Supplementary Information

Mechanistic study and computational prediction of iron, cobalt and manganese cyclopentadienone complexes for hydrogenation of carbon dioxide

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1. Computational Details

All DFT calculations in this study were performed by using the Gaussian 09 suite of programs[1] for the M06 functional[2] with the all-electron 6-31++G(d,p) basis set[3-5] for all atoms. All structures studied in this paper were fully optimized in water (ε = 78.3553) by using the integral equation formalism polarizable continuum model (IEFPCM)[6] with SMD[7] atomic radii solvent effect corrections. An ultrafine integration grid (99,590) was used for numerical integrations. The ground states of intermediates and transition states were confirmed as singlets through comparison with the optimized high-spin analogs. Thermal corrections were calculated within the harmonic potential approximation on optimized structures under T = 298.15 K and 1 atm pressure. Unless otherwise noted, the energies reported in the text are Gibbs free energies with solvent effect corrections. Calculating the harmonic vibrational frequencies for optimized structures and noting the number of imaginary frequency (IF) confirmed the nature of intermediate (no IF) and transition state (only one IF) structures. The latter were also confirmed to connect reactants and products by intrinsic reaction coordinate (IRC) calculations. The 3D molecular structure figures displayed in this paper were drawn by using the JIMP2 molecular visualizing and manipulating program[8]. The electrostatic potential maps shown in Figure S1 were drawn by using Molekel 4.3[9].

2. Evaluation of density functionals

In order to evaluate the dependency of the metal cyclopentadienone complexes to density functionals, we also calculated the relative energies between $\mathbf{TS_{5,6\text{-}Fe}}$ and $\mathbf{2_{Fe}'}$ in the reaction catalysed by $\mathbf{1_{Fe}}$, and the relative energies between $\mathbf{TS_{5,6\text{-}Co\text{-}a}}$ and $\mathbf{1_{Co\text{-}a}}$ in the reaction catalysed by $\mathbf{1_{Co\text{-}a}}$ using other eight widely-used and/or recently developed density functionals, including ωB97X-D[10], B3LYP[11, 12], B3PW91[13-15], HSE06[16, 17], PBEh1PBE[18], TPSSh[19], M06L[2], and TPSS[19]. All structures were independently optimized using these functionals with the same basis set. The calculation results are listed in Table S1 and S2. In general, pure functionals without Hartree-Fock exchange (M06L and TPSS) have obviously lower barriers. For the reaction catalysed by $\mathbf{1_{Fe}}$, the ωB97X-D functional has the highest free energy barrier of 30.0 kcal/mol, while the M06L functional has the lowest free energy barrier of 20.8 kcal/mol. For the reaction catalysed by $\mathbf{1_{Co\text{-}a}}$, the PBEh1PBE functional has the highest free energy barrier of 24.4 kcal/mol, while the TPSS functional has the lowest relative energy of 17.8 kcal/mol. Such results indicate that both the Fe and Co complexes have a moderate dependence of density functionals. The M06 results of 25.4 kcal/mol for $\mathbf{1_{Fe}}$ and 20.0 kcal/mol for $\mathbf{1_{Co\text{-}a}}$ are in the middle of them. Therefore, we believe the M06 functional is suitable for the study of this based catalytic system. In addition, it is worth to note that no matter which functional is used, $\mathbf{1_{Co\text{-}a}}$ always has a lower barrier than $\mathbf{1_{Fe}}$ for hydrogenation of CO_2.

Table S1. Absolute and relative free energies of rate-limiting states $\mathbf{2_{Fe}'}$ and $\mathbf{TS_{5,6\text{-}Fe}}$ obtained using different density functionals.

Density functionals	Absolute free energies (Hartree)		Total barriers (kcal/mol)
	$\mathbf{2_{Fe}'}$	$\mathbf{TS_{5,6\text{-}Fe}}$	$\mathbf{2_{Fe}'}\rightarrow\mathbf{TS_{5,6\text{-}Fe}}$
M06	-2920.547775	-2848.117626	25.4
ωB97X-D	-2921.022086	-2848.457731	30.0
B3LYP	-2921.383362	-2847.944322	28.7
B3PW91	-2920.83684	-2846.881292	27.3
HSE06	-2919.750637	-2846.907955	28.6
PBEh1PBE	-2919.777343	-2848.117626	28.7
TPSSh	-2921.472108	-2848.548697	25.7
TPSS	-2921.650806	-2848.721028	21.2
M06L	-2921.198186	-2848.268698	20.8

Table S2. Absolute and relative free energies of rate-limiting states $\mathbf{1}_{\mathbf{Co\text{-}a}}$ and $\mathbf{TS}_{\mathbf{5,6\text{-}Co\text{-}a}}$ obtained using different density functionals.

Density functionals	Absolute free energies (Hartree)		Total barriers (kcal/mol)
	$\mathbf{1}_{\mathbf{Co\text{-}a}}$	$\mathbf{TS}_{\mathbf{5,6\text{-}Co\text{-}a}}$	$\mathbf{1}_{\mathbf{Co\text{-}a}} \rightarrow \mathbf{TS}_{\mathbf{5,6\text{-}Co\text{-}a}}$
M06	-2827.220085	-2942.828032	20.0
ωB97X-D	-2827.643823	-2943.280862	22.9
B3LYP	-2827.946324	-2943.622994	23.0
B3PW91	-2827.483819	-2943.109842	26.3
HSE06	-2826.513527	-2942.061656	23.8
PBEh1PBE	-2826.537048	-2942.086321	24.4
TPSSh	-2828.018921	-2943.696014	21.5
TPSS	-2828.174331	-2943.869758	17.8
M06L	-2827.764667	-2943.424317	18.4

3. Electrostatic potential map analysis

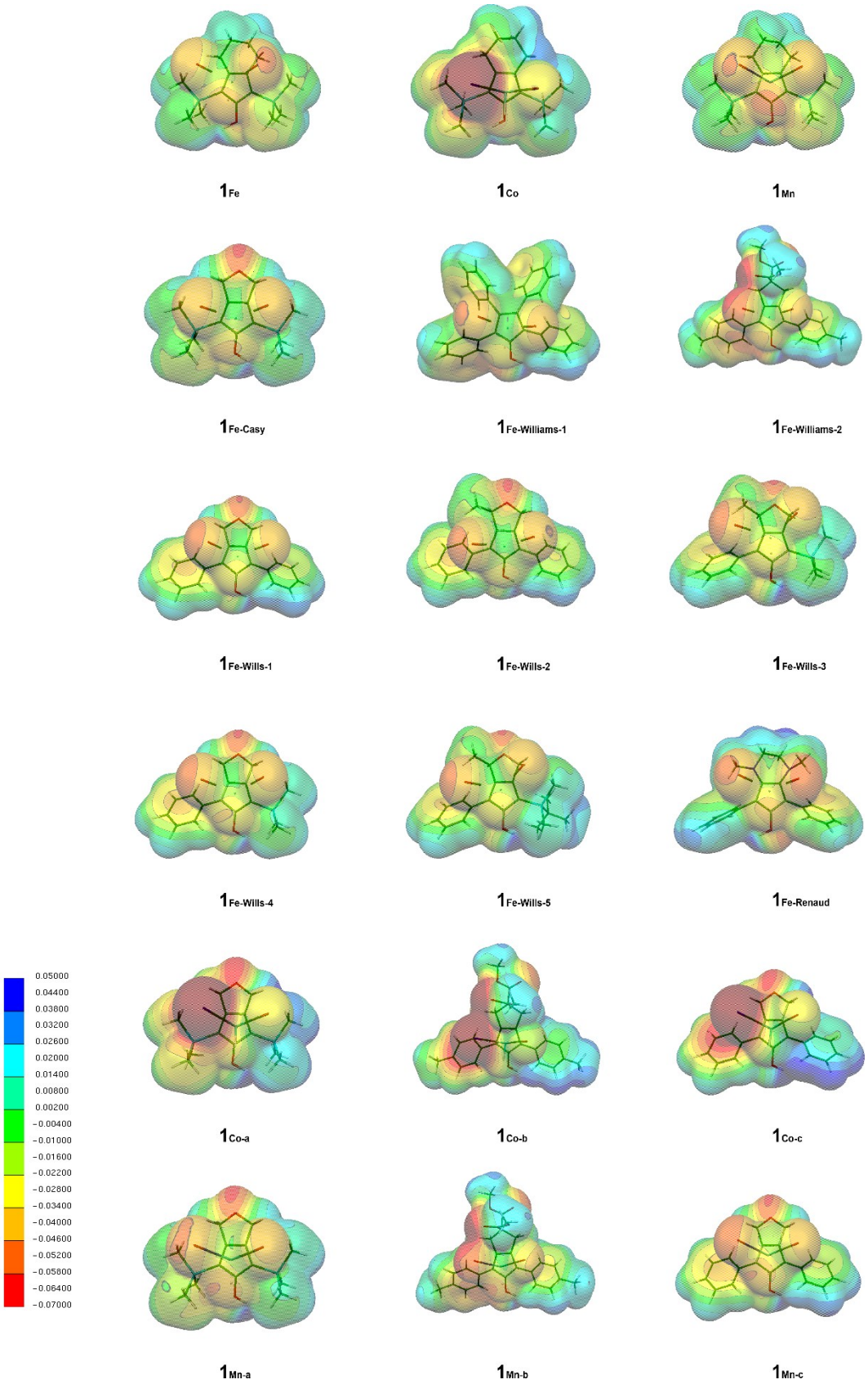

Fig. S1 Electrostatic potential maps of all metal complexes shown in Fig. 1

4. Absolute free energies (Hartree) and Cartesian coordinates (Ångström) of all structures optimized in water

1Co-a Gsolv= -2827.220085

C	-0.023977	1.264376	0.080647
O	-0.129224	2.450400	-0.543583
C	-1.202890	0.518898	0.418249
C	-0.705628	-0.599519	1.179295
C	0.693974	-0.577893	1.193357
C	1.177104	0.558245	0.440229
Si	-2.988485	1.051268	0.077192
C	-3.274835	2.685328	0.972414
H	-4.014562	2.567885	1.774102
H	-3.653236	3.444607	0.276320
H	-2.354507	3.074586	1.423762
C	-4.105613	-0.287212	0.759543
H	-3.922603	-0.455326	1.828939
H	-3.970151	-1.238964	0.230176
H	-5.155548	0.013060	0.647375
C	-3.229384	1.266347	-1.767198
H	-3.130135	0.311602	-2.298264
H	-2.500087	1.970926	-2.186609
H	-4.232499	1.665210	-1.967350
Si	2.981921	1.053705	0.123175
C	3.276733	2.659274	1.042596
H	4.311574	2.998073	0.905908
H	3.097588	2.539890	2.118198
H	2.614474	3.455160	0.676578
C	4.064032	-0.327039	0.766687
H	5.119711	-0.064013	0.621321
H	3.883129	-1.268805	0.232661
H	3.909322	-0.499716	1.839272
C	3.213043	1.304425	-1.719368
H	4.201623	1.738000	-1.918682
H	2.461808	1.984729	-2.142004
H	3.147972	0.354187	-2.264161
C	-1.333683	-1.818733	-1.364372
C	1.260417	-1.695159	-1.463427
O	2.052285	-2.356811	-1.965711
H	-0.039502	-0.022940	-2.082965
C	1.184614	-1.741288	1.987221
O	0.013348	-2.562823	2.124190
C	-1.178698	-1.775422	1.960705
H	1.541364	-1.410968	2.976146
H	1.970326	-2.338986	1.513092
H	-1.935422	-2.394784	1.467517
H	-1.566835	-1.457015	2.941529
H	0.734312	2.824175	-0.775775
N	-2.167650	-2.554858	-1.743371
Co	0.013512	-0.675188	-0.751010

1Co-a-triplet state Gsolv= -2827.180650

Co	-0.063461	-0.803303	-0.802156
C	0.032888	1.267417	-0.060806
O	-0.035123	2.421556	-0.738218
C	-1.189681	0.653311	0.429629
C	-0.726583	-0.390203	1.242060
C	0.704297	-0.450078	1.204334
C	1.225969	0.601370	0.423230
Si	-2.955597	1.167001	0.006223
C	-3.261239	2.897631	0.660708
H	-3.095698	2.946937	1.744178
H	-4.299754	3.195243	0.464816
H	-2.604997	3.634592	0.181751
C	-4.100342	-0.054242	0.845516
H	-3.943381	-0.067513	1.932009
H	-3.959351	-1.072891	0.462052
H	-5.145708	0.227726	0.664554
C	-3.146154	1.129291	-1.858135
H	-3.002087	0.114401	-2.250788
H	-2.414345	1.789118	-2.341566
H	-4.148364	1.467879	-2.151565
Si	3.037571	1.028416	0.100034
C	3.372056	2.671418	0.936676
H	4.409397	2.989906	0.772353
H	3.200656	2.610968	2.018550
H	2.714061	3.454106	0.535552
C	4.076132	-0.350747	0.817773
H	5.139493	-0.131821	0.655508
H	3.858933	-1.310858	0.331652
H	3.920914	-0.465286	1.897845

C	3.341229	1.188617	-1.744120
H	4.378379	1.506630	-1.915468
H	2.690353	1.935616	-2.217411
H	3.193695	0.234362	-2.265592
C	-1.591140	-2.157261	-1.148942
C	1.289640	-1.937982	-1.433842
O	2.113361	-2.594438	-1.880357
H	0.326150	0.047607	-2.010116
C	1.144246	-1.570632	2.083846
O	-0.062813	-2.317227	2.310364
C	-1.215081	-1.476872	2.133338
H	1.538868	-1.182873	3.037069
H	1.886293	-2.247828	1.647413
H	-2.027641	-2.089566	1.727874
H	-1.539162	-1.060418	3.101047
H	0.829734	2.698116	-1.078332
N	-2.457350	-2.925163	-1.356382

1Co-b Gsolv= -2969.987846

Co	0.068559	-0.623900	1.004918
H	0.133466	-1.846471	1.832906
H	1.083943	-3.598038	-0.694865
C	0.132273	-1.936386	-0.644546
O	0.168623	-3.273693	-0.688546
C	-1.098682	-1.199289	-0.592344
C	-0.725855	0.187274	-0.735413
C	0.669792	0.287888	-0.761984
C	1.246120	-1.027627	-0.634318
C	-1.367608	-0.162279	2.118692
C	1.337802	-0.051510	2.090671
O	2.195734	0.244647	2.793447
C	-2.457947	-1.754766	-0.544652
C	-3.474883	-1.172215	-1.309792
C	-2.771244	-2.853262	0.264419
C	-4.769388	-1.679789	-1.267992
H	-3.249017	-0.325832	-1.956752
C	-4.066807	-3.355018	0.299557
H	-1.998736	-3.302722	0.885963
C	-5.089121	-2.776681	-0.461612
H	-5.547923	-1.218005	-1.874377
H	-4.295435	-4.208008	0.937451
C	2.676372	-1.375428	-0.655719
C	3.525574	-0.745067	-1.572467
C	3.217935	-2.325983	0.219669
C	4.878812	-1.063913	-1.614557
H	3.121476	-0.004849	-2.261690
C	4.570142	-2.643725	0.165585
H	2.579368	-2.796604	0.968163
C	5.423315	-2.021152	-0.752376
H	5.527338	-0.561359	-2.331096
H	4.977683	-3.377942	0.859424
C	-6.491805	-3.297044	-0.396878
H	-6.522632	-4.319168	-0.004818
H	-7.112425	-2.673261	0.259808
H	-6.966291	-3.290383	-1.384781
C	6.874452	-2.383254	-0.820082
H	7.478682	-1.546977	-1.187991
H	7.257402	-2.684614	0.161104
H	7.036335	-3.226893	-1.503918
C	-1.364496	1.528464	-0.876389
C	1.111516	1.703616	-0.909916
H	-2.238258	1.697070	-0.239973
H	-1.675308	1.678798	-1.919289
H	1.356863	1.900322	-1.962863
H	1.981380	1.983904	-0.310315
C	-0.178887	2.477832	-0.532246
C	-0.259210	2.845760	0.958620
C	-0.237196	3.819629	-1.249258
O	-1.307337	3.113863	1.513658
O	0.753554	4.436919	-1.593426
O	0.924517	2.907699	1.550645
O	-1.479720	4.252189	-1.406471
C	0.913906	3.252742	2.947810
H	1.956651	3.231889	3.263838
H	0.492689	4.252052	3.085328
H	0.328023	2.517394	3.508940
C	-1.636934	5.545239	-2.018898
H	-1.236238	5.529287	-3.035718
H	-2.710275	5.731812	-2.037029
H	-1.127096	6.306915	-1.423376
N	-2.293347	0.085667	2.799594

1Co-b- triplet state Gsolv= -2969.948319

Co	0.102460	-0.486664	1.099244
H	0.184307	-1.906787	1.595902
H	1.139926	-3.528327	-0.712363
C	0.150380	-1.890228	-0.592705
O	0.217611	-3.225439	-0.690638

C	-1.115879	-1.185320	-0.711098
C	-0.762867	0.165200	-0.823044
C	0.665850	0.302098	-0.827529
C	1.264014	-0.962283	-0.712113
C	-1.448741	-0.230584	2.309075
C	1.672138	-0.187161	2.187017
O	2.610765	-0.145635	2.837250
C	-2.455389	-1.761384	-0.637451
C	-3.527005	-1.113076	-1.268362
C	-2.718923	-2.944580	0.069807
C	-4.813920	-1.635582	-1.201173
H	-3.347714	-0.203895	-1.840114
C	-4.007666	-3.460480	0.128843
H	-1.911111	-3.457695	0.587186
C	-5.078897	-2.818120	-0.503336
H	-5.629429	-1.121443	-1.708752
H	-4.190721	-4.381904	0.680936
C	2.692436	-1.289732	-0.731025
C	3.548814	-0.579941	-1.586717
C	3.243543	-2.288809	0.082900
C	4.906005	-0.869341	-1.630375
H	3.140220	0.193984	-2.234720
C	4.604097	-2.578576	0.024805
H	2.616226	-2.819443	0.800371
C	5.458104	-1.878043	-0.830992
H	5.554825	-0.307692	-2.302032
H	5.014100	-3.354939	0.669410
C	-6.467949	-3.370047	-0.414615
H	-6.463082	-4.465771	-0.396264
H	-6.967755	-3.034678	0.503843
H	-7.083904	-3.041128	-1.258718
C	6.920537	-2.190805	-0.903543
H	7.527470	-1.285012	-0.786516
H	7.216187	-2.904411	-0.127597
H	7.183482	-2.625088	-1.876539
C	-1.413984	1.504423	-0.919899
C	1.054107	1.735642	-0.955532
H	-2.293681	1.632753	-0.280052
H	-1.725685	1.694672	-1.956253
H	1.266229	1.969413	-2.008506
H	1.929946	2.031006	-0.371759
C	-0.248445	2.466184	-0.537144
C	-0.333033	2.767320	0.969117
C	-0.337483	3.834961	-1.196489
O	-1.378478	3.045170	1.524949
O	0.640845	4.487286	-1.511146
O	0.842751	2.739483	1.579468
O	-1.588214	4.248059	-1.340472
C	0.829887	3.017295	2.992051
H	1.872214	2.982437	3.308269
H	0.407178	4.008299	3.176102
H	0.244050	2.254227	3.515551
C	-1.768098	5.563468	-1.896557
H	-1.360055	5.601219	-2.909807
H	-2.844812	5.729537	-1.914250
H	-1.278166	6.308034	-1.263716
N	-2.399816	-0.107691	2.990289

1Co-c Gsolv= -2471.911339

C	0.023935	-1.153323	-0.404375
O	-0.005543	-2.463776	-0.140606
C	-1.165787	-0.363132	-0.568624
C	-0.706516	0.935051	-0.998768
C	0.687902	0.957717	-0.993171
C	1.186180	-0.318427	-0.551753
C	-1.446236	1.338140	1.775129
C	1.234037	1.293533	1.869771
O	2.061711	1.756231	2.515195
H	-0.046734	-0.472503	2.014516
C	1.156454	2.311553	-1.402365
O	-0.035671	3.106633	-1.303942
C	-1.202953	2.276681	-1.420311
H	1.527265	2.298295	-2.439388
H	1.926284	2.748488	-0.756749
H	-1.552224	2.250236	-2.464941
C	2.595520	-0.725960	-0.435089
C	3.049513	-1.483755	0.651799
C	3.499254	-0.352432	-1.436664
C	4.382468	-1.877358	0.722706
H	2.359963	-1.740863	1.456166
C	4.833377	-0.741172	-1.357811
H	3.149543	0.235245	-2.284295
C	5.276610	-1.507844	-0.281462
H	4.725946	-2.463459	1.571804
H	5.527435	-0.446741	-2.141445
H	6.318852	-1.812244	-0.221689
C	-2.560617	-0.806428	-0.451555
C	-2.938489	-1.803877	0.457023

