	0.316803	-0.270641
C	2.732281	1.660799	-2.241463
C	3.746642	-1.533234	0.448765
C	1.232231	-0.275329	0.570168
C	1.568099	-1.251965	1.706538
C	3.066652	-1.569694	1.807818
C	1.050896	-0.745675	3.068860
H	1.761325	-0.022395	3.486344
C	-0.314773	-0.068015	2.929830
H	3.260768	-2.233018	-0.244419
H	4.555437	2.180315	-1.204522
H	4.051629	-0.683556	-2.158431
H	2.475068	1.128130	-3.170471
H	3.196964	-2.539196	2.300186
H	-0.194121	1.011870	2.767744
N	1.845204	1.203189	-1.184445
P	-0.494849	-0.170251	0.328843
H	-0.934178	-0.203249	3.819870
H	0.997224	-1.590302	3.765441
H	1.051987	-2.203328	1.510667
H	2.521199	2.719965	-2.428792
H	4.796452	1.637814	-2.867170
H	0.596089	0.717884	-1.540542
H	-0.130244	0.184564	-1.574859
H	5.482669	-0.172753	-1.259711
H	4.118216	0.560631	0.622489
H	4.798031	-1.832518	0.530301
H	3.554637	-0.824461	2.450131
C	-1.550614	-1.377346	-0.520194
C	-2.930597	-1.140880	-0.512322
C	-1.010530	-2.479302	-1.177337

C	-3.755883	-2.040560	-1.188402
C	-1.849059	-3.379751	-1.823991
H	0.069014	-2.612842	-1.190428
C	-3.223890	-3.154003	-1.831652
H	-4.828484	-1.866009	-1.207215
H	-1.433598	-4.245223	-2.329631
H	-3.884470	-3.843151	-2.348270
C	-1.362659	1.406758	0.173728
C	-0.689212	2.628249	0.154494
C	-2.764567	1.347924	0.124729
C	-1.413699	3.813325	0.071072
H	0.396510	2.634358	0.176587
C	-3.468415	2.548338	0.026413
C	-2.803172	3.770657	0.001444
H	-0.894112	4.765787	0.054943
H	-4.553722	2.522507	-0.024855
H	-3.373033	4.691664	-0.072091
O	-1.033586	-0.637070	1.839526
C	-3.520049	0.035859	0.238156
H	-3.555746	-0.234785	1.302180
H	-4.552699	0.190161	-0.087636

M15OL3-Pr

SCF energy in gas phase: -1402.232916

SCF energy in solution: -1402.545541

Free energy in solution: -1402.119382

C	4.411789	2.136296	-1.270354
C	4.591046	0.633842	-1.071228
C	3.834645	0.155622	0.173842
C	2.373417	0.570297	0.098772
C	2.927715	2.460762	-1.361805
C	3.998814	-1.341638	0.405793
C	1.347342	-0.264842	0.383325
C	1.578181	-1.675579	0.928850
C	3.006632	-1.828963	1.451629
C	0.540501	-2.031981	2.011944
H	0.995551	-2.691614	2.760147
C	0.008420	-0.767620	2.662360
H	3.820683	-1.879148	-0.536227
H	4.844990	2.675661	-0.420151
H	4.201790	0.099180	-1.949082
H	2.519000	2.038359	-2.294463
H	3.187624	-2.878499	1.708912

H	0.848983	-0.139115	2.996972	C	1.350779	-1.173843	-0.275546
N	2.226004	1.932513	-0.189069	C	2.755606	-2.847627	0.735032
P	-0.419349	0.239688	0.100770	C	3.471830	-1.784345	-1.319488
H	-0.603293	-0.996692	3.541972	C	3.683266	-2.688766	-0.270752
H	-0.308573	-2.570701	1.576470	C	2.302195	-1.050920	-1.310848
H	1.458429	-2.391201	0.102775	C	1.547107	-2.097505	0.783471
H	2.769121	3.542509	-1.388589	H	4.585866	-3.292758	-0.253173
H	4.920606	2.477199	-2.177263	H	2.933236	-3.572505	1.524559
H	1.262209	2.238302	-0.165900	H	4.190746	-1.676739	-2.124709
H	0.010100	0.915151	-1.118938	N	0.681460	-2.331362	1.792304
H	5.650587	0.370470	-0.977504	P	0.053048	0.049133	-0.599877
H	4.253470	0.693749	1.038458	C	1.918644	-0.047102	-2.385123
H	5.032579	-1.550855	0.701515	H	2.201048	-0.396602	-3.381520
H	3.121724	-1.243319	2.374981	H	-0.272069	-1.897430	1.994364
C	-1.225619	-1.174910	-0.713604	H	-0.428685	0.049700	1.129565
C	-2.565477	-1.456881	-0.404714	C	0.537185	1.768887	-0.197468
C	-0.540184	-1.941379	-1.655938	C	0.160987	2.831943	-1.022354
C	-3.175445	-2.543211	-1.035131	C	1.366441	2.001994	0.900821
C	-1.161363	-3.021503	-2.274059	C	0.558810	4.128669	-0.706288
H	0.485506	-1.678763	-1.905997	C	1.789410	3.293889	1.193920
C	-2.481555	-3.325640	-1.953198	C	1.369699	4.360381	0.401097
H	-4.214232	-2.769661	-0.809383	C	-1.664795	-0.453135	-0.859037
H	-0.622889	-3.615867	-3.004933	C	-2.544809	0.389271	-1.546180
H	-2.978671	-4.163826	-2.431344	C	-2.098744	-1.687301	-0.370013
C	-1.863434	1.417798	0.163791	C	-3.867767	0.003911	-1.725061
C	-1.706877	2.776502	-0.090921	C	-3.423866	-2.068302	-0.565608
C	-3.150821	0.890010	0.355138	C	-4.306729	-1.224370	-1.231218
C	-2.804246	3.634863	-0.103946	H	1.684011	1.165502	1.517135
H	-0.716911	3.183316	-0.291595	H	2.444017	3.467988	2.041757
C	-4.246497	1.750274	0.307473	H	1.688037	5.370524	0.638250
C	-4.078450	3.117272	0.098088	H	0.249644	4.955614	-1.337284
H	-2.664659	4.695958	-0.284359	H	-4.555007	0.659310	-2.250014
H	-5.246470	1.342175	0.431619	H	-5.341037	-1.523315	-1.368860
H	-4.944403	3.771171	0.074281	H	-3.766766	-3.022245	-0.180086
O	-0.814531	-0.043989	1.770449	H	-1.418145	-2.337678	0.166937
C	-3.352289	-0.596767	0.566328	H	0.969019	-3.032394	2.457818
H	-3.040397	-0.842891	1.587922	H	2.440860	0.902765	-2.209489
H	-4.415470	-0.837798	0.473439	C	-1.222776	-0.003300	2.230985
				C	-2.302928	1.013265	1.866508
				H	-2.829839	1.279499	2.789993
				H	-1.888891	1.930173	1.432428
				H	-3.024302	0.564011	1.182054
				C	-0.247788	0.523656	3.293099
				H	0.053302	1.559431	3.120477
M4NL2-TS2							
SCF energy in gas phase: -1378.935965							
SCF energy in solution: -1379.257738							
Free energy in solution: -1378.885276							

H	-0.774644	0.469739	4.251908
H	0.634046	-0.119317	3.355391
H	-2.200516	1.343138	-1.932264
H	-0.406666	2.637433	-1.925413
N	0.474294	0.183544	-2.301227
H	-0.018297	-0.544350	-2.815051
O	-1.603188	-1.222233	2.377019

M4OL2-TS2

SCF energy in gas phase: -1398.809856

SCF energy in solution: -1399.140100

Free energy in solution: -1398.781089

C	1.427608	-1.076480	-0.273831
C	2.945237	-2.642352	0.744322
C	3.585410	-1.547813	-1.320268
C	3.860400	-2.422425	-0.259121
C	2.368996	-0.898966	-1.309486
C	1.677638	-1.989893	0.786782
H	4.806274	-2.955693	-0.232655
H	3.175133	-3.345069	1.540219
H	4.291751	-1.401608	-2.130051
N	0.822845	-2.286318	1.780242
P	0.079281	0.061325	-0.612363
C	1.904998	0.051410	-2.387869
H	2.088178	-0.349131	-3.388331
H	-0.205197	-1.945725	1.973516
H	-0.459178	0.012173	1.149685
C	0.401850	1.804172	-0.170356
C	-0.006258	2.834974	-1.022287
C	1.162926	2.099697	0.961593
C	0.283068	4.157623	-0.697555
C	1.474758	3.420298	1.266975
C	1.018229	4.450740	0.448092
C	-1.593749	-0.529137	-0.894658
C	-2.545883	0.292203	-1.505917
C	-1.926952	-1.819681	-0.479569
C	-3.838505	-0.178733	-1.694374
C	-3.225076	-2.282778	-0.678295
C	-4.177877	-1.465733	-1.276264
H	1.514414	1.290560	1.595038
H	2.071482	3.644351	2.145075
H	1.249837	5.482156	0.693922
H	-0.052222	4.957515	-1.349614

H	-4.581215	0.457277	-2.164465
H	-5.189989	-1.830858	-1.418674
H	-3.491065	-3.281037	-0.348614
H	-1.190342	-2.452640	0.002048
H	1.163125	-2.970240	2.440569
H	2.412741	1.023365	-2.298811
C	-1.230488	-0.146165	2.185103
C	-2.410668	0.768304	1.862220
H	-2.959777	0.942819	2.794205
H	-2.092987	1.739008	1.464513
H	-3.084034	0.275486	1.159062
C	-0.344855	0.422561	3.304311
H	-0.140475	1.489608	3.185738
H	-0.892871	0.275905	4.240890
H	0.593657	-0.134013	3.371116
H	-2.287250	1.297432	-1.821310
H	-0.521517	2.603360	-1.948399
O	-1.508966	-1.409997	2.290067
O	0.504910	0.216046	-2.223591

M5CL2-TS2

SCF energy in gas phase: -1440.280383

SCF energy in solution: -1440.610105

Free energy in solution: -1440.194797

C	1.358901	-0.293362	-0.791210
C	3.733890	-0.015579	-0.353894
C	3.023408	-1.547533	-2.069986
C	4.046057	-0.933762	-1.325257
C	2.385205	0.326877	-0.054138
H	5.086730	-1.171769	-1.530587
H	3.258833	-2.259214	-2.854723
N	2.347832	1.288281	0.906992
P	-0.447076	-0.134464	-0.664460
C	0.539720	-1.774956	-2.588835
C	4.638269	0.850061	0.491303
C	1.708380	-1.210741	-1.814503
C	3.661707	1.415426	1.539230
H	5.468853	0.303055	0.943212
H	0.234293	-2.739392	-2.161975
H	0.816872	-1.960307	-3.630799
H	5.061478	1.656343	-0.119410
H	1.529943	1.514823	1.513250
H	-0.267589	0.336409	1.002641

C	-1.373031	1.433953	-0.854987	C	3.692067	-0.209695	-0.280017
C	-2.458506	1.505472	-1.737666	C	2.940752	-1.574695	-2.123752
C	-0.986440	2.571641	-0.139689	C	3.977758	-1.054642	-1.322443
C	-3.161794	2.696096	-1.887726	C	2.352180	0.156218	0.041540
C	-1.679899	3.766596	-0.316522	H	5.010961	-1.315203	-1.538103
H	-0.178958	2.525418	0.583417	H	3.163170	-2.225058	-2.963468
C	-2.767571	3.830396	-1.182207	N	2.325881	0.999447	1.098640
H	-4.011827	2.738182	-2.560956	P	-0.478440	-0.228008	-0.662341
H	-1.371655	4.645794	0.239411	C	0.418351	-1.709817	-2.597526
H	-3.310002	4.762387	-1.306361	C	4.604557	0.427466	0.742619
C	-1.350858	-1.555753	0.063946	C	1.639192	-1.226981	-1.831666
C	-2.746467	-1.556389	0.121257	C	3.676447	1.454479	1.425749
C	-0.637391	-2.669357	0.512341	H	4.948576	-0.325779	1.461165
C	-3.420859	-2.657048	0.642990	H	0.143291	-2.717007	-2.257173
C	-1.317813	-3.771263	1.025187	H	0.608800	-1.768923	-3.672294
H	0.449844	-2.666555	0.475408	H	5.489667	0.893009	0.303035
C	-2.708223	-3.765052	1.094945	H	1.485327	1.530160	1.476101
H	-4.504694	-2.646712	0.698181	H	-0.356726	0.329664	1.041270
H	-0.758071	-4.633254	1.373988	C	-1.294632	1.369842	-0.891580
H	-3.235802	-4.622293	1.500412	C	-2.639363	1.434790	-1.268964
H	3.866905	2.456435	1.797679	C	-0.557728	2.537826	-0.683760
H	3.696467	0.823821	2.465771	C	-3.252144	2.673454	-1.419818
C	-0.307937	0.710308	2.427107	C	-1.178667	3.772980	-0.848173
O	0.312772	1.812516	2.549657	H	0.479274	2.485403	-0.373841
C	0.379779	-0.539532	2.975283	C	-2.521310	3.841725	-1.206519
H	0.449338	-0.417693	4.062384	H	-4.297963	2.727022	-1.704169
H	-0.172744	-1.455590	2.759379	H	-0.612276	4.681948	-0.676915
H	1.395988	-0.618798	2.578668	H	-3.001551	4.808196	-1.322037
C	-1.818853	0.741840	2.617522	C	-1.309739	-1.663519	0.109364
H	-2.299355	-0.201923	2.351694	C	-2.507439	-2.165644	-0.405655
H	-2.004334	0.941144	3.679345	C	-0.683487	-2.314309	1.173602
H	-2.252868	1.562079	2.041142	C	-3.105374	-3.274446	0.188630
H	-3.308333	-0.689154	-0.216960	C	-1.267943	-3.439146	1.744781
H	-2.760987	0.634125	-2.309170	H	0.267332	-1.939908	1.541800
C	-0.591633	-0.759354	-2.454630	C	-2.489221	-3.908178	1.264239
H	-0.425560	0.084278	-3.132761	H	-4.044879	-3.652889	-0.200813
H	-1.571870	-1.196683	-2.660754	H	-0.771466	-3.947241	2.565031
M5NL2-TS2				H	-2.952322	-4.778221	1.718658
SCF energy in gas phase: -1456.324540				H	3.847441	2.462360	1.022903
SCF energy in solution: -1456.664348				H	3.817669	1.500125	2.508340
Free energy in solution: -1456.257341				C	-0.531787	1.099685	2.168438
C	1.316780	-0.370320	-0.750182	O	0.170334	2.165450	2.036027
				C	-0.057339	0.111003	3.241934
				H	-0.113469	0.641926	4.198487

H	-0.683533	-0.781876	3.304040
H	0.985057	-0.170330	3.071495
C	-2.050194	1.270590	2.158820
H	-2.575584	0.338855	1.921768
H	-2.352224	1.587686	3.163703
H	-2.336810	2.054193	1.455586
H	-2.945119	-1.711737	-1.287885
H	-3.206062	0.524180	-1.435905
N	-0.693576	-0.795717	-2.314986
H	-0.639067	0.007873	-2.937421

M5OL2-TS2

SCF energy in gas phase: -1476.198764

SCF energy in solution: -1476.544093

Free energy in solution: -1476.150897

C	1.309155	-0.377359	-0.749793
C	3.684049	-0.260481	-0.264452
C	2.924540	-1.575743	-2.142477
C	3.962841	-1.091604	-1.317719
C	2.347898	0.134462	0.052064
H	4.992554	-1.369900	-1.527348
H	3.143547	-2.206442	-2.997519
N	2.323261	0.974507	1.103113
P	-0.471709	-0.239869	-0.680513
C	0.412649	-1.645104	-2.630966
C	4.598062	0.344674	0.775761
C	1.629718	-1.214581	-1.846149
C	3.681823	1.378613	1.466004
H	4.921969	-0.425289	1.485813
H	0.154500	-2.690945	-2.408511
H	0.562730	-1.544060	-3.709153
H	5.495680	0.799279	0.350307
H	1.469562	1.542175	1.481881
H	-0.363157	0.354102	1.063520
C	-1.279950	1.348680	-0.913219
C	-2.638767	1.428905	-1.230512
C	-0.515316	2.505937	-0.754898
C	-3.234981	2.674544	-1.381103
C	-1.122558	3.748732	-0.912676
H	0.533369	2.441945	-0.488770
C	-2.476559	3.833768	-1.218466
H	-4.290276	2.741419	-1.624103
H	-0.535067	4.650513	-0.779041

H	-2.945566	4.805973	-1.331877
C	-1.338075	-1.631737	0.120360
C	-2.530883	-2.130280	-0.412361
C	-0.733703	-2.280685	1.197748
C	-3.147916	-3.228352	0.181209
C	-1.339346	-3.393461	1.770811
H	0.215676	-1.914040	1.576482
C	-2.556276	-3.855907	1.274508
H	-4.083136	-3.603314	-0.221491
H	-0.861494	-3.897254	2.604539
H	-3.035543	-4.716500	1.729929
H	3.886217	2.392304	1.095345
H	3.803097	1.392626	2.552139
O	-0.657668	-0.790876	-2.250674
C	-0.505199	1.113474	2.122640
O	0.234836	2.168157	1.975705
C	-0.064049	0.153601	3.238316
H	-0.107357	0.722444	4.173026
H	-0.716827	-0.717792	3.332493
H	0.969983	-0.166761	3.084644
C	-2.013782	1.357442	2.140921
H	-2.588358	0.446372	1.938502
H	-2.279069	1.715439	3.142029
H	-2.278293	2.134733	1.422257
H	-2.957753	-1.681997	-1.303473
H	-3.231753	0.527969	-1.349281

M6CL2-TS2

SCF energy in gas phase: -1479.579664

SCF energy in solution: -1479.917921

Free energy in solution: -1479.472310

C	-1.146959	0.462828	-0.953613
C	-3.560604	0.319860	-0.705694
C	-2.586228	1.966277	-2.212175
C	-3.687436	1.374762	-1.590088
C	-2.268498	-0.178369	-0.362293
H	-4.688843	1.735251	-1.815741
H	-2.711363	2.763785	-2.936954
P	0.637559	0.158683	-0.717398
C	-0.060838	2.007051	-2.544076
H	0.311582	2.890354	-2.008963
C	-1.325265	1.493706	-1.898929
C	-3.282970	-1.806701	1.214518

C	-4.776377	-0.309835	-0.068607
C	-4.431257	-0.816052	1.329527
H	-3.644321	-2.723473	0.727750
H	-5.591445	0.420055	-0.038808
H	-5.291911	-1.299588	1.799613
N	-2.164597	-1.252690	0.460664
H	0.282138	-0.291461	0.999423
H	-1.282813	-1.466428	0.923843
H	-2.878579	-2.080466	2.193230
H	-4.133351	0.027460	1.963273
H	-5.127326	-1.155411	-0.675746
H	-0.249791	2.312288	-3.577281
C	1.485427	-1.463147	-0.879297
C	2.435624	-1.639885	-1.897874
C	1.222174	-2.522397	-0.002438
C	3.107774	-2.849370	-2.035199
H	2.667521	-0.837216	-2.586884
C	1.888230	-3.736273	-0.161590
H	0.533475	-2.421147	0.832547
C	2.828355	-3.905029	-1.171747
H	3.847161	-2.965320	-2.820924
H	1.668960	-4.548881	0.523145
H	3.346136	-4.852414	-1.284491
C	1.620517	1.440094	0.147051
C	3.005679	1.294494	0.245500
C	0.997346	2.570173	0.678118
C	3.759586	2.262498	0.902967
H	3.493412	0.415082	-0.167975
C	1.757956	3.538761	1.328407
H	-0.081629	2.682680	0.596375
C	3.136816	3.382429	1.448580
H	4.833970	2.138002	0.993070
H	1.270863	4.414238	1.745820
H	3.724951	4.134719	1.963964
C	0.146035	-0.624714	2.396407
O	-0.385266	-1.782548	2.466029
C	-0.721729	0.555338	2.839377
H	-0.915271	0.422887	3.910177
H	-0.234695	1.520821	2.691545
H	-1.682630	0.539900	2.318643
C	1.610651	-0.506630	2.814427
H	2.013131	0.499602	2.677088
H	1.659195	-0.765090	3.878364
H	2.224260	-1.227619	2.267020

C	0.947798	0.866549	-2.446698
H	0.718513	0.102218	-3.196328
H	1.978779	1.205630	-2.574068

M6NL2-TS2

SCF energy in gas phase: -1495.621449

SCF energy in solution: -1495.971710

Free energy in solution: -1495.539260

C	-1.180586	0.310872	-0.953032
C	-3.571487	0.072802	-0.584239
C	-2.753221	1.608532	-2.289237
C	-3.791551	1.024513	-1.560806
C	-2.239858	-0.339780	-0.255627
H	-4.820060	1.310855	-1.770549
H	-2.949013	2.325822	-3.079124
P	0.618006	0.252502	-0.732499
C	-0.253088	1.804269	-2.675977
H	-0.075085	2.836902	-2.328922
C	-1.460992	1.240014	-1.974446
C	-3.140004	-1.928809	1.406965
C	-4.740501	-0.529396	0.162981
C	-4.315514	-0.977364	1.558037
H	-3.481651	-2.846947	0.906273
H	-5.553054	0.202589	0.212022
H	-5.138621	-1.472459	2.080434
N	-2.054034	-1.316655	0.658218
H	0.469232	-0.391567	0.922620
H	-1.137703	-1.602411	1.077188
H	-2.714484	-2.220903	2.371669
H	-4.011275	-0.108549	2.153293
H	-5.130554	-1.398522	-0.383785
H	-0.419607	1.840782	-3.758235
N	0.831746	0.896479	-2.345390
H	1.749983	1.290973	-2.521315
C	1.639436	-1.231356	-0.950418
C	2.953218	-1.127944	-1.419966
C	1.096777	-2.485290	-0.660788
C	3.732384	-2.270672	-1.561691
H	3.376368	-0.161180	-1.678836
C	1.877269	-3.625857	-0.826082
H	0.083313	-2.574739	-0.289402
C	3.194288	-3.520438	-1.262528
H	4.755044	-2.185606	-1.914336

H	1.453495	-4.597889	-0.597834	H	-5.487276	0.803848	0.153284
H	3.802029	-4.412619	-1.374817	H	-5.304358	-1.024643	1.912462
C	1.310044	1.659520	0.215182	N	-2.176384	-1.113713	0.580042
C	2.668652	1.746613	0.532594	H	0.400110	-0.410804	1.026359
C	0.452398	2.707537	0.567940	H	-1.288513	-1.622162	0.925442
C	3.159253	2.861153	1.207190	H	-2.997104	-2.058211	2.205756
H	3.342368	0.931352	0.286244	H	-4.039259	0.200243	2.098676
C	0.950757	3.820809	1.239293	H	-5.226304	-0.792500	-0.539486
H	-0.608204	2.641436	0.338511	H	-0.012541	1.938446	-3.626325
C	2.302772	3.900196	1.561441	C	1.470970	-1.317164	-0.934058
H	4.213398	2.912776	1.460437	C	2.862560	-1.401533	-1.044775
H	0.276770	4.624875	1.516899	C	0.680604	-2.465132	-1.005184
H	2.687336	4.766926	2.089019	C	3.461863	-2.640816	-1.227051
C	0.576946	-0.993019	2.150062	H	3.477397	-0.510272	-0.975882
O	-0.031604	-2.120349	2.081319	C	1.292484	-3.702408	-1.190411
C	-0.092367	0.112658	2.973458	H	-0.397960	-2.397879	-0.916399
H	-0.057910	-0.190168	4.026254	C	2.675538	-3.791243	-1.295987
H	0.409532	1.078500	2.867896	H	4.541242	-2.710449	-1.312586
H	-1.141829	0.210499	2.680624	H	0.682255	-4.597658	-1.235448
C	2.090112	-1.066896	2.337362	H	3.146724	-4.759474	-1.431900
H	2.575259	-0.089379	2.304181	C	1.506215	1.576631	0.275193
H	2.260142	-1.503149	3.327833	C	2.740610	2.068884	-0.160430
H	2.532712	-1.737717	1.596885	C	0.873931	2.162893	1.372488

M6OL2-TS2

SCF energy in gas phase: -1515.499265

SCF energy in solution: -1515.853721

Free energy in solution: -1515.430996

C	-1.104176	0.493192	-0.912451	H	3.191074	1.675969	-1.065809
C	-3.510620	0.503657	-0.614623	C	1.492092	3.202440	2.059364
C	-2.474256	2.017038	-2.227686	H	-0.106228	1.808228	1.676006
C	-3.591250	1.520211	-1.544845	C	2.748369	3.653121	1.658605
C	-2.242795	-0.078087	-0.276324	H	4.335391	3.457281	0.217247
H	-4.574717	1.931375	-1.763478	H	0.992888	3.660013	2.907222
H	-2.573647	2.781683	-2.990422	H	3.235753	4.455731	2.202745
P	0.665622	0.269800	-0.686517	C	0.444027	-1.238283	2.017585
C	0.060894	1.900501	-2.536457	O	-0.212714	-2.308955	1.684754
H	0.385950	2.885743	-2.169939	C	-0.205310	-0.401245	3.132867
C	-1.244452	1.489422	-1.898991	H	-0.298439	-1.058917	4.003424
C	-3.347571	-1.652073	1.251595	H	0.390225	0.470077	3.418451
C	-4.757906	-0.008275	0.070550	H	-1.210483	-0.083701	2.838394
C	-4.419068	-0.589921	1.440321	C	1.945632	-1.421945	2.231127
H	-3.769590	-2.491145	0.677979	H	2.496840	-0.475529	2.190344
				H	2.091253	-1.862850	3.223665
				H	2.339378	-2.119442	1.490280
				O	1.020973	0.913391	-2.188023

M7OL2-TS2

SCF energy in gas phase: -1438.095179

SCF energy in solution: -1438.436980

Free energy in solution: -1438.048084

C	-0.705357	-2.365539	0.974320
C	-2.704733	-3.627741	0.373570
C	-2.356609	-1.451921	-0.596786
C	-3.147372	-2.578585	-0.433544
C	-1.100268	-1.354159	0.060129
C	-1.517455	-3.520394	1.062235
C	-1.871265	-0.000218	-2.586963
C	-2.857356	-0.328916	-1.468615
N	0.432648	-2.268822	1.730848
P	-0.070796	0.020377	-0.538929
H	-3.311063	-4.521943	0.483033
H	-4.105074	-2.637056	-0.939956
H	-1.198317	-4.315105	1.730513
H	-2.102211	0.981212	-3.019466
H	-3.817537	-0.604409	-1.912381
H	-3.030561	0.563867	-0.857777
H	0.574941	-3.098061	2.295400
H	0.485710	-1.390547	2.364185
H	0.777092	0.278685	1.051385
H	-1.937911	-0.753692	-3.377962
C	1.666548	-0.214941	-0.983018
C	2.229557	-1.490242	-0.972206
C	2.434115	0.902822	-1.317421
C	3.577195	-1.639261	-1.287761
H	1.630535	-2.349448	-0.688275
C	3.778899	0.741034	-1.631974
H	1.990621	1.895169	-1.318766
C	4.352167	-0.528926	-1.611828
H	4.024124	-2.628006	-1.271567
H	4.379348	1.607213	-1.890118
H	5.403534	-0.652796	-1.850068
C	-0.768306	1.639660	-0.104851
C	-0.808132	2.669243	-1.048820
C	-1.390154	1.790272	1.139685
C	-1.453776	3.863604	-0.737846
H	-0.351032	2.525496	-2.023980
C	-2.061632	2.973882	1.425473
H	-1.305768	1.001427	1.887210
C	-2.089535	4.009710	0.492297

H	-1.475179	4.671224	-1.462373
H	-2.549442	3.093937	2.387258
H	-2.608433	4.933947	0.725814
O	-0.520357	-0.003327	-2.147548
C	1.340410	0.497119	2.206724
O	0.569200	-0.051684	3.092497
C	1.469933	2.022011	2.250630
H	2.214789	2.264834	3.016584
H	1.814442	2.437551	1.297100
H	0.528785	2.489913	2.536306
C	2.720426	-0.151118	2.008670
H	3.310860	0.334555	1.226594
H	3.246237	-0.041774	2.963334
H	2.630377	-1.214393	1.783779

M8OL2-TS2

SCF energy in gas phase: -1515.487203

SCF energy in solution: -1515.842343

Free energy in solution: -1515.420961

C	-2.942258	-1.905081	1.978448
C	-4.170179	-1.585756	1.108887
C	-3.598640	-0.638085	0.083070
C	-2.170882	-0.688831	0.156159
C	-4.238971	0.126513	-0.848030
C	-1.396425	0.067567	-0.764906
C	-2.100858	0.820927	-1.767207
C	-3.482206	0.858354	-1.779103
C	-1.420517	1.543854	-2.915717
H	-2.053839	2.375147	-3.239367
C	-0.029192	2.038729	-2.599089
H	-5.324951	0.156816	-0.881297
H	-2.874660	-2.958598	2.259490
H	-4.546823	-2.488363	0.613715
H	-3.984906	1.440798	-2.544340
H	0.463234	2.446839	-3.485391
N	-1.800274	-1.523846	1.151126
P	0.400574	0.268040	-0.680360
H	-2.951156	-1.314211	2.905733
H	-4.993475	-1.154136	1.682663
H	-1.342070	0.846207	-3.758735
H	-0.046360	2.819063	-1.825991
H	-0.838117	-1.807099	1.542252
H	0.496811	-0.395787	1.010705