C	-3.540751	-0.200187	-1.245817
C	-4.270099	-2.191507	0.556148
H	-2.189562	-2.261710	1.099625
C	-4.873514	-0.589635	-1.142593
H	-3.258437	0.570461	-1.961273
C	-5.241599	-1.586755	-0.242242
H	-4.553108	-2.964065	1.267345
H	-5.624250	-0.112118	-1.767938
H	-6.282389	-1.890904	-0.159269
H	0.892472	-2.821008	-0.036451
Co	-0.013546	0.505005	0.902421
N	-2.370843	1.841625	2.298081
H	-1.995524	2.698380	-0.792986

1Co-c- triplet state Gsolv= -2471.869159

Co	-0.004983	0.606823	0.978724
N	-2.556044	1.613378	2.541600
H	-2.060836	2.683626	-0.709892
C	0.003672	-1.088156	-0.440124
O	-0.022474	-2.416178	-0.281677
C	-1.205683	-0.331243	-0.714216
C	-0.753391	0.956249	-1.033335
C	0.674743	0.998528	-1.001845
C	1.181757	-0.266326	-0.661492
C	-1.579293	1.249165	1.997263
C	1.550116	0.972257	2.080988
O	2.453168	1.023186	2.778195
H	-0.039472	-0.670227	1.778473
C	1.108771	2.388939	-1.314490
O	-0.092767	3.154208	-1.120703
C	-1.245372	2.326780	-1.349457
H	1.453043	2.475670	-2.357534
H	1.885061	2.787151	-0.651335
H	-1.564443	2.396482	-2.401889
C	2.585119	-0.673268	-0.555411
C	3.020161	-1.597468	0.406639
C	3.526079	-0.116449	-1.433324
C	4.359850	-1.969399	0.470772
H	2.320499	-1.999119	1.139952
C	4.865862	-0.482674	-1.358341
H	3.199232	0.593490	-2.191711
C	5.286443	-1.414238	-0.410074
H	4.682430	-2.684376	1.223980
H	5.583075	-0.043395	-2.047846
H	6.333458	-1.702358	-0.353974
C	-2.587510	-0.781542	-0.565872
C	-2.940071	-1.790014	0.344183
C	-3.599885	-0.162184	-1.313433
C	-4.269207	-2.172135	0.490538
H	-2.172658	-2.262800	0.952718
C	-4.928747	-0.545596	-1.161352
H	-3.342932	0.610668	-2.036269
C	-5.268834	-1.552839	-0.259664
H	-4.526939	-2.953073	1.202451
H	-5.700324	-0.058212	-1.753046
H	-6.307149	-1.853570	-0.140863
H	0.873904	-2.777861	-0.184213

1Co Gsolv= -2830.573354

C	0.005277	-1.276690	-0.369799
O	0.098090	-2.594951	-0.110576
H	-0.767566	-2.993649	0.062958
C	-1.179668	-0.483260	-0.493224
C	-0.707847	0.828490	-0.922044
C	-1.510183	2.040125	-1.274320
H	-2.370021	2.145568	-0.603019
H	-1.920713	1.902540	-2.287733
C	-0.636622	3.290399	-1.238651
H	-1.198844	4.142732	-1.637508
H	-0.386424	3.529392	-0.191753
C	0.645591	3.073497	-2.032716
H	1.214690	4.006035	-2.121502
H	0.378693	2.766451	-3.055658
C	1.524994	1.999621	-1.393965
H	2.281014	1.650591	-2.110618
H	2.084096	2.419515	-0.545750
C	0.705223	0.823337	-0.952570
C	1.180254	-0.477267	-0.513324
Si	-2.954414	-1.135492	-0.307449
C	-3.219826	-2.341504	-1.720411
H	-3.118874	-1.840046	-2.691259
H	-4.227820	-2.772914	-1.665613
H	-2.499460	-3.169674	-1.693779
C	-4.232730	0.225694	-0.387269
H	-4.217661	0.760757	-1.344122
H	-4.120632	0.953109	0.425879
H	-5.222742	-0.239593	-0.283337
C	-3.092704	-2.025034	1.339095

H	-2.945347	-1.325245	2.171807
H	-2.376207	-2.847665	1.463731
H	-4.098839	-2.455181	1.434374
Si	2.946689	-1.129758	-0.288700
C	3.302826	-2.275620	-1.727324
H	4.321131	-2.679039	-1.654629
H	3.218992	-1.742629	-2.683173
H	2.604344	-3.121428	-1.748119
C	4.174943	0.284512	-0.255541
H	5.171259	-0.133500	-0.056409
H	3.952547	1.001174	0.545573
H	4.227918	0.830614	-1.204432
C	3.056376	-2.043543	1.344366
H	4.056254	-2.485847	1.449324
H	2.320225	-2.851636	1.423894
H	2.905673	-1.359622	2.189919
C	-1.377950	1.212458	1.892729
C	1.241118	1.148215	1.932837
O	2.033205	1.646903	2.599073
H	-0.013097	-0.657957	2.050738
N	-2.232712	1.756215	2.489300
Co	0.005917	0.353739	0.963186

1Co- triplet state Gsolv= -2830.528250

Co	0.045412	0.604751	0.987690
C	-0.022778	-1.258839	-0.232044
O	0.094687	-2.551871	0.112402
H	-0.760947	-2.956947	0.319674
C	-1.227283	-0.545596	-0.539955
C	-0.771894	0.715802	-1.009850
C	-1.575643	1.902599	-1.436922
H	-2.460954	2.018031	-0.801238
H	-1.948049	1.721926	-2.458521
C	-0.724253	3.168248	-1.427656
H	-1.299872	4.001099	-1.848103
H	-0.483295	3.437913	-0.384846
C	0.563009	2.951724	-2.212251
H	1.112280	3.892782	-2.332171
H	0.303674	2.604487	-3.224327
C	1.463063	1.922798	-1.530976
H	2.249588	1.585000	-2.219402
H	1.982949	2.394236	-0.682142
C	0.679594	0.737911	-1.045778
C	1.165984	-0.481793	-0.521840
Si	-2.980952	-1.186788	-0.255734
C	-3.247907	-2.626702	-1.430809
H	-3.155759	-2.304821	-2.475907
H	-4.254040	-3.045214	-1.294519
H	-2.525880	-3.437122	-1.264515
C	-4.280241	0.124185	-0.565472
H	-4.237551	0.532384	-1.582099
H	-4.211006	0.952519	0.150920
H	-5.265843	-0.343892	-0.435326
C	-3.139228	-1.798164	1.514838
H	-3.010813	-0.975461	2.229898
H	-2.416759	-2.582926	1.774408
H	-4.143151	-2.219722	1.661038
Si	2.932443	-1.136285	-0.361925
C	3.219128	-2.270325	-1.827994
H	4.227166	-2.703634	-1.796559
H	3.117711	-1.717567	-2.771260
H	2.493887	-3.093920	-1.838647
C	4.177250	0.265693	-0.378733
H	5.177718	-0.165832	-0.236154
H	4.011638	0.982914	0.435569
H	4.186797	0.816694	-1.326455
C	3.123368	-2.075967	1.249719
H	4.155577	-2.442281	1.333742
H	2.455168	-2.942429	1.309346
H	2.928329	-1.433693	2.118440
C	-1.425964	1.436823	1.999387
C	1.581958	1.207519	2.054543
O	2.401588	1.333260	2.842326
H	0.087279	-0.541926	1.986005
N	-2.311715	1.950793	2.577951

1Fe-Casey Gsolv= -2728.685669

Fe	-0.000219	-0.707618	-0.775154
C	-0.020836	1.252458	0.033241
O	-0.132969	2.432528	-0.622131
C	-1.195526	0.536205	0.429721
C	-0.685993	-0.584291	1.176334
C	0.716501	-0.564323	1.160162
C	1.187695	0.568965	0.401424
Si	-2.984623	1.050574	0.122870
C	-3.298661	2.635034	1.076278
H	-3.112911	2.492893	2.148371
H	-4.339531	2.961618	0.954445

H	-2.648984	3.446289	0.724252
C	-4.074936	-0.332538	0.762629
H	-3.907765	-0.517946	1.831672
H	-3.901073	-1.270217	0.218770
H	-5.132098	-0.066415	0.633151
C	-3.265115	1.320448	-1.710438
H	-3.163568	0.382905	-2.271845
H	-2.554481	2.045187	-2.126610
H	-4.278160	1.707364	-1.882714
Si	2.982442	1.077543	0.097192
C	3.268909	2.686847	1.016186
H	4.300641	3.036404	0.882650
H	3.087064	2.567444	2.091545
H	2.597776	3.473650	0.646351
C	4.079650	-0.291791	0.746107
H	5.132874	-0.019256	0.599036
H	3.905627	-1.234918	0.212002
H	3.928741	-0.466232	1.818925
C	3.268697	1.330176	-1.739414
H	4.287542	1.704255	-1.906785
H	2.576890	2.059504	-2.181154
H	3.160668	0.388532	-2.292664
C	-1.292056	-1.699194	-1.417705
O	-2.153894	-2.350325	-1.840273
C	1.263737	-1.769135	-1.362278
O	2.107873	-2.469056	-1.739729
H	0.029994	-0.019134	-2.127573
C	1.222872	-1.703107	1.979834
O	0.053202	-2.516931	2.176907
C	-1.143944	-1.737561	2.002615
H	1.606713	-1.346079	2.949322
H	1.993482	-2.322128	1.506931
H	-1.902450	-2.378528	1.539413
H	-1.521902	-1.396360	2.980021
H	0.711470	2.716711	-1.000757

1Fe-Casey- triplet state Gsolv= -2728.641512

Fe	-0.015229	-0.768808	-0.772286
C	-0.070304	1.311951	-0.048770
O	-0.157671	2.411839	-0.841795
C	-1.244914	0.665897	0.426500
C	-0.730375	-0.406287	1.230885
C	0.677032	-0.350563	1.275258
C	1.150022	0.675129	0.414853
Si	-3.024254	1.055399	-0.023593
C	-3.465210	2.764007	0.614701
H	-3.346775	2.823540	1.703959
H	-4.508283	3.008300	0.374348
H	-2.827837	3.534785	0.163056
C	-4.104860	-0.247323	0.782712
H	-3.975588	-0.264863	1.872658
H	-3.882726	-1.249848	0.393900
H	-5.162693	-0.038279	0.576362
C	-3.228434	1.006100	-1.889366
H	-3.077741	-0.009628	-2.278640
H	-2.508374	1.668561	-2.386780
H	-4.237154	1.331333	-2.176688
Si	2.944614	1.155382	0.089553
C	3.243001	2.815090	0.910237
H	4.275512	3.151928	0.751406
H	3.066974	2.756848	1.991851
H	2.572362	3.583896	0.503362
C	4.044126	-0.164286	0.834675
H	5.095978	0.114370	0.687647
H	3.894357	-1.142777	0.359555
H	3.879252	-0.275205	1.913966
C	3.253105	1.293685	-1.756025
H	4.275367	1.653930	-1.932888
H	2.568399	1.996872	-2.247946
H	3.147053	0.321081	-2.253656
C	-1.160888	-2.078523	-1.175498
O	-1.956189	-2.901527	-1.375252
C	1.642950	-2.089281	-1.160685
O	2.289604	-2.693794	-1.886300
H	0.253999	-0.381853	-2.282453
C	1.174233	-1.451755	2.148867
O	-0.000036	-2.246807	2.398176
C	-1.194730	-1.485748	2.147237
H	1.575791	-1.062964	3.098652
H	1.933612	-2.102768	1.696152
H	-1.950757	-2.164794	1.736674
H	-1.581684	-1.062821	3.088939
H	0.717674	2.742170	-1.089562

1Fe Gsolv= -2732.034114

Fe	-0.003401	0.386970	0.990794
C	0.012292	-1.276086	-0.327353
O	0.105232	-2.597772	-0.035776

H	-0.759570	-2.979176	0.173641
C	-1.177307	-0.502006	-0.495805
C	-0.707556	0.808433	-0.921218
C	-1.515054	2.005951	-1.319513
H	-2.391743	2.124443	-0.671421
H	-1.905241	1.841971	-2.337464
C	-0.654233	3.265367	-1.302594
H	-1.216329	4.101361	-1.735673
H	-0.424052	3.537051	-0.259181
C	0.643415	3.037957	-2.068242
H	1.204341	3.973932	-2.175387
H	0.394795	2.700173	-3.086459
C	1.523504	1.990839	-1.386746
H	2.299966	1.642734	-2.081505
H	2.056618	2.442606	-0.537869
C	0.709163	0.811820	-0.933870
C	1.186556	-0.485988	-0.496688
Si	-2.944063	-1.155673	-0.322691
C	-3.233527	-2.349600	-1.741074
H	-3.149954	-1.838623	-2.708702
H	-4.236213	-2.791588	-1.675853
H	-2.502998	-3.169150	-1.730849
C	-4.218391	0.213739	-0.363796
H	-4.228429	0.757375	-1.315745
H	-4.081117	0.935496	0.451217
H	-5.208044	-0.245882	-0.233536
C	-3.108932	-2.050856	1.321857
H	-2.978904	-1.347752	2.155300
H	-2.399547	-2.875560	1.472265
H	-4.118679	-2.476841	1.398691
Si	2.944803	-1.143327	-0.282301
C	3.286177	-2.327246	-1.696965
H	4.301441	-2.738185	-1.620919
H	3.200771	-1.816722	-2.665023
H	2.580057	-3.167286	-1.695069
C	4.204107	0.245725	-0.308019
H	5.198196	-0.195150	-0.149483
H	4.037214	0.974719	0.494956
H	4.229652	0.783305	-1.263230
C	3.088974	-2.029760	1.365011
H	4.094406	-2.461369	1.463121
H	2.361241	-2.842943	1.468865
H	2.942122	-1.332816	2.200806
C	-1.287267	1.198594	1.858186
O	-2.147673	1.730614	2.428400
C	1.272191	1.187572	1.879939
O	2.123254	1.713777	2.469189
H	-0.013101	-0.651030	2.100604

1Fe-Renaud Gsolv= -2487.320959

Fe	0.008557	0.273783	1.129934
C	-0.010505	-1.270232	-0.280157
O	0.030790	-2.605233	-0.079738
H	-0.864129	-2.948455	0.074755
C	-1.177289	-0.459423	-0.412646
C	-0.713184	0.857862	-0.807337
C	-0.624855	3.190756	-1.119512
H	-1.189391	4.009705	-1.578240
H	-0.430179	3.461882	-0.063064
C	0.676485	2.975816	-1.856345
H	1.263473	3.899007	-1.860526
H	0.461479	2.721421	-2.902909
C	0.712622	0.841167	-0.819019
C	1.160703	-0.484238	-0.439116
C	-1.206857	1.016778	2.152960
O	-1.993345	1.416076	2.911773
C	2.535781	-1.024395	-0.440456
C	3.060645	-1.676438	0.681649
C	3.319217	-0.933084	-1.597492
C	4.343421	-2.216192	0.651232
H	2.456273	-1.754324	1.584515
C	4.606301	-1.464786	-1.623865
H	2.913395	-0.455140	-2.486310
C	5.122930	-2.106303	-0.499640
H	4.737114	-2.719231	1.531645
H	5.203563	-1.383365	-2.529374
H	6.128312	-2.520764	-0.520989
C	-2.547868	-1.018015	-0.417321
C	-3.225299	-1.150168	-1.636842
C	-3.169291	-1.459169	0.755777
C	-4.509246	-1.684965	-1.676810
H	-2.740401	-0.821910	-2.555437
C	-4.451771	-2.003210	0.713321
H	-2.642733	-1.367730	1.705017
C	-5.127286	-2.109677	-0.500369
H	-5.028000	-1.773154	-2.628736
H	-4.925710	-2.337717	1.633383
H	-6.132067	-2.524813	-0.531341

N	-1.445358	1.980684	-1.174148
N	1.493396	1.912250	-1.258783
C	2.510729	2.395869	-0.335822
H	2.063197	2.919700	0.527952
H	3.120294	1.566064	0.035930
H	3.175157	3.089553	-0.860906
C	-2.737517	2.197265	-0.542977
H	-3.377042	1.315163	-0.617507
H	-2.626375	2.467917	0.520537
H	-3.240582	3.024058	-1.053886
C	1.331897	0.817045	2.142068
O	2.202742	1.093067	2.861812
H	-0.084492	-0.861602	2.129269

1Fe-Renaud- triplet state Gsolv= -2487.274222

Fe	-0.007113	0.303803	1.208070
C	0.038768	-1.293710	-0.236446
O	0.038481	-2.633859	-0.022833
H	-0.870624	-2.960153	0.070203
C	-1.100555	-0.479593	-0.558974
C	-0.575100	0.806400	-0.886600
C	-0.339773	3.145444	-1.210523
H	-0.857953	3.991517	-1.675064
H	-0.119681	3.422276	-0.159904
C	0.942945	2.850600	-1.945217
H	1.586395	3.735570	-1.951685
H	0.722692	2.599339	-2.991655
C	0.879498	0.714148	-0.900920
C	1.255417	-0.587496	-0.491458
C	-1.802804	0.563334	2.279663
O	-2.486077	0.560421	3.202084
C	2.605999	-1.152381	-0.348719
C	2.991829	-1.804171	0.831071
C	3.531403	-1.058402	-1.397827
C	4.269587	-2.342146	0.959532
H	2.284853	-1.872183	1.657378
C	4.810082	-1.592005	-1.265814
H	3.242124	-0.570383	-2.326291
C	5.185243	-2.234751	-0.086406
H	4.553312	-2.840746	1.883974
H	5.514915	-1.509929	-2.090516
H	6.185051	-2.650589	0.016266
C	-2.476570	-0.995269	-0.610894
C	-3.273385	-0.767270	-1.743205
C	-3.004520	-1.770916	0.432716
C	-4.561634	-1.285384	-1.821645
H	-2.873871	-0.179339	-2.567954
C	-4.290945	-2.299997	0.346155
H	-2.410718	-1.948759	1.330327
C	-5.076484	-2.054643	-0.777318
H	-5.165188	-1.093392	-2.706056
H	-4.681474	-2.896754	1.167485
H	-6.083554	-2.460171	-0.840795
N	-1.236086	1.987255	-1.239316
N	1.686294	1.749154	-1.324600
C	2.794626	2.164776	-0.473676
H	2.465088	2.920298	0.257777
H	3.205270	1.312859	0.074052
H	3.594623	2.599766	-1.082355
C	-2.456360	2.289017	-0.503207
H	-3.161474	1.455259	-0.524383
H	-2.227699	2.532130	0.551181
H	-2.941384	3.156859	-0.961236
C	0.650503	1.743809	2.073159
O	1.061410	2.641624	2.693891
H	0.175660	-0.699062	2.441030

1Fe- triplet state Gsolv= -2731.986993

Fe	0.010187	0.459082	0.999188
C	0.058718	-1.339430	-0.264450
O	0.138311	-2.621393	0.185370
H	-0.737124	-3.001567	0.343981
C	-1.145407	-0.584199	-0.528134
C	-0.679980	0.652945	-1.084874
C	-1.478646	1.845071	-1.519690
H	-2.323557	2.014747	-0.838330
H	-1.919555	1.647798	-2.510175
C	-0.602456	3.092995	-1.594372
H	-1.160888	3.907116	-2.072026
H	-0.353095	3.429431	-0.573904
C	0.683354	2.800778	-2.355661
H	1.247957	3.722118	-2.542259
H	0.422519	2.383752	-3.341091
C	1.560011	1.806426	-1.596773
H	2.330347	1.395470	-2.263851
H	2.103800	2.322864	-0.792658
C	0.741750	0.675393	-1.040511
C	1.228362	-0.592247	-0.533181