C	1.456040	-1.169845	-0.994006	C	-2.423227	0.170290	1.046510
C	2.728364	-1.002695	-1.550677	H	-4.451836	-1.669840	-0.082486
C	0.991563	-2.442900	-0.658018	H	-4.309948	1.131055	1.124562
C	3.550776	-2.108625	-1.728614	H	-4.419905	-0.463630	-2.315012
H	3.058630	-0.018749	-1.865367	N	-1.946180	0.590820	2.223245
C	1.814391	-3.546218	-0.863224	H	-2.641853	0.751498	2.937066
H	0.006238	-2.575448	-0.227464	P	0.007157	-0.010336	-0.500387
C	3.095542	-3.379538	-1.380300	C	-1.631671	0.182574	-2.493460
H	4.542123	-1.980708	-2.151048	H	-1.833008	-0.210994	-3.494358
H	1.455331	-4.534816	-0.598941	H	-1.808241	1.270025	-2.491492
H	3.739477	-4.241859	-1.521761	H	-4.250926	-0.402323	1.981832
C	0.892666	1.747002	0.277340	H	-5.665114	-0.392568	-0.149414
C	2.204167	2.225173	0.235427	H	-3.997714	1.024512	-1.454385
C	-0.075584	2.435209	1.012099	H	-2.413263	-1.572856	-1.591706
C	2.551889	3.362225	0.959877	C	1.073837	-1.487661	-0.566710
H	2.958014	1.707441	-0.350388	C	2.415442	-1.392352	-0.935611
C	0.271242	3.587529	1.710833	C	0.505694	-2.735352	-0.305880
H	-1.096531	2.062609	1.039270	C	3.190993	-2.545940	-1.025182
C	1.586628	4.045511	1.695653	H	2.859144	-0.420930	-1.137207
H	3.576364	3.719544	0.940457	C	1.283988	-3.884776	-0.401300
H	-0.486388	4.121935	2.274715	H	-0.538717	-2.799634	-0.009034
H	1.858351	4.936522	2.252146	C	2.627732	-3.790521	-0.756901
O	0.741049	0.924822	-2.174694	H	4.236946	-2.470436	-1.304750
C	0.953077	-0.971795	2.135033	H	0.842016	-4.854120	-0.193808
O	0.450720	-2.159086	2.181101	H	3.234737	-4.687498	-0.825317
C	2.469247	-0.900619	1.976125	C	0.852916	1.609706	-0.547362
H	2.824178	0.089854	1.677959	C	1.498097	1.998391	-1.729301
H	2.902434	-1.133593	2.955488	C	0.818126	2.480455	0.546561
H	2.810805	-1.656223	1.266520	C	2.124563	3.238379	-1.803630
C	0.408190	0.030539	3.159414	H	1.494331	1.332729	-2.585071
H	0.638615	-0.371690	4.151762	C	1.429676	3.728377	0.452332
H	0.858632	1.021687	3.066632	H	0.360141	2.180185	1.484632
H	-0.679218	0.112383	3.070003	C	2.086256	4.106497	-0.715318
M10OL2-TS2				H	2.634444	3.529411	-2.716485
SCF energy in gas phase: -1401.214381				H	1.398813	4.400259	1.303765
SCF energy in solution: -1401.540980				H	2.567926	5.077425	-0.779046
Free energy in solution: -1401.136198				O	-0.286528	-0.107766	-2.168038
				H	-0.937184	0.728874	2.580025
				H	0.473895	-0.053191	1.202763
C	-1.737033	-0.136437	-0.110479	C	0.991036	-0.091469	2.461747
C	-3.949783	0.096286	1.053693	O	0.428881	0.855083	3.134622
C	-3.926193	-0.071185	-1.419473	C	2.480559	0.080153	2.191121
C	-4.588025	-0.583674	-0.148653	H	2.987041	0.002795	3.159626
C	-2.464476	-0.486668	-1.411071	H	2.881377	-0.687913	1.526997

H	2.683160	1.072895	1.783759
C	0.592480	-1.518257	2.844369
H	1.060729	-2.272718	2.209202
H	0.919038	-1.674714	3.878286
H	-0.494882	-1.628429	2.811461

M11OL2-TS2

SCF energy in gas phase: -1478.603729

SCF energy in solution: -1478.945158

Free energy in solution: -1478.505238

C	1.308731	-0.233672	-0.698867
C	3.710904	-0.730638	-0.122491
C	3.122760	0.443110	-2.300438
C	4.179934	-0.354368	-1.540216
C	2.290352	-0.301169	0.267441
H	5.113264	0.215540	-1.479614
H	3.404699	0.531126	-3.356350
N	2.275485	-0.089579	1.584226
P	-0.445997	0.036827	-0.619153
C	0.654999	0.551251	-2.881729
H	0.621639	0.346335	-3.955493
H	1.432823	0.152467	2.218282
H	-0.472916	-0.164007	1.112223
C	1.756601	-0.217831	-2.160697
H	0.793345	1.634536	-2.730262
C	3.572769	-0.307497	2.211913
C	4.542457	-0.181523	1.038902
H	3.738023	0.427568	3.003186
H	4.769557	0.874498	0.852078
H	3.627720	-1.308409	2.665092
H	5.481316	-0.718950	1.188313
H	4.408099	-1.265362	-2.102665
H	3.051469	1.458251	-1.889854
H	3.689498	-1.827062	-0.034938
H	1.801850	-1.234525	-2.584791
C	-1.132251	1.697350	-0.284332
C	-2.044521	2.251930	-1.190291
C	-0.705751	2.439638	0.821813
C	-2.546619	3.531846	-0.974397
H	-2.341623	1.681286	-2.063793
C	-1.198409	3.727521	1.016929
H	-0.023139	2.006539	1.549394
C	-2.121006	4.271430	0.126168

H	-3.262587	3.954270	-1.672211
H	-0.865758	4.302074	1.875379
H	-2.507605	5.272840	0.288503
C	-1.638539	-1.341808	-0.568835
C	-1.159021	-2.639302	-0.758674
C	-3.002926	-1.122640	-0.382326
C	-2.040353	-3.714971	-0.737264
H	-0.094578	-2.803155	-0.908351
C	-3.882052	-2.203530	-0.363616
H	-3.379830	-0.112802	-0.242904
C	-3.402251	-3.498982	-0.535073
H	-1.663744	-4.723120	-0.877720
H	-4.943102	-2.030399	-0.214618
H	-4.088525	-4.339374	-0.516368
O	-0.564343	0.122753	-2.308979
C	-0.618428	-0.337058	2.476799
O	0.249024	0.417962	3.054211
C	-0.373023	-1.846249	2.532763
H	-0.436292	-2.144457	3.585132
H	-1.112768	-2.410123	1.960065
H	0.630456	-2.086084	2.170582
C	-2.075411	0.052762	2.686401
H	-2.763273	-0.547234	2.088781
H	-2.293933	-0.121822	3.745911
H	-2.223647	1.114894	2.483554

M12NL2-TS2

SCF energy in gas phase: -1498.017257

SCF energy in solution: -1498.364096

Free energy in solution: -1497.883980

C	-0.940422	-1.134077	-0.268723
C	-3.412355	-1.190305	0.159011
C	-2.429744	-2.936970	-1.329029
C	-3.512028	-1.876789	-1.198853
C	-2.025438	-0.579710	0.375883
H	-4.506499	-2.323338	-1.306823
H	-2.512348	-3.473064	-2.282212
P	0.596881	-0.253087	-0.603426
C	-0.500356	-1.774853	-2.547399
C	-1.035258	-2.319853	-1.217866
C	-3.065100	1.290454	1.683604
C	-4.537138	-0.173108	0.357920
C	-4.383199	0.537490	1.695762

H	-2.791187	1.656668	2.676680	H	1.152702	-1.771067	2.479211
H	-4.509311	0.564778	-0.455919	H	0.638512	-1.082595	4.032842
H	-4.385384	-0.199129	2.508131	H	-0.537922	-1.234627	2.714935
N	-1.960684	0.454972	1.237127	N	0.648495	-0.934687	-2.234041
H	-0.210604	-2.578231	-3.233715	H	1.534375	-1.371549	-2.452484
H	0.736155	0.195487	1.075981	M12OL2-TS2			
H	-1.075523	0.770741	1.652339	SCF energy in gas phase: -1517.896101			
H	-1.285909	-1.182574	-3.039817	SCF energy in solution: -1518.248087			
H	-0.335823	-3.106435	-0.893228	Free energy in solution: -1517.779450			
H	-3.154716	2.167223	1.024144	C	-0.982855	-0.991315	-0.423351
H	-5.206107	1.235117	1.876874	C	-3.460543	-1.081359	-0.109256
H	-5.498785	-0.692274	0.287059	C	-2.455933	-2.562719	-1.843314
H	-3.525624	-1.959186	0.939833	C	-3.518430	-1.510051	-1.572306
H	-3.410622	-1.121869	-1.989006	C	-2.088406	-0.496339	0.244171
H	-2.569187	-3.679825	-0.535157	H	-4.516264	-1.903215	-1.795543
C	2.323822	-0.755143	-0.241645	H	-2.491778	-2.907019	-2.883980
C	2.594152	-2.037480	0.243337	P	0.597673	-0.173354	-0.595403
C	3.371945	0.138410	-0.467245	C	-0.417215	-1.315513	-2.725388
C	3.902109	-2.406689	0.542828	C	-1.055946	-2.029131	-1.537213
H	1.780285	-2.741726	0.401122	C	-3.199026	1.131329	1.788715
C	4.680549	-0.240751	-0.176862	C	-4.619624	-0.153658	0.252147
H	3.163934	1.134309	-0.849272	C	-4.481658	0.327742	1.688821
C	4.946798	-1.506480	0.337684	H	-2.928317	1.351580	2.825016
H	4.106055	-3.398264	0.934668	H	-4.625098	0.710723	-0.426337
H	5.492226	0.459472	-0.346939	H	-4.439552	-0.533889	2.365896
H	5.966207	-1.794893	0.572580	N	-2.057559	0.434201	1.210695
C	0.466878	1.532884	-1.011606	H	-0.086903	-2.010066	-3.505201
C	0.410647	1.914569	-2.358641	H	0.655714	0.136363	1.140951
C	0.406572	2.516796	-0.014965	H	-1.189049	0.733052	1.711095
C	0.303069	3.257850	-2.704658	H	-1.128867	-0.598096	-3.163381
H	0.461536	1.146019	-3.120896	H	-0.403466	-2.881232	-1.295609
C	0.296396	3.858791	-0.374194	H	-3.338539	2.095467	1.277177
H	0.424204	2.262365	1.041236	H	-5.331808	0.946509	1.989857
C	0.246800	4.233377	-1.713318	H	-5.560962	-0.690252	0.094114
H	0.266427	3.540749	-3.752100	H	-3.562989	-1.986209	0.511098
H	0.246719	4.612151	0.405635	H	-3.367147	-0.630132	-2.210622
H	0.163775	5.281676	-1.984033	H	-2.662616	-3.437103	-1.216199
C	0.867364	0.400443	2.521507	C	2.199508	-0.936674	-0.184945
O	0.053815	1.329301	2.826591	C	2.245136	-2.243985	0.301195
C	2.355102	0.727737	2.606537	C	3.381090	-0.217970	-0.368897
H	2.565727	0.949435	3.658830	C	3.467951	-2.817763	0.635057
H	2.998127	-0.094011	2.283241	H	1.323114	-2.803923	0.437732
H	2.583316	1.623936	2.023592				
C	0.508312	-1.022523	2.945887				

C	4.602228	-0.798640	-0.037049	H	-4.141856	-0.945410	1.543229
H	3.346920	0.797769	-0.753145	H	-3.703999	-2.424857	-1.094469
C	4.647295	-2.093303	0.472892	H	-2.734987	-2.761156	2.453526
H	3.500176	-3.831014	1.022803	H	-1.762324	1.541510	-2.369505
H	5.519885	-0.234966	-0.171669	H	-0.697179	-2.582686	2.698642
H	5.599727	-2.540403	0.738724	H	-0.013976	-1.044369	2.469947
C	0.705170	1.634479	-0.868375	H	0.836842	0.096964	1.013166
C	0.988996	2.095547	-2.163194	H	-1.371660	0.589221	-3.817412
C	0.510768	2.558078	0.166914	C	1.595869	-0.836605	-0.892210
C	1.086220	3.460129	-2.413951	C	1.679081	-2.207003	-0.648166
H	1.137269	1.379755	-2.961804	C	2.708813	-0.129809	-1.351173
C	0.600364	3.922634	-0.102348	C	2.886856	-2.867071	-0.855527
H	0.286670	2.242322	1.183316	H	0.812635	-2.742366	-0.271260
C	0.890063	4.376944	-1.384624	C	3.915310	-0.795776	-1.542767
H	1.315990	3.805103	-3.417087	H	2.639454	0.936155	-1.550557
H	0.443824	4.631360	0.704481	C	4.006278	-2.163726	-1.292399
H	0.963648	5.441939	-1.582845	H	2.955873	-3.933050	-0.663477
O	0.722599	-0.642230	-2.226174	H	4.784225	-0.246586	-1.891271
C	0.716616	0.280945	2.507927	H	4.948960	-2.680099	-1.441525
O	-0.127347	1.199221	2.825362	C	-0.142615	1.819032	-0.214631
C	2.193504	0.621068	2.685580	C	0.297570	2.781160	-1.126785
H	2.351575	0.801649	3.754440	C	-0.790179	2.209950	0.961796
H	2.858971	-0.181892	2.359208	C	0.114819	4.133603	-0.849199
H	2.438997	1.541555	2.148705	H	0.759537	2.466266	-2.058187
C	0.347873	-1.143247	2.926342	C	-0.998723	3.561536	1.215735
H	1.061379	-1.886818	2.567592	H	-1.073782	1.460053	1.697266
H	0.344124	-1.163281	4.021717	C	-0.539701	4.522954	0.316791
H	-0.657710	-1.394033	2.578887	H	0.470732	4.881320	-1.550750
M13OL2-TS2				H	-1.503417	3.864512	2.127311
SCF energy in gas phase: -1440.493861				H	-0.693957	5.577037	0.524790
SCF energy in solution: -1440.833392				O	-0.233342	0.143832	-2.208714
Free energy in solution: -1440.397398				C	1.512162	0.308731	2.182557
				O	0.614763	0.221716	3.098400
				C	2.160798	1.670679	1.944702
C	-1.469141	-1.702462	1.098044	H	2.950209	1.788034	2.695712
C	-3.990495	-1.853681	0.947262	H	2.623074	1.740413	0.954558
C	-2.702277	-0.542567	-0.801410	H	1.441298	2.477816	2.075942
C	-3.863896	-1.501067	-0.521249	C	2.546008	-0.823110	2.125701
C	-1.421439	-0.883760	-0.006497	H	3.249412	-0.723391	1.294874
C	-2.707369	-2.542308	1.382065	H	3.103706	-0.766763	3.067114
C	-1.489051	0.538776	-2.731050	H	2.061103	-1.799337	2.073162
C	-2.528847	-0.476592	-2.322891	H	-2.607319	-3.502879	0.859567
N	-0.462859	-1.895150	1.995193	H	-4.850750	-2.506737	1.123052
P	0.037125	0.034916	-0.553559	H	-4.784441	-1.045842	-0.902702

H	-3.021341	0.464023	-0.478279
H	-2.227491	-1.461186	-2.700280
H	-3.495792	-0.223993	-2.774830

M15OL2-TS2

SCF energy in gas phase: -1557.183337

SCF energy in solution: -1557.545790

Free energy in solution: -1557.049081

C	-4.176530	-1.822960	-1.432333
C	-4.453324	-0.443913	-0.858315
C	-3.553474	-0.188294	0.349214
C	-2.067571	-0.445680	0.060460
C	-2.741924	-1.836532	-1.916214
C	-3.764393	1.210759	0.914201
C	-1.127134	0.197044	0.857637
C	-1.511988	1.099404	2.049214
C	-3.019487	1.321984	2.228142
C	-0.928800	0.590860	3.380167
H	-1.491298	-0.291653	3.705486
C	0.554305	0.234063	3.235325
H	-3.403558	1.956561	0.193641
H	-4.323444	-2.583016	-0.655529
H	-4.265894	0.319852	-1.626086
H	-2.661361	-1.235505	-2.834259
H	-3.181005	2.293318	2.706927
H	0.685599	-0.850023	3.118075
N	-1.802891	-1.321317	-0.922110
P	0.646716	0.283026	0.614934
H	1.141971	0.545849	4.101937
H	-1.072887	1.368157	4.139694
H	-1.061753	2.085333	1.867719
H	-2.402066	-2.841788	-2.177848
H	-4.848358	-2.061367	-2.261869
H	-0.842607	-1.571031	-1.289435
H	0.572070	-0.251459	-1.096725
H	-5.496993	-0.335623	-0.545430
H	-3.843872	-0.910866	1.128069
H	-4.836150	1.388164	1.056265
H	-3.424830	0.564793	2.911916
C	1.224709	1.795894	-0.235625
C	0.256481	2.621958	-0.809918
C	2.571367	2.157509	-0.304365
C	0.632455	3.798198	-1.451223

H	-0.789669	2.328375	-0.765719
C	2.944767	3.323673	-0.966817
H	3.334146	1.527191	0.140032
C	1.977668	4.146323	-1.538556
H	-0.125821	4.437270	-1.892263
H	3.994570	3.591404	-1.030654
H	2.272142	5.056935	-2.050160
C	1.668540	-1.220600	0.743721
C	1.140357	-2.477605	0.440575
C	2.995973	-1.106711	1.173907
C	1.953735	-3.604926	0.524654
H	0.103975	-2.585484	0.147385
C	3.807146	-2.233844	1.234816
H	3.379150	-0.142984	1.491921
C	3.287696	-3.483177	0.899738
H	1.540666	-4.578904	0.284974
H	4.838909	-2.139791	1.557847
H	3.919962	-4.364134	0.947518
O	1.095016	0.909156	2.106555
C	0.824023	-0.808971	-2.279836
O	0.277965	-1.978265	-2.278285
C	2.349182	-0.786411	-2.344276
H	2.631533	-1.034185	-3.373836
H	2.773541	0.191251	-2.099237
H	2.761973	-1.554422	-1.686890
C	0.166406	0.253047	-3.170178
H	0.651984	1.229235	-3.091475
H	0.237209	-0.097687	-4.205549
H	-0.893292	0.356391	-2.916530

M4NL3-TS2

SCF energy in gas phase: -1417.039747

SCF energy in solution: -1417.374330

Free energy in solution: -1416.995767

C	-2.010532	-0.146296	-0.384116
C	-4.163236	-0.847009	0.434746
C	-4.050620	0.812815	-1.321819
C	-4.786438	0.035012	-0.420554
C	-2.675257	0.692580	-1.300330
C	-2.750136	-0.997649	0.478727
H	-5.870424	0.101853	-0.409059
H	-4.759293	-1.472165	1.093547
H	-4.539114	1.466275	-2.036611

N	-2.229272	-1.962623	1.266918	M4OL3-TS2			
P	-0.227240	0.088553	-0.582000	SCF energy in gas phase: -1436.919464			
C	-1.756088	1.395549	-2.268185	SCF energy in solution: -1437.256891			
H	-1.618764	2.446398	-1.957614	Free energy in solution: -1436.890078			
H	-1.223478	-2.098539	1.573182				
H	0.004860	-0.390094	1.071078	C	-2.004105	-0.109416	-0.375078
C	1.045455	-1.139945	-0.897613	C	-4.204174	-0.730064	0.379385
C	2.336563	-0.670567	-1.185285	C	-3.981725	0.859355	-1.436259
C	0.785321	-2.500758	-0.738020	C	-4.769885	0.125143	-0.536847
C	3.354504	-1.610745	-1.343338	C	-2.615171	0.712369	-1.346125
C	1.815816	-3.419558	-0.905368	C	-2.792759	-0.910978	0.498050
C	3.097516	-2.972806	-1.210208	H	-5.852055	0.209637	-0.577202
C	0.623630	1.574497	0.025537	H	-4.841199	-1.314286	1.037327
C	1.954945	1.760368	-0.377219	H	-4.428142	1.495019	-2.193027
C	-0.007432	2.493741	0.862862	N	-2.321736	-1.824295	1.360320
C	2.639847	2.875144	0.109016	P	-0.228800	0.104396	-0.557431
C	0.685694	3.610397	1.319148	C	-1.623079	1.370574	-2.274429
C	2.014948	3.793902	0.947282	H	-1.482008	2.430795	-2.013785
H	-0.211976	-2.835573	-0.469734	H	-1.288180	-2.053674	1.669981
H	1.620073	-4.478547	-0.778547	H	0.009093	-0.405608	1.140842
H	3.906482	-3.686148	-1.330512	C	1.008475	-1.141330	-0.893111
H	4.362507	-1.269339	-1.563663	C	2.281267	-0.662425	-1.245611
H	3.679064	3.022924	-0.173181	C	0.759271	-2.497989	-0.695392
H	2.568695	4.653014	1.311943	C	3.300220	-1.595738	-1.420121
H	0.195084	4.326526	1.970092	C	1.793293	-3.410481	-0.883431
H	-1.036594	2.318097	1.168480	C	3.057927	-2.957341	-1.243994
H	-2.895890	-2.456583	1.840841	C	0.638870	1.561320	0.070274
H	-2.192303	1.398964	-3.272772	C	1.946069	1.745311	-0.407106
C	0.473036	-0.980369	2.253729	C	0.068845	2.445639	0.982824
O	0.199568	-2.224844	2.186858	C	2.674568	2.828714	0.082668
C	-0.341496	-0.116662	3.224134	C	0.804963	3.533893	1.441644
H	-0.063314	-0.414148	4.241811	C	2.111373	3.716652	0.996243
H	-0.128190	0.948427	3.102816	H	-0.220622	-2.832697	-0.372647
H	-1.410415	-0.297732	3.095612	H	1.613362	-4.468403	-0.728531
C	1.950658	-0.608554	2.211729	H	3.868097	-3.666917	-1.378732
H	2.121946	0.458966	2.047623	H	4.295067	-1.252739	-1.690313
H	2.370654	-0.879172	3.187364	H	3.694985	2.979297	-0.259082
H	2.462536	-1.200740	1.450463	H	2.697062	4.554052	1.361696
C	2.652647	0.807599	-1.334216	H	0.365850	4.228121	2.150278
H	3.733154	0.942638	-1.230863	H	-0.942568	2.268781	1.341601
H	2.421164	1.114710	-2.366036	H	-3.030689	-2.297932	1.901607
N	-0.524534	0.620597	-2.230891	H	-1.944514	1.308744	-3.317411
H	0.256175	1.100497	-2.667148	C	0.428408	-1.008957	2.215946
				O	0.048021	-2.247081	2.153515

C	-0.263485	-0.131085	3.268591	H	-4.400966	1.990572	-1.483577
H	0.001243	-0.531799	4.253213	H	-0.923475	4.505014	-1.279761
H	0.063359	0.910999	3.217283	H	-3.371299	4.234661	-1.575941
H	-1.349008	-0.184498	3.159053	C	-1.317906	-1.429958	0.301842
C	1.936853	-0.786366	2.167211	C	-2.682888	-1.333079	-0.011194
H	2.208737	0.258466	1.985896	C	-0.858212	-2.313942	1.274433
H	2.335878	-1.081947	3.143937	C	-3.575732	-2.130975	0.703582
H	2.387420	-1.432841	1.411054	C	-1.763216	-3.118325	1.960319
C	2.545382	0.818220	-1.449559	H	0.204741	-2.356438	1.500275
H	3.624863	0.984308	-1.497287	C	-3.122929	-3.016684	1.678799
H	2.130520	1.104345	-2.425201	H	-4.638892	-2.058712	0.490914
O	-0.403122	0.665178	-2.135511	H	-1.409632	-3.811284	2.716444

M5OL3-TS2

SCF energy in gas phase: -1514.308478

SCF energy in solution: -1514.660619

Free energy in solution: -1514.260044

C	1.560386	-0.517509	-0.654565
C	3.944630	-0.313761	-0.229527
C	3.166250	-1.934159	-1.842519
C	4.213127	-1.318248	-1.119399
C	2.610248	0.138328	0.024645
H	5.240824	-1.631380	-1.285502
H	3.375615	-2.697877	-2.583925
N	2.602159	1.168869	0.881727
P	-0.216716	-0.329629	-0.618793
C	0.654636	-2.044457	-2.319562
C	4.872529	0.471390	0.667959
C	1.876908	-1.521458	-1.604330
C	3.963372	1.611447	1.179477
H	5.215672	-0.156436	1.498351
H	0.359337	-3.028581	-1.924787
H	0.821879	-2.139091	-3.395865
H	5.758590	0.844823	0.149349
H	1.735669	1.739311	1.243003
H	-0.081440	0.439650	0.983674
C	-1.160900	1.137580	-1.013540
C	-2.545833	0.962180	-1.162339
C	-0.570354	2.399123	-1.043650
C	-3.325763	2.097565	-1.368620
C	-1.370287	3.517246	-1.258276
H	0.494515	2.507515	-0.868519
C	-2.743371	3.363039	-1.419967

H	-4.400966	1.990572	-1.483577
H	-0.923475	4.505014	-1.279761
H	-3.371299	4.234661	-1.575941
C	-1.317906	-1.429958	0.301842
C	-2.682888	-1.333079	-0.011194
C	-0.858212	-2.313942	1.274433
C	-3.575732	-2.130975	0.703582
C	-1.763216	-3.118325	1.960319
H	0.204741	-2.356438	1.500275
C	-3.122929	-3.016684	1.678799
H	-4.638892	-2.058712	0.490914
H	-1.409632	-3.811284	2.716444
H	-3.836247	-3.628426	2.221664
H	4.176918	2.552234	0.654778
H	4.081609	1.796847	2.250394
O	-0.383885	-1.103612	-2.107112
C	-3.177429	-0.417095	-1.117202
C	-0.174887	1.260315	2.006352
O	0.507751	2.327445	1.737591
C	0.385112	0.340872	3.101319
H	0.358782	0.901308	4.042291
H	-0.210346	-0.568153	3.220502
H	1.423877	0.077550	2.889240
C	-1.682792	1.459567	2.128013
H	-2.239422	0.517378	2.098289
H	-1.867078	1.937694	3.096589
H	-2.037715	2.133736	1.346043
H	-4.262502	-0.310716	-1.034916
H	-2.972515	-0.913506	-2.075321

M6CL3-TS2

SCF energy in gas phase: -1517.687390

SCF energy in solution: -1518.034486

Free energy in solution: -1517.580078

C	1.379732	-0.683782	-0.818032
C	3.771766	-0.510508	-0.431629
C	2.868438	-2.393725	-1.689053
C	3.934849	-1.710701	-1.098895
C	2.470945	0.057821	-0.290136
H	4.940901	-2.117168	-1.179962
H	3.029210	-3.309519	-2.248289
P	-0.409745	-0.378853	-0.684288
C	0.362037	-2.484143	-2.169396

H	-0.034666	-3.271274	-1.513793	H	-2.237920	1.811762	1.470082
C	1.597189	-1.867460	-1.551673	C	-3.470731	-0.257666	-0.847459
C	3.414567	1.982657	0.951548	H	-4.500973	-0.023211	-0.564306
C	4.954666	0.213176	0.168743	H	-3.541402	-0.785370	-1.809439
C	4.516203	1.027235	1.384318	C	-0.650596	-1.349540	-2.293095
H	3.841238	2.745947	0.285018	H	-0.391860	-0.694578	-3.131939
H	5.728335	-0.513742	0.435993	H	-1.675261	-1.704508	-2.422274
H	5.353609	1.589920	1.805931				
N	2.330585	1.279784	0.279950	M6NL3-TS2			
H	-0.142356	0.386914	0.845725	SCF energy in gas phase: -1533.729709			
H	1.416757	1.662078	0.563579	SCF energy in solution: -1534.088075			
H	2.960645	2.502372	1.800969	Free energy in solution: -1533.646003			
H	4.138638	0.353406	2.162613				
H	5.399769	0.892630	-0.570834	C	-1.373775	0.620731	-0.839471
H	0.603467	-2.953769	-3.127507	C	-3.763610	0.475365	-0.450449
C	-1.324693	1.129734	-1.076005	C	-2.853555	2.305180	-1.781391
C	-2.726515	1.047433	-1.068827	C	-3.920515	1.653650	-1.155345
C	-0.675072	2.346813	-1.281301	C	-2.467204	-0.108100	-0.297399
C	-3.453431	2.217642	-1.288626	H	-4.923778	2.065207	-1.243871
C	-1.420875	3.498499	-1.509561	H	-3.010379	3.193824	-2.383613
H	0.409276	2.395922	-1.253801	P	0.411678	0.366095	-0.703148
C	-2.809868	3.431654	-1.511824	C	-0.348479	2.324329	-2.272170
H	-4.539384	2.175537	-1.278809	H	-0.014447	3.226534	-1.730980
H	-0.917008	4.446026	-1.665260	C	-1.591409	1.769548	-1.622444
H	-3.397096	4.329359	-1.676945	C	-3.435749	-1.998445	0.962978
C	-1.514559	-1.412304	0.328845	C	-4.953978	-0.215793	0.174310
C	-2.893727	-1.209793	0.185091	C	-4.520985	-1.024286	1.394975
C	-1.012342	-2.314948	1.265330	H	-3.874327	-2.754230	0.295293
C	-3.752682	-1.924096	1.023119	H	-5.709045	0.531054	0.440164
C	-1.885114	-3.033000	2.075912	H	-5.364696	-1.569718	1.826540
H	0.064245	-2.436439	1.366364	N	-2.337713	-1.314505	0.296519
C	-3.258150	-2.828622	1.957754	H	0.169535	-0.459876	0.833632
H	-4.824709	-1.764160	0.942261	H	-1.426198	-1.738603	0.577543
H	-1.496305	-3.738724	2.802527	H	-2.993084	-2.527619	1.812782
H	-3.945809	-3.372279	2.597474	H	-4.127697	-0.349927	2.165048
C	-0.205487	1.310561	1.988503	H	-5.421462	-0.894370	-0.552062
O	0.296737	2.407945	1.603500	H	-0.556668	2.613115	-3.307921
C	0.610831	0.432382	2.942439	N	0.613473	1.233427	-2.213553
H	0.652244	0.945762	3.910675	H	1.563901	1.528984	-2.411199
H	0.156318	-0.551134	3.087916	C	1.401069	-1.087974	-1.073673
H	1.632602	0.314709	2.574135	C	2.796799	-0.945306	-1.018979
C	-1.704142	1.288100	2.266315	C	0.807297	-2.331151	-1.290080
H	-2.103263	0.278811	2.396276	C	3.579107	-2.082422	-1.216860
H	-1.860492	1.844966	3.197840	C	1.608470	-3.450246	-1.488868

H	-0.274274	-2.423787	-1.291347	C	1.539916	-1.751655	-1.635046
C	2.993078	-3.323237	-1.453611	C	3.517608	1.918477	0.982135
H	4.661547	-1.994862	-1.174692	C	4.982831	0.136208	0.107297
H	1.150370	-4.419567	-1.651275	C	4.605406	0.924366	1.358330
H	3.622751	-4.195646	-1.596542	H	3.937435	2.671336	0.298742
C	1.427149	1.423341	0.370235	H	5.731077	-0.631063	0.330429
C	2.820476	1.310077	0.253476	H	5.471808	1.450009	1.769041
C	0.852899	2.307250	1.283186	N	2.375372	1.259670	0.367316
C	3.617304	2.087814	1.095810	H	-0.172675	0.482742	0.903059
C	1.664141	3.088884	2.099685	H	1.467219	1.748069	0.685759
H	-0.230614	2.363229	1.362463	H	3.128106	2.452814	1.854677
C	3.048856	2.970712	2.009448	H	4.229200	0.241682	2.129457
H	4.698716	1.996402	1.034852	H	5.440160	0.822687	-0.618004
H	1.218800	3.778017	2.809597	H	0.368556	-2.481657	-3.304123
H	3.688707	3.565209	2.653419	C	-1.379013	1.074226	-1.075894
C	0.223300	-1.360986	1.894068	C	-2.773347	0.900372	-1.090042
O	-0.307335	-2.453845	1.497381	C	-0.791987	2.326534	-1.246377
C	-0.560452	-0.511429	2.903212	C	-3.566059	2.025195	-1.301747
H	-0.595220	-1.068487	3.846639	C	-1.606574	3.434070	-1.462545
H	-0.083843	0.455558	3.085873	H	0.285714	2.437305	-1.192628
H	-1.586031	-0.355809	2.559576	C	-2.988255	3.280564	-1.488083
C	1.720728	-1.401156	2.182207	H	-4.647194	1.918637	-1.314557
H	2.164061	-0.408956	2.305365	H	-1.160912	4.414032	-1.591227
H	1.846842	-1.953620	3.120461	H	-3.626261	4.144754	-1.644334
H	2.235059	-1.955723	1.394620	C	-1.435080	-1.403101	0.412069
C	3.473036	0.391420	-0.765768	C	-2.821464	-1.311997	0.215413
H	4.504315	0.203403	-0.453255	C	-0.894600	-2.215262	1.405654
H	3.556353	0.930542	-1.722204	C	-3.651604	-2.041192	1.066532
M6OL3-TS2				C	-1.739450	-2.950829	2.231121
SCF energy in gas phase: -1553.609167				H	0.184178	-2.252837	1.539097
SCF energy in solution: -1553.970761				C	-3.118501	-2.853822	2.064169
Free energy in solution: -1553.540230				H	-4.729137	-1.970646	0.944927
				H	-1.324465	-3.587641	3.005199
				H	-3.783684	-3.412830	2.714438
C	1.358762	-0.618575	-0.816922	C	-0.208366	1.354765	1.858445
C	3.760147	-0.516171	-0.496918	O	0.387406	2.431482	1.445264
C	2.784751	-2.298874	-1.852268	C	0.514979	0.552894	2.951623
C	3.878793	-1.671785	-1.241002	H	0.560386	1.183797	3.846081
C	2.474580	0.085896	-0.278994	H	-0.009822	-0.372714	3.203972
H	4.874188	-2.090572	-1.374066	H	1.538292	0.321723	2.643467
H	2.913627	-3.171551	-2.483364	C	-1.703179	1.497318	2.133055
P	-0.415638	-0.376424	-0.673780	H	-2.202496	0.535637	2.289568
C	0.255887	-2.266999	-2.238169	H	-1.806590	2.093670	3.046359
H	-0.080950	-3.182877	-1.729291	H	-2.182611	2.045091	1.318554