Si	-2.911825	-1.220820	-0.314599
C	-3.146748	-2.651169	-1.509681
H	-2.992418	-2.327563	-2.546901
H	-4.167076	-3.049061	-1.428444
H	-2.451008	-3.476832	-1.310010
C	-4.190095	0.103277	-0.660948
H	-4.121234	0.509900	-1.676619
H	-4.127838	0.933534	0.054457
H	-5.183646	-0.353000	-0.549760
C	-3.171717	-1.837730	1.441907
H	-3.145889	-1.008544	2.160784
H	-2.428809	-2.578446	1.764478
H	-4.160467	-2.311520	1.514056
Si	2.975224	-1.169683	-0.148086
C	3.448025	-2.538093	-1.344606
H	4.456047	-2.915258	-1.127347
H	3.439165	-2.174808	-2.380347
H	2.749155	-3.381793	-1.277245
C	4.202967	0.242889	-0.283727
H	5.189320	-0.125965	0.030361
H	3.939121	1.079865	0.376004
H	4.302976	0.627704	-1.305743
C	3.032420	-1.804535	1.620093
H	4.034294	-2.191013	1.851198
H	2.310103	-2.610424	1.798380
H	2.813790	-0.991462	2.326456
C	-1.657894	1.624540	1.751427
O	-2.317135	1.961025	2.625461
C	1.188105	1.521973	1.801743
O	2.011747	2.193958	2.274808
H	-0.306444	-0.328156	2.338767

1Fe-williams-1 Gsolv= -2682.490340

Fe	0.023076	-0.705702	1.306296
C	0.027970	-1.766928	-0.545991
O	0.013515	-3.098200	-0.752372
H	0.915771	-3.455136	-0.762567
C	-1.161176	-0.996914	-0.396238
C	-0.748584	0.388068	-0.296225
C	0.673859	0.439694	-0.317544
C	1.165337	-0.920580	-0.434435
C	-1.107175	-0.146254	2.525679
O	-1.837096	0.203057	3.355733
C	1.368833	-0.640718	2.425725
O	2.250356	-0.663577	3.178594
H	-0.174824	-2.073449	1.911101
C	-2.537494	-1.517413	-0.524807
C	-3.548659	-1.192905	0.387100
C	-2.858851	-2.314162	-1.631253
C	-4.847882	-1.654581	0.197880
H	-3.321410	-0.576224	1.254292
C	-4.157354	-2.782522	-1.815910
H	-2.086802	-2.558588	-2.358391
C	-5.156653	-2.453396	-0.902397
H	-5.620603	-1.393539	0.917443
H	-4.388568	-3.401361	-2.680086
H	-6.171406	-2.817593	-1.045820
C	2.568507	-1.343762	-0.615360
C	3.142901	-2.350567	0.169755
C	3.334800	-0.751846	-1.628442
C	4.456876	-2.756633	-0.052985
H	2.558526	-2.808500	0.968441
C	4.649828	-1.152391	-1.843153
H	2.892931	0.023626	-2.252810
C	5.214370	-2.155734	-1.056174
H	4.890951	-3.538396	0.566053
H	5.234310	-0.682374	-2.630777
H	6.242381	-2.468058	-1.224836
C	1.502478	1.661975	-0.373488
C	2.589425	1.868480	0.482659
C	1.231279	2.617355	-1.361451
C	3.383138	3.005325	0.358609
H	2.818695	1.137583	1.255563
C	2.022883	3.756656	-1.483041
H	0.398320	2.459687	-2.045512
C	3.101701	3.954452	-0.622995
H	4.222185	3.151707	1.035083
H	1.797873	4.487861	-2.256215
H	3.720294	4.844008	-0.717122
C	-1.658114	1.551506	-0.278563
C	-2.610431	1.673900	-1.297179
C	-1.551387	2.566385	0.678545
C	-3.441735	2.789147	-1.357045
H	-2.689343	0.895730	-2.055536
C	-2.382475	3.681479	0.617101
H	-0.812827	2.479109	1.475378
C	-3.331439	3.794868	-0.398747
H	-4.175073	2.872019	-2.156064

H	-2.292271	4.462602	1.368655
H	-3.981937	4.665388	-0.443376

1Fe-williams-1-triplet state Gsolv= -2682.445754

Fe	0.028709	-0.666492	1.334196
C	0.007734	-1.731688	-0.652560
O	0.029221	-3.068112	-0.845911
H	0.941680	-3.398217	-0.827110
C	-1.175114	-0.967175	-0.576974
C	-0.749247	0.404336	-0.375689
C	0.681971	0.458787	-0.449754
C	1.163231	-0.881891	-0.525162
C	-1.245380	-0.404634	2.547912
O	-2.100325	-0.276340	3.323789
C	1.649297	-0.394218	2.661619
O	2.361248	-0.716388	3.497055
H	0.109734	-2.097794	1.976353
C	-2.550142	-1.485836	-0.627983
C	-3.582998	-0.927492	0.143370
C	-2.865458	-2.557957	-1.477119
C	-4.879722	-1.425659	0.067809
H	-3.374298	-0.093552	0.810564
C	-4.162923	-3.058689	-1.546706
H	-2.089160	-2.994313	-2.100872
C	-5.177262	-2.496703	-0.774358
H	-5.661146	-0.976872	0.677466
H	-4.381073	-3.889440	-2.214513
H	-6.190924	-2.887166	-0.829038
C	2.555374	-1.336052	-0.709175
C	3.134538	-2.288981	0.137920
C	3.314285	-0.822461	-1.769861
C	4.444784	-2.716813	-0.069111
H	2.554778	-2.685387	0.972333
C	4.625397	-1.242523	-1.968807
H	2.868189	-0.088720	-2.439777
C	5.194835	-2.190749	-1.118642
H	4.881864	-3.455789	0.598665
H	5.203354	-0.831901	-2.793724
H	6.219949	-2.518598	-1.275219
C	1.510495	1.677586	-0.410982
C	2.704352	1.738660	0.323096
C	1.134962	2.800234	-1.164498
C	3.487981	2.889210	0.314624
H	3.032677	0.877638	0.902682
C	1.919070	3.949701	-1.172599
H	0.226681	2.766779	-1.763585
C	3.097383	4.001258	-0.429485
H	4.408176	2.915501	0.894083
H	1.610270	4.805621	-1.768763
H	3.710456	4.899644	-0.435612
C	-1.645775	1.579619	-0.341575
C	-2.484177	1.827699	-1.434652
C	-1.641028	2.482278	0.726896
C	-3.297248	2.957431	-1.461102
H	-2.487660	1.133010	-2.273955
C	-2.449977	3.615232	0.698595
H	-0.992274	2.292812	1.582771
C	-3.280488	3.856551	-0.395428
H	-3.941900	3.137799	-2.318591
H	-2.435311	4.309693	1.535781
H	-3.914152	4.740366	-0.416216

1Fe-williams-2 Gsolv= -2871.449612

Fe	0.081599	-0.535535	1.136884
C	0.110371	-1.984198	-0.416886
O	0.162947	-3.327824	-0.306579
C	-1.124177	-1.253718	-0.440836
C	-0.747439	0.119984	-0.658112
C	-1.376460	1.445463	-0.946600
H	-2.250011	1.704915	-0.343510
H	-1.672672	1.490364	-2.004144
C	-0.188963	2.414626	-0.688529
C	1.094261	1.606748	-1.013083
H	1.318406	1.703528	-2.084430
H	1.974878	1.945038	-0.459716
C	0.652696	0.213920	-0.713881
C	1.226476	-1.088695	-0.520623
C	-1.142450	0.024157	2.261930
O	-1.939967	0.360405	3.033728
C	1.426077	0.110697	2.055439
O	2.350450	0.499694	2.637575
H	0.167413	-1.736371	2.051753
C	-0.238024	2.886615	0.774539
O	-1.264508	3.000116	1.416663
O	0.958916	3.229319	1.233415
C	-0.269157	3.688125	-1.515775
O	0.684488	4.208799	-2.062652

O	-1.500529	4.183963	-1.534081
C	1.010371	3.679036	2.598305
H	2.065919	3.843705	2.814198
H	0.446992	4.609759	2.707142
H	0.598940	2.911894	3.262045
C	-1.682729	5.422077	-2.244020
H	-2.736656	5.673484	-2.128947
H	-1.053996	6.201523	-1.805575
H	-1.436554	5.288230	-3.300610
C	2.654941	-1.446191	-0.564828
C	3.230515	-2.325921	0.362842
C	3.469527	-0.905898	-1.565540
C	4.575347	-2.664428	0.275348
H	2.627366	-2.721763	1.180566
C	4.819224	-1.240875	-1.639323
H	3.040646	-0.224484	-2.299160
C	5.394415	-2.127669	-0.725500
H	5.005709	-3.348594	1.006192
H	5.437391	-0.809366	-2.425658
C	-2.489416	-1.806066	-0.410226
C	-2.771009	-3.071714	-0.943729
C	-3.556187	-1.051665	0.094473
C	-4.072292	-3.561356	-0.962652
H	-1.968376	-3.672861	-1.363423
C	-4.855490	-1.548143	0.071056
H	-3.374251	-0.064243	0.515680
C	-5.138676	-2.812056	-0.454875
H	-4.267930	-4.545638	-1.387983
H	-5.667495	-0.941972	0.471202
C	6.846417	-2.488496	-0.793716
H	7.393449	-2.091346	0.070790
H	6.986445	-3.576170	-0.785114
H	7.316334	-2.090340	-1.699014
C	-6.534605	-3.354271	-0.479084
H	-7.257859	-2.612488	-0.124395
H	-6.826089	-3.657720	-1.492103
H	-6.626566	-4.243958	0.156640
H	1.081238	-3.627520	-0.212667

1Fe-williams-2- triplet state

Gsolv= -2871.450021

Fe	0.078310	-0.539455	1.131389
C	0.108780	-1.984845	-0.425578
O	0.159488	-3.328645	-0.317504
C	-1.125005	-1.252662	-0.449883
C	-0.746205	0.121171	-0.663696
C	-1.372133	1.448597	-0.950719
H	-2.247453	1.708616	-0.350538
H	-1.664229	1.496627	-2.009318
C	-0.183967	2.415196	-0.686698
C	1.098567	1.606309	-1.011035
H	1.324623	1.705723	-2.081740
H	1.978802	1.941533	-0.455157
C	0.654215	0.213361	-0.716464
C	1.226120	-1.090196	-0.524767
C	-1.147676	0.019015	2.255000
O	-1.947298	0.354482	3.024914
C	1.421424	0.103040	2.054604
O	2.344837	0.489208	2.640010
H	0.160592	-1.742850	2.043363
C	-0.235814	2.883146	0.777526
O	-1.263457	2.995745	1.417890
O	0.960410	3.224033	1.239556
C	-0.260775	3.691321	-1.510169
O	0.694311	4.211942	-2.054589
O	-1.491246	4.189423	-1.528139
C	1.009204	3.671155	2.605395
H	2.064366	3.834957	2.823800
H	0.446038	4.601955	2.714716
H	0.595922	2.903066	3.266869
C	-1.670554	5.430235	-2.234017
H	-2.724362	5.682618	-2.120006
H	-1.041686	6.207332	-1.791585
H	-1.422561	5.300023	-3.290630
C	2.654725	-1.447727	-0.566086
C	3.228347	-2.326910	0.363332
C	3.471532	-0.907279	-1.564869
C	4.573553	-2.664690	0.279426
H	2.622786	-2.723362	1.178979
C	4.821594	-1.241672	-1.635165
H	3.044175	-0.226154	-2.299653
C	5.394874	-2.127845	-0.719556
H	5.002474	-3.348374	1.011574
H	5.441578	-0.810086	-2.420029
C	-2.491230	-1.802347	-0.418191
C	-2.775438	-3.073007	-0.938381
C	-3.556530	-1.040876	0.078998
C	-4.077649	-3.560421	-0.951031

H	-1.974051	-3.680472	-1.351216
C	-4.856772	-1.534941	0.061384
H	-3.372098	-0.050267	0.491421
C	-5.142522	-2.803789	-0.450958
H	-4.275468	-4.549305	-1.364603
H	-5.667156	-0.923323	0.456486
C	6.847063	-2.488568	-0.784207
H	7.390496	-2.098317	0.085660
H	6.986603	-3.576374	-0.783112
H	7.320925	-2.084129	-1.684642
C	-6.539834	-3.342635	-0.472602
H	-7.253428	-2.620291	-0.062517
H	-6.855209	-3.588187	-1.494323
H	-6.619025	-4.266461	0.113918
H	1.077557	-3.630979	-0.230478
H	5.512015	-0.535558	-2.158075
H	6.311890	-1.876495	-0.223460
C	-2.567926	-0.813947	-0.440723
C	-2.973541	-1.739210	0.530777
C	-3.525325	-0.285532	-1.314943
C	-4.305082	-2.132153	0.614367
H	-2.244874	-2.136426	1.234602
C	-4.859098	-0.677023	-1.225574
H	-3.222015	0.425512	-2.082136
C	-5.252884	-1.602796	-0.262253
H	-4.606926	-2.848084	1.375566
H	-5.590218	-0.258206	-1.913413
H	-6.293879	-1.909452	-0.191243
H	0.886333	-2.808272	0.069577
H	-1.982467	2.695438	-0.863018

1Fe-wills-1 Gsolv= -2373.372682

Fe	-0.012537	0.550585	0.927984
C	0.017443	-1.149936	-0.339162
O	-0.014890	-2.459912	-0.028803
C	-1.169320	-0.371579	-0.549470
C	-0.703786	0.915338	-0.995204
C	0.695032	0.932820	-0.986623
C	1.185936	-0.336802	-0.529312
C	-1.342673	1.335443	1.759160
O	-2.261118	1.820014	2.273909
C	1.280591	1.363665	1.788011
O	2.173913	1.866822	2.328652
H	-0.012189	-0.447097	2.069890
C	1.166746	2.264695	-1.461187
O	-0.023052	3.070433	-1.400408
C	-1.194792	2.240539	-1.474585
H	1.534757	2.205488	-2.497924
H	1.938337	2.733849	-0.840182
H	-1.550049	2.176012	-2.515767
C	2.592318	-0.757806	-0.418244
C	3.053387	-1.501340	0.676114
C	3.491681	-0.412376	-1.434343
C	4.383401	-1.907197	0.740173
H	2.372167	-1.736230	1.494179
C	4.823702	-0.810600	-1.362185
H	3.138634	0.163064	-2.289108
C	5.271873	-1.563451	-0.278111
H	4.729495	-2.482131	1.596028

1Fe-wills-1- triplet state Gsolv= -2373.330641

Fe	-0.003491	0.530567	0.969283
C	0.089738	-1.177453	-0.441963
O	0.040124	-2.497260	-0.152046
C	-1.111213	-0.403305	-0.697173
C	-0.643322	0.865489	-1.118741
C	0.759844	0.900895	-1.027214
C	1.256684	-0.385275	-0.650039
C	-1.845093	1.339751	1.731259
O	-2.773430	1.319651	2.396808
C	1.166134	1.510661	1.889998
O	2.004427	2.096745	2.441250
H	-0.130791	-0.432462	2.207680
C	1.233408	2.249098	-1.449703
O	0.040226	3.048663	-1.383016
C	-1.128149	2.218969	-1.515787
H	1.620167	2.228369	-2.481578
H	1.992077	2.701513	-0.800936
H	-1.482239	2.229176	-2.559510
C	2.658811	-0.764566	-0.447338
C	3.053958	-1.563611	0.636842
C	3.639445	-0.308603	-1.340014
C	4.389971	-1.916967	0.805412
H	2.316322	-1.880128	1.375211
C	4.976259	-0.651006	-1.160118
H	3.345065	0.309188	-2.187599
C	5.355627	-1.463384	-0.091933
H	4.679262	-2.536238	1.651586

H	5.723711	-0.287856	-1.862107
H	6.399759	-1.734988	0.044888
C	-2.508726	-0.831318	-0.570940
C	-2.896875	-1.839750	0.324440
C	-3.501062	-0.167162	-1.305580
C	-4.238251	-2.177148	0.468610
H	-2.145557	-2.343803	0.927765
C	-4.843576	-0.503815	-1.154938
H	-3.219471	0.610985	-2.013449
C	-5.218253	-1.510372	-0.267274
H	-4.521384	-2.958407	1.170611
H	-5.598357	0.022582	-1.734965
H	-6.266800	-1.772493	-0.146529
H	0.935744	-2.855232	-0.043963
H	-1.919676	2.635884	-0.879266

1Fe-wills-2 Gsolv= -2412.638915

Fe	0.079346	0.396449	0.990573
C	0.135848	-1.212704	-0.385476
O	0.128368	-2.541139	-0.159196
C	-1.071548	-0.454314	-0.534818
C	-0.650071	0.873564	-0.899714
C	0.748143	0.918255	-0.913233
C	1.281667	-0.358879	-0.538392
C	-1.264914	0.880478	2.007557
O	-2.169062	1.122809	2.692192
C	1.312685	1.291757	1.857387
O	2.170874	1.845987	2.405307
H	0.256840	-0.681756	2.035427
C	1.190305	2.272049	-1.349435
O	-0.010607	3.050483	-1.262350
C	-1.184996	2.205370	-1.332106
H	1.555694	2.244239	-2.388653
H	1.959925	2.737059	-0.722185
H	-1.503768	2.129548	-2.387245
C	-2.277972	2.832070	-0.506386
H	-1.920858	3.011255	0.514762
H	-2.588653	3.787078	-0.942793
H	-3.153486	2.172967	-0.463564
C	-2.449287	-0.970629	-0.466539
C	-2.854076	-1.855075	0.541338
C	-3.379042	-0.572614	-1.434477
C	-4.159686	-2.334320	0.573798
H	-2.145376	-2.150087	1.313537
C	-4.687423	-1.049036	-1.396914
H	-3.070435	0.107910	-2.227182
C	-5.080620	-1.932996	-0.394288
H	-4.462610	-3.016861	1.364652
H	-5.399043	-0.729798	-2.155005
H	-6.102109	-2.305071	-0.363146
C	2.702170	-0.740804	-0.468045
C	3.197252	-1.546849	0.565562
C	3.582690	-0.293076	-1.460784
C	4.539959	-1.913073	0.591786
H	2.532881	-1.863852	1.369319
C	4.928074	-0.649262	-1.424198
H	3.207148	0.329672	-2.271652
C	5.409381	-1.465153	-0.401952
H	4.910437	-2.538940	1.400456
H	5.600746	-0.291949	-2.200604
H	6.459688	-1.745837	-0.375450
H	1.032159	-2.876935	-0.047238

1Fe-wills-2- triplet state Gsolv= -2412.593458

Fe	0.080697	0.495243	1.035378
C	0.079477	-1.223734	-0.448062
O	0.097996	-2.546519	-0.175458
C	-1.115748	-0.494222	-0.642246
C	-0.683421	0.852554	-0.936855
C	0.718552	0.884180	-1.016890
C	1.243540	-0.364281	-0.609269
C	-1.287317	0.956970	2.072005
O	-2.229043	1.148199	2.726836
C	1.743417	1.428205	1.953114
O	2.664877	1.454929	2.629067
H	0.349449	-0.577019	2.152012
C	1.159638	2.251758	-1.405065
O	-0.043087	3.028963	-1.304236
C	-1.220029	2.185851	-1.362805
H	1.540818	2.272847	-2.438730
H	1.920615	2.697029	-0.749770
H	-1.555497	2.119183	-2.413771
C	-2.297547	2.816954	-0.519088
H	-1.920774	2.995039	0.495697
H	-2.613766	3.772891	-0.949970
H	-3.173986	2.160451	-0.458205
C	-2.491014	-0.983654	-0.506000
C	-2.836443	-1.924212	0.476807

C	-3.496233	-0.503662	-1.357545
C	-4.146501	-2.377871	0.593898
H	-2.072992	-2.287403	1.162792
C	-4.807904	-0.954334	-1.234493
H	-3.242295	0.218848	-2.132459
C	-5.138299	-1.895078	-0.260031
H	-4.396324	-3.104886	1.363721
H	-5.573322	-0.571965	-1.906471
H	-6.162368	-2.248946	-0.164939
C	2.659848	-0.755254	-0.544270
C	3.153307	-1.577813	0.478717
C	3.549826	-0.285345	-1.519908
C	4.497810	-1.936782	0.510680
H	2.487112	-1.907472	1.276125
C	4.896763	-0.633990	-1.477282
H	3.178713	0.347399	-2.325000
C	5.374440	-1.465478	-0.465718
H	4.864497	-2.573487	1.312663
H	5.574021	-0.258584	-2.241174
H	6.426397	-1.739350	-0.433876
H	1.008652	-2.880044	-0.156300