O	-0.709628	-1.240471	-2.085053
C	-3.405245	-0.467137	-0.902265
H	-4.478518	-0.344103	-0.734774
H	-3.285492	-1.025820	-1.840078

M10OL3-TS2

SCF energy in gas phase: -1439.322460

SCF energy in solution: -1439.658147

Free energy in solution: -1439.244214

C	-1.941791	-0.249735	-0.182864
C	-4.224276	0.257369	0.723234
C	-4.034326	-0.656456	-1.575766
C	-4.761320	-0.788696	-0.243902
C	-2.563603	-0.981343	-1.370547
C	-2.704744	0.389316	0.771140
H	-4.597272	-1.794295	0.161389
H	-4.617783	1.246183	0.453254
H	-4.462235	-1.321475	-2.333317
N	-2.298356	1.194926	1.760560
H	-3.028058	1.546312	2.363243
P	-0.176584	-0.201875	-0.450201
C	-1.678434	-0.581793	-2.544939
H	-1.787144	-1.248064	-3.406656
H	-1.916519	0.447387	-2.857057
H	-4.569596	0.053622	1.743411
H	-5.841312	-0.659760	-0.361107
H	-4.135058	0.373560	-1.944628
H	-2.463518	-2.070404	-1.237340
C	1.041094	-1.509771	-0.138441
C	2.295350	-1.356743	-0.747062
C	0.773254	-2.586651	0.701348
C	3.280594	-2.303595	-0.465416
C	1.762274	-3.532005	0.954981
H	-0.206894	-2.673682	1.164496
C	3.020035	-3.381994	0.376192
H	4.264744	-2.192782	-0.912894
H	1.555406	-4.374608	1.606622
H	3.802141	-4.106180	0.580463
C	0.770720	1.303631	-0.729497
C	2.058246	1.146639	-1.270529
C	0.293955	2.553853	-0.341954
C	2.850205	2.283033	-1.417294
C	1.097935	3.677784	-0.509391

H	-0.691203	2.644029	0.104157
C	2.374720	3.538920	-1.042708
H	3.851729	2.183051	-1.827126
H	0.734184	4.653044	-0.204960
H	3.011172	4.410318	-1.161176
O	-0.347186	-0.668350	-2.081660
H	-1.303514	1.506181	2.048343
H	0.110375	0.135947	1.219128
C	0.588669	0.671923	2.403924
O	0.060934	1.833503	2.528444
C	2.094356	0.636879	2.180656
H	2.559222	0.900237	3.137648
H	2.459719	-0.348205	1.878240
H	2.383067	1.392576	1.447060
C	0.082075	-0.432522	3.338035
H	0.513848	-1.406591	3.096957
H	0.382249	-0.160526	4.356337
H	-1.008013	-0.490738	3.306257
C	2.572280	-0.213327	-1.705563
H	2.094980	-0.462770	-2.662245
H	3.648952	-0.148257	-1.885498

M12OL3-TS2

SCF energy in gas phase: -1556.003438

SCF energy in solution: -1556.364231

Free energy in solution: -1555.887515

C	-1.293812	-0.911675	-0.299631
C	-3.763402	-0.765833	-0.081320
C	-2.832927	-2.711810	-1.334824
C	-3.808219	-1.546448	-1.394124
C	-2.371436	-0.164793	0.135891
H	-4.827406	-1.909460	-1.566715
H	-2.841956	-3.285103	-2.269699
P	0.408543	-0.426394	-0.467355
C	-0.582729	-2.006678	-2.312651
C	-1.405211	-2.238028	-1.044437
C	-3.416834	1.887650	1.117256
C	-4.885312	0.266917	0.004003
C	-4.717480	1.119833	1.252610
H	-3.125267	2.380974	2.049369
H	-4.862568	0.910964	-0.885950
H	-4.684995	0.475513	2.139658
N	-2.300376	1.032416	0.735912

H	-0.276077	-2.948339	-2.782265	H	3.039492	-0.806910	-2.197366
H	0.353039	0.422507	1.022289				
H	-1.399924	1.513275	1.013207	M16			
H	-1.172251	-1.424807	-3.038240	SCF energy in gas phase:	-1229.802325		
H	-0.887290	-3.022791	-0.472434	SCF energy in solution:	-1230.079327		
H	-3.546516	2.679108	0.363796	Free energy in solution:	-1229.815026		
H	-5.548056	1.819757	1.380330				
H	-5.847012	-0.256277	-0.003755	C	-1.475791	-1.182198	-0.593530
H	-3.914432	-1.482555	0.741113	C	-2.912874	-1.610597	1.312373
H	-3.559348	-0.870299	-2.221780	C	-3.571141	-2.204434	-0.982908
H	-3.160935	-3.396232	-0.544791	C	-3.821422	-2.144499	0.392341
C	1.752664	-1.302291	0.373330	C	-2.373821	-1.698199	-1.504471
C	1.518373	-2.134585	1.464885	C	-1.702064	-1.154477	0.789948
C	3.053527	-1.063956	-0.090446	H	-4.769205	-2.524976	0.763177
C	2.587464	-2.739023	2.119133	H	-2.166183	-1.691010	-2.569649
H	0.497390	-2.291475	1.806403	H	-3.144690	-1.566335	2.370879
C	4.114919	-1.660625	0.590606	H	-4.318564	-2.625299	-1.645952
C	3.887320	-2.491352	1.684837	N	-0.537033	-0.611549	1.287885
H	2.407889	-3.390849	2.967896	P	0.043409	-0.224730	-0.477698
H	5.131990	-1.472208	0.257071	C	1.764472	-0.780503	-0.220441
H	4.727646	-2.946133	2.199522	C	2.138723	-1.520159	0.905943
C	1.120489	1.109860	-1.090158	C	2.741698	-0.411764	-1.154822
C	2.495239	1.081299	-1.384071	C	3.468578	-1.888752	1.091130
C	0.386338	2.290113	-1.186284	H	1.378577	-1.809970	1.621769
C	3.107641	2.269746	-1.775807	C	4.071300	-0.765154	-0.953700
C	1.016713	3.462600	-1.594225	H	2.452559	0.146154	-2.037042
H	-0.668792	2.296650	-0.935983	C	4.436569	-1.506644	0.167923
C	2.376534	3.451368	-1.882095	H	3.746799	-2.473930	1.961668
H	4.170684	2.268600	-2.001446	H	4.822129	-0.466596	-1.678257
H	0.448319	4.383420	-1.666934	H	5.474196	-1.787706	0.319480
H	2.875759	4.366176	-2.185704	C	-0.158280	1.563573	-0.250977
O	0.574849	-1.288153	-1.935972	C	-1.344601	2.177352	-0.659675
C	0.442518	1.368252	2.034717	C	0.834374	2.318429	0.377064
O	-0.285145	2.363290	1.691412	C	-1.537235	3.536480	-0.430973
C	1.948035	1.597774	2.072226	H	-2.115643	1.592085	-1.152739
H	2.157910	2.220290	2.949612	C	0.639394	3.679656	0.595409
H	2.517465	0.668091	2.161160	H	1.760399	1.845309	0.693929
H	2.261380	2.150233	1.183266	C	-0.546492	4.289027	0.195031
C	-0.082160	0.477108	3.165339	H	-2.461595	4.009098	-0.747484
H	0.535070	-0.412123	3.314201	H	1.415695	4.262838	1.080349
H	-0.068247	1.071216	4.086187	H	-0.698293	5.349502	0.368760
H	-1.115710	0.182261	2.964375	F	0.250453	-0.102673	-2.129648
C	3.297858	-0.205175	-1.315969	C	-0.500398	0.169543	2.501333
H	4.362968	0.032930	-1.383710	H	-1.078242	1.104325	2.433365

H	-0.887529	-0.417493	3.342617
H	0.537670	0.429774	2.730247

M16-TS

SCF energy in gas phase: -1230.925271

SCF energy in solution: -1231.203733

Free energy in solution: -1230.924633

C	-1.125526	-1.077843	-0.410864
C	-3.326658	-1.773054	0.362259
C	-2.095322	-3.151515	-1.222750
C	-3.238182	-2.883627	-0.435011
C	-1.058888	-2.250621	-1.201832
C	-2.266955	-0.801409	0.433428
H	-4.073035	-3.579333	-0.460624
H	-0.183499	-2.421751	-1.823625
H	-4.220275	-1.605787	0.952449
H	-2.049009	-4.034802	-1.848394
N	-2.254594	0.272113	1.205858
P	0.281050	-0.049571	-0.476453
H	-0.793557	0.233825	1.660802
H	0.034360	0.046542	1.649603
C	1.875560	-0.706165	0.078537
C	1.929279	-1.708889	1.047646
C	3.050050	-0.240117	-0.520684
C	3.158429	-2.239014	1.422857
H	1.007755	-2.062652	1.500933
C	4.278698	-0.758491	-0.123394
H	3.001013	0.518303	-1.296438
C	4.331647	-1.757759	0.845119
H	3.202019	-3.023792	2.170618
H	5.192416	-0.389462	-0.577314
H	5.290455	-2.165462	1.149229
C	0.086344	1.724744	-0.262286
C	-1.057075	2.329175	-0.786273
C	1.082665	2.488173	0.343797
C	-1.194393	3.710109	-0.708958
H	-1.839067	1.717701	-1.226350
C	0.937612	3.870212	0.415506
H	1.956276	2.006393	0.773305
C	-0.197839	4.479299	-0.111824
H	-2.084755	4.184667	-1.107372
H	1.708480	4.468715	0.889424
H	-0.310740	5.557058	-0.050670

F	0.645088	-0.065200	-2.054936
C	-3.354128	0.471848	2.120743
H	-4.297889	0.678755	1.594213
H	-3.535921	-0.390404	2.782176
H	-3.136315	1.336723	2.752164

M16-Pr

SCF energy in gas phase: -1230.997121

SCF energy in solution: -1231.277349

Free energy in solution: -1230.991272

C	-0.721862	-1.392120	-0.352574
C	-2.542440	-2.855554	0.288755
C	-0.867374	-3.637564	-1.271874
C	-2.020754	-3.853322	-0.524134
C	-0.237901	-2.401949	-1.185794
C	-1.905073	-1.607339	0.395614
H	-2.534866	-4.808304	-0.580346
H	0.654961	-2.200050	-1.767572
H	-3.454334	-3.045068	0.842475
H	-0.468951	-4.413482	-1.915639
N	-2.417884	-0.618721	1.216587
P	0.297195	0.103870	-0.131097
H	-2.176296	0.326486	0.957865
H	0.031124	0.104903	1.286191
C	2.095113	-0.086185	0.207584
C	2.507336	-0.140251	1.542399
C	3.060289	-0.184896	-0.803367
C	3.852141	-0.290260	1.867431
H	1.768383	-0.067727	2.334707
C	4.403894	-0.337566	-0.477126
H	2.749252	-0.138495	-1.838452
C	4.802850	-0.389954	0.856341
H	4.155537	-0.330466	2.908644
H	5.142966	-0.416014	-1.268228
H	5.852805	-0.508841	1.105469
C	-0.470734	1.776174	-0.265610
C	-0.782853	2.374563	-1.492423
C	-0.762195	2.464198	0.917763
C	-1.381321	3.630022	-1.525914
H	-0.549640	1.849014	-2.408978
C	-1.350917	3.725259	0.882348
H	-0.522526	2.007104	1.875017
C	-1.664055	4.307961	-0.341970

H	-1.624938	4.083516	-2.481493
H	-1.563172	4.250202	1.808183
H	-2.126914	5.289394	-0.375114
F	0.619437	0.122856	-1.809166
C	-3.721629	-0.759104	1.823610
H	-4.521276	-0.948314	1.092551
H	-3.720953	-1.579415	2.548429
H	-3.953920	0.160175	2.362782

M4CH₂-OL1

SCF energy in gas phase: -726.586623

SCF energy in solution: -726.750211

Free energy in solution: -726.634247

C	0.040759	-0.288781	-0.045344
C	2.430825	-0.155999	0.041970
C	1.038828	1.883429	0.013233
C	2.294474	1.208321	0.053525
C	-0.097667	1.116967	-0.038631
C	1.272602	-1.031645	-0.015307
H	3.195200	1.816247	0.097439
H	3.409857	-0.622143	0.078370
H	0.993397	2.966733	0.018050
P	-1.486098	-1.076589	-0.023512
C	-1.529734	1.605989	-0.152875
H	-1.737805	-1.993302	1.007595
H	-1.908190	-1.799664	-1.153862
H	-1.717034	2.464992	0.496523
H	-1.720296	1.932640	-1.180632
C	-2.494845	0.442119	0.203427
H	-3.404183	0.432892	-0.398728
H	-2.785634	0.479155	1.256219
O	1.279338	-2.276390	-0.028535

M4CH₂-OL1-TS1

SCF energy in gas phase: -727.735210

SCF energy in solution: -727.888960

Free energy in solution: -727.757611

C	-0.032521	0.273797	-0.036087
C	-2.434274	0.076184	0.055248
C	-1.039399	-1.924887	-0.031338
C	-2.297908	-1.292684	0.032146
C	0.087827	-1.134093	-0.067111

C	-1.299115	0.940648	0.024882
H	-3.192872	-1.908145	0.066716
H	-3.408482	0.549277	0.108285
H	-0.958911	-3.006534	-0.045474
P	1.561027	1.020853	-0.056430
C	1.504818	-1.663894	-0.170005
H	-0.239418	2.653030	-0.269251
H	0.640941	2.765534	-0.524313
H	1.951667	1.890082	0.961745
H	2.153798	1.452284	-1.248033
H	1.623267	-2.587611	0.402370
H	1.723801	-1.906673	-1.216625
C	2.455426	-0.561160	0.324613
H	3.447222	-0.602631	-0.130421
H	2.572393	-0.617197	1.411045
O	-1.424742	2.215290	0.067039

M4CH₂-OL1-Pr

SCF energy in gas phase: -727.762896

SCF energy in solution: -727.904105

Free energy in solution: -727.767022

C	0.015210	-0.268711	-0.026001
C	2.428474	-0.152250	0.058889
C	1.121157	1.886667	-0.042751
C	2.352085	1.232634	0.026047
C	-0.042380	1.130017	-0.065378
C	1.259504	-0.919491	0.022725
H	3.269168	1.813286	0.055764
H	3.378763	-0.671392	0.115247
H	1.068811	2.970700	-0.072624
P	-1.645534	-1.054842	-0.100709
C	-1.438990	1.712760	-0.160923
H	0.550995	-2.681295	-0.078669
H	-1.039808	-2.384384	-0.453671
H	-2.346191	-1.713919	0.949160
H	-2.349877	-1.116099	-1.332420
H	-1.495502	2.667740	0.371004
H	-1.658961	1.927070	-1.215338
C	-2.388603	0.652683	0.380854
H	-3.411127	0.747348	0.001954
H	-2.422765	0.702251	1.475957
O	1.412596	-2.260565	0.066688

M4NH-OL1

SCF energy in gas phase: -742.622773

SCF energy in solution: -742.794934

Free energy in solution: -742.690357

C	-0.030706	-0.282000	-0.015000
C	-2.413124	-0.204391	0.005388
C	-1.068889	1.869538	0.003746
C	-2.306060	1.165242	0.009001
C	0.082439	1.119398	-0.010295
C	-1.237304	-1.055348	-0.005438
H	-3.221164	1.752595	0.018270
H	-3.384136	-0.688406	0.012914
H	-1.047138	2.953296	0.010219
P	1.523930	-1.010178	-0.000479
C	1.514395	1.614283	-0.025624
H	1.906600	-1.789673	-1.108431
H	1.850552	-1.856885	1.069657
H	1.730901	2.152120	-0.955669
H	1.712008	2.286215	0.815583
O	-1.205053	-2.301936	-0.006948
N	2.376693	0.414477	0.083414
H	3.352484	0.497235	-0.154336

M4NH-OL1-TS1

SCF energy in gas phase: -743.777636

SCF energy in solution: -743.941368

Free energy in solution: -743.821595

C	0.018561	0.275373	-0.017427
C	2.423914	0.116359	0.004728
C	1.065797	-1.910238	-0.011813
C	2.313199	-1.254109	-0.003408
C	-0.069997	-1.132616	-0.021323
C	1.276251	0.970631	0.010610
H	3.220225	-1.852541	0.001965
H	3.391230	0.606145	0.018431
H	1.001708	-2.992949	-0.004639
P	-1.598991	0.955389	-0.015252
C	-1.476972	-1.685275	-0.028357
H	0.098439	2.683651	-0.125564
H	-0.767882	2.798050	-0.248487
H	-2.140609	1.546497	-1.163033
H	-2.029008	1.729276	1.063237

H	-1.673100	-2.202846	-0.976591
H	-1.608662	-2.409267	0.783230
O	1.388142	2.239911	0.043762
N	-2.369251	-0.539746	0.151274
H	-3.332356	-0.658662	-0.126836

M4NH-OL1-Pr

SCF energy in gas phase: -743.812447

SCF energy in solution: -743.966270

Free energy in solution: -743.839920

C	-0.007545	-0.269418	0.003689
C	-2.420179	-0.178742	-0.046848
C	-1.136083	1.876756	0.041311
C	-2.360195	1.207403	-0.009797
C	0.029451	1.125321	0.036028
C	-1.243124	-0.934834	-0.028300
H	-3.285028	1.776181	-0.025504
H	-3.366026	-0.707223	-0.089088
H	-1.095230	2.961324	0.072851
P	1.678546	-0.996878	0.097899
C	1.442889	1.687381	0.107173
H	-0.512259	-2.690393	0.011185
H	1.127988	-2.365880	0.275716
H	2.541207	-1.524410	-0.898539
H	2.225049	-1.067837	1.390584
H	1.551978	2.560098	-0.544177
H	1.627899	2.035846	1.133227
O	-1.385058	-2.277571	-0.060830
N	2.378797	0.632077	-0.242153
H	2.603827	0.688293	-1.232565

M4O-OL1

SCF energy in gas phase: -762.487288

SCF energy in solution: -762.662585

Free energy in solution: -762.569892

C	-0.026564	-0.293430	0.000075
C	-2.410248	-0.199147	-0.000450
C	-1.052372	1.868143	0.000415
C	-2.295159	1.168370	-0.000027
C	0.090890	1.109952	0.000435
C	-1.239358	-1.059976	-0.000093

H	-3.206602	1.761094	-0.000045
H	-3.384237	-0.677026	-0.000914
H	-1.025770	2.951527	0.000503
P	1.540510	-0.971398	0.000097
C	1.530655	1.573498	-0.000222
H	1.957963	-1.743108	-1.093941
H	1.959946	-1.741762	1.094344
H	1.786767	2.150751	-0.891646
H	1.787770	2.151042	0.890719
O	-1.217563	-2.304282	0.000250
O	2.396244	0.393531	-0.000410

M4O-OL1-TS1

SCF energy in gas phase: -763.649155

SCF energy in solution: -763.818249

Free energy in solution: -763.710613

C	0.016122	0.282583	-0.000050
C	2.421556	0.122185	0.000065
C	1.059154	-1.907651	0.000007
C	2.308679	-1.245388	0.000067
C	-0.071087	-1.127984	-0.000030
C	1.274260	0.989064	-0.000050
H	3.215493	-1.844194	0.000137
H	3.390712	0.608572	0.000135
H	0.998361	-2.990229	-0.000010
P	-1.610367	0.901639	0.000071
C	-1.486564	-1.653551	-0.000106
H	-0.033167	2.731556	0.000009
H	-0.861016	2.853187	0.000018
H	-2.125489	1.558762	-1.117084
H	-2.125326	1.558579	1.117414
H	-1.699508	-2.252904	-0.889965
H	-1.699539	-2.253124	0.889596
O	1.381124	2.247515	-0.000116
O	-2.385842	-0.528808	0.000023

M4O-OL1-Pr

SCF energy in gas phase: -763.694809

SCF energy in solution: -763.855531

Free energy in solution: -763.741217

C	0.006349	-0.265272	-0.008574
C	-2.405035	-0.195216	-0.017822

C	-1.138102	1.873572	0.028213
C	-2.355704	1.192220	0.007285
C	0.030658	1.128191	0.015203
C	-1.223677	-0.943261	-0.019455
H	-3.285767	1.752386	0.006856
H	-3.347382	-0.730881	-0.037408
H	-1.105407	2.958376	0.046072
P	1.682326	-0.971154	0.061489
C	1.439452	1.679880	0.042146
H	-0.483379	-2.698098	-0.007630
H	1.175649	-2.349239	0.214106
H	2.492057	-1.400002	-1.003282
H	2.308883	-1.097487	1.314329
H	1.565404	2.458901	-0.719940
H	1.631861	2.145166	1.022821
O	-1.357786	-2.286003	-0.045049
O	2.318978	0.624442	-0.209981

M7CH₂-OL1

SCF energy in gas phase: -765.894781

SCF energy in solution: -766.064292

Free energy in solution: -765.919827

C	1.478882	-0.972574	-0.026989
C	2.539124	1.219684	-0.026787
C	0.123871	1.166010	0.101577
C	1.291985	1.895472	0.048675
C	0.249563	-0.237347	0.071911
C	2.659487	-0.147377	-0.064726
C	-2.356936	1.019824	-0.484822
C	-1.239786	1.814147	0.203997
P	-1.066391	-1.360153	0.057966
H	3.443187	1.822777	-0.064224
H	1.260617	2.980101	0.062895
H	3.627287	-0.632321	-0.132517
H	-2.115823	0.895248	-1.547017
H	-1.095836	-2.295076	1.098791
H	-1.142629	-2.164760	-1.087611
H	-3.292987	1.583972	-0.434346
H	-1.189742	2.819049	-0.225491
H	-1.504451	1.942410	1.263195
O	1.417246	-2.228074	-0.077120
C	-2.591847	-0.357518	0.160898
H	-3.422023	-0.889750	-0.310394

H -2.835762 -0.236692 1.221797

M7CH₂-OL1-TS1

SCF energy in gas phase: -767.028146

SCF energy in solution: -767.191166

Free energy in solution: -767.031379

C 1.582387 -0.824654 0.034329

C 2.452358 1.443323 0.046211

C 0.052699 1.137102 -0.076034

C 1.156727 1.973108 -0.031571

C 0.261627 -0.266199 -0.068658

C 2.668320 0.085495 0.077813

C -2.533473 0.930203 -0.275050

C -1.311119 1.811698 -0.036196

P -1.132133 -1.369309 -0.097377

H 3.300848 2.120698 0.086258

H 1.006439 3.048565 -0.031432

H 3.663230 -0.339786 0.143758

H -2.590763 0.639318 -1.333556

H 0.833590 -2.561074 -0.584252

H 0.041246 -2.664004 -1.083102

H -1.043663 -2.445615 0.784315

H -1.784916 -1.711147 -1.289003

H -3.440074 1.505269 -0.066018

H -1.308119 2.639905 -0.752025

H -1.412967 2.271018 0.955953

O 1.787359 -2.098625 0.102132

C -2.479348 -0.325771 0.597336

H -3.417754 -0.888302 0.562519

H -2.265043 -0.072035 1.641099

M7CH₂-OL1-Pr

SCF energy in gas phase: -767.050381

SCF energy in solution: -767.201539

Free energy in solution: -767.036726

C 1.559483 -0.793069 0.006363

C 2.469635 1.432083 0.045059

C 0.064302 1.125284 -0.055222

C 1.185219 1.956924 -0.018260

C 0.241014 -0.276551 -0.061041

C 2.660218 0.061061 0.063215

C -2.514508 0.978329 -0.261547

C -1.278449 1.838695 -0.038765

P -1.180879 -1.443799 -0.144177

H 3.327320 2.096601 0.080180

H 1.036945 3.033020 -0.027291

H 3.645925 -0.386183 0.120685

H -2.569600 0.670956 -1.317493

H 1.091410 -2.618836 -0.260937

H -0.313160 -2.456988 -0.843209

H -1.330307 -2.382847 0.917268

H -2.002695 -1.527796 -1.314546

H -3.411395 1.577240 -0.073260

H -1.240953 2.652929 -0.770679

H -1.366977 2.320973 0.944106

O 1.849257 -2.112538 0.079340

C -2.447582 -0.259539 0.617571

H -3.403753 -0.797407 0.637832

H -2.179628 -0.003675 1.651040

M7NH-OL1

SCF energy in gas phase: -781.932487

SCF energy in solution: -782.109390

Free energy in solution: -781.930448

C -1.414264 -0.992406 0.024631

C -2.558652 1.146418 0.046320

C -0.147518 1.191773 -0.102949

C -1.345092 1.876652 -0.042072

C -0.230948 -0.205788 -0.064151

C -2.628527 -0.229182 0.082732

C 2.320884 1.025751 0.438259

C 1.211570 1.840468 -0.231193

P 1.090708 -1.320308 -0.061673

H -3.486670 1.711318 0.092088

H -1.361536 2.961455 -0.060192

H -3.578780 -0.747070 0.152586

H 2.136780 0.974915 1.520883

H 1.208633 -2.209186 -1.132526

H 1.130312 -2.148640 1.071550

H 3.281624 1.523652 0.287607

H 1.191169 2.841200 0.211466

H 1.463667 1.956889 -1.292403

O -1.250233 -2.248452 0.041721

N 2.437406 -0.321199 -0.158911

H 3.349490 -0.746022 -0.056825

M7NH-OL1-TS1

SCF energy in gas phase: -783.068744

SCF energy in solution: -783.243327

Free energy in solution: -783.049666

C	-1.568667	-0.849984	-0.046808
C	-2.464734	1.416623	0.002666
C	-0.062813	1.139794	0.055413
C	-1.171827	1.964816	0.049584
C	-0.253304	-0.268301	0.048718
C	-2.664440	0.059753	-0.047237
C	2.498877	0.926180	0.241492
C	1.297196	1.808039	-0.059540
P	1.170083	-1.314797	0.091493
H	-3.322771	2.083155	-0.004581
H	-1.033477	3.041604	0.046928
H	-3.656068	-0.374970	-0.100675
H	2.559221	0.718217	1.325188
H	-0.716899	-2.610379	0.530763
H	0.039138	-2.721159	0.983677
H	1.204929	-2.386073	-0.796395
H	1.711286	-1.667292	1.338680
H	3.418318	1.445738	-0.037633
H	1.319388	2.689429	0.588947
H	1.397555	2.164624	-1.091362
O	-1.766150	-2.113658	-0.141343
N	2.388119	-0.307278	-0.547432
H	3.278774	-0.782244	-0.658877

M7NH-OL1-Pr

SCF energy in gas phase: -783.100742

SCF energy in solution: -783.264339

Free energy in solution: -783.064305

C	-1.542130	-0.807281	-0.008517
C	-2.476204	1.410355	-0.020551
C	-0.069180	1.127072	0.030233
C	-1.195140	1.948838	0.016384
C	-0.229369	-0.278387	0.037470
C	-2.652133	0.038858	-0.038744
C	2.477388	0.948888	0.243477
C	1.271858	1.835729	-0.017729
P	1.213440	-1.401648	0.123952

H	-3.341615	2.065461	-0.036913
H	-1.056241	3.025999	0.021495
H	-3.634108	-0.418264	-0.078543
H	2.524538	0.696387	1.323738
H	-1.049007	-2.640371	0.168530
H	0.382989	-2.483176	0.721129
H	1.532042	-2.288694	-0.936494
H	1.909500	-1.424415	1.369561
H	3.395818	1.495406	0.010478
H	1.252259	2.676091	0.684726
H	1.374505	2.258620	-1.024075
O	-1.833816	-2.126311	-0.078155
N	2.346102	-0.227966	-0.593357
H	3.245006	-0.676500	-0.756311

M7O-OL1

SCF energy in gas phase: -801.804392

SCF energy in solution: -801.976289

Free energy in solution: -801.853585

C	-1.228601	-1.049862	0.025787
C	-2.662237	0.844623	0.033937
C	-0.282734	1.262899	-0.094579
C	-1.587326	1.755971	-0.045361
C	-0.210754	-0.109692	-0.063855
C	-2.540599	-0.549556	0.074504
C	2.179577	1.102275	0.420133
C	1.050278	1.969712	-0.174509
P	1.100175	-1.252115	-0.052296
H	-3.665570	1.260646	0.074568
H	-1.787839	2.822268	-0.057883
H	-3.413288	-1.188029	0.141209
H	1.983814	0.951242	1.492446
H	1.448470	-2.046834	-1.140546
H	1.442163	-1.887155	1.144903
H	3.134141	1.624226	0.325388
H	1.028781	2.923171	0.363679
H	1.286946	2.195485	-1.221036
O	-0.645492	-2.238209	0.048745
O	2.362259	-0.165731	-0.223075

M7O-OL1-TS1

SCF energy in gas phase: -802.943486

SCF energy in solution: -803.123290

Free energy in solution: -802.985746

C	-1.567078	-0.856875	-0.047592
C	-2.451612	1.420328	0.026208
C	-0.051820	1.140366	0.048285
C	-1.152986	1.968829	0.058127
C	-0.247992	-0.271256	0.038161
C	-2.659635	0.067799	-0.028714
C	2.489810	0.878023	0.242249
C	1.318758	1.782921	-0.089993
P	1.181733	-1.285401	0.066621
H	-3.306612	2.090874	0.032425
H	-1.013265	3.045259	0.053089
H	-3.655034	-0.359390	-0.074207
H	2.523765	0.648322	1.318942
H	-0.631466	-2.650953	0.563834
H	0.091217	-2.768992	0.983384
H	1.235996	-2.342239	-0.833289
H	1.749865	-1.650626	1.292891
H	3.441862	1.332500	-0.035880
H	1.367912	2.680236	0.534934
H	1.431629	2.111417	-1.129925
O	-1.764105	-2.109506	-0.145871
O	2.385788	-0.345020	-0.502366

M7O-OL1-Pr

SCF energy in gas phase: -802.986034

SCF energy in solution: -803.155831

Free energy in solution: -803.011971

C	-1.535492	-0.806280	0.001840
C	-2.464414	1.414373	-0.001688
C	-0.059698	1.124958	0.009150
C	-1.181165	1.950735	0.010866
C	-0.220194	-0.282428	0.021783
C	-2.643697	0.043922	-0.011606
C	2.457181	0.907422	0.271609
C	1.288569	1.815523	-0.058095
P	1.232903	-1.391958	0.080397
H	-3.328706	2.071064	-0.005980
H	-1.039377	3.027324	0.010615
H	-3.627611	-0.410307	-0.032612
H	2.447500	0.651417	1.347792
H	-1.044824	-2.648134	0.119481

H	0.427722	-2.509577	0.603525
H	1.575050	-2.169238	-1.043229
H	1.942309	-1.449861	1.303804
H	3.411601	1.402334	0.068021
H	1.278611	2.691713	0.599044
H	1.421278	2.184968	-1.082187
O	-1.839775	-2.122486	-0.051786
O	2.364319	-0.248974	-0.517888

M10CH₂-OL1

SCF energy in gas phase: -729.001127

SCF energy in solution: -729.154772

Free energy in solution: -728.992532

C	-0.075629	0.336769	-0.232014
C	2.395093	0.442998	0.142356
C	1.137675	-1.760312	0.264012
C	2.365399	-1.027568	-0.291531
C	-0.132899	-1.171832	-0.349555
C	1.053870	1.159567	-0.000701
H	2.341966	-1.088010	-1.387311
H	2.671016	0.519502	1.201731
H	1.201441	-2.834837	0.057898
P	-1.625831	1.010573	-0.051038
H	-2.227390	1.830641	-1.029385
H	-1.884627	1.777248	1.102626
C	-1.444628	-1.604883	0.332160
H	-1.750551	-2.617706	0.051724
H	-1.294306	-1.585714	1.418028
H	3.145256	1.013850	-0.412673
H	3.284571	-1.527673	0.029597
H	1.100133	-1.632106	1.354720
H	-0.173522	-1.493951	-1.404726
C	-2.542891	-0.584183	-0.039642
H	-3.392339	-0.582563	0.645305
H	-2.920680	-0.756014	-1.052672
O	0.968820	2.384426	0.155026

M10CH₂-OL1-TS1

SCF energy in gas phase: -730.140431

SCF energy in solution: -730.287208

Free energy in solution: -730.109669

C	0.088539	0.334502	0.142209
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C	-2.416703	0.394780	-0.060641
C	-1.186044	-1.784128	-0.285089
C	-2.395421	-1.081668	0.331472
C	0.090666	-1.182941	0.288920
C	-1.067779	1.088453	-0.024026
H	-2.338410	-1.175038	1.423019
H	-2.784081	0.514616	-1.087701
H	-1.215440	-2.861926	-0.089551
P	1.731209	0.938381	0.063678
H	0.082854	2.714594	-0.080867
H	1.029164	2.778974	0.043660
H	2.388786	1.571114	1.127376
H	2.259944	1.472354	-1.119204
C	1.380640	-1.687627	-0.369904
H	1.579388	-2.736338	-0.126807
H	1.272630	-1.610703	-1.459582
H	-3.093238	0.977809	0.571399
H	-3.328871	-1.560685	0.021251
H	-1.192032	-1.643964	-1.374750
H	0.136089	-1.461764	1.355982
C	2.502700	-0.761881	0.109743
H	3.412489	-0.817000	-0.492929
H	2.768830	-0.990266	1.147972
O	-1.115728	2.354447	-0.201317

M10CH₂-OL1-Pr

SCF energy in gas phase: -730.159771

SCF energy in solution: -730.298804

Free energy in solution: -730.115888

C	-0.095553	0.328220	-0.140316
C	2.413895	0.431469	0.022733
C	1.224491	-1.761434	0.316368
C	2.426706	-1.059160	-0.314089
C	-0.058673	-1.183978	-0.266463
C	1.040942	1.051105	-0.001706
H	2.380958	-1.190812	-1.401827
H	2.812569	0.605537	1.030730
H	1.265654	-2.841883	0.140053
P	-1.799651	0.982954	-0.031267
H	0.232429	2.753770	0.184389
H	-1.301798	2.406249	0.102028
H	-2.593171	1.443426	-1.118888
H	-2.443410	1.166527	1.224645

C	-1.354496	-1.699547	0.372973
H	-1.494442	-2.768783	0.179480
H	-1.285757	-1.569381	1.462930
H	3.052355	1.007304	-0.655759
H	3.368438	-1.503453	0.020778
H	1.229645	-1.604601	1.403663
H	-0.096445	-1.455735	-1.334536
C	-2.457143	-0.818403	-0.193784
H	-3.416973	-0.919840	0.323240
H	-2.616600	-1.048852	-1.255632
O	1.132539	2.380822	0.173676

M10NH-OL1

SCF energy in gas phase: -745.036214

SCF energy in solution: -745.199376

Free energy in solution: -745.048194

C	-0.085561	0.339856	-0.265052
C	2.368513	0.465684	0.192483
C	1.145389	-1.754543	0.218453
C	2.368731	-0.986942	-0.296522
C	-0.130631	-1.169839	-0.389215
C	1.027768	1.174445	0.011486
H	2.361193	-1.006487	-1.393912
H	2.599025	0.503772	1.264720
H	1.228314	-2.821376	-0.017326
P	-1.658846	0.941156	-0.093769
H	-2.425103	1.543606	-1.119759
H	-1.824241	1.878024	0.939843
C	-1.428446	-1.593757	0.332728
H	-1.841495	-2.534307	-0.040680
H	-1.224789	-1.710241	1.403207
H	3.134659	1.062845	-0.310165
H	3.289799	-1.486364	0.019797
H	1.095502	-1.660014	1.311989
H	-0.189129	-1.492058	-1.442394
O	0.931293	2.397687	0.159371
N	-2.450424	-0.525912	0.164714
H	-3.212991	-0.744280	-0.462928

M10NH-OL1-TS1

SCF energy in gas phase: -746.183613

SCF energy in solution: -746.341153

Free energy in solution: -746.174658

C	-0.098588	0.317988	-0.162330
C	2.387214	0.464178	0.103854
C	1.224133	-1.764866	0.254220
C	2.417294	-1.002883	-0.326063
C	-0.062318	-1.192199	-0.327033
C	1.018889	1.116328	0.041880
H	2.377941	-1.068287	-1.420376
H	2.724032	0.567092	1.143181
H	1.298288	-2.835393	0.032544
P	-1.756062	0.849600	-0.090966
H	-0.236735	2.688780	-0.032188
H	-1.133399	2.703284	-0.261063
H	-2.488078	1.397851	-1.148315
H	-2.220055	1.483258	1.071505
C	-1.346371	-1.708712	0.329789
H	-1.608975	-2.709883	-0.025903
H	-1.207637	-1.751490	1.422291
H	3.064151	1.079315	-0.496407
H	3.360987	-1.460949	-0.015272
H	1.211383	-1.651209	1.346578
H	-0.110723	-1.463022	-1.393478
O	1.000956	2.378845	0.232302
N	-2.376138	-0.746355	-0.070765
H	-3.306435	-0.908617	0.292428

M10NH-OL1-Pr

SCF energy in gas phase: -746.209357

SCF energy in solution: -746.361344

Free energy in solution: -746.188758

C	-0.109354	0.316668	-0.166055
C	2.388556	0.477643	0.042017
C	1.243505	-1.744988	0.315295
C	2.440250	-1.013035	-0.293341
C	-0.035589	-1.191039	-0.294804
C	1.003565	1.067672	-0.006557
H	2.417105	-1.145633	-1.381494
H	2.766008	0.660751	1.056582
H	1.314533	-2.823373	0.136211
P	-1.822108	0.911647	-0.037869
H	0.158623	2.758349	0.158225
H	-1.395654	2.346477	0.027602
H	-2.725065	1.295398	-1.054329

H	-2.381669	1.099986	1.254253
C	-1.342126	-1.695243	0.323669
H	-1.535939	-2.737776	0.046244
H	-1.254169	-1.653745	1.427874
H	3.026960	1.065469	-0.626111
H	3.385858	-1.435062	0.058717
H	1.227317	-1.590709	1.402605
H	-0.067594	-1.461315	-1.360234
O	1.061914	2.400166	0.174724
N	-2.336063	-0.796910	-0.227901
H	-3.280413	-0.982550	0.098067

M10O-OL1

SCF energy in gas phase: -764.904474

SCF energy in solution: -765.072360

Free energy in solution: -764.932953

C	-0.091527	0.335924	-0.311499
C	2.346513	0.499633	0.202349
C	1.154257	-1.737680	0.222683
C	2.371176	-0.953920	-0.284073
C	-0.124326	-1.175264	-0.404870
C	0.997706	1.186322	0.006089
H	2.374058	-0.976477	-1.381171
H	2.567236	0.544319	1.276274
H	1.255818	-2.804051	-0.005547
P	-1.674354	0.885881	-0.108695
H	-2.489485	1.442655	-1.110320
H	-1.865761	1.787293	0.952227
C	-1.412248	-1.576763	0.334591
H	-1.861552	-2.505115	-0.021519
H	-1.227502	-1.643348	1.412910
H	3.108552	1.106137	-0.295399
H	3.295110	-1.440515	0.042929
H	1.092860	-1.636529	1.314868
H	-0.187124	-1.525222	-1.446933
O	0.867786	2.403523	0.174746
O	-2.417312	-0.541882	0.112814

M10O-OL1-TS1

SCF energy in gas phase: -766.057701

SCF energy in solution: -766.220995

Free energy in solution: -766.065695

C	-0.102087	0.313506	-0.173086	H	-1.603103	-2.687751	0.059374
C	2.376961	0.493716	0.108856	H	-1.269426	-1.600644	1.430003
C	1.231328	-1.753749	0.251004	H	3.017961	1.082648	-0.620383
C	2.419261	-0.974204	-0.321307	H	3.383736	-1.415743	0.065190
C	-0.057170	-1.193855	-0.339873	H	1.220229	-1.589910	1.397753
C	1.002692	1.134405	0.041800	H	-0.073043	-1.466837	-1.365978
H	2.386828	-1.039455	-1.415827	O	1.033822	2.406607	0.182874
H	2.707298	0.598348	1.149976	O	-2.342521	-0.791327	-0.161354
H	1.324210	-2.822444	0.029139				
P	-1.761675	0.790277	-0.090970				
H	-0.359211	2.668525	-0.085858				
H	-1.211737	2.651802	-0.328940				
H	-2.533159	1.248266	-1.161981				
H	-2.249261	1.426444	1.054499				
C	-1.344348	-1.683880	0.328165				
H	-1.679844	-2.658384	-0.032622				
H	-1.214185	-1.725500	1.418342				
H	3.053630	1.112476	-0.487853				
H	3.365056	-1.424500	-0.006036				
H	1.208576	-1.640090	1.343194				
H	-0.100148	-1.473819	-1.404461				
O	0.948139	2.387933	0.234155				
O	-2.377232	-0.736866	0.005798				

M10O-OL1-Pr

SCF energy in gas phase: -766.093166

SCF energy in solution: -766.252783

Free energy in solution: -766.091245

C	-0.112910	0.314893	-0.175486
C	2.378861	0.492655	0.045102
C	1.242158	-1.740759	0.309935
C	2.437848	-0.998219	-0.291135
C	-0.036425	-1.189194	-0.301978
C	0.990956	1.074171	-0.007424
H	2.421319	-1.129425	-1.379491
H	2.751378	0.676883	1.061232
H	1.323202	-2.817620	0.127814
P	-1.834808	0.868780	-0.045295
H	0.131568	2.761192	0.157808
H	-1.468907	2.302157	-0.010774
H	-2.725788	1.139861	-1.097934
H	-2.400678	1.008816	1.239316
C	-1.353279	-1.656473	0.328208

M13CH₂-OL1

SCF energy in gas phase: -768.304812

SCF energy in solution: -768.466228

Free energy in solution: -768.275385

C	1.339362	1.086460	0.000246
C	2.573481	-1.129647	0.269470
C	0.058205	-1.174169	0.308268
C	1.318719	-1.811945	-0.280816
C	0.148269	0.323540	0.114622
C	2.652849	0.335243	-0.167973
C	-2.492082	-1.110325	0.276350
C	-1.223985	-1.769915	-0.279150
P	-1.214416	1.351406	0.058830
H	2.549457	-1.184393	1.365579
H	1.293090	-1.709871	-1.374637
H	2.911178	0.397293	-1.233076
H	-2.443887	-1.099673	1.373087
H	-1.206303	-1.660993	-1.372779
H	-1.251257	-2.843788	-0.060772
H	-1.166351	2.321734	-0.950631
H	3.428530	0.884244	0.372767
H	3.472667	-1.665161	-0.051238
H	1.330582	-2.883758	-0.049281
H	-3.374672	-1.699132	0.007714
H	0.051446	-1.422051	1.385331
H	-1.545251	2.156831	1.174964
O	1.313348	2.329885	-0.033442
C	-2.695107	0.319461	-0.250680
H	-3.576019	0.792847	0.191000
H	-2.842036	0.293489	-1.334963

M13CH₂-OL1-TS1

SCF energy in gas phase: -769.434048

SCF energy in solution: -769.591245

Free energy in solution: -769.385008

C	1.355636	0.977744	-0.165545
C	2.563874	-1.175646	0.363110
C	0.030740	-1.155147	0.359488
C	1.296961	-1.890822	-0.089808
C	0.153265	0.342978	0.085008
C	2.642251	0.194039	-0.300680
C	-2.524574	-1.174805	0.098775
C	-1.193651	-1.816721	-0.287836
P	-1.299898	1.336292	0.245102
H	2.544665	-1.054825	1.453216
H	1.294950	-1.956791	-1.186694
H	2.862919	0.088274	-1.370696
H	-2.619544	-1.155056	1.194503
H	-1.081292	-1.776429	-1.380066
H	-1.196710	-2.876421	-0.006311
H	-1.430208	2.421749	-0.623066
H	-0.173883	2.693952	1.067954
H	3.435095	0.817195	0.121719
H	3.451824	-1.767403	0.121095
H	1.264267	-2.916761	0.293627
H	-3.357407	-1.781881	-0.270837
H	-0.067955	-1.306090	1.448586
H	-1.902025	1.562796	1.496725
H	0.610257	2.662886	0.440220
O	1.471448	2.261867	-0.289564
C	-2.625329	0.244814	-0.458201
H	-3.598105	0.699417	-0.237862
H	-2.505003	0.227475	-1.547989

M13CH₂-OL1-Pr

SCF energy in gas phase: -769.448051

SCF energy in solution: -769.597721

Free energy in solution: -769.387442

C	1.318335	0.959099	-0.153450
C	2.590312	-1.129947	0.384734
C	0.053133	-1.156397	0.354940
C	1.340690	-1.873340	-0.066022
C	0.138762	0.352926	0.116014
C	2.631784	0.235945	-0.287570
C	-2.490209	-1.233034	0.036832
C	-1.140197	-1.842764	-0.323690

P	-1.360612	1.380004	0.334863
H	2.568694	-1.000394	1.473561
H	1.352666	-1.959988	-1.161359
H	2.869134	0.135702	-1.354670
H	-2.607648	-1.224300	1.132149
H	-1.004735	-1.791772	-1.412898
H	-1.113007	-2.904643	-0.050324
H	-1.732151	2.382043	-0.623812
H	-0.542949	2.453772	1.018636
H	3.401881	0.882945	0.142915
H	3.493206	-1.698735	0.144319
H	1.322954	-2.893104	0.333685
H	-3.300642	-1.860592	-0.351028
H	-0.074129	-1.305990	1.440302
H	-2.037390	1.227806	1.584898
H	0.723051	2.758538	0.024661
O	1.486623	2.286200	-0.349984
C	-2.581547	0.186322	-0.501213
H	-3.580169	0.616482	-0.344322
H	-2.388946	0.199712	-1.583233

M13NH-OL1

SCF energy in gas phase: -784.341044

SCF energy in solution: -784.511401

Free energy in solution: -784.332192

C	1.279707	1.091954	0.024785
C	2.583944	-1.080644	0.263045
C	0.074561	-1.212588	0.292131
C	1.353691	-1.784708	-0.323296
C	0.133438	0.288829	0.169816
C	2.628548	0.406925	-0.109710
C	-2.452437	-1.091238	0.275170
C	-1.213220	-1.771890	-0.318623
P	-1.229121	1.307051	0.023982
H	2.553498	-1.182766	1.355526
H	1.325766	-1.635242	-1.411449
H	2.934369	0.529631	-1.156442
H	-2.415550	-1.162949	1.369097
H	-1.204910	-1.623697	-1.407026
H	-1.274867	-2.850372	-0.129989
H	-1.285372	2.132436	-1.111673
H	3.359287	0.956187	0.491285
H	3.501220	-1.575085	-0.071569

H	1.406814	-2.864164	-0.137891
H	-3.367787	-1.597176	-0.042025
H	0.069938	-1.511186	1.355756
H	-1.462081	2.243610	1.048411
O	1.162653	2.333801	-0.072720
N	-2.600559	0.330592	-0.090002
H	-3.130219	0.470629	-0.939878

M13NH-OL1-TS1

SCF energy in gas phase: -785.479167

SCF energy in solution: -785.646377

Free energy in solution: -785.450803

C	1.346700	0.993353	-0.150214
C	2.557858	-1.170498	0.357177
C	0.030581	-1.159887	0.356930
C	1.294777	-1.883875	-0.112671
C	0.147553	0.341604	0.096305
C	2.637588	0.212858	-0.279393
C	-2.514129	-1.103632	0.087690
C	-1.207603	-1.802834	-0.285768
P	-1.328590	1.283642	0.225015
H	2.533119	-1.071443	1.449471
H	1.291307	-1.923349	-1.210821
H	2.871895	0.128907	-1.348422
H	-2.621801	-1.072193	1.181551
H	-1.096397	-1.781033	-1.378814
H	-1.252455	-2.857341	0.013110
H	-1.501621	2.348368	-0.656871
H	-0.263332	2.695242	1.023944
H	3.424451	0.829324	0.163750
H	3.448851	-1.755068	0.108911
H	1.268324	-2.918498	0.247545
H	-3.379577	-1.655257	-0.291694
H	-0.058096	-1.327249	1.444784
H	-1.916865	1.489094	1.480746
H	0.494142	2.668016	0.458627
N	-2.578816	0.276673	-0.403980
H	-2.569051	0.286549	-1.421945
O	1.443466	2.270256	-0.278946

M13NH-OL1-Pr

SCF energy in gas phase: -785.501904

SCF energy in solution: -785.662750

Free energy in solution: -785.461853

C	1.315558	0.961902	-0.128941
C	2.579869	-1.143193	0.373422
C	0.047635	-1.157190	0.347203
C	1.327652	-1.870207	-0.098333
C	0.135052	0.355816	0.128651
C	2.630142	0.241453	-0.260081
C	-2.488583	-1.152249	0.036003
C	-1.163869	-1.819554	-0.324689
P	-1.387767	1.342701	0.302749
H	2.556202	-1.044324	1.465422
H	1.336713	-1.923875	-1.195844
H	2.884200	0.172182	-1.325863
H	-2.608506	-1.143147	1.130522
H	-1.035577	-1.779924	-1.415584
H	-1.175138	-2.879954	-0.042036
H	-1.735428	2.248022	-0.742959
H	-0.642061	2.465198	0.948001
H	3.395171	0.874511	0.199679
H	3.481193	-1.708559	0.119669
H	1.307240	-2.901164	0.271451
H	-3.333983	-1.728055	-0.357791
H	-0.068168	-1.322952	1.431756
H	-2.021676	1.135530	1.555675
H	0.697338	2.759157	0.001682
O	1.484488	2.290492	-0.320326
N	-2.556634	0.221876	-0.430548
H	-2.501225	0.259107	-1.447978

M13O-OL1

SCF energy in gas phase: -804.211605

SCF energy in solution: -804.381382

Free energy in solution: -804.212659

C	1.107903	1.092763	0.081802
C	2.662568	-0.847675	0.217204
C	0.177086	-1.311504	0.327358
C	1.502178	-1.690707	-0.350534
C	0.115679	0.177127	0.309608
C	2.535145	0.660487	-0.086116
C	-2.342639	-1.143115	0.258107
C	-1.105298	-1.838404	-0.325752
P	-1.195980	1.248380	-0.028300
H	2.691588	-0.990240	1.304673

H	1.411209	-1.508449	-1.429971
H	2.820116	0.880848	-1.122295
H	-2.312953	-1.203937	1.355813
H	-1.079107	-1.656019	-1.407814
H	-1.208513	-2.918581	-0.172376
H	-1.312204	1.866253	-1.274065
H	3.195817	1.256599	0.551208
H	3.616064	-1.216797	-0.171366
H	1.716748	-2.756403	-0.213362
H	-3.255049	-1.640097	-0.079799
H	0.201617	-1.689185	1.362748
H	-1.645247	2.173416	0.921879
O	0.639611	2.286239	-0.079632
O	-2.491625	0.224143	-0.144223

M13O-OL1-TS1

SCF energy in gas phase: -805.354160

SCF energy in solution: -805.527403

Free energy in solution: -805.343620

C	1.329482	1.008645	-0.145530
C	2.557095	-1.150514	0.371438
C	0.034213	-1.167490	0.352988
C	1.306775	-1.874151	-0.117327
C	0.136477	0.334913	0.100684
C	2.629307	0.237873	-0.255194
C	-2.489355	-1.086558	0.062511
C	-1.197532	-1.793431	-0.313719
P	-1.344463	1.248980	0.197734
H	2.519662	-1.060385	1.464217
H	1.310891	-1.899836	-1.215600
H	2.877717	0.163218	-1.321586
H	-2.621870	-1.078879	1.157572
H	-1.085990	-1.745741	-1.403388
H	-1.268349	-2.850053	-0.028768
H	-1.548641	2.298505	-0.689359
H	-0.336118	2.690457	0.997892
H	3.403768	0.860535	0.200919
H	3.457049	-1.723398	0.128597
H	1.288699	-2.912871	0.231267
H	-3.360777	-1.579489	-0.373739
H	-0.061592	-1.348938	1.437875
H	-1.951297	1.485438	1.442994
H	0.393976	2.679208	0.463005

O	1.407521	2.277797	-0.289547
O	-2.493640	0.251178	-0.434581

M13O-OL1-Pr

SCF energy in gas phase: -805.384715

SCF energy in solution: -805.553485

Free energy in solution: -805.364171

C	1.293308	0.973071	-0.120873
C	2.579175	-1.124737	0.381251
C	0.053342	-1.164541	0.337022
C	1.339979	-1.858960	-0.113490
C	0.117532	0.349772	0.118676
C	2.618951	0.269882	-0.230329
C	-2.456269	-1.120357	0.025355
C	-1.158106	-1.825065	-0.329594
P	-1.412157	1.316823	0.280230
H	2.543673	-1.043993	1.474470
H	1.355471	-1.894264	-1.211336
H	2.894257	0.221476	-1.291879
H	-2.583674	-1.100227	1.125819
H	-1.041609	-1.790594	-1.419343
H	-1.194782	-2.879175	-0.028734
H	-1.869233	2.200382	-0.720496
H	-0.693556	2.436538	0.925344
H	3.365348	0.907922	0.252794
H	3.490275	-1.674145	0.127750
H	1.327556	-2.895402	0.240818
H	-3.321477	-1.649842	-0.386857
H	-0.055133	-1.331334	1.422221
H	-2.095031	1.127278	1.505284
H	0.649414	2.769965	-0.056540
O	1.455405	2.300859	-0.319811
O	-2.444984	0.180226	-0.501548

M4O-OL2

SCF energy in gas phase: -1224.446178

SCF energy in solution: -1224.726982

Free energy in solution: -1224.481965

C	-1.619048	0.000468	-0.016304
C	-3.530396	0.000831	-1.449231
C	-3.800828	0.000687	0.996900
C	-4.319767	0.000880	-0.321930

C	-2.430564	0.000482	1.130692	C	-2.361147	0.134480	-1.358989
C	-2.088695	0.000574	-1.370739	H	-5.396306	1.124010	-0.109801
H	-5.399820	0.001054	-0.447288	H	-4.321061	0.376537	-2.198707
H	-3.971980	0.000948	-2.440357	H	-4.101534	1.296514	2.016603
H	-4.460849	0.000770	1.856874	P	0.082245	0.066060	0.194579
P	0.034738	0.000043	0.496120	C	-1.351406	0.705347	2.256595
C	-1.640773	0.000217	2.420244	H	-1.678553	-0.034277	2.994871
H	-1.831126	-0.891101	3.023865	H	-0.454865	-0.207877	-2.148265
C	0.999743	1.463509	0.105081	H	0.318784	-0.105320	-1.801936
C	0.906733	2.002259	-1.183254	C	1.397152	1.272200	-0.159164
C	1.830655	2.034820	1.072631	C	2.481189	0.960781	-0.981214
C	1.664952	3.127539	-1.493365	C	1.316807	2.524005	0.452486
C	2.580325	3.159607	0.745996	C	3.484437	1.900848	-1.186097
C	2.497934	3.701525	-0.535402	C	2.309847	3.471390	0.222665
C	0.998965	-1.463892	0.104963	C	3.394756	3.158208	-0.591408
C	1.829330	-2.035908	1.072568	C	0.687145	-1.634821	0.140230
C	0.905914	-2.002324	-1.183500	C	1.717455	-2.005475	1.006527
C	2.578374	-3.161086	0.745879	C	0.076925	-2.577681	-0.690645
C	1.663528	-3.128001	-1.493678	C	2.152525	-3.327589	1.027220
C	2.495949	-3.702691	-0.535659	C	0.509729	-3.898162	-0.651547
H	1.875476	1.611735	2.072059	C	1.547684	-4.271104	0.201012
H	3.225077	3.614602	1.490620	H	0.482169	2.755786	1.106917
H	3.083465	4.580254	-0.786498	H	2.238448	4.450006	0.685487
H	1.598445	3.560328	-2.485958	H	4.172794	3.895116	-0.762750
H	0.241294	1.542053	-1.913431	H	4.331891	1.655014	-1.817152
H	1.874234	-1.613030	2.072080	H	2.532354	-0.012834	-1.461061
H	3.222688	-3.616617	1.490555	H	2.168823	-1.267430	1.663830
H	3.081025	-4.581712	-0.786795	H	2.958638	-3.620647	1.691580
H	1.596975	-3.560521	-2.486385	H	1.885631	-5.302331	0.221476
H	0.240903	-1.541601	-1.913742	H	0.039769	-4.636337	-1.292758
H	-1.830782	0.891469	3.024071	H	-0.717301	-2.269466	-1.367204
O	-0.221523	0.000000	2.093796	H	-1.300394	1.684899	2.745892
O	-1.303486	0.000468	-2.354149	O	-0.038474	0.357055	1.815627
				O	-1.840351	-0.321359	-2.432745

M4O-OL2-TS1

SCF energy in gas phase: -1225.591319

SCF energy in solution: -1225.871827

Free energy in solution: -1225.610421

C	-1.630505	0.320797	-0.134816
C	-3.746903	0.478057	-1.284298
C	-3.611899	1.006291	1.093202
C	-4.334731	0.891192	-0.110421
C	-2.266124	0.714929	1.057202

M4O-OL2-Pr

SCF energy in gas phase: -1225.635432

SCF energy in solution: -1225.912058

Free energy in solution: -1225.645105

C	-1.434524	0.898618	-0.128510
C	-3.350044	2.006742	-1.091280
C	-3.364470	1.398358	1.257482
C	-3.983663	1.968005	0.144011

C	-2.089603	0.876323	1.100317	C	-4.273869	0.002103	1.131728
C	-2.069538	1.465965	-1.243725	C	-2.768332	0.002004	-0.714399
H	-4.976886	2.395900	0.240664	C	-1.862038	0.001081	1.649474
H	-3.822781	2.454291	-1.958322	H	-5.297865	0.002362	1.497901
H	-3.862949	1.372960	2.221514	H	-3.463962	0.001382	3.118000
P	0.169972	0.030155	-0.067341	H	-4.913261	0.002656	-0.958466
C	-1.252417	0.214230	2.169361	P	-0.210821	0.000608	-0.603866
H	-1.669226	-0.779482	2.405229	C	-2.259678	0.002148	-2.139053
H	-0.651894	1.112658	-2.463085	H	-2.567997	0.892435	-2.694019
H	0.265315	0.006917	-1.533706	C	0.879123	-1.396866	-0.381603
C	1.819734	0.842413	-0.013891	C	1.917268	-1.272473	0.553937
C	2.664106	0.674159	-1.114993	C	0.675901	-2.577654	-1.098340
C	2.255064	1.615054	1.067440	C	2.747508	-2.375166	0.754496
C	3.928410	1.253400	-1.134250	C	1.517898	-3.661112	-0.886254
C	3.509473	2.216783	1.034935	C	2.550708	-3.554860	0.044143
C	4.349302	2.033415	-0.060416	C	0.881612	1.396081	-0.381299
C	0.105424	-1.810419	-0.096116	C	1.919496	1.269553	0.554226
C	0.368037	-2.576188	1.045612	C	0.680546	2.577436	-1.097762
C	-0.220766	-2.458278	-1.290550	C	2.751741	2.370709	0.755071
C	0.312750	-3.965604	0.983608	C	1.524505	3.659289	-0.885396
C	-0.298585	-3.846341	-1.345365	C	2.557118	3.550907	0.045006
C	-0.025296	-4.601826	-0.208142	H	-0.132996	-2.636093	-1.821082
H	1.606908	1.731870	1.926138	H	1.372064	-4.582142	-1.439964
H	3.833668	2.826139	1.872524	H	3.212867	-4.397866	0.214317
H	5.330508	2.497608	-0.078085	H	3.557449	-2.303969	1.474611
H	4.580308	1.102168	-1.988620	H	3.561497	2.297853	1.475222
H	2.331870	0.076723	-1.960227	H	3.220794	4.392671	0.215395
H	0.619230	-2.070031	1.970294	H	1.380404	4.580727	-1.438884
H	0.531843	-4.552327	1.870097	H	-0.128164	2.637469	-1.820577
H	-0.075377	-5.685389	-0.251007	H	-2.569009	-0.887389	-2.694646
H	-0.565732	-4.337501	-2.275495	O	-0.803664	0.001293	-2.110133
H	-0.422797	-1.871259	-2.182599	O	-0.870151	0.000351	2.412942
H	-1.250770	0.804053	3.093838	C	2.097815	-0.001684	1.351581
O	0.055309	0.108178	1.680862	H	3.077948	-0.002607	1.834938
O	-1.516707	1.546012	-2.474888	H	1.319285	-0.001066	2.132788

M4O-OL3

SCF energy in gas phase: -1262.551668

SCF energy in solution: -1262.845554

Free energy in solution: -1262.591551

M4O-OL3-TS1

SCF energy in gas phase: -1263.697150

SCF energy in solution: -1263.989350

Free energy in solution: -1263.721921

C	-1.724911	0.001516	0.222322	C	-1.829438	0.000268	0.238889
C	-3.253100	0.001549	2.053620	C	-3.851518	0.001880	1.571809
C	-4.072016	0.002323	-0.274835	C	-4.007163	-0.002056	-0.858742