1Fe-wills-3 Gsolv= -2590.295725

Fe	0.276369	0.430328	0.935642
C	0.129898	-1.297702	-0.279329
O	-0.020431	-2.587914	0.096673
C	-1.006829	-0.447757	-0.477428
C	-0.471881	0.789958	-0.975968
C	0.924646	0.691218	-1.016977
C	1.357218	-0.596488	-0.536309
Si	3.132529	-1.220383	-0.373730
C	3.356047	-2.633444	-1.586258
H	2.677056	-3.465608	-1.356183
H	4.382512	-3.019875	-1.544703
H	3.155526	-2.311986	-2.615849
C	4.272858	0.210801	-0.761602
H	5.315655	-0.121003	-0.673478
H	4.127947	1.041230	-0.058140
H	4.131620	0.588757	-1.781925
C	3.428775	-1.834175	1.373574
H	4.412317	-2.318214	1.438455
H	2.677302	-2.568168	1.693684
H	3.413147	-1.004086	2.091630
C	-1.000241	1.097517	1.930755
O	-1.861544	1.480608	2.606573
C	1.553914	1.374991	1.677578
O	2.412982	1.983144	2.164082
H	0.436247	-0.545905	2.080192
C	1.474361	1.947595	-1.605909
O	0.350662	2.839918	-1.597524
C	-0.899655	2.112719	-1.528155
H	1.816565	1.769965	-2.638315
H	2.291062	2.417111	-1.045940
H	-1.280225	1.963329	-2.554587
C	-2.425313	-0.820519	-0.341124
C	-2.896310	-1.541011	0.763670
C	-3.326908	-0.453181	-1.347251
C	-4.240035	-1.890542	0.854248
H	-2.207860	-1.808278	1.563842
C	-4.672028	-0.801562	-1.253267
H	-2.967994	0.100858	-2.213796
C	-5.132098	-1.522784	-0.153393
H	-4.593954	-2.445767	1.720038
H	-5.360635	-0.510011	-2.043120
H	-6.182660	-1.794110	-0.078557
C	-1.886798	2.920897	-0.726374
H	-1.466814	3.155990	0.259200
H	-2.126356	3.857733	-1.240605
H	-2.817872	2.357516	-0.587931
H	0.835321	-3.007869	0.270291

1Fe-wills-3- triplet state Gsolv= -2590.249351

Fe	0.292758	0.550855	0.933429
C	0.080152	-1.364690	-0.229906
O	-0.048025	-2.600699	0.313548
C	-1.043011	-0.562169	-0.531316
C	-0.485270	0.653484	-1.077900
C	0.909050	0.525533	-1.157662
C	1.329476	-0.681493	-0.531718
Si	3.098780	-1.303392	-0.328988
C	3.326853	-2.772489	-1.472826
H	2.641930	-3.591586	-1.214493
H	4.351191	-3.161490	-1.405526
H	3.136713	-2.495546	-2.517424
C	4.262941	0.088559	-0.790059
H	5.298614	-0.266769	-0.707251
H	4.155108	0.951978	-0.120568
H	4.112813	0.428308	-1.822601

C	3.393148	-1.839176	1.444716
H	4.379731	-2.313549	1.532999
H	2.644510	-2.563734	1.791880
H	3.369324	-0.979927	2.127899
C	-0.985058	1.332009	1.890723
O	-1.878329	1.745864	2.509420
C	1.880984	1.878834	1.575098
O	2.619342	2.263182	2.358008
H	0.697660	-0.230477	2.237474
C	1.468148	1.745989	-1.807306
O	0.344998	2.639536	-1.870286
C	-0.907253	1.922497	-1.748604
H	1.836276	1.524967	-2.822302
H	2.272909	2.248663	-1.254653
H	-1.280935	1.687995	-2.762224
C	-2.460185	-0.873696	-0.310227
C	-2.892176	-1.524705	0.854932
C	-3.415265	-0.509812	-1.269744
C	-4.239787	-1.813870	1.046250
H	-2.165848	-1.785430	1.623103
C	-4.764091	-0.795181	-1.074238
H	-3.093372	-0.009404	-2.182465
C	-5.181346	-1.451137	0.082970
H	-4.558060	-2.316916	1.956881
H	-5.490506	-0.507299	-1.831166
H	-6.234736	-1.674864	0.235719
C	-1.898506	2.803301	-1.032281
H	-1.491013	3.120980	-0.064732
H	-2.124732	3.694203	-1.628062
H	-2.836444	2.261963	-0.857599
H	0.807524	-3.050590	0.370856

1Fe-wills-4 Gsolv= -2551.029608

Fe	0.190538	-0.590353	-0.856957
C	0.029731	1.231407	0.223884
O	-0.162480	2.483985	-0.244445
C	-1.082349	0.371642	0.510254
C	-0.502561	-0.805754	1.093654
C	0.892403	-0.682232	1.085473
C	1.279415	0.579228	0.500771
Si	3.035136	1.236354	0.262281
C	3.245055	2.705445	1.406633
H	2.539558	3.508996	1.155467
H	4.259695	3.116531	1.327015
H	3.073667	2.424606	2.453239
C	4.223981	-0.142490	0.691617
H	5.254268	0.223129	0.590912
H	4.107832	-0.999699	0.015923
H	4.096684	-0.492277	1.723871
C	3.272105	1.779964	-1.517679
H	4.251520	2.263486	-1.631233
H	2.509458	2.499104	-1.844675
H	3.237986	0.923776	-2.203610
C	-1.084725	-1.503590	-1.634561
O	-1.970323	-2.071013	-2.122555
C	1.503441	-1.480233	-1.606942
O	2.377950	-2.056196	-2.105021
H	0.191052	0.288766	-2.091253
C	1.477542	-1.901373	1.720083
O	0.368757	-2.817096	1.762913
C	-0.876116	-2.099257	1.730987
H	1.828404	-1.679994	2.741056
H	2.291574	-2.380366	1.165421
H	-1.609810	-2.698981	1.180157
H	-1.250278	-1.940617	2.755608
C	-2.516120	0.658769	0.346290
C	-2.998851	1.410136	-0.734122
C	-3.428539	0.150289	1.278697
C	-4.361495	1.654566	-0.867827
H	-2.303198	1.786544	-1.481503
C	-4.793018	0.394358	1.140597
H	-3.068592	-0.428736	2.128097
C	-5.263940	1.148321	0.068383
H	-4.722172	2.235323	-1.713909
H	-5.488238	-0.006461	1.874842
H	-6.329216	1.338154	-0.041267
H	0.676944	2.926312	-0.439480

1Fe-wills-4- triplet state Gsolv= -2550.984484

Fe	-0.167070	-0.675440	0.845973
C	-0.004093	1.313182	-0.170668
O	0.155766	2.501388	0.461113
C	1.107461	0.530422	-0.580450
C	0.518689	-0.623235	-1.206698
C	-0.878620	-0.486992	-1.223894
C	-1.266894	0.674241	-0.500060
Si	-3.025628	1.282124	-0.179627
C	-3.265960	2.913761	-1.075968

H	-2.598131	3.692353	-0.682942
H	-4.296765	3.269714	-0.948587
H	-3.071641	2.815490	-2.151155
C	-4.201587	-0.021764	-0.826937
H	-5.236144	0.316394	-0.683777
H	-4.086181	-0.974206	-0.292823
H	-4.058506	-0.205644	-1.899357
C	-3.282467	1.549872	1.659652
H	-4.257371	2.023316	1.837136
H	-2.511296	2.201928	2.091207
H	-3.265638	0.599542	2.208566
C	1.102847	-1.754159	1.468386
O	2.010438	-2.399746	1.799161
C	-1.794668	-1.948952	1.444001
O	-2.487010	-2.431925	2.214800
H	-0.417213	-0.078544	2.285841
C	-1.460324	-1.666900	-1.929024
O	-0.343736	-2.566163	-2.063449
C	0.897001	-1.846405	-1.968157
H	-1.844369	-1.388715	-2.923891
H	-2.255173	-2.196614	-1.388861
H	1.635441	-2.493282	-1.480148
H	1.266399	-1.590174	-2.975101
C	2.533936	0.754915	-0.328791
C	2.981164	1.421860	0.823056
C	3.489092	0.252108	-1.224435
C	4.341548	1.590297	1.060455
H	2.256455	1.792836	1.544909
C	4.849995	0.418638	-0.981697
H	3.162685	-0.261692	-2.127902
C	5.282872	1.089882	0.160580
H	4.668973	2.105529	1.961056
H	5.574616	0.023642	-1.690498
H	6.345814	1.219666	0.350897
H	-0.692933	2.947106	0.595794

1Fe-wills-5 Gsolv= -2708.065367

Fe	0.447662	0.964186	-0.892856
C	0.023591	-1.023838	-0.319058
O	-0.016743	-2.130669	-1.094909
C	1.249651	-0.584960	0.278867
C	0.890459	0.538120	1.101065
C	-0.482004	0.778512	0.953676
C	-1.069154	-0.156813	0.031136
Si	-2.888209	-0.267590	-0.466449
C	-3.662134	1.428066	-0.271523
H	-4.738357	1.361079	-0.481463
H	-3.234186	2.146323	-0.982245
H	-3.548428	1.835452	0.740610
C	-3.011813	-0.800165	-2.263161
H	-4.043791	-0.659598	-2.611891
H	-2.757139	-1.853008	-2.444413
H	-2.362091	-0.176972	-2.892416
C	-3.731395	-1.525767	0.687078
C	2.004122	1.502259	-1.483129
O	3.041863	1.807538	-1.901572
C	-0.387572	2.426762	-1.384994
O	-0.936409	3.391739	-1.719546
H	0.258766	0.466284	-2.308955
C	-0.871377	1.904019	1.852449
O	0.388198	2.447012	2.273500
C	1.461461	1.489039	2.104886
H	-1.440399	1.527740	2.718814
H	-1.450064	2.706139	1.379640
H	1.610255	0.952959	3.059336
C	-5.183393	-1.720523	0.248235
H	-5.691231	-2.425959	0.925551
H	-5.753614	-0.780959	0.268734
H	-5.254415	-2.134550	-0.767449
C	2.569805	-1.229726	0.168908
C	3.065778	-1.690099	-1.057719
C	3.348007	-1.394943	1.320874
C	4.311856	-2.304698	-1.126629
H	2.479488	-1.543253	-1.963394
C	4.597056	-2.007251	1.249026
H	2.967448	-1.048677	2.281151
C	5.081623	-2.465259	0.025749
H	4.687863	-2.652088	-2.086342
H	5.190864	-2.127636	2.152324
H	6.057388	-2.942112	-0.032104
C	2.717925	2.231922	1.731159
H	2.544368	2.836855	0.832646
H	3.029456	2.893340	2.546669
H	3.533745	1.526656	1.530516
H	-0.869384	-2.205456	-1.549656
C	-3.004596	-2.869500	0.629005
H	-3.510233	-3.600126	1.280611
H	-2.993415	-3.292167	-0.385825

H	-1.964123	-2.790319	0.974945
C	-3.698639	-0.999985	2.122566
H	-2.670051	-0.835368	2.476109
H	-4.248087	-0.054108	2.228327
H	-4.165744	-1.729060	2.804132

1Fe-wills-5- triplet state Gsolv= -2629.502326

Fe	0.092895	0.541542	0.958867
C	0.006724	-1.225959	-0.444152
O	0.032719	-2.528908	-0.070154
C	-1.205177	-0.514920	-0.591671
C	-0.799801	0.813947	-0.992768
C	0.593626	0.842547	-1.149041
C	1.163868	-0.384398	-0.706585
Si	2.993795	-0.841694	-0.668717
C	3.298513	-2.197630	-1.931558
H	4.373535	-2.395690	-2.034870
H	2.913009	-1.911709	-2.918161
H	2.813161	-3.138610	-1.638146
C	3.974880	0.695254	-1.098029
H	5.047992	0.462626	-1.091752
H	3.805683	1.503161	-0.373722
H	3.726213	1.069930	-2.099155
C	3.459922	-1.458650	1.050261
H	2.727420	-2.211717	1.380437
H	3.356748	-0.613828	1.749058
C	-1.215986	1.029839	2.059134
O	-2.120807	1.246217	2.756376
C	1.565134	1.940093	1.641874
O	2.361281	2.322973	2.366433
H	0.613803	-0.359289	2.135140
C	0.994605	2.183790	-1.661821
O	-0.210824	2.958330	-1.560704
C	-1.379871	2.108068	-1.470530
H	1.324628	2.127419	-2.711789
H	1.777921	2.694620	-1.085939
H	-1.793278	1.966725	-2.485960
C	4.872538	-2.035747	1.112785
H	5.150826	-2.327208	2.133327
H	4.969611	-2.929199	0.482478
H	5.622712	-1.310972	0.767672
C	-2.570449	-1.001502	-0.361493
C	-2.870625	-1.864976	0.703009
C	-3.610968	-0.595268	-1.209267
C	-4.171568	-2.315923	0.904225
H	-2.079201	-2.166260	1.387438
C	-4.913060	-1.043406	-1.003276
H	-3.393166	0.067307	-2.046259
C	-5.198109	-1.908233	0.052152
H	-4.386783	-2.982341	1.736824
H	-5.706311	-0.718741	-1.673240
H	-6.214867	-2.259641	0.212676
C	-2.400566	2.789103	-0.595123
H	-1.963821	3.016101	0.385268
H	-2.739480	3.723646	-1.055043
H	-3.274218	2.142038	-0.449523
H	0.938736	-2.869822	-0.059650

1Mn-a Gsolv= -2632.572704

C	-0.018402	1.262384	0.026533
O	-0.113040	2.446025	-0.621562
C	-1.199418	0.572161	0.441281
C	-0.702013	-0.550525	1.184155
C	0.701740	-0.565625	1.152455
C	1.181249	0.557113	0.386484
Si	-2.985664	1.076622	0.094938
C	-3.325505	2.677354	1.009913
H	-3.152077	2.564579	2.087345
H	-4.367723	2.990245	0.865853
H	-2.679158	3.485661	0.645102
C	-4.077589	-0.307156	0.728335
H	-3.930993	-0.486055	1.801318
H	-3.884755	-1.245911	0.192095
H	-5.133930	-0.050686	0.575060
C	-3.230273	1.311101	-1.747867
H	-3.119867	0.361671	-2.287288
H	-2.512832	2.027331	-2.166907
H	-4.240345	1.694051	-1.944983
Si	2.982202	1.074714	0.118373
C	3.223218	2.695377	1.029698
H	4.255186	3.052355	0.918248
H	3.017846	2.582180	2.101517
H	2.555599	3.474464	0.638447
C	4.072212	-0.268909	0.828912
H	5.125500	0.022256	0.724003
H	3.939376	-1.225039	0.307093
H	3.877862	-0.426610	1.897512
C	3.315726	1.316615	-1.710895

H	4.335101	1.698889	-1.854130
H	2.627571	2.039397	-2.169104
H	3.229036	0.373322	-2.264712
C	1.367107	-1.701663	-1.389029
O	2.270301	-2.334066	-1.744606
H	0.091275	0.096452	-2.089648
C	1.190252	-1.707614	1.978706
O	0.004969	-2.497320	2.184236
C	-1.179227	-1.701167	2.002820
H	1.584128	-1.353945	2.945243
H	1.945622	-2.344483	1.504960
H	-1.943944	-2.328713	1.530332
H	-1.561647	-1.355706	2.976728
H	0.732485	2.712059	-1.011774
Mn	-0.042009	-0.748921	-0.803306
N	-1.196761	-1.759738	-1.351280
O	-2.065699	-2.486134	-1.680078

1Mn-a- triplet state Gsolv= -2632.570121

Mn	0.010559	-0.796283	-0.739158
N	-0.930175	-2.238455	-1.066533
O	-1.758356	-3.105727	-1.183326
C	-0.172032	1.373825	-0.110307
O	-0.305764	2.422802	-0.957217
C	-1.317419	0.708636	0.410670
C	-0.761345	-0.269449	1.287681
C	0.648249	-0.164184	1.316638
C	1.076563	0.822309	0.394740
Si	-3.106794	0.935997	-0.119228
C	-3.685250	2.664483	0.319909
H	-3.644601	2.838366	1.402356
H	-4.721981	2.815522	-0.008133
H	-3.065703	3.426839	-0.169168
C	-4.115813	-0.366975	0.773069
H	-4.003796	-0.299372	1.862879
H	-3.817168	-1.376201	0.457508
H	-5.181839	-0.248728	0.539710
C	-3.219147	0.665917	-1.973615
H	-2.966982	-0.372783	-2.228373
H	-2.533356	1.325379	-2.520718
H	-4.236884	0.864471	-2.334963
Si	2.847461	1.374317	0.038741
C	3.012810	3.155209	0.604952
H	4.032003	3.522220	0.427157
H	2.798466	3.254276	1.676313
H	2.322320	3.813800	0.061492
C	3.999046	0.251360	0.995027
H	5.037353	0.570433	0.835798
H	3.918076	-0.791219	0.660399
H	3.803485	0.286489	2.074265
C	3.205503	1.265640	-1.799213
H	4.206260	1.669522	-2.003489
H	2.487717	1.837918	-2.401890
H	3.183663	0.224276	-2.146033
C	2.220942	-2.461211	-1.033918
O	2.759886	-3.273346	-1.619976
H	0.316163	-0.271283	-2.252707
C	1.186504	-1.183277	2.263413
O	0.049269	-2.020729	2.542577
C	-1.179104	-1.335801	2.240676
H	1.547397	-0.715645	3.193744
H	1.987000	-1.818150	1.863562
H	-1.888523	-2.070424	1.841243
H	-1.608719	-0.900909	3.157843
H	0.550238	2.704178	-1.312097

1Mn-b Gsolv= -2775.338442

Mn	0.069969	-0.509692	1.197013
O	-1.825499	0.480962	3.022577
N	-1.027184	0.052005	2.268135
H	0.370541	-1.807744	1.967975
H	1.109587	-3.637420	-0.227651
C	0.126592	-1.997926	-0.406321
O	0.189587	-3.340145	-0.311258
C	-1.112522	-1.284225	-0.446428
C	-0.752058	0.090419	-0.653295
C	0.648481	0.208602	-0.698539
C	1.234335	-1.086476	-0.500447
C	1.543298	0.141989	1.994126
O	2.519226	0.552662	2.463313
C	-2.470320	-1.849812	-0.407928
C	-3.532324	-1.123973	0.153276
C	-2.749677	-3.094986	-0.981923
C	-4.824524	-1.630945	0.137489
H	-3.344595	-0.156095	0.615896
C	-4.049107	-3.596943	-0.992334
H	-1.950117	-3.671998	-1.439888
C	-5.108316	-2.877209	-0.436038

H	-5.633964	-1.052886	0.582761
H	-4.244079	-4.567052	-1.448189
C	2.666690	-1.430262	-0.551620
C	3.473683	-0.859085	-1.541427
C	3.253661	-2.325800	0.353594
C	4.826531	-1.178256	-1.626003
H	3.037081	-0.167441	-2.260518
C	4.601554	-2.648276	0.255020
H	2.658727	-2.747517	1.164002
C	5.413066	-2.079908	-0.734434
H	5.437774	-0.722929	-2.404240
H	5.040226	-3.345394	0.968438
C	-6.509469	-3.405403	-0.453228
H	-6.550361	-4.418304	-0.867158
H	-6.936363	-3.432866	0.556775
H	-7.165711	-2.767217	-1.058515
C	6.868724	-2.423046	-0.812501
H	7.327949	-2.020131	-1.721151
H	7.416530	-2.017752	0.047807
H	7.021787	-3.508873	-0.803006
C	-1.403132	1.405220	-0.940897
C	1.065355	1.605874	-1.014581
H	-2.277178	1.650105	-0.332218
H	-1.709098	1.437357	-1.995926
H	1.283247	1.693623	-2.087946
H	1.942182	1.966697	-0.469954
C	-0.230122	2.396711	-0.696844
C	-0.291913	2.892014	0.758675
C	-0.328433	3.657896	-1.541699
O	-1.329320	3.040694	1.375610
O	0.622257	4.190412	-2.082496
O	0.902141	3.214203	1.238739
O	-1.568436	4.129012	-1.581604
C	0.930981	3.673935	2.601110
H	1.984834	3.804876	2.845890
H	0.396748	4.624155	2.686845
H	0.472041	2.928515	3.258890
C	-1.764801	5.356035	-2.307324
H	-1.504007	5.214583	-3.359403
H	-2.824433	5.589196	-2.207264
H	-1.155329	6.151381	-1.870434