C	-4.600077	-0.000257	0.420819
C	-2.633451	-0.001726	-0.921875
C	-2.417166	0.002474	1.558969
H	-5.684086	-0.000464	0.499317
H	-4.319110	0.003421	2.550237
H	-4.611261	-0.003431	-1.759660
P	-0.137697	-0.000127	-0.254351
C	-1.841344	-0.003177	-2.204072
H	-2.054250	0.883690	-2.811210
H	-0.416449	0.002234	2.200828
H	0.322211	-0.000019	1.772890
C	0.936342	-1.434009	-0.110858
C	2.236905	-1.293292	0.388256
C	0.475406	-2.657703	-0.600119
C	3.062627	-2.419750	0.384874
C	1.305423	-3.769986	-0.576682
C	2.603481	-3.645092	-0.084835
C	0.936374	1.433796	-0.112148
C	2.236911	1.293468	0.387155
C	0.475459	2.657073	-0.602467
C	3.062638	2.419919	0.382867
C	1.305498	3.769360	-0.579936
C	2.603523	3.644866	-0.087905
H	-0.534943	-2.732477	-0.993829
H	0.947410	-4.725073	-0.945273
H	3.263104	-4.506700	-0.072163
H	4.077411	-2.331275	0.762791
H	4.077401	2.331757	0.760913
H	3.263149	4.506480	-0.075909
H	0.947509	4.724143	-0.949338
H	-0.534857	2.731487	-0.996317
H	-2.052287	-0.892726	-2.808016
O	-0.455693	-0.000953	-1.870518
O	-1.758177	0.004871	2.643873
C	2.740607	0.000340	0.986100
H	3.834272	0.000335	0.965637
H	2.444957	0.000799	2.046937

M4O-OL3-Pr

SCF energy in gas phase: -1263.734898

SCF energy in solution: -1264.021218

Free energy in solution: -1263.746789

C	-1.951691	-0.000250	0.235000
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C	-4.057355	-0.000285	1.423646
C	-4.046776	0.000108	-1.000291
C	-4.735675	-0.000041	0.212211
C	-2.660503	0.000015	-0.964617
C	-2.659632	-0.000406	1.453099
H	-5.821460	0.000045	0.215853
H	-4.585571	-0.000407	2.370488
H	-4.579248	0.000292	-1.946371
P	-0.141198	-0.000045	0.000696
C	-1.750888	0.000211	-2.168611
H	-1.947954	0.886228	-2.790572
H	-1.123037	-0.000524	2.570203
H	0.059337	-0.000187	1.471279
C	0.971798	-1.435072	-0.083318
C	2.227660	-1.284832	0.521736
C	0.627694	-2.613884	-0.739098
C	3.123962	-2.352134	0.457444
C	1.520269	-3.679942	-0.765769
C	2.770619	-3.544803	-0.167062
C	0.971507	1.435228	-0.083052
C	2.227478	1.285006	0.521775
C	0.627190	2.614117	-0.738594
C	3.123696	2.352391	0.457461
C	1.519671	3.680248	-0.765264
C	2.770158	3.545106	-0.166832
H	-0.335060	-2.684723	-1.237292
H	1.250172	-4.604366	-1.265548
H	3.479288	-4.366273	-0.198620
H	4.109777	-2.245261	0.902513
H	4.109578	2.245556	0.902390
H	3.478774	4.366620	-0.198440
H	1.249411	4.604742	-1.264824
H	-0.335689	2.684984	-1.236542
H	-1.948043	-0.885504	-2.790966
O	-0.430724	0.000022	-1.721411
O	-2.086795	-0.000769	2.673517
C	2.610713	0.000096	1.232584
H	3.689500	0.000159	1.412373
H	2.128971	0.000004	2.222115

M7O-OL2

SCF energy in gas phase: -1263.750615

SCF energy in solution: -1264.040681

Free energy in solution: -1263.766583

				SCF energy in solution: -1265.175664		
				Free energy in solution: -1264.885535		
C	1.682621	-0.143164	-1.586712			
C	4.097180	-0.137435	-1.268174			
C	2.712299	0.020380	0.702023	C	2.066328	-0.837912
C	3.971548	-0.021862	0.136017	C	4.350253	-0.321155
C	1.604342	-0.032284	-0.164427	C	2.534430	0.304346
C	3.015154	-0.200342	-2.115360	C	3.886962	0.248573
C	1.167671	0.744575	2.557189	C	1.602042	-0.184426
C	2.496467	0.099323	2.196847	C	3.479861	-0.848383
P	-0.051764	-0.024031	0.394321	C	0.681552	1.149654
H	5.097282	-0.174807	-1.693357	C	2.133880	0.752463
H	4.855636	0.028258	0.763437	P	-0.128514	-0.018928
H	3.138055	-0.292537	-3.189186	H	5.419153	-0.355509
H	1.112831	1.774763	2.182761	H	4.592914	0.610369
H	1.002646	0.754209	3.635819	H	3.821103	-1.311929
C	-1.042757	-1.501201	0.100628	H	0.468199	2.096358
C	-1.665565	-1.697055	-1.136945	H	0.142419	-0.596033
C	-1.180085	-2.444066	1.124195	H	-0.426476	-0.012215
C	-2.424191	-2.843508	-1.341177	H	0.408715	1.265895
H	-1.519592	-0.972462	-1.929331	C	-1.176635	-1.486685
C	-1.942429	-3.587294	0.905621	C	-2.322726	-1.514286
H	-0.700173	-2.277893	2.082188	C	-0.834517	-2.582847
C	-2.563065	-3.786351	-0.324513	C	-3.132309	-2.644282
H	-2.903398	-3.003361	-2.301232	H	-2.569944	-0.659325
H	-2.051602	-4.321435	1.696982	C	-1.639550	-3.717837
H	-3.154988	-4.680561	-0.493277	H	0.055413	-2.546943
C	-1.028821	1.455131	0.013743	C	-2.787662	-3.746591
C	-1.841409	1.959680	1.036715	H	-4.025954	-2.668096
C	-0.979460	2.094996	-1.230016	H	-1.369281	-4.578365
C	-2.604955	3.100833	0.815186	H	-3.414886	-4.632202
H	-1.869775	1.461664	2.001054	C	-0.989518	1.542417
C	-1.747246	3.237253	-1.436534	C	-2.153745	1.846777
H	-0.356350	1.678438	-2.014834	C	-0.470416	2.450814
C	-2.557730	3.739199	-0.421421	C	-2.812621	3.049945
H	-3.234909	3.490627	1.608020	H	-2.536718	1.146851
H	-1.710755	3.736499	-2.399286	C	-1.117307	3.662336
H	-3.153418	4.630185	-0.594106	H	0.429798	2.195080
O	0.065989	-0.015116	2.013427	C	-2.292726	3.957871
O	0.606733	-0.181522	-2.256305	H	-3.726463	3.280867
H	2.519349	-0.907917	2.631416	H	-0.709959	4.372053
H	3.306443	0.669034	2.663827	H	-2.802911	4.898741
M7O-OL2-TS1				O	-0.156504	0.114001
SCF energy in gas phase: -1264.881659				O	1.285488	-1.389734
				H	2.332813	-0.082319

H 2.774450 1.581755 2.502088

M7O-OL2-Pr

SCF energy in gas phase: -1264.921645

SCF energy in solution: -1265.207968

Free energy in solution: -1264.912741

H -3.817150 4.335673 -0.773930

O -0.200570 0.087528 1.686225

O 1.737538 -0.856458 -2.415036

H 2.134367 0.116448 2.930608

H 2.459587 1.830569 2.670858

C 2.328109 -0.262504 -1.352636

C 4.461174 0.433052 -0.472302

C 2.472427 0.630072 0.894750

C 3.844685 0.788937 0.722355

C 1.666003 0.129540 -0.159310

C 3.708814 -0.098304 -1.500848

C 0.435921 1.209921 2.253367

C 1.926412 0.964123 2.265497

P -0.173826 -0.028002 -0.031729

H 5.532227 0.561713 -0.594643

H 4.433798 1.186818 1.543265

H 4.151779 -0.415386 -2.438146

H 0.208149 2.126136 1.688050

H 0.779380 -0.885679 -2.282382

H -0.256283 -0.107098 -1.489306

H 0.043262 1.346056 3.266931

C -0.908386 -1.713455 0.059409

C -1.565071 -2.206082 -1.071537

C -0.826560 -2.518329 1.201776

C -2.138868 -3.473648 -1.066455

H -1.642410 -1.586224 -1.961599

C -1.381329 -3.794120 1.198230

H -0.332516 -2.133559 2.084450

C -2.040164 -4.272983 0.068298

H -2.656320 -3.836456 -1.948625

H -1.304037 -4.415385 2.084929

H -2.476897 -5.266818 0.073485

C -1.319340 1.417700 -0.219556

C -2.289502 1.709189 0.744361

C -1.262877 2.185249 -1.384397

C -3.194092 2.746120 0.536579

H -2.328938 1.114161 1.650510

C -2.143301 3.246327 -1.575393

H -0.523561 1.948212 -2.146482

C -3.116654 3.521262 -0.618071

H -3.958255 2.951197 1.279692

H -2.078946 3.848693 -2.475941

M7O-OL3

SCF energy in gas phase: -1301.856526

SCF energy in solution: -1302.159104

Free energy in solution: -1301.876216

C 1.470539 0.173437 -1.747629

C 3.905241 0.142408 -1.909593

C 2.934842 -0.105069 0.284890

C 4.058147 -0.036891 -0.511077

C 1.677118 0.026107 -0.336724

C 2.681403 0.247216 -2.523644

C 1.867195 0.368375 2.508866

C 2.994957 -0.340006 1.775382

P 0.163704 -0.018897 0.517133

H 4.803140 0.194298 -2.520807

H 5.047297 -0.125445 -0.073617

H 2.592899 0.372536 -3.597549

H 1.935260 1.450929 2.350966

H 1.896948 0.169530 3.581398

C -0.897163 -1.440078 0.282473

C -2.060385 -1.323008 -0.489892

C -0.540206 -2.650575 0.882439

C -2.855189 -2.461332 -0.642885

C -1.341989 -3.769710 0.714168

H 0.360637 -2.701998 1.487244

C -2.502054 -3.669073 -0.052759

H -3.763753 -2.394669 -1.234645

H -1.070105 -4.711439 1.178434

H -3.139240 -4.537588 -0.187012

C -0.941820 1.379382 0.312155

C -2.116491 1.235487 -0.439300

C -0.637687 2.583508 0.951165

C -2.971846 2.334982 -0.530716

C -1.497952 3.667294 0.842895

H 0.274725 2.673198 1.533334

C -2.668289 3.537021 0.098468

H -3.887983 2.243634 -1.107387

H	-1.261303	4.603651	1.336288
H	-3.351280	4.376033	0.010977
O	0.568376	-0.097837	2.086270
O	0.292857	0.217490	-2.194005
H	2.930001	-1.414484	1.991830
H	3.951130	0.010660	2.176860
C	-2.439858	-0.036862	-1.181749
H	-3.506125	-0.056718	-1.423379
H	-1.868745	-0.001576	-2.119650

M7O-OL3-TS1

SCF energy in gas phase: -1302.982198

SCF energy in solution: -1303.283643

Free energy in solution: -1302.986525

C	-3.018544	2.519546	-0.576522
C	-1.056723	3.889831	-0.294391
H	0.785450	2.820234	-0.002538
C	-2.428947	3.776580	-0.495561
H	-4.083080	2.435953	-0.778923
H	-0.582900	4.865371	-0.270543
H	-3.038074	4.666928	-0.613147
O	0.139812	0.098335	1.848549
O	1.324266	-1.307755	-2.331972
H	2.697552	-0.238125	2.712513
H	3.149100	1.438130	2.429548
C	-2.919502	0.028151	-0.763042
H	-3.991766	0.099223	-0.557283
H	-2.821770	-0.087728	-1.854905

C	2.151589	-0.771963	-1.514809
C	4.472249	-0.261809	-0.955218
C	2.755860	0.281379	0.660883
C	4.087413	0.254861	0.293770
C	1.760272	-0.173109	-0.256802
C	3.543538	-0.765355	-1.827458
C	1.037785	1.052361	2.407869
C	2.465036	0.646608	2.107098
P	0.053646	-0.010531	0.204658
H	5.525199	-0.276593	-1.223562
H	4.839680	0.593665	0.999406
H	3.822422	-1.191526	-2.784596
H	0.806487	2.054905	2.029831
H	0.207822	-0.617059	-2.089696
H	-0.393579	-0.050305	-1.779756
H	0.850348	1.055857	3.483907
C	-1.040938	-1.426874	0.175751
C	-2.386418	-1.249138	-0.157694
C	-0.553372	-2.656190	0.619105
C	-3.240655	-2.344783	-0.016986
C	-1.415122	-3.739468	0.727202
H	0.498419	-2.755571	0.871816
C	-2.763364	-3.576549	0.416143
H	-4.292432	-2.228968	-0.264480
H	-1.040453	-4.701733	1.058564
H	-3.447430	-4.413857	0.509664
C	-0.895137	1.482224	-0.164728
C	-2.265305	1.353029	-0.436786
C	-0.291096	2.741424	-0.127544

M7O-OL3-Pr

SCF energy in gas phase: -1303.017358

SCF energy in solution: -1303.313766

Free energy in solution: -1303.009973

C	2.363721	0.616396	-1.407960
C	4.602711	-0.187734	-1.018769
C	2.806484	-0.888231	0.438052
C	4.149645	-0.913981	0.080250
C	1.871412	-0.146317	-0.321176
C	3.719343	0.581434	-1.751230
C	1.372446	-0.703888	2.428872
C	2.373146	-1.584886	1.701841
P	0.055387	-0.161475	0.013330
H	5.653347	-0.209906	-1.291095
H	4.845828	-1.490596	0.681256
H	4.037165	1.177841	-2.598904
H	1.823586	0.283247	2.617202
H	0.676336	1.294189	-1.996479
H	-0.127976	0.043306	-1.441794
H	1.092660	-1.133419	3.396888
C	-1.308502	-1.376280	-0.161666
C	-2.488394	-0.889238	-0.743469
C	-1.220138	-2.701620	0.256264
C	-3.565240	-1.764081	-0.894718
C	-2.287157	-3.571653	0.059482
H	-0.318685	-3.042848	0.755023
C	-3.463717	-3.098450	-0.514669
H	-4.494094	-1.391658	-1.319071

H	-2.208806	-4.607903	0.372022	C	-2.425192	-1.627859	1.042463
H	-4.308698	-3.765275	-0.653768	C	-2.987913	-1.995455	-1.671451
C	-0.777782	1.423106	0.312902	H	-1.169779	-0.871749	-2.038866
C	-2.030222	1.603711	-0.291482	C	-3.556714	-2.341474	0.654530
C	-0.231409	2.405992	1.135554	H	-2.187711	-1.486026	2.092286
C	-2.719521	2.791509	-0.044153	C	-3.836754	-2.521308	-0.697818
C	-0.918255	3.595967	1.348483	H	-3.206469	-2.148003	-2.723205
H	0.732334	2.234593	1.607232	H	-4.217918	-2.758700	1.407074
C	-2.166799	3.783806	0.759996	H	-4.718669	-3.079900	-0.995297
H	-3.699481	2.939441	-0.490287	C	-0.544075	1.581178	0.199583
H	-0.489110	4.367321	1.979380	C	-1.862897	2.018356	0.350320
H	-2.715183	4.704267	0.933160	C	0.466481	2.491418	-0.120462
O	0.197080	-0.602293	1.667686	C	-2.165582	3.367172	0.196948
O	1.617225	1.452469	-2.162473	H	-2.650320	1.305769	0.579070
H	1.892895	-2.547570	1.486409	C	0.156415	3.837078	-0.282179
H	3.248510	-1.788336	2.325903	H	1.482365	2.130778	-0.250267
C	-2.614988	0.548979	-1.211050	C	-1.156674	4.273574	-0.120519
H	-3.671265	0.773567	-1.384427	H	-3.188076	3.709695	0.316387
H	-2.115302	0.633211	-2.188426	H	0.937378	4.544191	-0.541337

M100-OL2

SCF energy in gas phase: -1226.854591

SCF energy in solution: -1227.135175

Free energy in solution: -1226.844593

C	1.423985	-0.631261	-0.090258
C	3.381218	-0.542437	-1.632551
C	3.686457	-0.917761	0.868178
C	4.095851	-1.354468	-0.545090
C	2.201951	-1.214234	1.069648
C	1.882891	-0.349421	-1.393286
H	3.852867	-2.418206	-0.663095
H	3.811535	0.465963	-1.694736
H	4.295197	-1.431976	1.620555
P	-0.107028	-0.150288	0.472121
C	1.567058	-0.571185	2.308454
H	1.657172	-1.165325	3.219633
H	1.983374	0.430061	2.476508
H	3.511758	-0.992175	-2.620992
H	5.179930	-1.266554	-0.668654
H	3.854856	0.162324	0.980909
H	2.074315	-2.306700	1.143067
C	-1.584455	-1.096082	0.063807
C	-1.855629	-1.280109	-1.297247

H	-1.395790	5.324630	-0.248837
O	0.138764	-0.433064	2.059323
O	1.158847	0.102049	-2.295628

M100-OL2-TS1

SCF energy in gas phase: -1227.997914

SCF energy in solution: -1228.274086

Free energy in solution: -1227.966366

C	1.505674	-0.531117	-0.175971
C	3.726476	-0.566491	-1.338751
C	3.604723	-0.810581	1.164438
C	4.236981	-1.341630	-0.124295
C	2.103607	-1.060914	1.114590
C	2.236696	-0.272958	-1.327115
H	3.982677	-2.403551	-0.229140
H	4.224837	0.408646	-1.409768
H	4.046385	-1.291949	2.043980
P	-0.166034	-0.109303	0.113804
H	0.437257	0.162542	-2.156546
H	-0.370436	0.058243	-1.800898
C	1.289574	-0.360774	2.200864
H	1.321023	-0.867629	3.168743
H	1.631163	0.677280	2.322041
H	3.945248	-1.086200	-2.276511

H	5.328337	-1.281049	-0.076292
H	3.789974	0.268912	1.247450
H	1.930857	-2.145442	1.212860
C	-1.607560	-1.192418	-0.155583
C	-2.644130	-0.828486	-1.016714
C	-1.665654	-2.405257	0.533317
C	-3.735011	-1.673804	-1.184911
H	-2.590208	0.114175	-1.554589
C	-2.747605	-3.259858	0.342860
H	-0.871786	-2.668472	1.224016
C	-3.782765	-2.893412	-0.512303
H	-4.544460	-1.384494	-1.846955
H	-2.785256	-4.207578	0.869973
H	-4.629484	-3.557583	-0.654124
C	-0.643120	1.645788	0.084711
C	-1.580877	2.081275	1.024195
C	-0.042089	2.557024	-0.787222
C	-1.933196	3.427019	1.076223
H	-2.021641	1.368919	1.715387
C	-0.386372	3.902626	-0.716008
H	0.687242	2.210340	-1.514595
C	-1.334921	4.336466	0.208333
H	-2.668669	3.765803	1.798636
H	0.082287	4.613291	-1.388877
H	-1.606249	5.386561	0.253114
O	-0.071399	-0.373543	1.758072
O	1.767500	0.246518	-2.397936

M100-OL2-Pr

SCF energy in gas phase: -1228.032945

SCF energy in solution: -1228.307668

Free energy in solution: -1227.993668

C	1.379202	-0.822823	-0.169512
C	3.575326	-1.428600	-1.226767
C	3.427410	-1.095580	1.263518
C	4.002519	-1.961005	0.141090
C	1.909063	-1.162584	1.204646
C	2.149425	-0.944788	-1.271364
H	3.634824	-2.986531	0.265068
H	4.200561	-0.576736	-1.524892
H	3.791456	-1.433349	2.239804
P	-0.265686	-0.047273	-0.085808
H	0.879585	-0.337406	-2.544264

H	-0.366582	0.051271	-1.551723
C	1.153903	-0.191343	2.112517
H	1.172938	-0.497989	3.163702
H	1.601646	0.815195	2.035900
H	3.701084	-2.183710	-2.009897
H	5.094030	-2.005666	0.193755
H	3.750090	-0.054043	1.131686
H	1.586115	-2.179033	1.478242
C	-1.857762	-0.973511	-0.098503
C	-2.689359	-0.837846	-1.213561
C	-2.258978	-1.808356	0.950133
C	-3.904904	-1.511257	-1.280362
H	-2.383655	-0.194420	-2.034268
C	-3.463301	-2.501229	0.871258
H	-1.623894	-1.899972	1.821469
C	-4.289814	-2.351358	-0.239174
H	-4.546245	-1.385922	-2.146950
H	-3.759969	-3.155669	1.684817
H	-5.232226	-2.887611	-0.293146
C	-0.336367	1.797409	-0.016220
C	-0.734812	2.479099	1.138816
C	0.023776	2.533085	-1.148105
C	-0.782626	3.870069	1.150000
H	-1.002417	1.906081	2.018688
C	0.001585	3.924297	-1.128551
H	0.334687	2.013548	-2.050790
C	-0.410241	4.594522	0.020163
H	-1.106253	4.390357	2.046116
H	0.297989	4.483341	-2.010304
H	-0.440331	5.679559	0.035141
O	-0.176951	-0.190161	1.659195
O	1.806649	-0.622515	-2.536840

M100-OL3

SCF energy in gas phase: -1264.962381

SCF energy in solution: -1265.250859

Free energy in solution: -1264.950000

C	-1.611749	-0.373331	0.229728
C	-3.312678	0.211586	1.953949
C	-4.004611	-0.439040	-0.405283
C	-4.258009	-0.637210	1.095213
C	-2.606401	-0.950680	-0.750488
C	-1.848987	0.148375	1.517542

H	-4.117135	-1.699045	1.334928	C	-3.965651	-0.372377	-0.876403
H	-3.603079	1.268825	1.904324	C	-4.540859	-0.718989	0.498525
H	-4.767189	-0.958264	-0.996598	C	-2.512547	-0.825242	-0.933490
P	-0.111229	-0.195458	-0.553020	C	-2.307266	0.116864	1.447696
C	-2.073816	-0.514758	-2.121311	H	-4.426510	-1.797095	0.666106
H	-2.343395	-1.183175	-2.941231	H	-4.161273	1.094838	1.630058
H	-2.405817	0.504865	-2.351996	H	-4.547529	-0.844688	-1.675576
H	-3.362320	-0.073462	3.008794	P	-0.049724	-0.147378	-0.193016
H	-5.298008	-0.396863	1.337415	H	-0.427638	0.291558	2.133194
H	-4.065396	0.631200	-0.645739	H	0.324308	-0.031246	1.739417
H	-2.624278	-2.053177	-0.719820	C	-1.729512	-0.318169	-2.143796
C	1.262292	-1.315752	-0.253756	H	-1.886031	-0.918277	-3.044136
C	2.227012	-0.920273	0.686043	H	-2.003019	0.724604	-2.361515
C	1.331439	-2.559890	-0.883123	H	-4.021338	-0.361140	2.592335
C	3.262213	-1.808218	0.977698	H	-5.613068	-0.504904	0.537640
C	2.371683	-3.429671	-0.579387	H	-4.010845	0.714701	-1.029433
H	0.576497	-2.829226	-1.615867	H	-2.498616	-1.927580	-0.957991
C	3.334011	-3.050237	0.354055	C	1.272630	-1.367043	-0.017639
H	4.022103	-1.518449	1.698101	C	2.518503	-0.979204	0.490824
H	2.435921	-4.395537	-1.069175	C	1.054498	-2.670948	-0.465315
H	4.151628	-3.723135	0.592640	C	3.534470	-1.935730	0.543110
C	0.703152	1.401458	-0.454936	C	2.069284	-3.615187	-0.382366
C	0.305866	2.446314	-1.289115	H	0.090716	-2.935437	-0.890912
C	1.742335	1.561819	0.471771	C	3.313343	-3.241948	0.121808
C	0.945394	3.677001	-1.202753	H	4.510812	-1.648048	0.923746
H	-0.494271	2.288648	-2.007155	H	1.897308	-4.631290	-0.721243
C	2.367405	2.805239	0.549583	H	4.117360	-3.968802	0.178616
C	1.973312	3.852242	-0.278354	C	0.784626	1.450983	-0.181543
H	0.646891	4.494269	-1.850418	C	0.142920	2.547713	-0.757936
H	3.170759	2.951962	1.265734	C	2.089396	1.558610	0.316585
H	2.476255	4.811388	-0.205308	C	0.793580	3.771883	-0.840456
O	-0.617146	-0.514214	-2.067223	H	-0.872573	2.439142	-1.129027
O	-0.958012	0.595636	2.257742	C	2.734119	2.792255	0.209592
C	2.131274	0.421300	1.382843	C	2.095771	3.888839	-0.359664
H	3.078096	0.645739	1.880859	H	0.292649	4.627200	-1.281118
H	1.345619	0.356272	2.152148	H	3.748483	2.892652	0.586037
M100-OL3-TS1				H	2.616681	4.838555	-0.428236
SCF energy in gas phase: -1266.102821				O	-0.341633	-0.394963	-1.814965
SCF energy in solution: -1266.390300				O	-1.671081	0.601987	2.440714
Free energy in solution: -1266.074255				C	2.771750	0.411416	1.026020
C	-1.728710	-0.300783	0.253723	H	3.849886	0.594711	1.050265
C	-3.816246	0.053496	1.600821	H	2.423216	0.426375	2.070458
				M100-OL3-Pr			

SCF energy in gas phase: -1266.131052
 SCF energy in solution: -1266.416502
 Free energy in solution: -1266.094723

C	-1.832811	-0.279876	0.269100
C	-4.009201	0.036903	1.480933
C	-3.995489	-0.251927	-1.016320
C	-4.679793	-0.650506	0.291966
C	-2.548299	-0.720729	-0.983531
C	-2.506785	0.078217	1.384956
H	-4.609730	-1.738340	0.410585
H	-4.346893	1.077778	1.570354
H	-4.519462	-0.679925	-1.877655
P	-0.040328	-0.131811	0.021275
H	-1.007776	0.551154	2.445761
H	0.175232	-0.036835	1.493353
C	-1.653133	-0.182764	-2.103418
H	-1.804749	-0.721804	-3.045373
H	-1.893342	0.880088	-2.281907
H	-4.270568	-0.446951	2.428119
H	-5.744249	-0.400037	0.274646
H	-4.018947	0.840946	-1.125703
H	-2.531456	-1.820445	-1.044129
C	1.270947	-1.398818	0.000034
C	2.495455	-1.038417	0.579355
C	1.097138	-2.655188	-0.575963
C	3.532665	-1.971505	0.574711
C	2.129769	-3.586230	-0.542077
H	0.157514	-2.885153	-1.068305
C	3.349418	-3.240725	0.034129
H	4.494584	-1.698190	1.000835
H	1.991007	-4.569362	-0.980079
H	4.166256	-3.955387	0.049721
C	0.859657	1.441470	-0.155490
C	0.340896	2.533193	-0.847622
C	2.136210	1.501246	0.422834
C	1.077066	3.708745	-0.952310
H	-0.641372	2.459697	-1.304692
C	2.874393	2.676882	0.283276
C	2.348178	3.776388	-0.388362
H	0.666920	4.562810	-1.481381
H	3.872501	2.731346	0.710246
H	2.935077	4.685255	-0.476052
O	-0.323603	-0.347820	-1.689374

O	-1.976091	0.559398	2.523695
C	2.701698	0.329217	1.201754
H	3.771530	0.489917	1.362895
H	2.232511	0.324523	2.197328

M13O-OL2

SCF energy in gas phase: -1266.157753
 SCF energy in solution: -1266.446296
 Free energy in solution: -1266.126211

C	1.625958	0.049801	-1.478281
C	3.991174	1.003199	-1.243067
C	2.451772	1.142303	0.733366
C	3.853846	0.758032	0.260587
C	1.429018	0.433433	-0.132568
C	3.039945	0.110751	-2.043101
C	0.802647	1.162773	2.638791
C	2.230412	0.851330	2.218170
P	-0.149645	0.069888	0.437285
H	3.764196	2.057455	-1.447349
H	4.025477	-0.305044	0.480587
H	3.409003	-0.923586	-2.050166
H	0.529326	2.188361	2.352738
H	2.435738	-0.205289	2.431993
H	2.913210	1.457358	2.825577
H	2.969951	0.420074	-3.089682
H	5.023375	0.836410	-1.567224
H	4.602969	1.335679	0.815646
H	0.664319	1.055060	3.716418
H	2.363191	2.237251	0.613156
C	-0.675489	-1.642471	0.216933
C	-2.026601	-1.984612	0.277720
C	0.295993	-2.630618	0.046429
C	-2.403875	-3.320996	0.179060
H	-2.780279	-1.211339	0.395370
C	-0.086504	-3.961869	-0.057239
H	1.341350	-2.340858	-0.011432
C	-1.435441	-4.306688	0.011150
H	-3.453798	-3.590683	0.226590
H	0.665475	-4.731053	-0.198654
H	-1.732579	-5.347391	-0.072243
C	-1.534906	1.120342	-0.085519
C	-2.346721	1.734421	0.872805
C	-1.767428	1.334103	-1.450615

C	-3.390034	2.563578	0.468316
H	-2.161987	1.555626	1.927447
C	-2.813338	2.162837	-1.842133
H	-1.124523	0.847490	-2.179084
C	-3.622450	2.777147	-0.887291
H	-4.021039	3.039556	1.212101
H	-2.997884	2.330978	-2.898224
H	-4.436909	3.422577	-1.201118
O	-0.137650	0.243501	2.053492
O	0.704926	-0.408216	-2.186342

M13O-OL2-TS1

SCF energy in gas phase: -1267.291610

SCF energy in solution: -1267.580566

Free energy in solution: -1267.244574

C	1.754017	-1.318590	-1.202139
C	4.196475	-0.741546	-0.857799
C	2.489458	0.152122	0.776906
C	3.849845	-0.529556	0.611181
C	1.440109	-0.485065	-0.133643
C	3.193104	-1.705828	-1.479597
C	0.728228	0.796813	2.479378
C	2.072797	0.129798	2.251493
P	-0.226811	-0.006737	0.142675
H	4.157302	0.221425	-1.382902
H	3.819808	-1.505286	1.115962
H	3.349500	-2.719697	-1.089335
H	0.751551	1.842835	2.137255
H	2.009825	-0.910749	2.593199
H	2.835169	0.637081	2.855617
H	-0.416607	-0.043558	-1.787341
H	3.294897	-1.771334	-2.566269
H	5.215469	-1.125283	-0.967270
H	4.613360	0.071667	1.117870
H	0.453299	0.795149	3.537220
H	2.615427	1.213334	0.496385
H	0.007685	-0.818020	-2.000420
C	-1.591770	-1.200573	0.023482
C	-2.652296	-0.997275	-0.857754
C	-1.587863	-2.301876	0.879649
C	-3.711177	-1.897132	-0.883956
H	-2.639064	-0.141397	-1.526546
C	-2.637585	-3.214765	0.829998

H	-0.767852	-2.438395	1.576661
C	-3.699371	-3.010827	-0.046572
H	-4.539261	-1.735464	-1.566021
H	-2.626983	-4.083419	1.480069
H	-4.519247	-3.721358	-0.079236
C	-0.687570	1.725128	-0.216092
C	-1.690565	2.341263	0.536019
C	-0.000250	2.450082	-1.190652
C	-2.021806	3.671476	0.289350
H	-2.201589	1.779340	1.312316
C	-0.314402	3.785699	-1.414528
H	0.770331	1.952769	-1.774542
C	-1.331831	4.393686	-0.681101
H	-2.813556	4.145760	0.860296
H	0.225883	4.349267	-2.168101
H	-1.586477	5.432358	-0.866815
O	-0.306858	0.089211	1.801781
O	0.882860	-1.787231	-2.018019

M13O-OL2-Pr

SCF energy in gas phase: -1267.322914

SCF energy in solution: -1267.607859

Free energy in solution: -1267.264748

C	1.557219	-1.688909	-1.053246
C	4.039193	-1.503619	-0.741771
C	2.466027	-0.252026	0.790189
C	3.706607	-1.144183	0.700181
C	1.344337	-0.720304	-0.133515
C	2.894982	-2.323224	-1.322753
C	0.786933	0.751191	2.375672
C	1.995373	-0.156513	2.243394
P	-0.289334	0.095867	-0.057652
H	4.169701	-0.585645	-1.327926
H	3.517898	-2.068628	1.263548
H	2.891086	-3.337510	-0.903023
H	1.042082	1.759663	2.010571
H	1.728512	-1.157373	2.605312
H	2.816751	0.218995	2.866499
H	-0.390575	-0.007063	-1.513637
H	2.982675	-2.440175	-2.407939
H	4.976830	-2.063562	-0.803309
H	4.545928	-0.637652	1.188764
H	0.486121	0.852399	3.425066

H	2.755577	0.765755	0.478465	H	0.136057	-2.167131	1.811090
H	-0.253447	-1.882049	-1.684702	H	-0.371706	-0.080610	1.115979
C	-1.843133	-0.909040	0.046455	C	0.306950	1.857113	-0.047337
C	-2.654445	-0.962823	-1.091958	C	-0.077852	2.887018	-0.912114
C	-2.217779	-1.642546	1.179208	C	0.994317	2.163462	1.128334
C	-3.823704	-1.719691	-1.101002	C	0.162187	4.213235	-0.562388
H	-2.371037	-0.397160	-1.976757	C	1.260338	3.488021	1.459743
C	-3.371552	-2.419556	1.159952	C	0.826871	4.514493	0.623461
H	-1.598248	-1.592769	2.064984	C	-1.654287	-0.473236	-0.844403
C	-4.178899	-2.456130	0.024578	C	-2.653324	0.438192	-1.194548
H	-4.449683	-1.737346	-1.987270	C	-1.944400	-1.834089	-0.736933
H	-3.644811	-2.996717	2.037735	C	-3.947460	-0.012956	-1.427178
H	-5.081668	-3.058858	0.018150	C	-3.243245	-2.276530	-0.972715
C	-0.345601	1.926668	-0.280999	C	-4.243183	-1.369998	-1.311632
C	-0.989483	2.767702	0.630159	H	1.341304	1.358876	1.768881
C	0.238447	2.473659	-1.425192	H	1.807309	3.717913	2.368192
C	-1.055118	4.137708	0.389771	H	1.023317	5.548798	0.887228
H	-1.432987	2.335764	1.521385	H	-0.155165	5.010774	-1.226367
C	0.206482	3.846899	-1.646069	H	-4.724992	0.694777	-1.695620
H	0.716567	1.812570	-2.144780	H	-5.254920	-1.720880	-1.488367
C	-0.449692	4.679057	-0.741616	H	-3.472326	-3.332839	-0.881145
H	-1.574178	4.784409	1.090272	H	-1.170843	-2.539675	-0.455585
H	0.678419	4.266375	-2.528878	H	2.212876	1.250208	-2.333738
H	-0.492168	5.748852	-0.920942	C	-1.085986	-0.586989	2.229347
O	-0.316091	0.223907	1.676153	C	-2.393005	0.178583	2.124094
O	0.626528	-2.239683	-1.865584	H	-2.872136	0.135084	3.109026

M4O-OL2-TS2

SCF energy in gas phase: -1418.682048

SCF energy in solution: -1419.018083

Free energy in solution: -1418.671279

C	1.461538	-0.994078	-0.350337
C	3.161840	-2.483722	0.492078
C	3.573146	-1.269388	-1.555139
C	3.989787	-2.163456	-0.562866
C	2.318062	-0.709618	-1.435606
C	1.869862	-1.920749	0.643893
H	4.969828	-2.626703	-0.630010
H	3.465367	-3.193467	1.253538
H	4.206870	-1.030169	-2.402960
P	0.026201	0.107102	-0.512460
C	1.733866	0.263236	-2.430292
H	1.863791	-0.084790	-3.459247

H	0.136057	-2.167131	1.811090
H	-0.371706	-0.080610	1.115979
C	0.306950	1.857113	-0.047337
C	-0.077852	2.887018	-0.912114
C	0.994317	2.163462	1.128334
C	0.162187	4.213235	-0.562388
C	1.260338	3.488021	1.459743
C	0.826871	4.514493	0.623461
C	-1.654287	-0.473236	-0.844403
C	-2.653324	0.438192	-1.194548
C	-1.944400	-1.834089	-0.736933
C	-3.947460	-0.012956	-1.427178
C	-3.243245	-2.276530	-0.972715
C	-4.243183	-1.369998	-1.311632
H	1.341304	1.358876	1.768881
H	1.807309	3.717913	2.368192
H	1.023317	5.548798	0.887228
H	-0.155165	5.010774	-1.226367
H	-4.724992	0.694777	-1.695620
H	-5.254920	-1.720880	-1.488367
H	-3.472326	-3.332839	-0.881145
H	-1.170843	-2.539675	-0.455585
H	2.212876	1.250208	-2.333738
C	-1.085986	-0.586989	2.229347
C	-2.393005	0.178583	2.124094
H	-2.872136	0.135084	3.109026
H	-2.234284	1.230854	1.868461
H	-3.054404	-0.293669	1.397709
C	-0.169649	-0.083904	3.343487
H	-0.131932	1.006571	3.384345
H	-0.598062	-0.450945	4.282777
H	0.832691	-0.504172	3.244026
H	-2.431606	1.498332	-1.267176
H	-0.539254	2.644391	-1.863719
O	-1.142758	-1.855642	2.044090
O	0.352934	0.353785	-2.154932
O	1.199946	-2.326381	1.697578

M4O-OL3-TS2

SCF energy in gas phase: -1456.791337

SCF energy in solution: -1457.134737

Free energy in solution: -1456.779602

C	-1.980126	-0.173869	-0.417708
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C	-4.213539	-0.736975	0.292571	C	2.597144	0.896779	-1.343637
C	-3.916993	0.723449	-1.610600	H	3.670389	1.105543	-1.354048
C	-4.746471	0.048246	-0.707434	H	2.207237	1.153879	-2.337512
C	-2.553492	0.588344	-1.457327	O	-0.303883	0.567451	-2.121036
C	-2.816500	-0.888069	0.479115	O	-2.472442	-1.690209	1.460433
H	-5.825579	0.124081	-0.804351				
H	-4.848302	-1.288594	0.976870				
H	-4.328557	1.317220	-2.420340				
P	-0.183221	0.063011	-0.498194	M10O-OL2-TS2			
C	-1.527484	1.221040	-2.366322	SCF energy in gas phase:	-1421.084816		
H	-1.440094	2.299622	-2.159143	SCF energy in solution:	-1421.417836		
H	-1.465596	-1.977281	1.679504	Free energy in solution:	-1421.026277		
H	-0.037052	-0.375667	1.064288	C	-1.726748	-0.149353	-0.123637
C	1.122125	-1.126955	-0.839051	C	-3.955461	-0.127934	1.039831
C	2.384634	-0.592958	-1.142185	C	-3.897057	0.141978	-1.428458
C	0.923541	-2.499669	-0.701780	C	-4.606160	-0.548199	-0.270430
C	3.448532	-1.480723	-1.295403	C	-2.454289	-0.330739	-1.458683
C	1.997859	-3.366919	-0.876137	C	-2.435521	-0.028974	1.043722
C	3.258947	-2.854655	-1.165065	H	-4.525842	-1.634291	-0.400734
C	0.605361	1.588057	0.085839	H	-4.310126	0.865513	1.341848
C	1.922798	1.814432	-0.340838	H	-4.383149	-0.078754	-2.385225
C	-0.034961	2.472125	0.951904	P	0.041624	0.003917	-0.476864
C	2.587088	2.938400	0.151387	C	-1.571758	0.395015	-2.462449
C	0.634796	3.603416	1.408806	H	-1.793785	0.123364	-3.498947
C	1.951015	3.827315	1.014158	H	-1.681934	1.486372	-2.349309
H	-0.053888	-2.885866	-0.434236	H	-4.222202	-0.798896	1.861955
H	1.850928	-4.436231	-0.770276	H	-5.672972	-0.307137	-0.249550
H	4.102398	-3.526883	-1.286541	H	-3.923966	1.230634	-1.284869
H	4.436908	-1.089792	-1.521535	H	-2.444613	-1.395003	-1.743846
H	3.614240	3.122490	-0.152185	C	1.126639	-1.456657	-0.641659
H	2.486583	4.697936	1.379019	C	2.510197	-1.328671	-0.762245
H	0.136372	4.299121	2.075655	C	0.542328	-2.724984	-0.637596
H	-1.054367	2.265788	1.271063	C	3.306775	-2.468100	-0.860819
H	-1.792627	1.093929	-3.420126	H	2.968056	-0.342745	-0.777215
C	0.296906	-1.091346	2.255382	C	1.341955	-3.859508	-0.730902
O	-0.192828	-2.257987	2.077209	H	-0.536977	-2.821552	-0.546409
C	-0.410559	-0.145189	3.221201	C	2.725435	-3.732604	-0.839422
H	-0.233291	-0.530050	4.232055	H	4.383151	-2.364732	-0.955628
H	-0.010153	0.869071	3.158905	H	0.884921	-4.843916	-0.719578
H	-1.486856	-0.143461	3.042948	H	3.348340	-4.618341	-0.910698
C	1.808448	-0.960403	2.251306	C	0.858642	1.642025	-0.492140
H	2.131620	0.058661	2.017506	C	1.582619	2.040808	-1.621813
H	2.155677	-1.205271	3.261751	C	0.734515	2.508582	0.598004
H	2.251141	-1.670684	1.551720	C	2.203262	3.286105	-1.644718

SCF energy in gas phase: -1421.084816

SCF energy in solution: -1421.417836

Free energy in solution: -1421.026277

H	1.641634	1.376095	-2.476909	C	1.136243	-1.493127	-0.236296
C	1.336020	3.763720	0.555633	C	2.385348	-1.232857	-0.818059
H	0.190399	2.199525	1.485932	C	0.918534	-2.645140	0.514810
C	2.076409	4.149599	-0.559268	C	3.413565	-2.153095	-0.603936
H	2.776044	3.586440	-2.516321	C	1.948010	-3.563761	0.696261
H	1.229985	4.437485	1.399649	H	-0.058150	-2.815891	0.962215
H	2.551522	5.125432	-0.584222	C	3.199617	-3.309127	0.141652
O	-0.256850	-0.017873	-2.160689	H	4.393656	-1.961581	-1.032971
H	-1.068751	0.425102	2.605159	H	1.776579	-4.467202	1.272330
H	0.455012	-0.074675	1.089376	H	4.012953	-4.011840	0.291342
C	0.893295	-0.180239	2.511949	C	0.736258	1.354678	-0.619804
O	0.168793	0.679911	3.110076	C	2.032491	1.293080	-1.156752
C	2.365996	0.139251	2.372457	C	0.194718	2.559664	-0.176863
H	2.808852	0.017208	3.367785	C	2.772769	2.472345	-1.224041
H	2.872826	-0.538338	1.684131	C	0.944843	3.729230	-0.267661
H	2.504820	1.176438	2.063134	H	-0.799295	2.577615	0.258934
C	0.551217	-1.652406	2.680232	C	2.235416	3.680958	-0.784669
H	1.119385	-2.288474	1.999291	H	3.782312	2.443150	-1.625406
H	0.806171	-1.921065	3.711954	H	0.527934	4.668372	0.079837
H	-0.520243	-1.814466	2.542943	H	2.830934	4.586620	-0.842889
O	-2.053289	0.195677	2.274830	O	-0.284750	-0.560562	-2.093981

M100-OL3-TS2

SCF energy in gas phase: -1459.192837

SCF energy in solution: -1459.533884

Free energy in solution: -1459.132749

C	-1.930837	-0.304328	-0.212943
C	-4.235600	-0.029269	0.738935
C	-3.984556	-0.414414	-1.705495
C	-4.767286	-0.807543	-0.457522
C	-2.534042	-0.822894	-1.515955
C	-2.724260	0.113409	0.822848
H	-4.650274	-1.884791	-0.288582
H	-4.629176	0.994932	0.736139
H	-4.394582	-0.891009	-2.602504
P	-0.141069	-0.211452	-0.418040
C	-1.580889	-0.300102	-2.583367
H	-1.700284	-0.808120	-3.545469
H	-1.739495	0.781187	-2.731403
H	-4.559055	-0.467742	1.688228
H	-5.837652	-0.617092	-0.578185
H	-4.044289	0.672919	-1.850750
H	-2.473936	-1.922069	-1.540647

C	1.136243	-1.493127	-0.236296
C	2.385348	-1.232857	-0.818059
C	0.918534	-2.645140	0.514810
C	3.413565	-2.153095	-0.603936
C	1.948010	-3.563761	0.696261
H	-0.058150	-2.815891	0.962215
C	3.199617	-3.309127	0.141652
H	4.393656	-1.961581	-1.032971
H	1.776579	-4.467202	1.272330
H	4.012953	-4.011840	0.291342
C	0.736258	1.354678	-0.619804
C	2.032491	1.293080	-1.156752
C	0.194718	2.559664	-0.176863
C	2.772769	2.472345	-1.224041
C	0.944843	3.729230	-0.267661
H	-0.799295	2.577615	0.258934
C	2.235416	3.680958	-0.784669
H	3.782312	2.443150	-1.625406
H	0.527934	4.668372	0.079837
H	2.830934	4.586620	-0.842889
O	-0.284750	-0.560562	-2.093981
H	-1.471847	1.100180	2.208850
H	0.072025	-0.025358	1.163582
C	0.477628	0.542603	2.500312
O	-0.254094	1.574396	2.610805
C	1.960300	0.751078	2.279643
H	2.410344	0.908399	3.267050
H	2.437263	-0.120070	1.822130
H	2.130092	1.643426	1.674874
C	0.104036	-0.704223	3.290664
H	0.674196	-1.576361	2.965668
H	0.344130	-0.500779	4.340943
H	-0.967485	-0.897668	3.216919
O	-2.421217	0.684508	1.962675
C	2.612940	-0.007257	-1.683023
H	2.151815	-0.204714	-2.659408
H	3.686335	0.121104	-1.848657

M4CH₂-PL1

SCF energy in gas phase: -993.277579

SCF energy in solution: -993.440798

Free energy in solution: -993.320305

C	0.054569	-0.049500	-0.057765
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C	-1.826750	1.403077	0.076216
C	0.451775	2.315363	-0.004262
C	-0.958964	2.467395	0.075122
C	0.956126	1.039405	-0.069522
C	-1.366734	0.047444	-0.008309
H	-1.367863	3.472295	0.139468
H	-2.896016	1.580548	0.137110
H	1.104897	3.181023	-0.006213
P	0.924216	-1.545718	0.012403
C	2.419161	0.661274	-0.190993
H	0.874962	-2.418788	-1.090223
H	0.564144	-2.392006	1.075040
H	2.743987	0.796049	-1.228128
H	3.050073	1.301657	0.430304
P	-2.302416	-1.437935	-0.059632
H	-3.576905	-0.852793	0.151660
C	2.597471	-0.825204	0.214013
H	2.866543	-0.918362	1.269108
H	3.349251	-1.350353	-0.376681

M4CH₂-PL1-TS1

SCF energy in gas phase: -994.417520

SCF energy in solution: -994.569796

Free energy in solution: -994.435140

C	0.071023	-0.054038	0.012546
C	-1.801973	1.430705	0.075889
C	0.454334	2.331122	0.043116
C	-0.937848	2.507669	0.111530
C	0.959450	1.047742	0.007891
C	-1.337097	0.098294	-0.023916
H	-1.344727	3.513392	0.162513
H	-2.874713	1.601724	0.083414
H	1.121645	3.186854	0.006793
P	1.058107	-1.523770	0.281914
C	2.437226	0.705906	-0.053563
H	-1.255341	-2.078047	0.928772
H	-0.442327	-2.149560	1.286535
H	0.767336	-2.686057	-0.436560
H	1.674714	-1.880704	1.504053
H	2.966387	1.387189	-0.725426
H	2.891289	0.820659	0.938903
P	-2.407057	-1.324530	-0.299370
H	-3.524912	-0.798891	0.399327

C	2.545781	-0.755898	-0.517126
H	3.479786	-1.238431	-0.221996
H	2.429742	-0.822636	-1.602690

M4CH₂-PL1-Pr

SCF energy in gas phase: -994.462401

SCF energy in solution: -994.604034

Free energy in solution: -994.465424

C	0.117654	-0.035305	-0.031988
C	-1.771655	1.432618	0.035656
C	0.465611	2.352247	-0.042555
C	-0.912908	2.530049	0.001656
C	0.982523	1.059708	-0.050774
C	-1.273947	0.125479	0.010335
H	-1.329240	3.532729	0.023046
H	-2.843686	1.600288	0.092125
H	1.134764	3.208172	-0.060794
P	1.018939	-1.654141	-0.155370
C	2.460451	0.722739	-0.102579
H	-2.039350	-1.990730	1.093034
H	-0.232012	-2.314783	-0.570452
H	1.619561	-2.044220	-1.385108
H	1.201211	-2.653873	0.846945
H	2.800739	0.784877	-1.145219
H	3.043270	1.458719	0.461081
P	-2.483092	-1.280368	-0.049056
H	-3.486908	-0.577743	0.668243
C	2.597155	-0.700682	0.421983
H	2.602411	-0.698665	1.518866
H	3.502233	-1.208256	0.074214

M4NH-PL1

SCF energy in gas phase: -1009.313684

SCF energy in solution: -1009.484270

Free energy in solution: -1009.375419

C	0.054225	-0.030678	-0.064166
C	-1.784804	1.451017	0.092858
C	0.513968	2.314982	-0.032309
C	-0.886944	2.497336	0.069569
C	0.984077	1.020511	-0.093913
C	-1.354911	0.093047	-0.005997
H	-1.270676	3.511870	0.135914

H	-2.848108	1.656482	0.168477
H	1.187092	3.165080	-0.026122
P	0.888105	-1.544745	0.098148
C	2.430294	0.573711	-0.107388
H	0.807198	-2.522728	-0.907563
H	0.558500	-2.256731	1.260431
H	2.904694	0.813806	-1.066145
H	2.997213	1.065230	0.689427
P	-2.272726	-1.413961	-0.123199
H	-3.496961	-0.932906	0.408373
N	2.422418	-0.889156	0.104501
H	3.238005	-1.414973	-0.170465

M4NH-PL1-TS1

SCF energy in gas phase: -1010.457797

SCF energy in solution: -1010.621071

Free energy in solution: -1010.496660

C	0.086057	-0.066584	0.016894
C	-1.782493	1.422149	0.139680
C	0.469210	2.326118	0.035418
C	-0.921497	2.497918	0.165533
C	0.963075	1.042859	-0.020898
C	-1.329034	0.083937	-0.003512
H	-1.328679	3.501183	0.249198
H	-2.853915	1.594342	0.185152
H	1.133674	3.181478	-0.038188
P	1.084897	-1.520702	0.230851
C	2.420872	0.699389	-0.219907
H	-1.223942	-2.154811	0.897337
H	-0.436041	-2.254301	1.203011
H	0.773118	-2.604473	-0.593411
H	1.594315	-2.085485	1.422978
H	2.797286	1.184030	-1.127464
H	3.023771	1.054781	0.626189
P	-2.427780	-1.297051	-0.311239
H	-3.568621	-0.698753	0.284985
N	2.488418	-0.759769	-0.355809
H	3.376204	-1.168036	-0.092552

M4NH-PL1-Pr

SCF energy in gas phase: -1010.520279

SCF energy in solution: -1010.670754

Free energy in solution: -1010.543240

C	-0.123617	-0.016617	0.000626
C	1.845909	1.363860	0.009036
C	-0.338132	2.399309	-0.003753
C	1.047336	2.508314	0.011125
C	-0.905330	1.128077	-0.010972
C	1.273547	0.088075	-0.001520
H	1.515417	3.487810	0.018095
H	2.927257	1.471395	0.010594
H	-0.964378	3.287931	-0.007751
P	-1.137960	-1.622657	0.024166
C	-2.389225	0.842988	-0.022825
H	-2.873378	1.289572	0.856203
H	-2.857481	1.276952	-0.916628
P	2.326101	-1.432566	0.076824
N	-2.499969	-0.599581	-0.013967
H	-3.413986	-1.028479	-0.017510
H	2.240610	-1.808592	-1.288920
H	3.563026	-0.763274	-0.088463
H	-0.448156	-2.137923	1.156050
H	-2.079766	-2.735328	0.020242
H	-0.394425	-2.198673	-1.049289

M4O-PL1

SCF energy in gas phase: -1029.190511

SCF energy in solution: -1029.353439

Free energy in solution: -1029.255491

C	0.120568	-0.032476	-0.028603
C	1.299990	1.982248	0.005076
C	2.448505	-0.216676	0.002926
C	2.459759	1.187959	0.011218
C	1.212713	-0.861351	-0.019780
C	0.055472	1.347653	-0.006990
H	3.423534	1.689351	0.027031
H	1.391402	3.063450	0.013118
H	3.386276	-0.763642	0.021302
P	-1.466923	-0.794103	0.020072
C	0.744353	-2.309639	0.003343
H	-2.315102	-1.074772	-1.055969
H	-2.177147	-0.965778	1.211415
H	1.119143	-2.859202	-0.868532
H	1.110991	-2.818268	0.903865
P	-1.774057	1.711252	-0.103089

H	-1.946845	2.031385	1.271532
O	-0.678214	-2.330758	-0.010205

M4O-PL1-TS

SCF energy in gas phase: -1030.328492

SCF energy in solution: -1030.498314

Free energy in solution: -1030.386050

C	-0.081934	-0.079372	0.022334
C	1.762052	1.435668	0.133806
C	-0.509527	2.308979	0.044308
C	0.886000	2.494461	0.165470
C	-0.977699	1.020555	-0.015143
C	1.336606	0.079793	-0.005694
H	1.280621	3.502930	0.246520
H	2.829861	1.627938	0.175419
H	-1.182665	3.156922	-0.028550
P	-1.109480	-1.486778	0.225660
C	-2.422460	0.627708	-0.225009
H	-2.819076	1.046634	-1.152898
H	1.182600	-2.209564	0.986458
H	0.435972	-2.350146	1.275054
H	-3.064258	0.937048	0.607253
O	-2.480688	-0.806221	-0.340940
P	2.447378	-1.275238	-0.302120
H	3.609970	-0.592412	0.140023
H	-1.590884	-1.951856	1.461296
H	-0.863331	-2.614235	-0.556594

M4O-PL1-Pr

SCF energy in gas phase: -1030.394465

SCF energy in solution: -1030.556153

Free energy in solution: -1030.440793

C	0.129798	-0.047024	0.004099
C	-1.729021	1.455284	0.012642
C	0.526438	2.337084	-0.032632
C	-0.849094	2.537637	-0.019952
C	1.005017	1.031833	-0.009930
C	-1.260933	0.137242	0.018341
H	-1.249364	3.546900	-0.022936
H	-2.797892	1.645963	0.039301
H	1.212201	3.179459	-0.048754
P	1.033665	-1.640903	-0.100940

C	2.458313	0.608154	-0.012536
H	-2.156156	-1.900130	1.145278
H	-0.198769	-2.385076	-0.313998
H	1.506127	-2.039471	-1.365556
H	1.418505	-2.515726	0.930820
H	2.906051	0.845537	-0.992844
H	3.024643	1.163155	0.746394
O	2.502577	-0.756758	0.265510
P	-2.488772	-1.249018	-0.066723
H	-3.542466	-0.498989	0.512956

M7CH₂-PL1

SCF energy in gas phase: -1032.579935

SCF energy in solution: -1032.751546

Free energy in solution: -1032.602136

C	-1.555885	-0.047502	0.007322
C	-1.500316	2.398436	0.058287
C	0.609998	1.237048	-0.126760
C	-0.087698	2.419718	-0.049240
C	-0.124951	0.021061	-0.089496
C	-2.205573	1.225160	0.087649
C	2.829100	0.133339	0.504193
C	2.118462	1.253688	-0.260253
P	0.700150	-1.513058	-0.062906
H	-2.035842	3.341774	0.121599
H	-3.288132	1.243548	0.166662
H	2.540328	0.166452	1.560669
H	0.373977	-2.381048	-1.119794
H	0.323390	-2.278142	1.058404
H	3.912344	0.279160	0.460200
H	2.486610	2.222148	0.088993
H	2.394905	1.181048	-1.321950
P	-2.356207	-1.622260	0.009647
H	-3.663170	-1.134166	0.250179
H	0.446320	3.364381	-0.068057
C	2.504146	-1.244283	-0.086763
H	2.990042	-2.056025	0.460696
H	2.836376	-1.299353	-1.128350

M7CH₂-PL1-TS1

SCF energy in gas phase: -1033.711564

SCF energy in solution: -1033.872959

Free energy in solution: -1033.711137

C	1.516731	0.076951	-0.090616
C	1.325184	2.505889	-0.057277
C	-0.676476	1.192417	0.240160
C	-0.062685	2.427074	0.124499
C	0.125972	0.027683	0.155567
C	2.092233	1.362777	-0.165036
C	-2.783038	0.157435	-0.679933
C	-2.174809	1.067257	0.402373
P	-0.769792	-1.489766	0.475802
H	1.799862	3.479627	-0.133594
H	3.162799	1.441979	-0.330385
H	-2.570163	0.609489	-1.652582
H	0.694803	-1.820858	1.635743
H	-1.489300	-1.638162	1.679458
H	-0.223644	-2.673517	-0.036699
H	-3.870673	0.141175	-0.569196
H	-2.628821	2.060285	0.345106
H	-2.423800	0.675989	1.399124
P	2.448173	-1.463257	-0.311816
H	3.650748	-0.987523	0.269036
H	1.499089	-1.894499	1.141715
H	-0.662425	3.331426	0.167305
C	-2.231603	-1.289507	-0.659267
H	-1.904942	-1.594108	-1.657858
H	-2.998301	-2.003819	-0.339788

M7CH₂-PL1-Pr

SCF energy in gas phase: -1033.710159

SCF energy in solution: -1033.899856

Free energy in solution: -1033.733853

C	1.540681	0.039049	0.048944
C	1.428495	2.466230	-0.098663
C	-0.645008	1.213637	-0.047840
C	0.030755	2.423246	-0.082838
C	0.120295	0.014089	-0.059512
C	2.162966	1.301916	-0.009102
C	-2.980208	0.027461	-0.063564
C	-2.152264	1.290556	0.165385
P	-0.791127	-1.509481	-0.348552
H	1.936814	3.424811	-0.143610
H	-0.540945	3.347235	-0.064277
H	3.246951	1.346309	0.040287

H	-3.089910	-0.164630	-1.140121
H	1.441050	-1.987025	-1.075515
H	0.643512	-1.912853	-1.511348
H	-0.243034	-2.642011	0.263795
H	-1.475159	-1.779913	-1.558229
H	-3.991265	0.189249	0.321233
H	-2.552219	2.106040	-0.445362
H	-2.295777	1.598186	1.210100
C	-2.339563	-1.193802	0.600889
H	-2.988337	-2.073386	0.536116
H	-2.108881	-1.001747	1.654206
P	2.481893	-1.484349	0.316849
H	3.658818	-1.037112	-0.333921

M7NH-PL1

SCF energy in gas phase: -1048.626547

SCF energy in solution: -1048.793034

Free energy in solution: -1048.654253

C	-1.510343	-0.040185	0.017399
C	-1.689684	2.353173	0.043100
C	0.522107	1.358158	-0.108654
C	-0.299950	2.482357	-0.047007
C	-0.124117	0.118726	-0.062765
C	-2.307681	1.105056	0.071485
C	2.688180	0.206252	0.424998
C	2.026187	1.440787	-0.186680
P	0.602978	-1.547043	0.000363
H	-2.298407	3.251633	0.089498
H	0.148643	3.472338	-0.056434
H	-3.388894	1.027807	0.123984
H	2.466541	0.178318	1.506402
H	0.804391	-2.612387	-0.903711
H	0.631272	-2.063415	1.309459
H	3.774080	0.286886	0.323249
H	2.372711	2.347601	0.320205
H	2.332549	1.511103	-1.237270
N	2.235675	-0.996700	-0.269294
H	2.927829	-1.737547	-0.285450
P	-1.871907	-1.838848	-0.099295
H	-2.214692	-2.043007	1.267840

M7NH-PL1-TS1

SCF energy in gas phase: -1049.749719

SCF energy in solution: -1049.924201

Free energy in solution: -1049.770602

C	-1.539449	0.017261	-0.043561
C	-1.434887	2.449472	0.138675
C	0.642271	1.216149	0.035302
C	-0.033123	2.420230	0.091875
C	-0.116481	0.009512	0.058153
C	-2.162487	1.284797	0.044407
C	2.942603	0.006930	0.019700
C	2.136704	1.271176	-0.250917
P	0.836174	-1.466205	0.338054
H	-1.949809	3.403351	0.204198
H	0.530831	3.348212	0.057140
H	-3.246972	1.326197	0.010129
H	3.093809	-0.121399	1.107577
H	-1.369635	-2.032266	1.102781
H	-0.615151	-1.970772	1.518367
H	0.370519	-2.640842	-0.252111
H	1.436953	-1.675067	1.604260
H	3.932154	0.102051	-0.433044
H	2.582057	2.105882	0.299264
H	2.235986	1.500929	-1.318597
N	2.252698	-1.148349	-0.570519
H	2.862232	-1.958958	-0.640820
P	-2.473488	-1.492342	-0.341986
H	-3.683057	-1.023832	0.231663

M7NH-PL1-Pr

SCF energy in gas phase: -1049.801403

SCF energy in solution: -1049.965560

Free energy in solution: -1049.809007

C	-1.466308	0.091559	0.009139
C	-1.339313	2.509471	0.013665
C	0.707092	1.208487	0.016913
C	0.044950	2.438616	0.022494
C	-0.057276	0.024149	0.045470
C	-2.089791	1.340695	-0.015448
C	2.918518	-0.069184	0.191288
C	2.219945	1.253774	-0.079285
P	0.739015	-1.629810	0.193000
H	-1.837227	3.474194	0.012792
H	0.636202	3.350536	0.020708

H	-3.173527	1.401264	-0.059606
H	2.888445	-0.285222	1.280322
H	-0.483898	-2.143803	0.812472
H	0.628594	-2.626296	-0.818270
H	1.401911	-1.908201	1.427676
H	3.975403	0.011950	-0.080028
H	2.596395	2.032802	0.593009
H	2.464884	1.563836	-1.102436
N	2.255959	-1.092165	-0.594790
H	2.862150	-1.895718	-0.746202
P	-2.593585	-1.383850	0.036092
H	-3.553902	-0.783447	-0.821035
H	-2.005496	-2.127254	-1.017664