1Mn-b- triplet state Gsolv=

Mn	0.046445	-0.445447	1.236099
O	-1.705802	0.420890	3.362271
N	-1.260204	-0.022809	2.328784
H	0.406926	-1.717316	2.135212
H	1.063067	-3.622474	-0.206595
C	0.104008	-1.972052	-0.416441
O	0.146780	-3.314579	-0.288097
C	-1.144222	-1.246808	-0.501769
C	-0.772790	0.108630	-0.730374
C	0.638046	0.194003	-0.775617
C	1.218701	-1.089209	-0.591179
C	1.581680	0.145666	2.244054
O	2.550304	0.348832	2.816664
C	-2.502290	-1.803761	-0.465380
C	-3.569254	-1.051052	0.049794
C	-2.781213	-3.072383	-0.988567
C	-4.864162	-1.551932	0.034415
H	-3.378315	-0.068351	0.477075
C	-4.082831	-3.567151	-1.000330
H	-1.976876	-3.671437	-1.408894
C	-5.147027	-2.818398	-0.492706
H	-5.677390	-0.951275	0.441727
H	-4.276782	-4.553638	-1.420277
C	2.644191	-1.441407	-0.635455
C	3.466024	-0.871389	-1.616045
C	3.221246	-2.342097	0.273155
C	4.817335	-1.196553	-1.689294
H	3.037758	-0.178162	-2.338752
C	4.569195	-2.669937	0.185865
H	2.618707	-2.762598	1.078816
C	5.392186	-2.103665	-0.795095
H	5.437353	-0.744533	-2.462720
H	4.998522	-3.371261	0.900986
C	-6.551442	-3.337905	-0.515739
H	-6.591328	-4.366381	-0.889680
H	-6.998085	-3.322656	0.485992
H	-7.192054	-2.721085	-1.158785
C	6.846607	-2.454769	-0.864388
H	7.313768	-2.052455	-1.769366
H	7.391842	-2.054427	-0.000065
H	6.994137	-3.541400	-0.856702
C	-1.389420	1.432850	-1.052879
C	1.073365	1.585662	-1.092699
H	-2.281212	1.700288	-0.480974
H	-1.644926	1.478785	-2.121293

H	1.268109	1.665565	-2.171967
H	1.968894	1.932077	-0.570159
C	-0.200346	2.393063	-0.751845
C	-0.263494	2.805559	0.728871
C	-0.256549	3.697707	-1.530661
O	-1.296502	3.118980	1.287909
O	0.714964	4.234297	-2.029249
O	0.940213	2.992092	1.256735
O	-1.483140	4.202838	-1.558009
C	0.975741	3.444818	2.623709
H	2.031893	3.505623	2.885588
H	0.506922	4.428591	2.708483
H	0.461164	2.725085	3.268845
C	-1.637436	5.478205	-2.206393
H	-1.360196	5.399314	-3.260716
H	-2.693043	5.730225	-2.109421
H	-1.018188	6.228749	-1.708164
H	6.300056	-1.884961	-0.242161
C	-2.582226	-0.834806	-0.432579
C	-2.964439	-1.823556	0.485041
C	-3.563737	-0.238546	-1.234612
C	-4.296611	-2.209781	0.586284
H	-2.217012	-2.278065	1.131533
C	-4.896906	-0.625742	-1.128282
H	-3.281390	0.522686	-1.960077
C	-5.267527	-1.614197	-0.219411
H	-4.579806	-2.976108	1.304279
H	-5.646053	-0.155025	-1.760861
H	-6.308319	-1.918271	-0.135943
H	0.873527	-2.828194	0.058160
H	-2.003500	2.663244	-0.857470
N	-1.213717	1.395846	1.747752
O	-2.123212	1.980232	2.218002
Mn	-0.035133	0.586363	0.963631

1Mn-c Gsolv= -2277.260685

C	0.000908	-1.168062	-0.335839
O	-0.027726	-2.477845	-0.032508
C	-1.185456	-0.398303	-0.560338
C	-0.722639	0.885219	-1.003663
C	0.677979	0.914207	-0.992084
C	1.168669	-0.350843	-0.527208
C	1.405256	1.335500	1.739182
O	2.358954	1.803284	2.199594
H	0.141014	-0.545159	1.997557
C	1.138725	2.241227	-1.491845
O	-0.052893	3.042843	-1.421679
C	-1.222165	2.209147	-1.478354
H	1.489071	2.169861	-2.533972
H	1.918571	2.721898	-0.890530
H	-1.591110	2.138877	-2.514372
C	2.576168	-0.771771	-0.418189
C	3.033470	-1.558731	0.647591
C	3.482952	-0.381145	-1.411397
C	4.364290	-1.962477	0.703992
H	2.352908	-1.827266	1.455476
C	4.816236	-0.776113	-1.345301
H	3.136905	0.227179	-2.245829
C	5.259374	-1.573427	-0.291752
H	4.705530	-2.571540	1.537882
H	5.509047	-0.464069	-2.123379

1Mn-c- triplet state Gsolv= -2277.255471

Mn	-0.068202	0.585332	1.037397
C	-0.249488	-1.255346	-0.301095
O	-0.331378	-2.549753	0.068131
C	-1.412318	-0.455089	-0.558263
C	-0.906196	0.771115	-1.043997
C	0.508606	0.716917	-1.123296
C	0.955844	-0.535207	-0.656179
C	2.659988	1.279093	1.361522
O	3.739974	1.458509	1.670533
H	0.046500	-0.393080	2.342684
C	1.002208	2.015468	-1.666901
O	-0.144212	2.877349	-1.568325
C	-1.355050	2.104257	-1.535718
H	1.309988	1.913386	-2.720164
H	1.827678	2.475107	-1.109588
H	-1.783910	2.027316	-2.548091
C	2.342410	-0.997619	-0.530548
C	2.759194	-1.805696	0.539121
C	3.298038	-0.567942	-1.462268
C	4.093504	-2.180466	0.663070
H	2.051522	-2.101460	1.312966
C	4.633652	-0.932978	-1.326898
H	2.988895	0.052387	-2.302294
C	5.036379	-1.742487	-0.265304
H	4.400084	-2.800851	1.502083

H	5.362503	-0.585586	-2.055565
H	6.080608	-2.026834	-0.159686
C	-2.812037	-0.801095	-0.297113
C	-3.171233	-1.683104	0.733354
C	-3.827018	-0.229379	-1.078611
C	-4.508667	-1.986208	0.968303
H	-2.398531	-2.119540	1.362866
C	-5.163821	-0.531834	-0.837670
H	-3.566355	0.445372	-1.893003
C	-5.510496	-1.413203	0.185424
H	-4.770240	-2.668677	1.773991
H	-5.936767	-0.080800	-1.456104
H	-6.555123	-1.650916	0.372607
H	0.547094	-2.961826	0.071414
H	-2.076915	2.618497	-0.889850
N	-0.572785	2.116509	1.730510
O	-1.021069	3.188079	2.047867

1Mn Gsolv= -2635.920814

C	0.008801	-1.286796	-0.330396
O	0.108109	-2.608286	-0.050050
H	-0.755120	-2.998733	0.149431
C	-1.180279	-0.522398	-0.521251
C	-0.713628	0.786806	-0.939589
C	-1.524765	1.984028	-1.330405
H	-2.392260	2.103927	-0.670334
H	-1.928827	1.815052	-2.341912
C	-0.664945	3.244594	-1.328920
H	-1.230912	4.074931	-1.767489
H	-0.430995	3.527370	-0.289386
C	0.630179	3.012366	-2.096973
H	1.186741	3.948969	-2.219296
H	0.379403	2.658806	-3.109283
C	1.516507	1.978891	-1.402838
H	2.289953	1.621064	-2.096126
H	2.052782	2.445338	-0.564212
C	0.704927	0.805146	-0.931215
C	1.180850	-0.487001	-0.482421
Si	-2.949298	-1.164608	-0.308053
C	-3.269872	-2.380292	-1.699711
H	-3.193245	-1.890520	-2.678635
H	-4.276179	-2.810126	-1.612408
H	-2.548165	-3.207594	-1.682248
C	-4.214110	0.213283	-0.340991
H	-4.236505	0.752815	-1.294889
H	-4.058829	0.937345	0.469233
H	-5.204222	-0.239846	-0.192520
C	-3.083773	-2.030662	1.353990
H	-2.941229	-1.312214	2.172288
H	-2.370461	-2.851685	1.505021
H	-4.091627	-2.456193	1.454902
Si	2.942341	-1.148426	-0.283400
C	3.261142	-2.326776	-1.707636
H	4.278028	-2.736309	-1.647029
H	3.161684	-1.812831	-2.672532
H	2.556296	-3.167709	-1.698055
C	4.202835	0.238728	-0.323628
H	5.196687	-0.203269	-0.166859
H	4.041607	0.975366	0.473267
H	4.224289	0.767108	-1.284098
C	3.104202	-2.044651	1.356294
H	4.113035	-2.471157	1.440842
H	2.382508	-2.863568	1.457993
H	2.961047	-1.357989	2.200981
C	1.363650	1.168468	1.858465
O	2.262735	1.676666	2.386150
H	0.101784	-0.760999	2.015662
O	-2.084203	1.794390	2.368368
N	-1.203498	1.210563	1.839410
Mn	-0.038753	0.415864	1.024791

1Mn- triplet state Gsolv= -2635.932235

Mn	-0.058547	0.104954	1.110374
C	0.100279	-0.979638	-0.865518
O	0.268859	-2.319646	-0.988184
H	-0.577582	-2.776362	-1.098364
C	-1.120776	-0.257957	-0.865766
C	-0.720133	1.130890	-0.736979
C	-1.588108	2.352384	-0.715229
H	-2.482671	2.183345	-0.104130
H	-1.948494	2.546262	-1.738796
C	-0.819339	3.568578	-0.205208
H	-1.415583	4.474091	-0.369816
H	-0.672412	3.477659	0.883737
C	0.538143	3.687938	-0.886463
H	1.031676	4.627280	-0.609750
H	0.388684	3.715157	-1.977374
C	1.437958	2.509586	-0.525247

H	2.337411	2.504835	-1.157201
H	1.796016	2.624723	0.510719
C	0.697910	1.209885	-0.673535
C	1.238360	-0.114589	-0.672007
Si	-2.845137	-1.023170	-0.816238
C	-3.171097	-1.926124	-2.430525
H	-3.175040	-1.232768	-3.280844
H	-4.150344	-2.421541	-2.392432
H	-2.416450	-2.698142	-2.631412
C	-4.186539	0.248559	-0.514650
H	-4.230226	1.022949	-1.289139
H	-4.075278	0.735085	0.463221
H	-5.149976	-0.279739	-0.513063
C	-2.889301	-2.251427	0.610230
H	-2.672589	-1.743911	1.561304
H	-2.176047	-3.078920	0.499041
H	-3.891937	-2.693653	0.689598
Si	3.072008	-0.559561	-0.580873
C	3.866440	-0.111485	-2.221540
H	4.944898	-0.316600	-2.197068
H	3.730664	0.952796	-2.453786
H	3.431281	-0.695073	-3.042740
C	3.861165	0.432515	0.805682
H	4.857625	0.026018	1.025455
H	3.266802	0.379654	1.728431
H	3.984700	1.489118	0.538567
C	3.327947	-2.388455	-0.255455
H	4.404582	-2.570658	-0.134058
H	2.976169	-3.007575	-1.088869
H	2.830165	-2.730956	0.660195
C	0.712630	-1.492783	2.127866
O	1.570455	-1.415182	2.995431
H	0.298198	-2.512784	1.884318
O	-2.129107	1.097503	2.936563
N	-1.193093	0.703631	2.290009

2'Co-a Gsolv= -3015.726857

C	0.050607	-0.053576	1.379059
O	0.136928	0.912100	2.278865
H	-0.726394	1.275717	2.535390
C	-1.151359	-0.585368	0.775012
C	-0.656189	-1.612316	-0.094535
C	0.756451	-1.592193	-0.111696
C	1.242091	-0.561899	0.760411
Si	-2.974859	-0.175916	1.158423
C	-3.216158	-0.517472	2.983710
H	-2.993288	-1.564317	3.223980
H	-4.258099	-0.320038	3.266943
H	-2.576495	0.118582	3.609227
C	-4.029835	-1.306306	0.112484
H	-3.819803	-2.362716	0.322880
H	-3.885250	-1.125347	-0.959729
H	-5.088084	-1.126304	0.341955
C	-3.282319	1.630328	0.777965
H	-3.133530	1.848031	-0.287305
H	-2.626256	2.292830	1.358031
H	-4.319306	1.884737	1.033618
Si	3.030308	-0.025613	1.128703
C	3.379450	-0.423076	2.922375
H	4.425308	-0.192590	3.162639
H	3.209561	-1.484937	3.137653
H	2.743003	0.168928	3.591524
C	4.123023	-1.010547	-0.025933
H	5.175266	-0.756883	0.156181
H	3.906728	-0.793052	-1.080109
H	4.010432	-2.090306	0.135266
C	3.175158	1.810918	0.801855
H	4.202509	2.142156	1.001969
H	2.505794	2.391606	1.448154
H	2.941704	2.057115	-0.242372
C	-1.363826	0.273067	-2.049309
C	1.271341	0.377534	-2.051495
O	2.043450	0.487812	-2.881707
C	-1.117707	-2.727132	-0.968901
O	0.052445	-3.050835	-1.732081
C	1.231490	-2.689071	-1.001890
H	-1.929467	-2.489782	-1.662070
H	-1.422357	-3.579633	-0.340210
H	1.587959	-3.529964	-0.384961
H	2.015754	-2.423276	-1.717242
H	-0.259719	2.711711	-2.287846
C	-0.261324	3.033619	-1.226040
O	-0.101859	2.117307	-0.340372
O	-0.410874	4.230401	-0.951346
Co	0.011613	0.205791	-0.749119
N	-2.205983	0.337063	-2.863204

2Co-a Gsolv= -3015.707702

C	-0.035559	-0.555789	-1.135537
O	-0.055657	-1.845724	-1.428873
H	0.328983	-2.432432	-0.702776
C	-1.256501	0.184627	-0.873444
C	-0.807436	1.505135	-0.603871
C	0.616752	1.538441	-0.606443
C	1.144017	0.240162	-0.889919
Si	-3.026000	-0.513709	-0.972930
C	-3.277616	-1.042724	-2.750296
H	-3.114615	-0.207168	-3.441964
H	-4.302391	-1.407613	-2.895720
H	-2.589651	-1.852629	-3.022411
C	-4.181026	0.879443	-0.504190
H	-4.025091	1.760479	-1.140186
H	-4.051252	1.180073	0.542957
H	-5.222094	0.556393	-0.632025
C	-3.171377	-1.970985	0.188986
H	-2.947720	-1.690793	1.226307
H	-2.496751	-2.784642	-0.104547
H	-4.197445	-2.360500	0.160107
Si	2.970047	-0.270080	-1.095376
C	3.170057	-0.751277	-2.890952
H	4.207991	-1.045707	-3.091581
H	2.920242	0.082262	-3.558590
H	2.523767	-1.600345	-3.145989
C	3.987178	1.233479	-0.651419
H	5.053297	1.002025	-0.771831
H	3.830826	1.536046	0.392245
H	3.759007	2.088856	-1.299883
C	3.367358	-1.704997	0.033353
H	4.443736	-1.914757	-0.023010
H	2.831748	-2.614068	-0.264375
H	3.123864	-1.489707	1.082366
C	-1.406711	0.620347	2.066009
C	1.225296	0.659377	2.040267
O	2.008719	0.948358	2.813721
H	-0.166221	-1.386894	1.337418
C	0.303902	-2.442646	1.672061
O	0.414862	-2.540733	2.886953
O	0.523563	-3.187430	0.706505
C	-1.305144	2.875486	-0.314558
O	-0.145096	3.551265	0.188153
C	1.044130	2.935971	-0.321216
H	-2.101422	2.943224	0.432451
H	-1.654037	3.339480	-1.251597
H	1.364864	3.414795	-1.261166
H	1.840679	3.051301	0.420612
Co	-0.053165	0.226824	0.808804
N	-2.230936	0.864418	2.863871

2'Co-b Gsolv= -3158.491979

C	-0.546269	-1.593276	-0.999395
O	-0.860915	-2.871041	-1.090043
H	-1.814288	-3.022121	-0.960942
C	-1.458240	-0.477913	-0.833645
C	-0.626430	0.680655	-0.800062
C	0.728143	0.285108	-0.816469
C	0.809505	-1.150888	-0.899539
C	-1.079977	0.656998	2.025238
C	1.324785	-0.484833	1.822987
O	2.291580	-0.473996	2.425337
C	-2.924897	-0.549529	-0.903973
C	-3.735655	0.206778	-0.046670
C	-3.535551	-1.340154	-1.885365
C	-5.116875	0.161628	-0.167809
H	-3.279406	0.826404	0.722546
C	-4.922759	-1.378905	-1.997303
H	-2.926781	-1.900426	-2.593729
C	-5.736342	-0.634436	-1.140541
H	-5.733862	0.754508	0.506503
H	-5.380639	-1.992129	-2.771936
C	2.024352	-1.974211	-0.959501
C	3.149017	-1.499555	-1.644029
C	2.092203	-3.222324	-0.327543
C	4.308255	-2.265298	-1.707113
H	3.114292	-0.533313	-2.144352
C	3.255470	-3.978381	-0.395318
H	1.237848	-3.591504	0.236338
C	4.380512	-3.517885	-1.089946
H	5.174962	-1.884333	-2.245666
H	3.298760	-4.943258	0.108090
C	-7.228658	-0.678189	-1.246764
H	-7.670852	-1.174915	-0.373866
H	-7.652045	0.332547	-1.285731
H	-7.551141	-1.221208	-2.141011
C	5.619097	-4.352237	-1.188379
H	5.605932	-4.964492	-2.099773
H	6.519519	-3.729654	-1.231432

H	5.708889	-5.036933	-0.338164
C	-0.759943	2.161410	-0.824026
C	1.632100	1.467099	-0.871916
H	-1.513118	2.573105	-0.146609
H	-1.030003	2.467533	-1.843733
H	1.981307	1.584067	-1.908734
H	2.518820	1.409817	-0.234770
C	0.681199	2.647698	-0.502441
C	0.753776	3.099914	0.957053
C	1.069524	3.863328	-1.335949
O	0.021156	3.973567	1.385167
O	0.456105	4.280156	-2.296427
O	1.679299	2.486116	1.672716
O	2.209115	4.381713	-0.890436
H	-0.466870	-1.563024	3.570521
C	-0.976733	-2.316398	2.935422
O	-0.991298	-2.095611	1.668289
O	-1.492424	-3.308821	3.460904
C	1.771210	2.852380	3.061532
H	2.620712	2.295354	3.456388
H	1.943391	3.927253	3.157706
H	0.849788	2.566277	3.579386
C	2.717947	5.525600	-1.600853
H	1.986871	6.337659	-1.571315
H	3.629327	5.814710	-1.078374
H	2.940173	5.254634	-2.636216
N	-1.615033	1.343975	2.811007
Co	-0.197033	-0.523561	0.822284

2Co-b Gsolv= -3158.467511

C	0.235989	-1.624333	-0.957355
O	0.391603	-2.927012	-0.999760
H	-0.169602	-3.402942	-0.307973
C	-1.020810	-0.889930	-0.864299
C	-0.638988	0.482612	-0.804986
C	0.778813	0.580434	-0.816486
C	1.353781	-0.722231	-0.849300
C	-1.267440	-0.049434	2.020531
C	1.422341	0.106584	1.967974
O	2.249265	0.479528	2.656922
C	-2.370075	-1.458028	-0.954371
C	-2.593633	-2.664256	-1.632356
C	-3.473528	-0.777334	-0.418382
C	-3.880967	-3.174317	-1.758346
H	-1.763929	-3.200674	-2.085603
C	-4.753358	-1.295831	-0.547865
H	-3.331475	0.157556	0.118144
C	-4.981635	-2.505862	-1.215640
H	-4.035658	-4.108468	-2.296316
H	-5.596829	-0.752950	-0.123415
C	2.779182	-1.077886	-0.844505
C	3.683750	-0.312776	-1.586136
C	3.258210	-2.165466	-0.100102
C	5.038384	-0.634603	-1.591312
H	3.327677	0.528266	-2.178714
C	4.610366	-2.475576	-0.109928
H	2.569422	-2.755129	0.502804
C	5.524073	-1.717486	-0.855156
H	5.730541	-0.033621	-2.179240
H	4.973001	-3.319119	0.476526
C	-6.363951	-3.066468	-1.328545
H	-7.095192	-2.281151	-1.551522
H	-6.422875	-3.829939	-2.111191
H	-6.674425	-3.534208	-0.385180
C	6.980859	-2.061074	-0.842306
H	7.413965	-1.899940	0.153073
H	7.142216	-3.117089	-1.090022
H	7.543206	-1.450916	-1.556425
C	-1.255203	1.838277	-0.840490
C	1.224160	1.992822	-0.865266
H	-2.110826	1.990575	-0.179848
H	-1.596093	2.023735	-1.870213
H	1.511184	2.222692	-1.901190
H	2.080186	2.231988	-0.226426
C	-0.056410	2.780412	-0.495775
C	0.012525	3.196911	0.974922
C	-0.190669	4.048741	-1.332865
O	1.031080	3.654382	1.463202
O	0.334221	4.212624	-2.415286
O	-1.118439	3.040275	1.635906
O	-1.006325	4.920195	-0.754339
C	-1.264031	6.138886	-1.477417
H	-1.740747	5.911403	-2.434218
H	-1.934847	6.719180	-0.844887
H	-0.328725	6.680715	-1.639092
C	-1.089410	3.375044	3.034001
H	-0.839905	4.431714	3.161917
H	-2.092888	3.172301	3.407112

H	-0.355367	2.747079	3.549069
C	-0.330611	-3.022832	2.056063
O	-0.424549	-2.989910	3.275777
H	0.219608	-2.052211	1.604403
O	-0.642571	-3.846226	1.179719
N	-2.128305	0.156779	2.789612
Co	0.138221	-0.503597	0.827341

2'Co-c Gsolv= -2660.412206

C	0.002146	0.183014	-1.348175
O	-0.034344	1.277835	-2.076380
H	0.857368	1.596439	-2.304375
C	1.176454	-0.468458	-0.813666
C	0.683293	-1.638474	-0.156361
C	-0.723679	-1.627904	-0.174302
C	-1.189855	-0.453785	-0.855204
C	1.385431	-0.098508	2.072952
C	-1.324139	-0.084893	2.064095
O	-2.161028	-0.176742	2.830595
C	2.581378	-0.096356	-1.026924
C	3.509248	-1.095607	-1.343222
C	3.009872	1.231983	-0.905007
C	4.845327	-0.767940	-1.550326
H	3.180145	-2.128905	-1.441538
C	4.346454	1.554245	-1.118544
H	2.304172	2.007156	-0.606521
C	5.265198	0.556792	-1.442244
H	5.559130	-1.549901	-1.797603
H	4.673665	2.586167	-1.018175
H	6.309898	0.811128	-1.604568
C	-2.584113	-0.052954	-1.074647
C	-3.581127	-1.035502	-1.114811
C	-2.940687	1.295260	-1.213718
C	-4.912407	-0.677440	-1.302856
H	-3.314430	-2.086724	-1.018637
C	-4.272721	1.646821	-1.402920
H	-2.177193	2.067578	-1.159967
C	-5.261121	0.663811	-1.447565
H	-5.677517	-1.449227	-1.337782
H	-4.541243	2.695237	-1.508169
H	-6.301620	0.943429	-1.594774
C	1.137802	-2.883879	0.522272
O	-0.044071	-3.323953	1.203604
C	-1.204728	-2.870639	0.497708
H	1.448871	-3.620904	-0.235432
H	-1.509697	-3.602520	-0.268006
H	-2.025226	-2.744078	1.210872
H	0.049230	2.155323	2.825877
C	0.074904	2.698492	1.858906
O	0.029833	1.982720	0.790422
O	0.142884	3.931806	1.850833
H	1.943559	-2.758205	1.251109
Co	-0.012773	0.028816	0.802071
N	2.280285	-0.157403	2.829503

2Co-c Gsolv= -2660.390312

C	-0.026746	-0.819765	-0.927429
O	-0.010484	-2.128077	-0.828813
H	0.612719	-2.441119	-0.099974
C	-1.254995	-0.056012	-0.888231
C	-0.847233	1.305912	-0.960110
C	0.571942	1.376407	-0.979495
C	1.123377	0.068655	-0.931653
C	-1.605387	0.943385	1.777198
C	0.964278	1.443361	1.874928
O	1.579775	2.078517	2.591048
C	-2.624197	-0.581149	-0.825478
C	-3.642287	0.086477	-1.514641
C	-2.934421	-1.710904	-0.056967
C	-4.953859	-0.375413	-1.445136
H	-3.407004	0.960093	-2.120257
C	-4.245722	-2.165945	0.010598
H	-2.152303	-2.214842	0.506972
C	-5.257648	-1.500506	-0.682281
H	-5.738590	0.147111	-1.986740
H	-4.481727	-3.037722	0.616114
H	-6.282966	-1.858046	-0.623139
C	2.535571	-0.334655	-0.978515
C	3.530103	0.459405	-0.391812
C	2.905092	-1.503736	-1.657081
C	4.865985	0.085627	-0.476412
H	3.262449	1.369515	0.142275
C	4.244297	-1.872238	-1.739914
H	2.147133	-2.119392	-2.135437
C	5.227030	-1.082560	-1.147406
H	5.628056	0.707366	-0.012940
H	4.518895	-2.779426	-2.272740
H	6.272674	-1.374282	-1.209715

C	-1.384934	2.688864	-1.052399
O	-0.247261	3.503234	-0.746600
C	0.956710	2.810738	-1.092179
H	-2.190892	2.921947	-0.349627
H	-1.738129	2.877251	-2.079216
H	1.250933	3.016592	-2.134413
H	1.757424	3.147438	-0.427792
C	0.769940	-1.721791	2.217655
O	1.180220	-2.596200	1.436006
H	-0.029048	-0.982416	1.707513
O	0.955212	-1.478683	3.404524
Co	-0.099274	0.471557	0.742779
N	-2.558614	1.233236	2.396476

2'Co Gsolv= -3019.079269

C	-0.031773	-0.525280	1.289395
O	-0.091156	-1.742367	1.810172
H	0.780615	-2.152884	1.928684
C	1.142142	0.210662	0.902388
C	0.633043	1.485073	0.444313
C	1.388184	2.705577	0.036410
H	2.294068	2.438709	-0.516910
H	1.721219	3.203696	0.961308
C	0.503557	3.656327	-0.762763
H	1.039566	4.597686	-0.927182
H	0.300210	3.224023	-1.755944
C	-0.805334	3.905927	-0.026726
H	-1.396495	4.680552	-0.527378
H	-0.575381	4.283072	0.980977
C	-1.639491	2.630914	0.086463
H	-2.406514	2.741073	0.864439
H	-2.190307	2.451376	-0.846645
C	-0.793632	1.445381	0.441399
C	-1.228788	0.139081	0.882518
Si	2.947133	-0.352658	1.170001
C	3.111817	-0.683734	3.008850
H	2.865008	0.210436	3.594912
H	4.150578	-0.957600	3.236540
H	2.471337	-1.503221	3.359449
C	4.174126	0.963493	0.666582
H	4.020402	1.909658	1.198494
H	4.170580	1.158440	-0.412423
H	5.173996	0.593185	0.932167
C	3.255034	-1.921753	0.192322
H	3.208376	-1.731119	-0.887780
H	2.547133	-2.728128	0.423875
H	4.263809	-2.288178	0.425763
Si	-2.976507	-0.596635	1.070854
C	-3.295997	-0.781068	2.905716
H	-4.306552	-1.173528	3.077417
H	-3.217801	0.185977	3.418167
H	-2.582091	-1.472332	3.369884
C	-4.239678	0.539643	0.285904
H	-5.218592	0.044051	0.338315
H	-4.024775	0.732519	-0.772765
H	-4.327114	1.501305	0.804840
C	-3.027750	-2.249486	0.191610
H	-4.029547	-2.684824	0.306281
H	-2.302450	-2.966424	0.593365
H	-2.836914	-2.134346	-0.884144
C	1.373279	0.349770	-2.035438
C	-1.281977	0.205712	-2.062859
H	0.260048	-1.922922	-3.079566
C	0.309072	-2.557108	-2.170689
O	0.156889	-1.970229	-1.040876
O	0.497664	-3.775077	-2.288643
N	2.217684	0.548617	-2.825650
Co	-0.006297	-0.031676	-0.789851
O	-2.072142	0.356423	-2.871021

2Co Gsolv= -3019.058251

C	0.003756	-0.618051	-1.127580
O	-0.034901	-1.896980	-1.481022
H	-0.346123	-2.516308	-0.746097
C	-1.143497	0.207956	-0.834431
C	-0.598079	1.501345	-0.533401
C	-1.306051	2.774541	-0.225861
H	-2.216196	2.584538	0.352098
H	-1.633353	3.197948	-1.189952
C	-0.380234	3.763824	0.473648
H	-0.889558	4.728727	0.571257
H	-0.163571	3.407789	1.493944
C	0.915976	3.916604	-0.310199
H	1.538584	4.713354	0.110643
H	0.672534	4.213506	-1.341126
C	1.715288	2.615008	-0.331421
H	2.470009	2.633353	-1.129369
H	2.279590	2.497772	0.604149

C	0.839938	1.424959	-0.561937
C	1.231167	0.076368	-0.861889
Si	-2.956637	-0.328107	-1.096185
C	-3.081064	-0.702855	-2.927400
H	-2.840642	0.179302	-3.533751
H	-4.102953	-1.015716	-3.178340
H	-2.399035	-1.512449	-3.215404
C	-4.140660	1.045054	-0.636794
H	-3.974523	1.960802	-1.216163
H	-4.105615	1.292299	0.431389
H	-5.156762	0.691256	-0.859694
C	-3.351159	-1.852912	-0.087448
H	-3.163880	-1.701837	0.983727
H	-2.782366	-2.728411	-0.420461
H	-4.419107	-2.078207	-0.211639
Si	2.954521	-0.728348	-0.995980
C	3.249458	-1.033603	-2.817949
H	4.241732	-1.473722	-2.978983
H	3.201389	-0.093530	-3.382022
H	2.501885	-1.719946	-3.234545
C	4.249994	0.420702	-0.285467
H	5.208748	-0.114768	-0.267650
H	4.021443	0.719063	0.745558
H	4.385275	1.327212	-0.886952
C	2.939233	-2.319068	-0.009665
H	3.929554	-2.789608	-0.070528
H	2.201260	-3.036312	-0.386776
H	2.726410	-2.127402	1.050986
C	-1.313084	0.525493	2.087991
C	1.327062	0.371242	2.097152
O	2.120160	0.538464	2.898155
H	-0.037333	-1.525323	1.339473
C	-0.399201	-2.631045	1.614409
O	-0.544255	-2.795716	2.818831
O	-0.518555	-3.352034	0.612380
N	-2.142063	0.768172	2.882156
Co	0.042371	0.105058	0.835709

2'Fe-Casey Gsolv= -2917.197036

Fe	-0.000199	-0.219702	-0.791042
C	-0.055756	0.013076	1.354465
O	-0.137954	-0.982132	2.246441
H	0.730018	-1.359404	2.458766
C	1.142241	0.579350	0.799552
C	0.644022	1.604535	-0.081610
C	-0.762736	1.571676	-0.115394
C	-1.246298	0.530499	0.750431
Si	2.949888	0.177595	1.203343
C	3.194113	0.465262	3.038004
H	2.969166	1.503976	3.310007
H	4.233685	0.257904	3.322577
H	2.548314	-0.188973	3.638534
C	4.017531	1.321753	0.180221
H	3.809179	2.376659	0.399236
H	3.877647	1.155088	-0.895431
H	5.074892	1.135817	0.409077
C	3.290636	-1.616152	0.775917
H	3.160575	-1.804673	-0.298248
H	2.635805	-2.309437	1.320583
H	4.327294	-1.866887	1.037256
Si	-3.028089	0.019844	1.130056
C	-3.366009	0.401300	2.932556
H	-4.411984	0.177230	3.179097
H	-3.186400	1.460459	3.155058
H	-2.729058	-0.199308	3.593886
C	-4.134636	1.041399	0.016968
H	-5.186316	0.801193	0.220701
H	-3.947972	0.841233	-1.046020
H	-4.000810	2.116288	0.194891
C	-3.241450	-1.809705	0.792449
H	-4.269973	-2.113748	1.027658
H	-2.565001	-2.416430	1.407005
H	-3.054575	-2.049344	-0.262250
C	1.300644	-0.205370	-2.017245
O	2.140063	-0.127205	-2.800817
C	-1.290393	-0.384960	-2.018089
O	-2.124067	-0.465408	-2.806827
C	1.108403	2.753976	-0.913894
O	-0.058313	3.098430	-1.676303
C	-1.244173	2.692104	-0.974784
H	1.925354	2.549291	-1.613392
H	1.406187	3.590846	-0.261595
H	-1.623655	3.514309	-0.346842
H	-2.008899	2.435352	-1.715224
H	0.327945	-2.736912	-2.331809
C	0.303968	-3.068745	-1.271106
O	0.104899	-2.161804	-0.389854
O	0.462612	-4.269682	-1.009474

2Fe-Casey Gsolv= -2917.176158

Fe	-0.060543	-0.212753	-0.847858
C	-0.055101	0.621376	1.091071
O	-0.031093	1.940650	1.349283
H	0.321860	2.464783	0.577256
C	-1.283111	-0.093848	0.861053
C	-0.855115	-1.437072	0.616849
C	0.557106	-1.503346	0.633242
C	1.106948	-0.205587	0.903907
Si	-3.033347	0.623139	0.948209
C	-3.314678	1.186022	2.711727
H	-3.194332	0.352964	3.415453
H	-4.328947	1.587140	2.833232
H	-2.604372	1.973723	2.992351
C	-4.203791	-0.761526	0.481673
H	-4.105495	-1.615515	1.164384
H	-4.028297	-1.115420	-0.542537
H	-5.241902	-0.409444	0.536917
C	-3.167328	2.054844	-0.250313
H	-3.056945	1.715274	-1.288634
H	-2.403918	2.817946	-0.054433
H	-4.151127	2.532986	-0.156361
Si	2.927605	0.260259	1.160634
C	3.113699	0.713554	2.967209
H	4.153310	0.988277	3.187311
H	2.842504	-0.126959	3.618063
H	2.476242	1.567406	3.229172
C	3.941861	-1.253848	0.733477
H	5.006186	-1.033715	0.888940
H	3.815585	-1.546594	-0.316877
H	3.687400	-2.112821	1.367392
C	3.418264	1.695432	0.066224
H	4.492857	1.885575	0.189716
H	2.882835	2.614775	0.332110
H	3.234218	1.482926	-0.995371
C	-1.340822	-0.697704	-2.006445
O	-2.171158	-1.047357	-2.719074
C	1.281578	-0.716538	-1.934131
O	2.148242	-1.073842	-2.597331
H	-0.201554	1.364709	-1.518717
C	0.469521	2.301199	-1.856691
O	0.781754	2.269461	-3.043003
O	0.624522	3.125684	-0.944017
C	-1.386603	-2.813297	0.402246
O	-0.239829	-3.541394	-0.060316
C	0.962047	-2.924191	0.425499
H	-2.183856	-2.914509	-0.341103
H	-1.746809	-3.222159	1.360278
H	1.266216	-3.370694	1.386076
H	1.756489	-3.095090	-0.308012

2'Fe Gsolv= -2920.547775

Fe	-0.007627	-0.031598	0.827842
C	0.051702	-0.545428	-1.265437
O	0.119144	-1.781492	-1.780278
H	-0.752700	-2.191327	-1.885851
C	-1.123510	0.200408	-0.937793
C	-0.615484	1.476787	-0.461265
C	-1.378846	2.715888	-0.111017
H	-2.307982	2.479850	0.419782
H	-1.682755	3.195690	-1.055287
C	-0.512046	3.681858	0.689743
H	-1.044482	4.631783	0.814899
H	-0.339128	3.274833	1.699608
C	0.820888	3.902434	-0.012650
H	1.399441	4.690938	0.482202
H	0.622097	4.250949	-1.037689
C	1.651194	2.620687	-0.064426
H	2.446932	2.717649	-0.814682
H	2.163413	2.465032	0.894892
C	0.804611	1.431367	-0.421517
C	1.243773	0.122522	-0.859516
Si	-2.915711	-0.364488	-1.211886
C	-3.115477	-0.717161	-3.042836
H	-2.916046	0.179243	-3.643321
H	-4.144267	-1.039951	-3.250120
H	-2.442750	-1.511291	-3.391731
C	-4.147301	0.938530	-0.676986
H	-4.026536	1.887655	-1.211919
H	-4.105625	1.133903	0.402192
H	-5.151705	0.553905	-0.901904
C	-3.231989	-1.923808	-0.214806
H	-3.189860	-1.713143	0.862788
H	-2.523794	-2.735881	-0.424777
H	-4.240312	-2.294907	-0.443379
Si	2.986194	-0.599126	-1.048575
C	3.329807	-0.773351	-2.883233

H	4.344441	-1.159178	-3.047353
H	3.251676	0.196383	-3.391245
H	2.625089	-1.464911	-3.361234
C	4.263350	0.529658	-0.268800
H	5.239522	0.029554	-0.333207
H	4.061675	0.723205	0.792203
H	4.350286	1.491985	-0.787007
C	3.068608	-2.264488	-0.191775
H	4.076269	-2.684517	-0.313460
H	2.352287	-2.985585	-0.602693
H	2.876562	-2.166539	0.885312
C	-1.316017	0.399943	1.964422
O	-2.159620	0.733556	2.674937
C	1.276348	0.185494	2.052363
O	2.105104	0.348004	2.835345
H	-0.531324	-1.937815	3.075094
C	-0.418780	-2.585160	2.179030
O	-0.134929	-1.999692	1.078669
O	-0.567682	-3.810679	2.297508

2Fe Gsolv= -2920.525996

Fe	0.051656	0.094916	0.871481
C	0.021448	-0.708993	-1.073626
O	-0.036376	-2.024863	-1.365146
H	-0.337737	-2.564258	-0.583433
C	-1.110585	0.140585	-0.867931
C	-0.545980	1.442778	-0.583747
C	-1.248340	2.741605	-0.346647
H	-2.164101	2.595611	0.237143
H	-1.568540	3.133269	-1.325751
C	-0.316536	3.746917	0.321255
H	-0.812339	4.722653	0.377757
H	-0.112511	3.429588	1.357260
C	0.987785	3.851659	-0.457748
H	1.615793	4.659687	-0.066042
H	0.750492	4.112060	-1.500346
C	1.774633	2.541243	-0.428602
H	2.512730	2.524631	-1.241634
H	2.357589	2.466401	0.499080
C	0.879240	1.348594	-0.595439
C	1.255909	-0.020542	-0.839122
Si	-2.916835	-0.359044	-1.177022
C	-3.047980	-0.666434	-3.020999
H	-2.770854	0.230179	-3.589941
H	-4.077556	-0.933348	-3.292707
H	-2.390923	-1.486284	-3.337230
C	-4.094926	1.006392	-0.668139
H	-3.942598	1.936920	-1.227216
H	-4.036322	1.227649	0.405371
H	-5.116014	0.657263	-0.875379
C	-3.366894	-1.900460	-0.214128
H	-3.229473	-1.759229	0.866481
H	-2.788308	-2.777540	-0.525577
H	-4.429481	-2.118577	-0.388211
Si	2.961420	-0.842487	-0.951259
C	3.236632	-1.291894	-2.749421
H	4.224277	-1.750529	-2.887234
H	3.190000	-0.397835	-3.384462
H	2.480254	-2.001369	-3.107510
C	4.294139	0.335664	-0.361797
H	5.249199	-0.206854	-0.347323
H	4.103598	0.695331	0.657576
H	4.414246	1.204571	-1.019588
C	2.977066	-2.358367	0.150348
H	3.940086	-2.876628	0.049518
H	2.181570	-3.067927	-0.107187
H	2.859065	-2.075328	1.205286
C	-1.293690	0.578157	1.956335
O	-2.167987	0.921655	2.619106
C	1.327679	0.541455	2.046965
O	2.153507	0.863217	2.779657
H	0.190642	-1.489463	1.519540
C	-0.477842	-2.427105	1.851449
O	-0.804124	-2.398500	3.034759
O	-0.616342	-3.254579	0.938516