M7O-PL1

SCF energy in gas phase: -1068.504600

SCF energy in solution: -1068.677190

Free energy in solution: -1068.549896

C	-1.506253	-0.082143	0.012239
C	-1.756973	2.300755	0.026885
C	0.484557	1.377467	-0.106472
C	-0.370974	2.476909	-0.047802
C	-0.129315	0.124204	-0.081364
C	-2.341405	1.033967	0.056415
C	2.621957	0.211704	0.457548
C	1.989099	1.467213	-0.144169
P	0.649643	-1.504836	-0.061508
H	-2.393442	3.179912	0.069880
H	0.043998	3.481281	-0.046064
H	-3.419774	0.926776	0.113280
H	2.326089	0.123370	1.516923
H	0.873960	-2.389816	-1.125116
H	0.849780	-2.106898	1.193221
H	3.712944	0.278455	0.425063
H	2.327032	2.358499	0.395275
H	2.331354	1.563290	-1.181512
O	2.246619	-0.943075	-0.268349
P	-1.755688	-1.911108	-0.045316
H	-1.978370	-2.091564	1.348518

M7O-PL1-TS1

SCF energy in gas phase: -1069.629796

SCF energy in solution: -1069.808198

Free energy in solution: -1069.667206

C	-1.508729	0.050627	0.074539
C	-1.324881	2.489785	0.000674
C	0.688711	1.192027	-0.219168
C	0.074688	2.422046	-0.132991
C	-0.105756	0.013541	-0.150680
C	-2.084686	1.347754	0.105221
C	2.695096	0.042529	0.735076
C	2.191765	1.051436	-0.298001
P	0.834658	-1.456409	-0.424918
H	-1.809344	3.460456	0.049217
H	0.671263	3.328873	-0.153138
H	-3.159166	1.427091	0.240620
H	2.406865	0.367343	1.740104
H	-0.638006	-1.896800	-1.616822
H	1.481043	-1.637837	-1.657972
H	0.348994	-2.650453	0.097324
H	3.782669	-0.053902	0.691171
H	2.668679	2.018150	-0.114972
H	2.512459	0.730686	-1.299274
O	2.159744	-1.273712	0.525406
P	-2.448628	-1.456748	0.319615
H	-3.694463	-0.913391	-0.083180
H	-1.396639	-1.951647	-1.204807

M7O-PL1-Pr

SCF energy in gas phase: -1069.686381

SCF energy in solution: -1069.856938

Free energy in solution: -1069.711298

C	-1.459759	0.100835	0.011598
C	-1.303239	2.518352	0.023852
C	0.725615	1.193649	0.001215
C	0.080081	2.431777	0.016560
C	-0.050429	0.015416	0.030198
C	-2.067420	1.358407	0.000773
C	2.883225	-0.124607	0.226147
C	2.237599	1.209597	-0.100152
P	0.746537	-1.638984	0.136668
H	-1.790238	3.488571	0.031924
H	0.682269	3.336308	0.011517
H	-3.150541	1.433217	-0.027821
H	2.795427	-0.329383	1.310314

H	-0.474289	-2.196536	0.690146
H	0.688568	-2.526113	-0.958365
H	1.408759	-1.973312	1.344156
H	3.951842	-0.109130	-0.010201
H	2.636428	2.003044	0.541590
H	2.495605	1.472987	-1.133320
O	2.260549	-1.129721	-0.525674
P	-2.605608	-1.360795	0.057229
H	-3.615342	-0.715849	-0.703677
H	-2.100874	-2.069908	-1.060467

M10CH₂-PL1

SCF energy in gas phase: -995.687785

SCF energy in solution: -995.841227

Free energy in solution: -995.673902

C	0.092795	-0.144237	-0.157792
C	-1.985920	1.151147	0.237872
C	0.260672	2.309921	0.199230
C	-1.189608	2.348891	-0.289232
C	0.966881	1.080294	-0.368069
C	-1.298519	-0.184786	0.000566
H	-1.198846	2.340137	-1.386664
H	-2.120305	1.260478	1.322876
H	0.796194	3.221671	-0.088186
P	1.070642	-1.546811	-0.006967
H	1.166139	-2.558063	-0.991370
H	0.778765	-2.325776	1.132530
C	2.321806	0.771158	0.293552
H	3.110337	1.451898	-0.041086
H	2.212692	0.887417	1.377840
H	-2.986850	1.132400	-0.200134
H	-1.673686	3.278672	0.025999
H	0.270802	2.252065	1.296372
H	1.142195	1.259942	-1.443020
P	-2.128075	-1.713051	-0.027904
H	-3.364904	-1.241822	0.492668
C	2.699118	-0.690232	-0.021514
H	3.408545	-1.122346	0.686037
H	3.117064	-0.791675	-1.028479

M10CH₂-PL1-TS1

SCF energy in gas phase: -996.813750

SCF energy in solution: -996.959498

Free energy in solution: -996.778621

C	0.088992	-0.167345	-0.122174
C	-1.976797	1.214638	0.151341
C	0.301441	2.293311	0.377240
C	-1.128250	2.455607	-0.138036
C	0.933410	1.096417	-0.319407
C	-1.282299	-0.124510	-0.061141
H	-1.090162	2.626233	-1.221031
H	-2.286178	1.221735	1.206852
H	0.887649	3.199823	0.184971
P	1.194914	-1.537796	0.237979
H	-1.050882	-2.281884	0.837989
H	-0.187020	-2.292231	1.152333
H	1.096333	-2.717114	-0.508070
H	1.841107	-1.869700	1.464147
C	2.381869	0.790055	0.071383
H	3.073479	1.532368	-0.337852
H	2.483179	0.817654	1.166228
H	-2.900113	1.244286	-0.433706
H	-1.606760	3.335519	0.303176
H	0.298425	2.123196	1.462203
H	0.936340	1.310327	-1.400808
P	-2.281414	-1.595655	-0.234503
H	-3.368224	-1.141098	0.564020
C	2.666287	-0.626774	-0.439396
H	3.607792	-1.046451	-0.077071
H	2.654616	-0.649300	-1.534392

M10CH₂-PL1-Pr

SCF energy in gas phase: -996.854781

SCF energy in solution: -996.995084

Free energy in solution: -996.810749

C	0.139462	-0.104421	-0.172788
C	-1.987193	1.180562	-0.021474
C	0.205557	2.354772	0.312597
C	-1.161567	2.420797	-0.365586
C	0.971501	1.156809	-0.230629
C	-1.196404	-0.117725	-0.045249
H	-1.016767	2.476918	-1.451324
H	-2.415011	1.282594	0.985437
H	0.774992	3.275819	0.147810
P	1.196387	-1.642991	-0.142238

H	-1.802870	-2.181235	1.283200
H	-0.020631	-2.464798	-0.267839
H	1.796074	-2.449833	-1.164167
H	1.460270	-2.207105	1.133159
C	2.289092	0.828961	0.489138
H	3.013908	1.641849	0.370656
H	2.086454	0.725498	1.564637
H	-2.847286	1.091538	-0.697453
H	-1.711007	3.319552	-0.069517
H	0.075865	2.239441	1.397356
H	1.220952	1.357545	-1.285841
P	-2.262875	-1.634687	0.061238
H	-3.342440	-0.944188	0.677589
C	2.750355	-0.496785	-0.093431
H	3.549429	-0.981374	0.476897
H	3.110566	-0.354881	-1.121070

M10NH-PL1

SCF energy in gas phase: -1011.723776

SCF energy in solution: -1011.885517

Free energy in solution: -1011.729260

C	0.091982	-0.148586	-0.174606
C	-1.951528	1.169503	0.301143
C	0.306379	2.304213	0.158261
C	-1.163276	2.353177	-0.270138
C	0.981416	1.059066	-0.415262
C	-1.294148	-0.170716	0.016438
H	-1.220445	2.334131	-1.365885
H	-2.020959	1.278662	1.392366
H	0.836974	3.207486	-0.162463
P	1.082028	-1.531298	0.010311
H	1.347916	-2.529597	-0.956625
H	0.700315	-2.312975	1.116131
C	2.326390	0.712784	0.253426
H	3.171586	1.253026	-0.179763
H	2.273366	0.958275	1.320050
H	-2.974838	1.169305	-0.081403
H	-1.620749	3.291999	0.057342
H	0.358282	2.262707	1.254840
H	1.149911	1.219634	-1.493344
P	-2.131033	-1.690188	-0.073652
H	-3.331114	-1.264616	0.560686
N	2.574867	-0.745445	0.121818

H 3.257485 -1.004272 -0.580120

M10NH-PL1-TS1

SCF energy in gas phase: -1012.853575

SCF energy in solution: -1013.011526

Free energy in solution: -1012.840895

C 0.085664 -0.177528 -0.118556

C -1.947136 1.238805 0.175377

C 0.359123 2.280080 0.363788

C -1.078428 2.463620 -0.125986

C 0.949660 1.069023 -0.342017

C -1.288941 -0.117286 -0.054638

H -1.055625 2.635779 -1.209131

H -2.232145 1.247927 1.237520

H 0.954333 3.177416 0.156562

P 1.210778 -1.508486 0.243294

H -1.007491 -2.306332 0.816411

H -0.179060 -2.362614 1.111097

H 1.201621 -2.705958 -0.476483

H 1.784896 -1.745861 1.512550

C 2.392819 0.697813 0.029553

H 3.130726 1.355671 -0.436106

H 2.529738 0.767960 1.118220

H -2.881788 1.293943 -0.388807

H -1.533814 3.351178 0.324123

H 0.374055 2.113135 1.449081

H 0.942197 1.279540 -1.424378

P -2.311258 -1.561624 -0.240120

H -3.404895 -1.078084 0.531448

N 2.627545 -0.705134 -0.364602

H 2.655076 -0.763271 -1.382628

M10NH-PL1-Pr

SCF energy in gas phase: -1012.905772

SCF energy in solution: -1013.059094

Free energy in solution: -1012.884516

C 0.143413 -0.100189 -0.186738

C -1.988183 1.171225 -0.019839

C 0.206263 2.352510 0.317665

C -1.166933 2.418402 -0.352116

C 0.966602 1.161503 -0.243993

C -1.190729 -0.123113 -0.053288

H -1.027394 2.488438 -1.437667

H -2.416511 1.263267 0.987749

H 0.767757 3.279096 0.157188

P 1.232723 -1.609685 -0.132342

H -1.721768 -2.217598 1.243623

H 0.066511 -2.462861 -0.375316

H 1.956137 -2.361192 -1.104616

H 1.394240 -2.136548 1.163584

C 2.282907 0.781995 0.466200

H 3.065167 1.529514 0.300977

H 2.097969 0.737954 1.549544

H -2.847287 1.086131 -0.697597

H -1.718289 3.311433 -0.042761

H 0.083751 2.226207 1.402012

H 1.218426 1.367723 -1.297403

P -2.235871 -1.651007 0.052940

H -3.304809 -0.995773 0.721218

N 2.682127 -0.531899 -0.004954

H 3.138397 -0.456107 -0.912170

M10O-PL1

SCF energy in gas phase: -1031.592578

SCF energy in solution: -1031.758246

Free energy in solution: -1031.613742

C 0.087802 -0.141560 -0.216559

C -1.911434 1.214939 0.313754

C 0.379070 2.291650 0.161594

C -1.094152 2.383581 -0.249873

C 1.015820 1.035884 -0.437802

C -1.288702 -0.135677 0.008010

H -1.163581 2.381487 -1.344840

H -1.974433 1.312210 1.406430

H 0.927783 3.185676 -0.152701

P 1.046029 -1.537279 0.001133

H 1.343202 -2.542590 -0.935054

H 0.662308 -2.273207 1.137252

C 2.328637 0.619847 0.242609

H 3.217508 1.084800 -0.186054

H 2.282401 0.831879 1.317303

H -2.935803 1.245955 -0.064714

H -1.520383 3.330415 0.095450

H 0.440131 2.234042 1.256722

H 1.203653 1.207270 -1.508907

O	2.505897	-0.813133	0.067767
P	-2.135635	-1.652993	-0.077676
H	-3.288116	-1.250779	0.654723

M10O-PL1-TS1

SCF energy in gas phase: -1032.728177

SCF energy in solution: -1032.892538

Free energy in solution: -1032.733364

C	0.090392	-0.184643	-0.105139
C	-1.910372	1.257860	0.230859
C	0.411564	2.278223	0.331003
C	-1.037931	2.466569	-0.120753
C	0.963832	1.046429	-0.369004
C	-1.289887	-0.110685	-0.035170
H	-1.046069	2.617392	-1.207197
H	-2.132336	1.275171	1.307720
H	1.008647	3.164779	0.086839
P	1.203231	-1.508380	0.204933
H	-0.979828	-2.341135	0.811878
H	-0.180838	-2.426651	1.086668
H	1.190283	-2.682129	-0.549201
H	1.760414	-1.830181	1.463705
C	2.394210	0.652385	-0.010316
H	3.149713	1.219755	-0.556315
H	2.572591	0.773708	1.070644
H	-2.873114	1.331335	-0.280743
H	-1.470227	3.367172	0.325934
H	0.456010	2.133822	1.418654
H	0.942507	1.232319	-1.453405
O	2.540215	-0.728740	-0.370239
P	-2.336868	-1.521309	-0.242903
H	-3.445752	-0.996939	0.477417

M10O-PL1-Pr

SCF energy in gas phase: -1032.788690

SCF energy in solution: -1032.949563

Free energy in solution: -1032.786683

C	0.149014	-0.107760	-0.203207
C	-1.948198	1.208122	-0.008688
C	0.273891	2.339729	0.321151
C	-1.101840	2.438992	-0.339219
C	0.999787	1.135997	-0.256279

C	-1.183904	-0.105049	-0.053174
H	-0.968207	2.512698	-1.425062
H	-2.368577	1.303012	1.002046
H	0.854212	3.254171	0.160641
P	1.210735	-1.611720	-0.142687
H	1.895372	-2.284469	-1.175692
H	1.460145	-2.134353	1.143186
C	2.292764	0.697758	0.443618
H	3.119391	1.391236	0.257659
H	2.120117	0.657465	1.535475
H	-2.813161	1.145748	-0.681289
H	-1.632138	3.341122	-0.020142
H	0.155349	2.210487	1.405482
H	1.260450	1.337070	-1.306096
O	2.607167	-0.560519	-0.083414
P	-2.264351	-1.608275	0.055034
H	-3.322693	-0.929468	0.714701
H	-1.763196	-2.176007	1.250408
H	0.060750	-2.491363	-0.304419

M13CH₂-PL1

SCF energy in gas phase: -1034.982503

SCF energy in solution: -1035.146291

Free energy in solution: -1034.952414

C	1.456634	-0.290792	-0.201891
C	1.794088	2.131135	0.361050
C	-0.546485	1.264762	-0.286929
C	0.264064	2.314586	0.495694
C	0.064238	-0.105943	-0.067429
C	2.180153	0.981104	-0.584058
C	-2.883574	0.246013	-0.539111
C	-2.031288	1.359322	0.074885
P	-0.878992	-1.511082	0.192274
H	2.261962	3.055845	0.009845
H	-0.021866	2.234676	1.550530
H	3.261705	0.831875	-0.576189
H	-2.648816	0.144659	-1.605710
H	-0.649782	-2.237691	1.382119
H	-0.635809	-2.536126	-0.753598
H	-3.946748	0.495435	-0.468961
H	-2.407240	2.335619	-0.249283
H	-2.140057	1.327790	1.168878
P	2.222346	-1.830446	0.061538

H	3.534690	-1.430087	-0.295375
H	1.895183	1.247307	-1.611611
H	2.225038	1.914122	1.342938
H	-0.039328	3.313735	0.161215
H	-0.466278	1.516288	-1.358993
C	-2.659185	-1.092602	0.177452
H	-3.207796	-1.910405	-0.296958
H	-2.997038	-1.025640	1.215993

M13CH₂-PL1-TS1

SCF energy in gas phase: -1036.106178

SCF energy in solution: -1036.262898

Free energy in solution: -1036.054598

C	1.431830	-0.175693	-0.269764
C	1.671225	2.221087	0.358642
C	-0.635646	1.229274	-0.254230
C	0.141288	2.404906	0.381681
C	0.091178	-0.092191	-0.029925
C	2.105298	1.129597	-0.628287
C	-2.995315	0.194295	-0.442576
C	-2.079674	1.211467	0.256328
P	-0.917047	-1.456601	0.523084
H	2.166752	3.166291	0.118121
H	-0.197445	2.521413	1.417537
H	3.192098	1.010808	-0.628520
H	-3.286301	0.585494	-1.422879
H	0.481023	-1.768093	1.679043
H	-1.669102	-1.478593	1.724336
H	-0.510191	-2.731703	0.107379
H	-3.918773	0.105335	0.137829
H	-2.510514	2.213770	0.156361
H	-2.051733	1.008268	1.337178
P	2.330921	-1.729331	-0.172498
H	3.539488	-1.168683	0.319288
H	1.341989	-1.945461	1.236835
H	1.818395	1.416573	-1.650144
H	2.021494	1.922922	1.351556
H	-0.146093	3.322645	-0.143668
H	-0.664369	1.398635	-1.342984
C	-2.358552	-1.203006	-0.626863
H	-1.945482	-1.311161	-1.635653
H	-3.099135	-1.997900	-0.490431

M13CH₂-PL1-Pr

SCF energy in gas phase: -1036.134283

SCF energy in solution: -1036.284926

Free energy in solution: -1036.073650

C	1.382919	-0.143032	-0.155536
C	1.623046	2.306850	0.257141
C	-0.670506	1.207634	-0.192084
C	0.093503	2.384982	0.448181
C	0.060892	-0.101046	0.089035
C	2.028908	1.135258	-0.648698
C	-3.003200	0.165601	-0.450318
C	-2.122969	1.191045	0.285221
P	-0.943011	-1.581355	0.552683
H	2.011683	3.240797	-0.158712
H	-0.145880	2.396037	1.517174
H	3.119492	1.043366	-0.685689
H	-3.403887	0.614376	-1.366417
H	0.033376	-1.952003	1.594698
H	-1.955751	-1.535602	1.567580
H	-0.706634	-2.837722	-0.092173
H	-3.871296	-0.062341	0.178481
H	-2.550257	2.195101	0.185017
H	-2.114097	0.975642	1.362509
P	2.490729	-1.608169	-0.178455
H	3.457939	-1.092713	0.721501
H	1.846307	-2.415503	0.785738
H	1.697738	1.331254	-1.678178
H	2.110576	2.166320	1.226221
H	-0.303679	3.316413	0.031481
H	-0.666193	1.357951	-1.284587
C	-2.246170	-1.128777	-0.782325
H	-1.712324	-1.038117	-1.738165
H	-2.941423	-1.971489	-0.883609

M13NH-PL1

SCF energy in gas phase: -1051.018567

SCF energy in solution: -1051.191197

Free energy in solution: -1051.009063

C	1.429616	-0.291530	-0.220884
C	1.803592	2.136597	0.275236
C	-0.561558	1.272435	-0.238022
C	0.286397	2.290618	0.542310

C	0.044665	-0.106940	-0.073763	H	-3.955187	0.140666	-0.211153
C	2.138048	0.965556	-0.669823	H	-2.560858	2.166929	-0.018375
C	-2.875269	0.238914	-0.465970	H	-2.168604	1.029519	1.250795
C	-2.035407	1.345129	0.166326	P	2.328530	-1.728915	-0.206468
P	-0.901576	-1.516815	0.145911	H	3.562348	-1.174675	0.227046
H	2.214289	3.059158	-0.146069	H	1.303090	-1.959857	1.230530
H	0.082313	2.140055	1.608158	H	1.802277	1.434272	-1.635200
H	3.218549	0.813918	-0.710563	H	2.027524	1.919206	1.369119
H	-2.753725	0.251785	-1.558931	H	-0.184693	3.322182	-0.036565
H	-0.816019	-2.271336	1.334178	H	-0.603698	1.414660	-1.337893
H	-0.542975	-2.501989	-0.804219	N	-2.364348	-1.237323	-0.428802
H	-3.933925	0.398524	-0.245796	H	-2.256352	-1.697678	-1.325880
H	-2.441370	2.318933	-0.128244				
H	-2.127983	1.263827	1.256713	M13NH-PL1-Pr			
P	2.200412	-1.807781	0.158794	SCF energy in gas phase: -1052.187697			
H	3.452907	-1.523641	-0.444164	SCF energy in solution: -1052.350012			
H	1.800740	1.215925	-1.685272	Free energy in solution: -1052.151120			
H	2.324476	1.962102	1.220993				
H	-0.050878	3.303818	0.293686	C	1.383363	-0.115774	-0.166530
H	-0.511161	1.547749	-1.305842	C	1.582032	2.341685	0.256077
N	-2.510378	-1.060600	0.115223	C	-0.693985	1.206006	-0.206472
H	-3.205642	-1.790360	0.045771	C	0.049102	2.402611	0.423147

SCF energy in gas phase: -1052.187697

Free energy in solution: -1052.151120

M13NH-PL1-TS1

SCF energy in gas phase: -1052.151036

SCF energy in solution: -1052.318515

Free energy in solution: -1052.121279

C	1.435097	-0.180103	-0.273768
C	1.656262	2.217311	0.383996
C	-0.629114	1.225184	-0.252237
C	0.122320	2.382551	0.436837
C	0.092548	-0.098604	-0.020628
C	2.093944	1.137430	-0.617433
C	-2.920992	0.122359	-0.574456
C	-2.103329	1.188594	0.164744
P	-0.948305	-1.410585	0.543667
H	2.135696	3.169872	0.140074
H	-0.206220	2.437131	1.481047
H	3.181815	1.030557	-0.622727
H	-2.950067	0.387827	-1.637824
H	0.481764	-1.797075	1.657683
H	-1.611580	-1.325206	1.779459
H	-0.630608	-2.712904	0.151158

N -2.227798 -1.181435 -0.669307
H -1.889466 -1.223648 -1.628234

M13O-PL1

SCF energy in gas phase: -1070.899070

SCF energy in solution: -1071.070170

Free energy in solution: -1070.897514

C -1.317112 -0.543244 0.031199
C -2.299900 1.772622 0.256950
C 0.192596 1.487670 0.237976
C -0.984618 2.252174 -0.372338
C -0.093690 0.011842 0.114398
C -2.570704 0.282134 -0.013133
C 2.613472 0.884576 0.315766
C 1.579836 1.825390 -0.300979
P 1.090484 -1.356010 0.028553
H -2.241976 1.936274 1.340025
H -1.000607 2.081821 -1.456817
H -3.013827 0.141932 -1.008019
H 2.506412 0.887209 1.414047
H 1.552674 -2.157016 -1.029558
H 1.406025 -1.960364 1.254632
H 3.630374 1.216476 0.087660
H 1.828284 2.866215 -0.064609
H 1.613742 1.710994 -1.391203
O 2.494170 -0.427191 -0.202491
P -1.116678 -2.360865 -0.162877
H -1.470167 -2.695565 1.176723
H -3.306332 -0.116534 0.694829
H -3.140476 2.371153 -0.106485
H -0.858022 3.328431 -0.211001
H 0.214167 1.720642 1.315526

M13O-PL1-TS1

SCF energy in gas phase: -1072.027378

SCF energy in solution: -1072.201080

Free energy in solution: -1072.015816

C 1.418591 -0.189117 -0.296601
C 1.650296 2.190630 0.431821
C -0.624605 1.240161 -0.256863
C 0.116071 2.356544 0.501610
C 0.067367 -0.102579 -0.054073

C 2.078342 1.138078 -0.604313
C -2.835707 0.075742 -0.668778
C -2.114994 1.190068 0.084464
P -0.960883 -1.395244 0.540439
H 2.130425 3.147795 0.208811
H -0.211195 2.344910 1.547506
H 3.165564 1.030055 -0.618654
H -2.731367 0.236173 -1.748757
H 0.479172 -1.783431 1.641718
H -1.588503 -1.338742 1.798887
H -0.666239 -2.702855 0.166224
H -3.902769 0.071503 -0.426455
H -2.587382 2.146057 -0.165781
H -2.248268 1.056613 1.167808
O -2.329597 -1.230811 -0.373697
P 2.317354 -1.723468 -0.228072
H 3.570438 -1.152656 0.117804
H 1.282515 -1.947687 1.242437
H 1.781620 1.466088 -1.610678
H 2.029853 1.865506 1.405127
H -0.192323 3.323105 0.086913
H -0.553998 1.467572 -1.332448

M13O-PL1-Pr

SCF energy in gas phase: -1072.070330

SCF energy in solution: -1072.240546

Free energy in solution: -1072.050733

C 1.376566 -0.142176 -0.132772
C 1.585209 2.316724 0.271890
C -0.688289 1.194570 -0.213241
C 0.051072 2.386418 0.425581
C 0.048320 -0.108654 0.078468
C 2.021024 1.142101 -0.614467
C -2.931445 0.031593 -0.444479
C -2.140085 1.146378 0.257688
P -0.973320 -1.570266 0.467243
H 1.977893 3.249790 -0.141860
H -0.210792 2.413771 1.488958
H 3.112849 1.060541 -0.625042
H -3.329032 0.401025 -1.396529
H -1.964871 -1.477424 1.476829
H -0.848801 -2.750605 -0.293040
H -3.796234 -0.250894 0.178907

H	-2.626844	2.112489	0.085077	C	-4.076043	1.751272	-3.888728
H	-2.139218	0.995342	1.345505	H	-6.601730	-1.281118	0.822427
O	-2.136261	-1.091752	-0.737648	H	-5.916846	-2.765036	2.674008
P	2.502211	-1.592483	-0.152825	H	-3.597633	-2.654683	3.565744
H	3.461030	-1.056945	0.744049	H	-1.939317	-1.167156	2.485662
H	1.712406	1.326343	-1.652978	H	-1.024297	1.483418	-2.414289
H	2.050161	2.187306	1.253560	H	-2.073565	2.114349	-4.594473
H	-0.342516	3.308871	-0.013671	H	-4.541632	1.988075	-4.840297
H	-0.682286	1.327444	-1.306484	H	-5.945179	1.277296	-2.938349
H	-0.028046	-2.061650	1.456861	C	0.678231	-1.552997	0.756654
H	1.876802	-2.411885	0.812762	C	-1.308007	-2.870349	0.344230

M5OL3_dim1

SCF energy in gas phase: -2640.141749

SCF energy in solution: -2640.714560

Free energy in solution: -2640.079064

C	-0.678206	1.552834	0.756920	H	2.924835	-3.425709	2.334899
C	1.307998	2.870259	0.344584	O	3.106231	-2.032433	0.843381
C	-0.243610	3.617939	2.009432	C	1.054836	-2.549729	1.681056
C	0.936162	3.808730	1.280763	H	2.695048	-1.738040	2.857540
C	0.591406	1.656082	0.163841	C	-2.170224	-1.658187	-1.468621
N	1.282398	0.761939	-0.673054	C	-2.472922	-2.895566	-0.602744
P	-2.175212	0.680603	0.135578	H	-2.492031	-3.810257	-1.201531
C	-2.516738	2.454928	2.035252	H	-3.430558	-2.817489	-0.075140
H	-2.924726	3.425376	2.335484	C	3.340018	0.391116	1.045831
O	-3.106152	2.032391	0.843669	C	4.672532	0.372843	0.590128
C	-1.054751	2.549428	1.681500	C	2.964130	1.188395	2.124468
H	-2.695053	1.737578	2.857763	C	5.574849	1.258006	1.178673
C	2.170156	1.658382	-1.468474	C	3.894874	2.032898	2.727618
C	2.472931	2.895594	-0.602379	C	5.191736	2.088918	2.231729
H	2.492158	3.810372	-1.201014	C	2.909493	-1.137392	-1.456095
H	3.430534	2.817304	-0.074741	C	2.105198	-1.493754	-2.534609
C	-3.340050	-0.391230	1.045816	C	4.301293	-1.051382	-1.575246
C	-2.964230	-1.188700	2.124305	C	2.692209	-1.821405	-3.752693
C	-4.672567	-0.372936	0.590037	C	4.868053	-1.354929	-2.814505
C	-3.894966	-2.033375	2.727243	C	4.076105	-1.750498	-3.889045
C	-5.574853	-1.258303	1.178305	H	1.939196	1.166825	2.485758
C	-5.191775	-2.089409	2.231237	H	3.597552	2.654059	3.566233
C	-2.909530	1.137588	-1.455879	H	5.916829	2.764378	2.674728
C	-2.105183	1.494097	-2.534309	H	6.601754	1.280833	0.822882
C	-4.301330	1.051709	-1.575082	H	1.024314	-1.483254	-2.414581
C	-2.692144	1.822024	-3.752342	H	2.073673	-2.113643	-4.594884
C	-4.868041	1.355533	-2.814282	H	4.541722	-1.987054	-4.840662

H	5.945186	-1.276580	-2.938548	C	-1.803782	4.250863	-0.656981
H	0.585904	-4.361536	2.722301	H	-3.546314	4.322577	0.605803
H	-1.537907	-4.702310	1.425407	H	-0.090196	3.891420	-1.920321
H	1.537992	4.702039	1.426030	H	-1.632812	5.320986	-0.595529
H	-0.585778	4.361080	2.723012	C	-3.328798	-0.624442	0.785084
C	-5.193540	0.640490	-0.418702	C	-4.122627	0.376905	1.357659
H	-6.141477	0.272631	-0.823618	C	-3.132695	-1.856208	1.405327
H	-5.414460	1.550308	0.152988	C	-4.737814	0.097975	2.579715
H	1.614358	1.958185	-2.365559	C	-3.759240	-2.114369	2.617121
H	3.073810	1.154131	-1.802162	H	-2.471951	-2.586429	0.947350
H	-3.073943	-1.153909	-1.802099	C	-4.561438	-1.134023	3.200450
H	-1.614549	-1.957790	-2.365847	H	-5.349548	0.861159	3.052324
C	5.193495	-0.640390	-0.418819	H	-3.613144	-3.068045	3.112503
H	5.414423	-1.550351	0.152650	H	-5.042136	-1.326105	4.154307
H	6.141409	-0.272456	-0.823712	H	2.420477	-2.914429	-0.274408

M5OL3_dim2

SCF energy in gas phase: -2640.124079

SCF energy in solution: -2640.709622

Free energy in solution: -2640.079301

C	-1.617105	-1.379555	-1.717425	C	1.912141	3.580297	0.208794
C	-0.078004	-3.135844	-2.373898	C	0.208650	3.024210	1.843471
C	-2.028646	-2.728756	-3.726880	C	1.132781	3.952878	1.255567
C	-0.849438	-3.448670	-3.462784	C	1.814548	2.252267	-0.401610
C	-0.408953	-2.067364	-1.485130	H	1.177041	4.973150	1.633181
H	-0.546622	-4.258076	-4.121235	H	-0.466742	3.338901	2.633207
H	-2.649566	-2.969515	-4.583090	N	2.326774	2.153279	-1.594816
N	0.545750	-1.938382	-0.522533	P	1.149468	-0.491825	0.350693
P	-2.574087	-0.211695	-0.779825	C	-0.674076	0.620824	1.895880
C	-3.649372	-0.914706	-3.010251	C	2.865946	4.355380	-0.664218
C	1.224503	-3.748940	-1.927955	C	0.208257	1.736057	1.385507
C	-2.393065	-1.728175	-2.857311	C	2.938178	3.443941	-1.924359
C	1.388104	-3.155786	-0.523721	H	2.519905	5.369335	-0.888003
H	1.197729	-4.840584	-1.914279	H	-1.711092	0.959523	2.006770
H	-4.517112	-1.536056	-3.245555	H	-0.335924	0.268546	2.882844
H	-3.536964	-0.152434	-3.791022	H	3.850430	4.446199	-0.189043
H	2.043870	-3.433525	-2.584278	C	1.753460	-1.240526	1.915270
C	-2.200641	1.525146	-0.740096	C	3.031938	-0.911961	2.389999
C	-3.102335	2.315575	-0.005703	C	0.956180	-2.139948	2.629335
C	-1.133148	2.081708	-1.444286	C	3.481815	-1.494867	3.575923
C	-2.879513	3.688781	0.027939	C	1.420788	-2.720651	3.804776
C	-0.941110	3.457861	-1.405780	H	-0.040213	-2.356817	2.254617
H	-0.425651	1.458872	-1.986435	C	2.688100	-2.393680	4.280084