2'Fe-Renaud Gsolv= -2675.830860

Fe	0.030105	-0.162518	0.918351
C	0.044323	-0.665389	-1.155571
O	0.043962	-1.899172	-1.666867
H	-0.860584	-2.254985	-1.702402
C	-1.110048	0.108133	-0.813578
C	-0.613571	1.413923	-0.445287
C	-0.509287	3.532391	0.578743
H	-1.040905	4.488842	0.583170
H	-0.420552	3.185138	1.625139
C	0.857128	3.708938	-0.043448
H	1.442597	4.418344	0.548624

H	0.738560	4.137882	-1.047282
C	0.817090	1.338350	-0.363037
C	1.231596	0.015678	-0.798670
C	-1.059514	0.452445	2.187006
O	-1.737315	0.862262	3.028605
C	1.398362	-0.264533	2.060102
O	2.259697	-0.414288	2.813205
H	-0.826678	-1.989902	3.135287
C	-0.762216	-2.656147	2.247747
O	-0.377439	-2.121946	1.152477
O	-1.057800	-3.854719	2.376447
C	2.598854	-0.478835	-1.054680
C	3.044490	-1.684585	-0.501457
C	3.453575	0.243270	-1.895500
C	4.323405	-2.157498	-0.780556
H	2.383878	-2.248233	0.156525
C	4.734838	-0.229097	-2.169448
H	3.109632	1.174935	-2.340442
C	5.173278	-1.428918	-1.611861
H	4.658689	-3.094603	-0.341951
H	5.391112	0.341709	-2.822574
H	6.174409	-1.796591	-1.825152
C	-2.492045	-0.318951	-1.132719
C	-3.344086	-0.870595	-0.171474
C	-2.948401	-0.169190	-2.448061
C	-4.644623	-1.233258	-0.512856
H	-2.989730	-1.004651	0.849822
C	-4.248392	-0.533038	-2.788419
H	-2.279886	0.251485	-3.198536
C	-5.100355	-1.060596	-1.818797
H	-5.303331	-1.653354	0.243783
H	-4.597216	-0.403409	-3.810377
H	-6.117421	-1.342128	-2.082016
N	1.613171	2.451524	-0.132488
N	-1.291500	2.575072	-0.203597
C	2.678656	2.323989	0.849595
H	2.279085	2.335478	1.879218
H	3.242110	1.398684	0.696823
H	3.376587	3.159291	0.736625
C	-2.716843	2.555266	0.093031
H	-3.271891	2.047085	-0.699352
H	-2.941585	2.070868	1.055198
H	-3.067439	3.589803	0.139590

2Fe-Renaud Gsolv= -2675.812467

Fe	-0.016637	-0.225401	0.945062
C	-0.033706	-0.594010	-1.125297
O	0.002179	-1.801971	-1.693025
H	-0.893725	-2.167656	-1.797296
C	-1.182597	0.141655	-0.738371
C	-0.679804	1.396698	-0.205753
C	-0.521771	3.493570	0.876634
H	-1.082055	4.427422	0.988074
H	-0.297099	3.108680	1.889505
C	0.759334	3.753436	0.126344
H	1.394870	4.422876	0.713617
H	0.557120	4.241042	-0.836972
C	0.761325	1.412704	-0.352416
C	1.166801	0.086455	-0.748809
C	-1.367704	-0.297914	2.111253
O	-2.232342	-0.403087	2.869024
C	1.189007	0.242857	2.175790
O	1.977466	0.594318	2.941673
H	0.438791	-1.924248	1.037711
C	0.113001	-2.870431	1.663211
O	0.664624	-2.957805	2.770451
O	-0.663344	-3.618812	1.052028
C	2.521589	-0.402104	-1.090627
C	3.181470	-1.345967	-0.299083
C	3.145202	0.082885	-2.245831
C	4.452786	-1.792002	-0.653321
H	2.699855	-1.720904	0.603594
C	4.417657	-0.360107	-2.595418
H	2.631016	0.820800	-2.860993
C	5.073988	-1.298331	-1.798873
H	4.960059	-2.523697	-0.028696
H	4.897917	0.026636	-3.491347
H	6.068659	-1.643943	-2.071102
C	-2.562924	-0.235330	-1.111526
C	-3.209462	-1.334668	-0.538949
C	-3.215603	0.502129	-2.108151
C	-4.496363	-1.682422	-0.945580
H	-2.702472	-1.916957	0.230484
C	-4.503387	0.158168	-2.505313
H	-2.707920	1.348514	-2.568371
C	-5.147543	-0.933641	-1.923128
H	-4.991751	-2.537357	-0.491373
H	-5.003949	0.741419	-3.274706

H	-6.154859	-1.201019	-2.233900
N	1.493518	2.504243	-0.090859
N	-1.370876	2.534042	0.168039
C	2.928239	2.501429	0.152903
H	3.301195	1.483433	0.281385
H	3.473277	2.976742	-0.671929
H	3.133894	3.059640	1.073552
C	-2.651668	2.377674	0.846093
H	-3.264733	1.605643	0.377396
H	-2.504295	2.122185	1.907894
H	-3.195609	3.325631	0.795711

2'Fe-williams-1 Gsolv= -2870.993084

Fe	-0.065894	-0.679732	0.999965
C	-0.075045	-1.362813	-1.069600
O	-0.147246	-2.638169	-1.451324
H	-1.068691	-2.948173	-1.453385
C	-1.180237	-0.503875	-0.768781
C	-0.623488	0.770662	-0.396900
C	0.798554	0.635269	-0.335907
C	1.146318	-0.711894	-0.763491
C	-1.104148	0.054921	2.259975
O	-1.750202	0.523485	3.088332
C	1.320068	-0.801504	2.134340
O	2.195038	-0.896320	2.873242
C	-2.597607	-0.849063	-1.000466
C	-3.565761	-0.748521	0.004582
C	-2.989716	-1.254070	-2.283316
C	-4.898812	-1.036305	-0.269993
H	-3.276172	-0.446019	1.008893
C	-4.323654	-1.548015	-2.554886
H	-2.245598	-1.318291	-3.076647
C	-5.281348	-1.438240	-1.549196
H	-5.640241	-0.952771	0.521168
H	-4.613789	-1.857705	-3.556169
H	-6.323520	-1.666254	-1.760145
C	2.503567	-1.246570	-0.986873
C	3.597118	-0.836387	-0.209043
C	2.732669	-2.141821	-2.040992
C	4.874635	-1.318854	-0.470126
H	3.458558	-0.131624	0.607833
C	4.013585	-2.622483	-2.300719
H	1.907478	-2.454854	-2.674775
C	5.089138	-2.216413	-1.515228
H	5.706754	-0.990813	0.148559
H	4.168359	-3.314898	-3.125004
H	6.089137	-2.593578	-1.716261
C	-1.393585	2.023443	-0.265238
C	-1.225216	2.918629	0.797117
C	-2.289709	2.349864	-1.292498
C	-1.942800	4.110887	0.833144
H	-0.542922	2.679596	1.609575
C	-3.003735	3.543742	-1.255428
H	-2.418474	1.669638	-2.132717
C	-2.833906	4.426587	-0.190867
H	-1.806289	4.793068	1.668906
H	-3.692507	3.783964	-2.061896
H	-3.394699	5.357785	-0.158235
C	1.767584	1.743128	-0.181185
C	2.084013	2.325345	1.048571
C	2.400398	2.208217	-1.340059
C	3.026027	3.349185	1.118949
H	1.601992	1.967910	1.957556
C	3.342206	3.230451	-1.269022
H	2.157770	1.753034	-2.299827
C	3.659694	3.801113	-0.037275
H	3.268703	3.791107	2.082632
H	3.829867	3.579260	-2.176367
H	4.398855	4.596754	0.021391
H	-0.566644	-2.404648	3.401601
C	-0.812400	-3.051167	2.532171
O	-0.676628	-2.532015	1.367163
O	-1.192356	-4.212000	2.731795

2Fe-Williams-1 Gsolv= -2870.973689

Fe	0.043887	-0.693817	1.008181
C	0.085639	-1.374271	-1.007353
O	0.209888	-2.648366	-1.375088
H	0.937611	-3.086059	-0.854129
C	-1.167394	-0.776870	-0.704382
C	-0.899433	0.593756	-0.329341
C	0.517312	0.801602	-0.385711
C	1.147944	-0.436766	-0.750011
C	-1.316723	-0.927270	2.162604
O	-2.177216	-1.106975	2.901267
C	1.083435	0.049780	2.281808
O	1.727749	0.530926	3.100515
C	-2.486111	-1.418679	-0.869359

C	-2.766280	-2.654802	-0.275788
C	-3.464436	-0.800557	-1.657117
C	-4.004838	-3.260259	-0.463129
H	-2.012361	-3.135279	0.346762
C	-4.704222	-1.407927	-1.840626
H	-3.251124	0.155213	-2.133916
C	-4.977350	-2.637439	-1.244620
H	-4.212699	-4.218427	0.007466
H	-5.457002	-0.918437	-2.454164
H	-5.946856	-3.109218	-1.387232
C	2.581864	-0.687691	-0.997585
C	3.572577	-0.362292	-0.064408
C	2.959558	-1.245923	-2.224423
C	4.913801	-0.588379	-0.354804
H	3.299036	0.067891	0.896829
C	4.302878	-1.475293	-2.511823
H	2.196970	-1.491820	-2.961117
C	5.283302	-1.147609	-1.577947
H	5.672863	-0.332507	0.380644
H	4.582005	-1.908692	-3.469402
H	6.332466	-1.327720	-1.800418
C	-1.906755	1.667809	-0.191987
C	-2.890662	1.683654	0.798861
C	-1.900799	2.678827	-1.162353
C	-3.854354	2.689086	0.818009
H	-2.914180	0.911897	1.563384
C	-2.866185	3.680573	-1.144666
H	-1.140698	2.668617	-1.942885
C	-3.846981	3.687597	-0.153679
H	-4.612868	2.689896	1.597260
H	-2.852898	4.455308	-1.907746
H	-4.601711	4.470401	-0.137534
C	1.187718	2.099423	-0.181610
C	0.847324	2.940829	0.884223
C	2.123767	2.535472	-1.126225
C	1.439657	4.192878	1.007224
H	0.116714	2.612610	1.622840
C	2.710479	3.792371	-1.003670
H	2.380420	1.896322	-1.969538
C	2.372693	4.621980	0.063466
H	1.172413	4.835162	1.842929
H	3.431738	4.123260	-1.747126
H	2.834315	5.601908	0.159699
C	1.528484	-2.886964	1.552341
O	2.019978	-2.800710	2.672090
H	0.469044	-2.301893	1.440606
O	1.819636	-3.522258	0.528537

2'Fe-williams-2 Gsolv= -3059.961875

Fe	-0.189329	-0.502431	0.858749
C	-0.565529	-1.582548	-0.978958
O	-0.875657	-2.875639	-1.068854
H	-1.822252	-3.024966	-0.905200
C	-1.477913	-0.481680	-0.818221
C	-0.646313	0.685098	-0.779291
C	0.706741	0.299214	-0.825949
C	0.789611	-1.136288	-0.906240
C	-1.045573	0.563193	2.022993
O	-1.576833	1.242033	2.784841
C	1.357721	-0.457962	1.758961
O	2.390687	-0.432592	2.264455
C	-2.947330	-0.554822	-0.891794
C	-3.765138	0.191242	-0.032605
C	-3.559439	-1.342043	-1.874618
C	-5.147261	0.142272	-0.151563
H	-3.318187	0.816267	0.737753
C	-4.947367	-1.393305	-1.981539
H	-2.947900	-1.898182	-2.584145
C	-5.765182	-0.657567	-1.121582
H	-5.764987	0.731543	0.525403
H	-5.402487	-2.009810	-2.755557
C	2.006851	-1.958263	-0.991737
C	3.115227	-1.488433	-1.706264
C	2.099145	-3.198977	-0.349213
C	4.278847	-2.246700	-1.784583
H	3.063877	-0.527823	-2.216470
C	3.265198	-3.951295	-0.435216
H	1.259412	-3.567001	0.237383
C	4.373406	-3.492256	-1.155686
H	5.131889	-1.865725	-2.345199
H	3.323158	-4.911422	0.076146
C	-7.258121	-0.720718	-1.217854
H	-7.683992	-1.276399	-0.372579
H	-7.701144	0.281832	-1.194600
H	-7.579151	-1.218952	-2.138528
C	5.620910	-4.312970	-1.266962
H	5.678108	-4.813219	-2.242539
H	6.518267	-3.690307	-1.175595

H	5.658703	-5.090064	-0.496226
C	-0.787719	2.168719	-0.829477
C	1.602540	1.488375	-0.925132
H	-1.531542	2.596033	-0.150521
H	-1.060947	2.466413	-1.850201
H	1.906281	1.616276	-1.974969
H	2.513751	1.447908	-0.322109
C	0.653140	2.657365	-0.515014
C	0.743833	3.055152	0.958984
C	1.029025	3.889510	-1.328049
O	-0.067413	3.808563	1.468569
O	0.455752	4.265883	-2.329997
O	1.773121	2.533786	1.604557
O	2.113988	4.469935	-0.825624
H	-0.261941	-1.705165	3.586311
C	-0.797167	-2.439811	2.947258
O	-0.897557	-2.154379	1.701387
O	-1.258695	-3.467327	3.461435
C	1.876734	2.844264	3.005101
H	2.787669	2.353867	3.347682
H	1.946683	3.925303	3.149379
H	1.006006	2.448022	3.537371
C	2.610853	5.622834	-1.529256
H	1.853506	6.410912	-1.534420
H	3.493318	5.945942	-0.978001
H	2.878907	5.350200	-2.553158

2Fe-Williams-2 Gsolv= -3059.938687

Fe	0.148069	-0.522272	0.880798
C	0.272995	-1.653393	-0.901740
O	0.443263	-2.976043	-0.925046
H	-0.088034	-3.407853	-0.198528
C	-0.983664	-0.945637	-0.857359
C	-0.622753	0.441700	-0.789791
C	0.784448	0.562133	-0.784050
C	1.377796	-0.737654	-0.805452
C	-1.220095	-0.036628	1.958028
O	-2.106035	0.249565	2.629156
C	1.445150	0.163255	1.918212
O	2.320426	0.593892	2.524851
C	-2.330037	-1.527768	-0.976676
C	-2.530578	-2.742547	-1.644299
C	-3.452016	-0.858415	-0.467441
C	-3.809752	-3.272846	-1.782442
H	-1.684529	-3.274011	-2.072930
C	-4.724828	-1.393772	-0.610948
H	-3.335183	0.088783	0.055277
C	-4.928300	-2.615049	-1.264482
H	-3.942931	-4.217003	-2.309242
H	-5.580948	-0.855199	-0.206222
C	2.812217	-1.065185	-0.819991
C	3.688089	-0.288354	-1.583632
C	3.331997	-2.136959	-0.080479
C	5.050141	-0.579145	-1.612578
H	3.303133	0.541498	-2.174238
C	4.690307	-2.420551	-0.116896
H	2.667495	-2.738560	0.537891
C	5.574127	-1.647963	-0.882762
H	5.717322	0.034604	-2.216441
H	5.080995	-3.254589	0.465444
C	-6.300868	-3.200068	-1.385563
H	-7.046804	-2.427354	-1.603882
H	-6.343692	-3.957090	-2.175745
H	-6.605871	-3.684189	-0.448571
C	7.038220	-1.962223	-0.900284
H	7.486487	-1.811629	0.089975
H	7.217141	-3.009483	-1.172510
H	7.575193	-1.327494	-1.612722
C	-1.265777	1.787360	-0.874451
C	1.210196	1.985554	-0.867198
H	-2.137678	1.946227	-0.236045
H	-1.585085	1.952426	-1.914142
H	1.499303	2.205990	-1.903564
H	2.052657	2.261058	-0.224778
C	-0.090411	2.753680	-0.522559
C	-0.044487	3.186217	0.944150
C	-0.240979	4.020636	-1.356304
O	0.938513	3.725779	1.420867
O	0.378413	4.262925	-2.371973
O	-1.153408	2.944707	1.621789
O	-1.187601	4.804507	-0.851410
C	-1.474502	6.016711	-1.573385
H	-1.815592	5.778249	-2.584060
H	-2.265815	6.512395	-1.012123
H	-0.582945	6.647700	-1.613882
C	-1.132921	3.286574	3.018990
H	-0.945012	4.356086	3.143400
H	-2.119901	3.025881	3.400769

H	-0.358084	2.705118	3.529239
C	-0.283395	-2.832036	2.181607
O	-0.436039	-2.677565	3.389944
H	0.442557	-2.004630	1.692186
O	-0.634518	-3.706968	1.374740

2'Fe-wills-1 Gsolv= -2561.882793

Fe	-0.012992	0.067094	0.843068
C	0.025499	0.173086	-1.320084
O	-0.013039	1.269115	-2.074381
H	0.882340	1.578513	-2.292925
C	1.197366	-0.467097	-0.793161
C	0.707050	-1.622292	-0.097313
C	-0.695325	-1.624494	-0.122732
C	-1.164797	-0.469844	-0.838111
C	1.303724	-0.017316	2.054812
O	2.183842	-0.120379	2.787593
C	-1.356240	-0.052731	2.022666
O	-2.249441	-0.174281	2.736189
C	2.604381	-0.103124	-1.025101
C	3.525178	-1.104906	-1.354906
C	3.045236	1.222231	-0.911927
C	4.861123	-0.785380	-1.578835
H	3.188754	-2.136789	-1.445113
C	4.379909	1.539030	-1.148312
H	2.348170	2.002130	-0.605493
C	5.290308	0.537294	-1.482048
H	5.567457	-1.572247	-1.832823
H	4.712435	2.570272	-1.056304
H	6.333925	0.786084	-1.659713
C	-2.564344	-0.102086	-1.092565
C	-3.542549	-1.104320	-1.116839
C	-2.951709	1.231816	-1.280474
C	-4.878939	-0.782875	-1.336691
H	-3.256304	-2.146194	-0.981522
C	-4.288029	1.547962	-1.503501
H	-2.206737	2.022895	-1.239332
C	-5.255987	0.544152	-1.532034
H	-5.625697	-1.573279	-1.357320
H	-4.576074	2.586817	-1.647385
H	-6.299668	0.795888	-1.705238
C	1.172921	-2.862982	0.587537
O	-0.009908	-3.317737	1.261526
C	-1.173733	-2.867479	0.552764
H	1.502028	-3.604196	-0.158312
H	-1.478548	-3.611427	-0.201209
H	-1.990969	-2.739062	1.270097
H	-0.032723	2.289294	2.791004
C	-0.056019	2.801590	1.805273
O	-0.055988	2.049093	0.767175
O	-0.081750	4.038680	1.764952
H	1.969524	-2.730467	1.326900