H	4.471608	-1.239915	3.945180	C	1.531257	0.200880	-2.709171
H	0.795093	-3.419512	4.351147	C	2.268113	2.876190	-2.943078
H	3.059272	-2.838163	5.198457	C	1.477243	0.824160	-3.949026
C	2.806196	-0.578054	-0.549142	H	1.236155	-0.839596	-2.600938
C	3.976907	-0.270778	0.152768	C	1.841481	2.165262	-4.060064
C	2.887422	-0.807199	-1.923532	H	2.560744	3.917509	-3.042751
C	5.199720	-0.230801	-0.518797	H	1.155642	0.267723	-4.823173
C	4.105483	-0.770158	-2.591692	H	1.796671	2.659933	-5.025226
H	1.977219	-0.991783	-2.491498	C	1.856907	1.420696	1.176585
C	5.269325	-0.483159	-1.884069	C	2.213199	2.726592	0.818693
H	6.104343	0.001680	0.037804	C	1.355728	1.124104	2.444325
H	4.144690	-0.944118	-3.662683	C	1.994764	3.742724	1.753297
H	6.227261	-0.450397	-2.394241	C	1.143691	2.146066	3.360025
H	3.970295	3.301032	-2.265315	H	1.136268	0.091013	2.699993
H	2.398278	3.899847	-2.769985	C	1.454978	3.459439	3.003244
O	-0.593765	-0.441320	0.968441	H	2.258103	4.764788	1.496189
C	3.905813	0.053565	1.628408	H	0.745479	1.926031	4.345105
H	4.910167	0.064492	2.062235	H	1.287051	4.265117	3.710714
H	3.489633	1.066400	1.738339	H	7.262635	0.829114	-0.712709

M5OL3_dim3

SCF energy in gas phase: -2640.123110

SCF energy in solution: -2640.714502

Free energy in solution: -2640.097006

C	3.434446	-0.929932	0.247519	C	-5.185222	2.994738	0.721666
C	5.729327	-1.635806	0.552655	C	-4.771059	0.612705	0.296354
C	3.894009	-3.247491	0.762682	H	-5.879215	3.809461	0.917424
C	5.292859	-2.904867	0.782644	H	-3.432412	4.316718	0.794629
C	4.805365	-0.554028	0.270473	N	-5.309377	-0.565762	0.161346
H	6.012775	-3.693202	0.992338	P	-2.086442	-0.122708	-0.021379
H	3.578274	-4.265990	0.958855	C	-1.398425	2.325913	0.303613
N	5.309284	0.630763	0.072808	C	-7.046229	1.129679	0.585584
P	2.093949	0.098522	-0.008523	C	-2.909854	2.269679	0.405265
C	1.480312	-2.349865	0.438114	C	-6.758899	-0.389211	0.332024
C	7.100360	-1.000915	0.518957	H	-7.543802	1.296026	1.546350
C	2.991965	-2.251168	0.497169	H	-0.918094	2.663674	1.228808
C	6.766926	0.497697	0.208913	H	-1.050933	2.950105	-0.525441
H	7.626452	-1.113263	1.472331	H	-7.691139	1.556492	-0.189403
H	1.033012	-2.660715	1.388783	C	-2.002966	-1.012198	-1.571134
H	1.129355	-3.017441	-0.354591	C	-2.420097	-2.350625	-1.608200
H	7.736110	-1.444556	-0.254132	C	-1.608546	-0.341111	-2.730119
C	1.948640	0.922763	-1.589915	C	-2.397218	-3.009312	-2.838468
C	2.338122	2.266393	-1.689572	C	-1.599394	-1.012788	-3.945403

H	-1.299293	0.699198	-2.672534	H	-3.563790	-2.923859	2.215981
C	-1.989312	-2.350599	-3.993675	H	-4.227726	-2.522383	-0.201580
H	-2.712389	-4.047604	-2.889108	N	-1.379613	-0.574810	-0.077869
H	-1.295662	-0.496005	-4.849757	H	-2.553445	-1.338142	-1.656304
H	-1.981327	-2.883120	-4.939431	H	-2.607853	-3.232055	-0.125732
C	-1.852751	-1.402160	1.211562	H	-3.649045	-1.182914	1.903628
C	-2.241901	-2.713456	0.913782	H	3.275255	-2.036470	2.392883
C	-1.320167	-1.065769	2.456295	N	2.815243	-2.590088	0.394649
C	-2.023533	-3.696148	1.883556	H	2.617589	-3.473209	-0.059031
C	-1.110205	-2.054447	3.408223	C	3.016770	-0.139201	0.794783
H	-1.075434	-0.028185	2.666368	C	2.606997	0.717201	1.822566
C	-1.453307	-3.374704	3.110365	C	4.380294	-0.156592	0.477388
H	-2.311694	-4.722024	1.672316	C	3.502381	1.573911	2.456405
H	-0.689396	-1.802830	4.376290	H	1.565332	0.726997	2.128562
H	-1.287595	-4.155063	3.846187	C	5.282137	0.704931	1.099827
H	-7.289472	-0.747148	-0.559745	H	4.754202	-0.882101	-0.239616
H	-7.115159	-1.002127	1.170403	C	4.843226	1.586885	2.083024
O	-0.901517	0.979443	0.044071	H	3.145007	2.239248	3.237156
C	-2.960478	-3.035281	-0.374912	H	6.332756	0.675474	0.824442
H	-2.986720	-4.116919	-0.530007	H	5.542746	2.260250	2.568721
H	-3.998779	-2.677861	-0.248353	C	0.803148	-2.520118	-1.367676
H	3.943398	2.677844	-0.383857	C	0.214745	-2.206987	-2.597828
H	2.895838	4.084970	-0.697054	C	0.445248	-3.768697	-0.825303

M6NHL2_dim1

SCF energy in gas phase: -2602.722119

SCF energy in solution: -2603.284598

Free energy in solution: -2602.581621

C	0.538411	-1.481336	1.133671	H	-0.644191	-5.605518	-1.014185
C	-1.649192	-2.007234	1.933836	H	-1.611505	-5.008740	-3.234242
C	0.315870	-2.867720	3.092229	C	0.358205	1.838645	-0.095456
C	-1.067450	-2.728860	2.967936	C	2.548147	2.267181	-1.056936
C	-0.841163	-1.306815	0.998298	C	1.619635	3.845396	0.517778
H	-1.722956	-3.250633	3.661350	C	2.636855	3.446204	-0.335235
H	0.740214	-3.504857	3.862816	C	1.468260	1.364800	-0.851074
P	1.766763	-1.289073	-0.166476	H	3.507840	4.079793	-0.485956
C	2.576030	-2.682737	1.853209	H	1.667636	4.793651	1.044816
H	2.756737	-3.711865	2.178877	P	-1.461829	1.357001	-0.035296
C	1.120473	-2.293597	2.120581	C	-0.861548	3.674849	1.011815
C	-2.667884	-1.115995	-0.588317	H	-0.833454	4.767827	0.978955
C	-3.117425	-2.106294	1.642068	C	0.458630	3.093200	0.540981
C	-3.200609	-2.347771	0.134586	C	2.582121	-0.196952	-2.423213
H	-3.456100	-0.354456	-0.507664	C	3.587531	1.999417	-2.119319

C	2.991247	1.063869	-3.155343	H	-3.381160	4.576230	-1.450741
H	3.497496	-0.609972	-1.974256	H	-4.174184	2.994978	-3.203989
H	3.892990	2.952902	-2.562028	P	-3.248760	-0.890600	-0.676811
H	3.711893	0.807667	-3.937119	C	-4.047661	0.150261	-2.957662
N	1.533387	0.047503	-1.388293	H	-3.361967	0.057485	-3.809433
H	2.217733	-0.952048	-3.119491	C	-3.597652	1.268920	-2.046612
H	2.119498	1.526052	-3.634372	C	-1.689684	2.085907	2.357082
H	4.484247	1.540723	-1.683762	C	-2.305377	4.082482	0.981550
H	-1.106466	3.384193	2.040130	C	-1.232912	3.467944	1.882697
N	-1.854972	3.134439	0.095829	H	-2.575338	2.209848	3.002544
H	-1.699714	3.580144	-0.808938	H	-1.951051	5.011129	0.520989
C	-2.335597	1.206116	1.599587	H	-1.026306	4.119200	2.738689
C	-1.665877	0.854246	2.772928	N	-1.984439	1.161001	1.269941
C	-3.707408	1.480691	1.659628	H	-0.911997	1.634082	2.986617
C	-2.362222	0.740321	3.975356	H	-0.290093	3.365238	1.329278
H	-0.598041	0.656722	2.758169	H	-3.172559	4.350650	1.600458
C	-4.405101	1.342481	2.854482	H	-5.053913	0.336639	-3.345820
H	-4.231005	1.814785	0.770393	N	-4.033636	-1.087117	-2.151416
C	-3.733435	0.966916	4.016764	H	-3.852376	-1.945414	-2.654948
H	-1.824551	0.463947	4.876676	C	-4.351875	-1.381511	0.664535
H	-5.471511	1.543250	2.880486	C	-5.642581	-1.822367	0.365339
H	-4.274556	0.867136	4.952276	C	-3.916048	-1.301962	1.994352
C	-2.204077	1.362630	-1.726019	C	-6.500559	-2.193253	1.397115
C	-3.402270	2.016276	-2.024876	H	-5.965944	-1.865368	-0.669901
C	-1.458907	0.784887	-2.752596	C	-4.784794	-1.669671	3.015940
C	-3.870234	2.042442	-3.336231	H	-2.920666	-0.923182	2.208155
H	-3.954907	2.522345	-1.240511	C	-6.071169	-2.117650	2.719041
C	-1.916210	0.837120	-4.066245	H	-7.503356	-2.538239	1.167791
H	-0.525640	0.296451	-2.495271	H	-4.456948	-1.604499	4.048197
C	-3.130585	1.452519	-4.358424	H	-6.741663	-2.405281	3.522730
H	-4.810752	2.535854	-3.559989	C	-1.815125	-1.979854	-0.610271
H	-1.324388	0.390649	-4.860445	C	-1.854741	-3.191276	0.089473
H	-3.495917	1.482006	-5.380118	C	-0.674686	-1.620794	-1.340042
M6NHL2_dim2				C	-0.746340	-4.033780	0.069220
SCF energy in gas phase: -2602.806860				H	-2.738152	-3.466455	0.657142
SCF energy in solution: -2603.377066				C	0.425473	-2.470921	-1.355399
Free energy in solution: -2602.689098				H	-0.646836	-0.676026	-1.880490
				C	0.393486	-3.671235	-0.644605
				H	-0.767733	-4.965572	0.624647
C	-3.014731	0.828020	-0.847610	H	1.320605	-2.185681	-1.897005
C	-2.728658	3.099237	-0.084517	H	1.272032	-4.307217	-0.631474
C	-3.728978	2.619188	-2.289502	C	2.834148	-0.997804	0.541856
C	-3.277452	3.505260	-1.280872	C	4.548479	-2.686302	0.349921
C	-2.542218	1.688164	0.190750	C	2.574443	-3.042385	1.787076

C	3.812737	-3.448246	1.226134	M6NHL2_dim3		
C	4.092563	-1.360861	-0.041857	SCF energy in gas phase: -2602.791660		
H	4.212021	-4.423519	1.504607	SCF energy in solution: -2603.369430		
H	2.029741	-3.685871	2.469633	Free energy in solution: -2602.682536		
P	2.024196	0.531444	0.349445			
C	0.796656	-1.177578	1.884106	C	2.862074	-0.870054
H	0.747908	-1.139732	2.979107	C	3.643144	-3.150512
C	2.098285	-1.799045	1.428379	C	2.325139	-2.375999
C	5.978726	-0.935701	-1.393215	C	3.035808	-3.370114
C	5.867497	-3.142464	-0.223707	C	3.580701	-1.836666
C	6.746073	-1.922845	-0.509221	H	3.100959	-4.371573
H	5.844832	-1.393764	-2.389555	H	1.867810	-2.608038
H	6.361076	-3.840905	0.461387	P	2.673834	0.793115
H	7.683454	-2.218717	-0.992141	C	1.582462	0.099337
N	4.697303	-0.518270	-0.849959	H	0.515409	-0.074715
H	6.592114	-0.040522	-1.559930	C	2.257762	-1.116443
H	6.999691	-1.430048	0.436910	C	4.762789	-2.512546
H	5.705943	-3.685446	-1.166287	C	4.385378	-4.219281
H	-0.056658	-1.769233	1.529676	C	4.274064	-3.934507
N	0.723485	0.182652	1.324484	H	5.848565	-2.468479
C	1.462398	0.956787	-1.319288	H	3.995941	-5.211807
C	2.034595	0.360374	-2.446752	H	4.846875	-4.663114
C	0.367035	1.814252	-1.449659	N	4.076508	-1.482098
C	1.473962	0.601637	-3.699332	H	4.637767	-2.293432
H	2.920948	-0.259268	-2.322878	H	3.222676	-4.016156
C	-0.190498	2.047226	-2.703175	H	5.447934	-4.214756
H	-0.078380	2.278899	-0.574012	H	2.041483	0.355198
C	0.360031	1.430863	-3.826058	N	1.747989	1.225338
H	1.910094	0.140434	-4.579915	H	0.916486	1.782385
H	-1.059782	2.691863	-2.789672	C	4.151133	1.833096
H	-0.075286	1.605086	-4.805662	C	4.330212	2.824307
C	2.871976	1.995860	0.990565	C	5.108573	1.628821
C	2.378698	2.612739	2.141894	C	5.467825	3.626202
C	4.010363	2.494741	0.345938	H	3.581245	2.954938
C	3.012031	3.746590	2.642867	C	6.243540	2.432047
H	1.505108	2.196218	2.635066	H	4.962630	0.824550
C	4.641570	3.621318	0.862695	C	6.420487	3.430864
H	4.401469	1.970950	-0.522950	H	5.610156	4.399662
C	4.140575	4.249870	2.002544	H	6.995423	2.277206
H	2.625699	4.232053	3.533384	H	7.308056	4.055107
H	5.529786	4.010920	0.375804	C	1.801367	1.152913
H	4.636397	5.132406	2.395029	C	1.645440	2.479527
H	-0.235457	0.514318	1.107825	C	1.287116	0.100658
				C	0.943527	2.755732

H	2.081375	3.290677	1.070666	C	0.085803	-2.813369	0.297214
C	0.593865	0.385610	3.167333	H	-0.232512	-1.296773	-1.182550
H	1.457156	-0.924157	1.676026	C	-1.342172	-2.709422	2.248459
C	0.419699	1.706722	3.576465	H	-2.793689	-1.111295	2.271470
H	0.813444	3.782431	3.144665	C	-0.307918	-3.318263	1.533154
H	0.195241	-0.429438	3.761735	H	0.895179	-3.273254	-0.262461
H	-0.118472	1.922035	4.494459	H	-1.660446	-3.119797	3.201615
C	-3.952105	0.730729	0.525980	H	0.186065	-4.195296	1.94001
C	-6.325771	0.345496	0.668497	H	-0.754904	1.669500	1.214320
C	-5.235374	2.133206	1.989437				
C	-6.368621	1.374363	1.575097	M12OL3_dim1			
C	-5.058031	-0.055962	0.071437	SCF energy in gas phase:	-1072.070330		
H	-7.337834	1.627925	2.003743	SCF energy in solution:	-1072.240546		
H	-5.338332	2.934568	2.712313	Free energy in solution:	-1072.050733		
P	-2.335480	0.488961	-0.014085				
C	-2.667123	2.401474	1.751253	C	0.690281	1.156383	1.349216
H	-2.374412	2.194758	2.788394	C	-1.220111	1.381508	2.942995
C	-4.019395	1.788352	1.448013	C	0.558251	3.143025	2.932903
C	-5.998608	-1.796402	-1.197329	C	-0.246630	2.190068	3.795402
C	-7.540765	-0.436951	0.237407	C	-0.552391	0.748848	1.706856
C	-7.117335	-1.855741	-0.152037	H	-0.807349	2.721929	4.571648
H	-6.416333	-1.391350	-2.135272	H	1.200370	3.795362	3.536045
H	-8.294202	-0.447120	1.033097	P	1.993923	0.067834	0.675978
H	-7.969327	-2.425315	-0.538100	C	2.662562	1.692674	2.654314
N	-4.840546	-1.020107	-0.787176	C	1.419962	2.329606	1.973399
H	-5.667528	-2.815727	-1.433370	C	-2.014263	-1.188465	1.876951
H	-6.744308	-2.378743	0.736930	C	-1.891184	0.319408	3.819383
H	-8.007551	0.042298	-0.634810	C	-2.825926	-0.544085	2.994399
H	-2.681926	3.488195	1.615844	H	-2.665291	-1.802268	1.255228
N	-1.682562	1.794943	0.824186	H	-1.112092	-0.313794	4.267573
C	-1.984822	0.718217	-1.772007	H	-3.647610	0.055547	2.587865
C	-2.311808	-0.287814	-2.689368	N	-1.252470	-0.262474	1.011737
C	-1.449091	1.931899	-2.213551	H	3.579514	2.225870	2.355251
C	-2.059714	-0.081981	-4.043203	H	2.574938	1.762125	3.746406
H	-2.795327	-1.193490	-2.332976	H	1.753337	2.998045	1.168203
C	-1.196657	2.125886	-3.569690	H	-1.300339	-1.881586	2.349084
H	-1.250568	2.716466	-1.487554	H	-3.269874	-1.336978	3.606697
C	-1.495277	1.115437	-4.481517	H	-2.413997	0.818828	4.643021
H	-2.311653	-0.856986	-4.759621	H	-2.016627	2.054693	2.603398
H	-0.777420	3.065725	-3.914529	H	0.433388	1.497413	4.309283
H	-1.300443	1.266908	-5.538510	H	-0.122272	3.793709	2.368938
C	-1.568640	-1.064100	0.500244	C	3.547491	0.736695	-0.018365
C	-0.547130	-1.683692	-0.219585	C	4.710308	-0.031496	0.145585
C	-1.975841	-1.585638	1.734006	C	3.604930	1.964367	-0.675789

SCF energy in gas phase: -1072.070330

SCF energy in solution: -1072.240546

Free energy in solution: -1072.050733

C	5.884759	0.410359	-0.468510	H	2.016900	2.056010	-2.602063
C	4.796267	2.418404	-1.233728	H	-0.432394	1.499714	-4.309244
H	2.706379	2.569005	-0.757154	H	0.122059	3.795252	-2.367583
C	5.932750	1.619333	-1.156907	C	-3.547304	0.737056	0.018636
H	6.784139	-0.194144	-0.382208	C	-4.710214	-0.030966	-0.145344
H	4.831595	3.380112	-1.735451	C	-3.604419	1.964377	0.676763
H	6.861976	1.944668	-1.613709	C	-5.884428	0.410605	0.469410
C	2.253017	-1.700797	1.019226	C	-4.795553	2.418197	1.235299
C	1.177823	-2.574169	1.143926	H	-2.705770	2.568860	0.758271
C	3.571107	-2.164353	1.123354	C	-5.932110	1.619246	1.158433
C	1.395249	-3.928549	1.377663	H	-6.783870	-0.193809	0.383109
H	0.175351	-2.178386	1.042114	H	-4.830630	3.379615	1.737593
C	3.771698	-3.530774	1.331574	H	-6.861150	1.944365	1.615765
C	2.698702	-4.407665	1.463648	C	-2.253330	-1.700191	-1.020097
H	0.549270	-4.601473	1.478353	C	-1.178299	-2.573708	-1.145110
H	4.788271	-3.910643	1.394105	C	-3.571516	-2.163485	-1.124367
H	2.884262	-5.464325	1.629137	C	-1.395937	-3.927962	-1.379411
O	2.719556	0.339215	2.292537	H	-0.175783	-2.178115	-1.043098
C	4.769921	-1.243604	1.055596	C	-3.772313	-3.529783	-1.333142
H	5.655924	-1.833468	0.801272	C	-2.699466	-4.406799	-1.465607
H	4.918449	-0.850501	2.069768	H	-0.550078	-4.600996	-1.480377
C	-0.690262	1.157155	-1.348910	H	-4.788942	-3.909486	-1.395808
C	1.220478	1.382983	-2.942188	H	-2.885243	-5.463344	-1.631580
C	-0.558124	3.144467	-2.931826	O	-2.719459	0.340324	-2.292588
C	0.247272	2.192030	-3.794466	C	-4.770155	-1.242567	-1.056033
C	0.552384	0.749650	-1.706627	H	-5.656253	-1.832393	-0.801956
H	0.808351	2.724499	-4.570045	H	-4.918681	-0.848838	-2.069957
H	-1.200329	3.796730	-3.534965				
P	-1.993923	0.068314	-0.676147	M12OL3_dim2			
C	-2.662378	1.693874	-2.653987	SCF energy in gas phase: -2723.540306			
C	-1.419840	2.330602	-1.972678	SCF energy in solution: -2724.135995			
C	2.013325	-1.188075	-1.877910	Free energy in solution: -2723.363052			
C	1.891915	0.321488	-3.819102				
C	2.825826	-0.543237	-2.994434	C	-3.442294	-0.038469	-1.181234
H	2.663426	-1.803337	-1.256626	C	-3.856946	-2.483447	-1.474107
H	1.112939	-0.310982	-4.268532	C	-5.640344	-0.858945	-2.184137
H	3.647710	0.055546	-2.587099	C	-5.315207	-2.053483	-1.292638
N	1.252184	-0.262225	-1.011959	C	-2.912321	-1.362165	-1.022182
H	-3.579365	2.227027	-2.354942	H	-5.978190	-2.892856	-1.533529
H	-2.574510	1.763623	-3.746038	H	-6.694525	-0.570425	-2.087021
H	-1.753351	2.998717	-1.167265	P	-2.960534	1.299561	-0.266913
H	1.298734	-1.879824	-2.351060	C	-5.391207	1.356076	-0.927973
H	3.269523	-1.335819	-3.607328	C	-4.737417	0.352756	-1.883471
H	2.415476	0.821555	-4.641868	C	-1.301531	-2.876030	-0.128416

C	-3.532905	-3.783515	-0.745841	H	4.656978	3.813949	-0.742473
C	-2.032128	-4.027728	-0.815296	H	2.757443	4.042934	0.847976
H	-0.234978	-2.932790	-0.362251	P	1.869231	-0.413007	0.653054
H	-3.841941	-3.694622	0.306223	C	1.182660	1.985648	0.968720
H	-1.723185	-4.078742	-1.867661	C	2.646860	1.950515	1.422818
N	-1.762641	-1.539594	-0.460557	C	5.788336	-0.929708	-1.232491
H	-6.100374	2.029202	-1.416326	C	5.940964	1.533526	-1.551270
H	-5.889158	0.827907	-0.103892	C	6.747107	0.247752	-1.410512
H	-4.547125	0.883870	-2.829132	H	6.351886	-1.824465	-0.938419
H	-1.368192	-3.000035	0.967149	H	5.260786	1.446376	-2.410682
H	-1.753173	-4.977718	-0.347232	H	7.399179	0.327509	-0.531249
H	-4.105830	-4.610818	-1.179892	N	4.717626	-0.729944	-0.273735
H	-3.685417	-2.641734	-2.551119	H	0.533924	2.564492	1.632008
H	-5.484105	-1.802207	-0.236693	H	1.112368	2.381975	-0.052814
H	-5.498097	-1.161226	-3.227481	H	2.659634	1.947697	2.524003
C	-1.740376	2.511781	-0.825634	H	5.334912	-1.170314	-2.208761
C	-1.435708	3.590835	0.014370	H	7.391978	0.079640	-2.279679
C	-1.132125	2.374395	-2.071172	H	6.585546	2.400343	-1.737223
C	-0.533081	4.552301	-0.437427	H	5.811623	1.986492	0.539139
C	-0.213308	3.328643	-2.501349	H	3.385056	2.667538	-1.180355
H	-1.382016	1.510704	-2.683902	H	4.194790	3.445528	1.666992
C	0.075367	4.421032	-1.685076	C	1.708818	-1.201406	-0.957982
H	-0.283905	5.396455	0.200450	C	2.120549	-2.532309	-1.107568
H	0.272435	3.223370	-3.466047	C	1.117521	-0.502895	-2.006320
H	0.789957	5.168688	-2.015130	C	1.956765	-3.137927	-2.351745
C	-2.540450	1.174628	1.480333	C	0.946131	-1.126243	-3.238247
C	-2.646296	-0.030073	2.174597	H	0.778012	0.517402	-1.845705
C	-2.136711	2.353521	2.127832	C	1.373269	-2.440427	-3.408195
C	-2.342020	-0.073218	3.530432	H	2.274850	-4.167674	-2.489867
H	-2.942357	-0.925126	1.637953	H	0.475038	-0.594143	-4.058638
C	-1.829074	2.288746	3.487028	H	1.240914	-2.932221	-4.367038
C	-1.928040	1.086285	4.182398	C	1.487993	-1.805078	1.735297
H	-2.414754	-1.011176	4.071574	C	0.752480	-1.622431	2.906153
H	-1.509777	3.189235	4.005093	C	1.939731	-3.078616	1.352712
H	-1.678813	1.056625	5.238746	C	0.460548	-2.714276	3.716934
O	-4.340486	2.187868	-0.388582	H	0.390833	-0.629727	3.157325
C	-2.071567	3.677684	1.385887	C	1.634913	-4.161081	2.177435
H	-1.536774	4.411802	1.995537	C	0.903677	-3.982679	3.349193
H	-3.098368	4.051305	1.266282	H	-0.113862	-2.578003	4.628104
C	3.176002	0.659776	0.836406	H	1.965368	-5.155865	1.891363
C	5.118733	1.750768	-0.284606	H	0.670781	-4.840847	3.972065
C	3.432690	3.180344	0.925627	O	0.660409	0.637056	0.972488
C	4.127999	2.913182	-0.408233	C	2.721521	-3.267450	0.068200
C	4.376108	0.465052	0.095345	H	2.810584	-4.333483	-0.157626

H	3.731201	-2.849670	0.208983	C	1.383435	1.962770	-0.875707
				C	2.128264	0.426976	-2.603224
M12OL3_dim3				C	1.127360	2.937694	-1.834961
SCF energy in gas phase: -2723.546477				H	1.216054	2.168530	0.178527
SCF energy in solution: -2724.142802				C	1.865223	1.412219	-3.556053
Free energy in solution: -2723.369626				C	1.360097	2.653815	-3.179459
				H	0.753812	3.912365	-1.535995
C	3.334797	-0.192473	1.131344	H	2.071370	1.206018	-4.602943
C	5.090192	1.463683	1.746798	H	1.160771	3.405921	-3.936378
C	3.445629	0.673118	3.499487	O	0.870419	-0.641121	1.078221
C	4.028309	1.884535	2.770205	C	2.798140	-0.867662	-2.989090
C	4.464342	0.550291	0.690267	H	3.859403	-0.741276	-2.720878
H	4.471784	2.577702	3.494945	H	2.740235	-1.014669	-4.071318
H	2.723883	0.989435	4.262927	C	-3.336249	-0.201216	-1.130626
P	2.111602	-0.545598	0.014012	C	-5.092909	1.451706	-1.751811
C	1.271723	-0.103683	2.362334	C	-3.449300	0.654364	-3.502286
C	2.784440	-0.330770	2.531794	C	-4.031872	1.868622	-2.777727
C	5.785190	1.424336	-1.094203	C	-4.465867	0.542950	-0.691974
C	5.772705	2.651167	1.073805	H	-4.476068	2.558665	-3.505006
C	6.654169	2.142154	-0.060749	H	-2.728414	0.967675	-4.267778
H	6.424372	0.889190	-1.808129	P	-2.111816	-0.546963	-0.012318
H	5.003885	3.322831	0.665391	C	-1.273925	-0.115757	-2.363409
H	7.394859	1.442453	0.346921	C	-2.786617	-0.344912	-2.530827
N	4.815176	0.486429	-0.557674	C	-5.785081	1.424441	1.090001
H	0.660702	-0.619850	3.108233	C	-5.775276	2.641807	-1.083312
H	1.029163	0.968600	2.379786	C	-6.655404	2.137399	0.054335
H	2.924145	-1.344817	2.937265	H	-6.423276	0.892444	1.807148
H	5.240978	2.179167	-1.686978	H	-5.006348	3.315628	-0.678678
H	7.206224	2.958658	-0.538169	H	-7.396218	1.435653	-0.349585
H	6.346491	3.226752	1.808964	N	-4.815533	0.484373	0.556535
H	5.858305	0.880123	2.279204	H	-0.663154	-0.635171	-3.107226
H	3.231503	2.432278	2.248086	H	-1.032222	0.956624	-2.386388
H	4.259239	0.168378	4.032078	H	-2.925753	-1.360766	-2.931951
C	1.965881	-2.082419	-0.915830	H	-5.240353	2.182128	1.678658
C	2.298299	-2.104857	-2.277950	H	-7.207307	2.955766	0.528736
C	1.584503	-3.251373	-0.254592	H	-6.350044	3.213879	-1.820436
C	2.213857	-3.319549	-2.960740	H	-5.861200	0.865671	-2.281235
C	1.520825	-4.454727	-0.946214	H	-3.234877	2.418749	-2.258390
H	1.313851	-3.205484	0.796600	H	-4.263162	0.146923	-4.031913
C	1.830983	-4.484832	-2.304305	C	-1.860529	0.716597	1.254077
H	2.457899	-3.349728	-4.019255	C	-2.128143	0.440008	2.599649
H	1.225452	-5.362412	-0.429659	C	-1.386693	1.967233	0.863128
H	1.775201	-5.418780	-2.854811	C	-1.866347	1.431089	3.546738
C	1.859452	0.710744	-1.259354	C	-1.131704	2.947982	1.816704

H	-1.220291	2.167240	-0.192367
C	-1.363421	2.671373	3.162910
H	-2.071604	1.230418	4.594876
H	-0.759826	3.921513	1.512023
H	-1.164981	3.428044	3.915497
C	-1.963029	-2.078517	0.925740
C	-1.579885	-3.250443	0.270844
C	-2.294110	-2.093830	2.288301
C	-1.513358	-4.449756	0.969218
H	-1.309926	-3.209875	-0.780750
C	-2.206823	-3.304495	2.977861
C	-1.822363	-4.472764	2.327696
H	-1.216507	-5.359756	0.457601
H	-2.449864	-3.329151	4.036750
H	-1.764480	-5.403486	2.883427
O	-0.871252	-0.646417	-1.076932
C	-2.795320	-0.853654	2.993294
H	-2.735717	-0.994737	4.076216
H	-3.857154	-0.730646	2.725834