2Fe-wills-1 Gsolv= -2561.860385

Fe	-0.081288	0.433375	0.813753
C	-0.058813	-0.827466	-0.887136
O	-0.068747	-2.158151	-0.817072
H	0.489578	-2.471487	-0.049505
C	-1.266928	-0.046946	-0.844951
C	-0.834214	1.312834	-0.903155
C	0.574638	1.360495	-0.914519
C	1.103654	0.030570	-0.899474
C	-1.461880	1.044444	1.784241
O	-2.383185	1.444866	2.339712
C	1.165683	1.252064	1.826972
O	1.958539	1.805871	2.444737
C	-2.651639	-0.545052	-0.815654
C	-3.622143	0.084822	-1.602589
C	-3.020880	-1.627340	-0.006337
C	-4.939662	-0.367272	-1.590313
H	-3.342064	0.923469	-2.238376
C	-4.336637	-2.077181	0.000867
H	-2.278053	-2.103038	0.631216
C	-5.298776	-1.450432	-0.791698
H	-5.684958	0.128072	-2.208210
H	-4.614528	-2.915648	0.635309
H	-6.327328	-1.803511	-0.781336
C	2.515797	-0.373904	-0.997941
C	3.535266	0.498231	-0.590601
C	2.869106	-1.610679	-1.554098
C	4.871157	0.137215	-0.723877
H	3.291556	1.466240	-0.156965
C	4.207916	-1.968178	-1.686755
H	2.095921	-2.293395	-1.896453
C	5.213486	-1.099167	-1.269948
H	5.647399	0.825478	-0.397809
H	4.463684	-2.931021	-2.122949
H	6.258730	-1.381206	-1.372182

C	-1.358490	2.700978	-1.032550
O	-0.211903	3.509817	-0.742779
C	0.988459	2.788263	-1.050475
H	-2.164831	2.971274	-0.342754
H	-1.705092	2.871141	-2.064629
H	1.310323	2.979901	-2.086978
H	1.773102	3.133768	-0.371205
C	0.667928	-1.674960	2.271244
O	1.077283	-2.578081	1.524302
H	-0.182690	-0.992186	1.757699
O	0.866084	-1.389774	3.448605

2'Fe-wills-2 Gsolv= -2601.146442

Fe	0.082680	0.014855	0.826002
C	0.046223	-0.513708	-1.277387
O	0.146580	-1.731205	-1.806694
H	-0.731341	-2.121481	-1.961499
C	-1.159590	0.143701	-0.876789
C	-0.746826	1.440500	-0.412951
C	0.652979	1.525819	-0.480432
C	1.198107	0.284389	-0.945378
C	-1.288888	-0.031787	1.983156
O	-2.187447	-0.116614	2.695007
C	1.295004	0.614658	1.999645
O	2.094265	1.049153	2.703395
C	-2.531094	-0.363005	-1.051159
C	-3.498473	0.456689	-1.644601
C	-2.882777	-1.657427	-0.647705
C	-4.794719	-0.013213	-1.834598
H	-3.228240	1.462716	-1.963219
C	-4.178030	-2.126897	-0.847599
H	-2.146624	-2.288234	-0.149222
C	-5.136103	-1.306364	-1.440687
H	-5.539605	0.631861	-2.294732
H	-4.441418	-3.132115	-0.527175
H	-6.149153	-1.672385	-1.590313
C	2.618754	-0.044664	-1.127694
C	3.555295	0.992071	-1.241006
C	3.073021	-1.371151	-1.163424
C	4.910515	0.712124	-1.385827
H	3.225613	2.029097	-1.236050
C	4.429042	-1.646323	-1.310089
H	2.366828	-2.190576	-1.063628
C	5.353454	-0.608701	-1.419902
H	5.620851	1.530718	-1.475977
H	4.765131	-2.680499	-1.331891
H	6.412532	-0.828320	-1.533070
C	-1.297700	2.784881	-0.043790
O	-0.126574	3.464104	0.460680
C	1.056791	2.918780	-0.127979
H	-1.622346	3.276898	-0.978922
H	1.323973	3.464574	-1.048348
H	1.881565	3.018414	0.585617
C	-2.390573	2.864993	0.987321
H	-2.732444	3.898899	1.099038
H	-3.247682	2.251802	0.684545
H	-2.026323	2.513736	1.959306
H	0.488116	-1.812158	3.140525
C	0.615245	-2.465707	2.250968
O	0.479734	-1.909165	1.104090
O	0.872558	-3.665911	2.413069

2Fe-wills-2 Gsolv= -2601.119287

Fe	0.003591	0.309128	0.864268
C	0.059248	-0.883288	-0.881111
O	0.107710	-2.219346	-0.874635
H	0.469241	-2.569273	-0.011163
C	-1.178759	-0.133624	-0.829772
C	-0.788855	1.237541	-0.830456
C	0.620266	1.316938	-0.828265
C	1.187610	0.003435	-0.854381
C	-1.161590	1.022570	2.036385
O	-1.869629	1.448780	2.833209
C	1.421775	0.906653	1.794225
O	2.356966	1.321589	2.314577
C	-2.527606	-0.724892	-0.905011
C	-3.564900	-0.315592	-0.058836
C	-2.787063	-1.703984	-1.872301
C	-4.834791	-0.870675	-0.180409
H	-3.380048	0.434969	0.706684
C	-4.057919	-2.260010	-1.990328
H	-1.991881	-2.021139	-2.543760
C	-5.084983	-1.845683	-1.144926
H	-5.629326	-0.544257	0.486553
H	-4.244965	-3.018029	-2.747355
H	-6.077422	-2.281025	-1.235881
C	2.620334	-0.327217	-0.962506
C	3.399140	0.397043	-1.874144

C	3.223278	-1.333924	-0.198959
C	4.754106	0.114982	-2.024306
H	2.937888	1.173715	-2.482269
C	4.577685	-1.613500	-0.353070
H	2.636657	-1.883805	0.534110
C	5.346497	-0.892106	-1.265238
H	5.346292	0.682800	-2.738113
H	5.035849	-2.393711	0.250348
H	6.405426	-1.111620	-1.380259
C	-1.322547	2.629000	-1.010439
O	-0.196172	3.440302	-0.618883
C	1.018603	2.750341	-0.926678
H	-1.480602	2.743317	-2.099786
H	1.344886	2.978562	-1.954587
H	1.798860	3.073357	-0.229528
C	-2.548925	3.093390	-0.276845
H	-2.759150	4.135070	-0.539453
H	-3.414524	2.488881	-0.567680
H	-2.416078	3.030796	0.808277
C	0.384166	-1.896633	2.321856
O	0.484746	-1.628420	3.514087
H	-0.323428	-1.129172	1.714759
O	0.756419	-2.844326	1.613046

2'Fe-wills-3 Gsolv= -2778.805872

Fe	0.239004	-0.017847	0.804691
C	0.058925	-0.503158	-1.291972
O	0.118283	-1.724137	-1.827514
H	-0.758743	-2.142846	-1.864503
C	-1.111600	0.166941	-0.805289
C	-0.639850	1.448318	-0.354324
C	0.755984	1.496703	-0.511567
C	1.249559	0.252045	-1.028001
Si	3.037558	-0.247083	-1.392056
C	3.199572	-0.549494	-3.233212
H	4.241013	-0.783793	-3.489066
H	2.901953	0.336194	-3.808236
H	2.577266	-1.392189	-3.558708
C	4.107919	1.188884	-0.844000
H	5.163721	0.960888	-1.039785
H	4.003367	1.377285	0.232953
H	3.862567	2.112293	-1.384045
C	3.480177	-1.783077	-0.415669
H	4.491812	-2.115239	-0.683778
H	2.789961	-2.614013	-0.608793
H	3.470189	-1.573437	0.662986
C	-1.046472	-0.050735	2.054057
O	-1.887208	-0.145338	2.831952
C	1.519499	0.537624	1.922297
O	2.340055	0.963998	2.608419
C	-2.505868	-0.299343	-0.894087
C	-3.482002	0.552125	-1.425585
C	-2.873624	-1.583173	-0.472182
C	-4.801488	0.123723	-1.538439
H	-3.200636	1.550809	-1.757435
C	-4.192707	-2.011494	-0.594728
H	-2.128481	-2.237700	-0.019625
C	-5.158719	-1.160098	-1.128324
H	-5.551881	0.793926	-1.951427
H	-4.467581	-3.009347	-0.261044
H	-6.189597	-1.494486	-1.218380
C	-1.130574	2.799541	0.067323
O	0.088379	3.445020	0.498388
C	1.218435	2.874270	-0.171148
H	-1.504171	3.310539	-0.839004
H	1.440715	3.424021	-1.100469
H	2.087576	2.948019	0.490273
C	-2.151270	2.892916	1.169247
H	-3.045172	2.312351	0.911346
H	-1.736410	2.510309	2.108739
H	-2.451217	3.934345	1.323475
H	1.304156	-1.877244	2.891711
C	1.016080	-2.538435	2.046839
O	0.488258	-1.973260	1.025998
O	1.213209	-3.757781	2.140532

2Fe-wills-3 Gsolv= -2778.774140

Fe	0.167298	0.318993	0.840018
C	0.019389	-0.960070	-0.823596
O	0.003784	-2.296160	-0.721652
H	0.518119	-2.613996	0.072221
C	-1.172286	-0.148954	-0.735149
C	-0.701302	1.203098	-0.833686
C	0.700753	1.185474	-0.979829
C	1.206103	-0.152484	-0.926331
Si	3.003929	-0.711346	-1.189128
C	3.016611	-1.751364	-2.744784
H	4.038804	-2.071712	-2.983601

H	2.627817	-1.190933	-3.603833
H	2.403078	-2.652485	-2.619333
C	4.021758	0.846603	-1.387277
H	5.083928	0.576111	-1.449488
H	3.905131	1.521479	-0.528815
H	3.767027	1.399118	-2.299959
C	3.656853	-1.698295	0.258862
H	4.726662	-1.885324	0.093421
H	3.156413	-2.668267	0.357310
H	3.554201	-1.160122	1.210605
C	-1.028495	0.926120	2.036451
O	-1.779465	1.277055	2.830942
C	1.557760	1.095252	1.679186
O	2.454212	1.614250	2.174372
C	-2.562143	-0.635679	-0.694321
C	-3.579247	0.113860	-0.087497
C	-2.901986	-1.840797	-1.324384
C	-4.895117	-0.335589	-0.097334
H	-3.347255	1.054920	0.405566
C	-4.219833	-2.289290	-1.331579
H	-2.134514	-2.424871	-1.824072
C	-5.220797	-1.541876	-0.715364
H	-5.668220	0.259533	0.383142
H	-4.463752	-3.226359	-1.826875
H	-6.249653	-1.894077	-0.719361
C	-1.198621	2.608079	-1.040280
O	-0.041695	3.267336	-1.608474
C	1.168704	2.568415	-1.292686
H	-1.986112	2.614585	-1.807005
H	1.819648	2.593116	-2.174055
H	1.696919	3.054122	-0.458386
C	-1.646587	3.378672	0.183192
H	-1.891325	4.405018	-0.108923
H	-2.537767	2.938794	0.643181
H	-0.838387	3.412531	0.925935
C	0.848215	-1.834145	2.344018
O	1.215847	-1.470423	3.456014
H	0.069113	-1.077142	1.818135
O	1.013190	-2.857206	1.665776

2'Fe-wills-4 Gsolv= -2739.543089

Fe	0.181271	-0.152361	0.809695
C	-0.018675	-0.054455	-1.344369
O	-0.040461	-1.085827	-2.190058
H	-0.946817	-1.391461	-2.362747
C	-1.144495	0.537283	-0.678252
C	-0.585466	1.621378	0.079401
C	0.812909	1.607401	-0.057582
C	1.219032	0.516581	-0.902677
Si	2.964527	-0.004538	-1.414498
C	3.119803	0.225473	-3.266462
H	4.135074	-0.023987	-3.600770
H	2.915999	1.264561	-3.553737
H	2.419874	-0.420759	-3.810588
C	4.143591	1.123198	-0.495750
H	5.178434	0.888779	-0.776916
H	4.060334	0.996381	0.591606
H	3.964257	2.179378	-0.735279
C	3.256797	-1.791417	-0.932427
H	4.253231	-2.108310	-1.267949
H	2.520968	-2.468948	-1.383641
H	3.214412	-1.919336	0.157869
C	-1.089689	-0.217287	2.066524
O	-1.951886	-0.211697	2.827466
C	1.539382	-0.099345	1.978168
O	2.409691	-0.007262	2.725138
C	-2.570967	0.203158	-0.828637
C	-3.500318	1.234136	-1.009758
C	-3.021040	-1.122843	-0.777652
C	-4.854427	0.943396	-1.149595
H	-3.156814	2.266705	-1.050501
C	-4.374891	-1.410182	-0.925745
H	-2.311434	-1.929495	-0.593562
C	-5.294116	-0.378855	-1.112515
H	-5.567430	1.752510	-1.289716
H	-4.713492	-2.442631	-0.881550
H	-6.352175	-0.605063	-1.222209
C	-0.979336	2.806797	0.892933
O	0.261946	3.209273	1.492423
C	1.361461	2.791577	0.668333
H	-1.707299	2.618840	1.689330
H	-1.369218	3.603692	0.239443
H	1.625634	3.580137	-0.054705
H	2.225175	2.607192	1.314894
H	0.576032	-2.582425	2.477297
C	0.468727	-2.973924	1.442847
O	0.214670	-2.116000	0.527309
O	0.592185	-4.190144	1.240676

2Fe-wills-4 Gsolv= -2739.519608

Fe	0.247163	0.073065	0.858074
C	0.067219	-0.435923	-1.182076
O	-0.015637	-1.686155	-1.660301
H	-0.278183	-2.340388	-0.952463
C	-1.043501	0.388853	-0.779379
C	-0.442142	1.612651	-0.341374
C	0.961304	1.511751	-0.448840
C	1.327155	0.219199	-0.937136
Si	3.047529	-0.514748	-1.241400
C	3.224522	-0.810422	-3.081412
H	4.218307	-1.217024	-3.308505
H	3.105883	0.123619	-3.644512
H	2.476846	-1.525431	-3.446394
C	4.281411	0.759649	-0.643774
H	5.303151	0.407761	-0.835735
H	4.191300	0.941496	0.435097
H	4.156134	1.716407	-1.167405
C	3.206426	-2.115317	-0.281583
H	4.183379	-2.576056	-0.477975
H	2.431575	-2.836411	-0.570448
H	3.129239	-1.941343	0.799890
C	-1.055294	0.358418	2.065635
O	-1.922756	0.581930	2.783543
C	1.591791	0.380930	2.012453
O	2.460642	0.603595	2.729019
C	-2.486966	0.120919	-0.888524
C	-3.333665	1.164927	-1.283428
C	-3.040860	-1.134368	-0.607437
C	-4.704974	0.956721	-1.402333
H	-2.915343	2.142693	-1.517389
C	-4.411659	-1.338861	-0.729972
H	-2.404856	-1.949255	-0.269143
C	-5.247953	-0.296357	-1.126961
H	-5.348626	1.776878	-1.711653
H	-4.829235	-2.317386	-0.504198
H	-6.319265	-0.460123	-1.217558
C	-0.787121	2.984876	0.127381
O	0.464800	3.483250	0.619184
C	1.550386	2.822929	-0.048009
H	-1.527843	3.037972	0.932503
H	-1.141076	3.594652	-0.719550
H	1.850795	3.379818	-0.950314
H	2.402863	2.781392	0.637085
C	-0.196497	-2.547485	1.476915
O	-0.501857	-3.197392	0.464626
H	0.480892	-1.589654	1.223444
O	-0.362078	-2.717897	2.680683

2'Fe-wills-5 Gsolv= -2896.574186

Fe	0.437467	1.099856	0.023618
C	-0.021138	-0.923000	-0.594335
O	-0.214524	-1.339085	-1.846076
H	0.613926	-1.646607	-2.250272
C	1.233337	-0.856659	0.096210
C	0.906989	-0.362062	1.406652
C	-0.472232	-0.096209	1.455165
C	-1.086963	-0.360493	0.187840
Si	-2.914985	-0.162157	-0.261086
C	-3.677982	0.986988	1.011225
H	-4.726255	1.176878	0.745000
H	-3.167602	1.958232	1.030791
H	-3.663724	0.569981	2.026389
C	-3.063414	0.623258	-1.956500
H	-4.113689	0.645379	-2.276266
H	-2.482881	0.103165	-2.727582
H	-2.708221	1.662562	-1.907913
C	-3.736788	-1.877647	-0.162108
C	2.053589	1.872887	0.040259
O	3.099020	2.348676	-0.004686
C	-0.384371	2.538886	0.699268
O	-0.892675	3.440522	1.203334
C	2.538359	-1.349546	-0.377970
C	3.276548	-2.211975	0.441726
C	3.053209	-0.987638	-1.629115
C	4.504244	-2.708604	0.014656
H	2.879389	-2.497538	1.414913
C	4.278217	-1.492653	-2.056762
H	2.504551	-0.285439	-2.257558
C	5.006057	-2.353214	-1.236808
H	5.069569	-3.376452	0.660481
H	4.670355	-1.201938	-3.028496
H	5.965540	-2.741927	-1.569836
C	1.485427	-0.194880	2.778297
O	0.437662	0.525231	3.466888
C	-0.832405	0.278652	2.852966
H	1.579004	-1.202082	3.223713

H	-1.345817	-0.569831	3.335867
H	-1.453885	1.172550	2.970991
C	2.778884	0.559339	2.932466
H	3.564624	0.097041	2.322963
H	2.652933	1.601950	2.618217
H	3.104310	0.549705	3.977575
C	-5.252503	-1.706608	-0.282389
H	-5.541777	-1.219180	-1.224563
H	-5.745247	-2.691831	-0.259079
H	-5.667584	-1.114372	0.544551
H	0.216082	3.552281	-1.668820
C	0.106077	2.708935	-2.383587
O	0.214422	1.528277	-1.900817
O	-0.104673	2.952780	-3.579934
C	-3.242474	-2.781085	-1.290939
H	-3.442971	-2.350532	-2.282570
H	-2.163731	-2.974469	-1.219623
H	-3.754929	-3.755528	-1.244826
C	-3.407088	-2.526212	1.183398
H	-2.327740	-2.700114	1.302640
H	-3.747063	-1.916842	2.032971
H	-3.906834	-3.505055	1.264120

2Fe-wills-5 Gsolv= -2896.549613

Fe	0.407363	1.073803	-0.180386
C	-0.032937	-1.007719	-0.398454
O	-0.180542	-1.658404	-1.551926
H	0.663161	-2.021545	-1.871001
C	1.181767	-0.820569	0.335377
C	0.801195	-0.054764	1.491101
C	-0.583690	0.207648	1.423297
C	-1.134517	-0.295811	0.208771
Si	-2.932200	-0.187278	-0.389977
C	-3.695536	1.345130	0.373312
H	-4.732529	1.443437	0.025819
H	-3.161701	2.250414	0.056380
H	-3.711343	1.318880	1.469945
C	-2.962084	-0.019157	-2.254807
H	-4.000129	0.064187	-2.603252
H	-2.494700	-0.862642	-2.775186
H	-2.441102	0.900192	-2.556474
C	-3.822175	-1.755366	0.218173
C	2.054732	1.769159	-0.372820
O	3.122291	2.173628	-0.502543
C	-0.336685	2.667216	0.171923
O	-0.787150	3.690286	0.437445
C	2.500125	-1.406212	0.037741
C	3.206090	-2.046989	1.063298
C	3.054076	-1.357187	-1.247747
C	4.440982	-2.634055	0.804425
H	2.780559	-2.092150	2.064956
C	4.285549	-1.953049	-1.504470
H	2.536305	-0.819642	-2.042967
C	4.981217	-2.592789	-0.480114
H	4.981307	-3.127664	1.608790
H	4.706496	-1.905460	-2.505891
H	5.945669	-3.053376	-0.680813
C	1.324956	0.424405	2.809820
O	0.246454	1.261790	3.284964
C	-0.997261	0.887443	2.683502
H	1.416817	-0.453366	3.474323
H	-1.542975	0.170110	3.318799
H	-1.613328	1.785233	2.566343
C	2.601708	1.222773	2.823200
H	2.884083	1.472137	3.850926
H	3.417436	0.645864	2.371204
H	2.470123	2.155500	2.261685
C	-5.299777	-1.666542	-0.167139
H	-5.438305	-1.590122	-1.255016
H	-5.830113	-2.572503	0.167319
H	-5.798640	-0.805530	0.299037
C	0.451619	1.561452	-2.844829
O	0.536678	2.779463	-3.001504
H	-0.073136	1.255122	-1.789991
O	0.692888	0.570639	-3.532996
C	-3.209520	-3.001970	-0.419893
H	-3.274777	-2.978616	-1.516704
H	-2.152626	-3.130478	-0.147334
H	-3.745608	-3.901455	-0.077525
C	-3.701210	-1.856171	1.739231
H	-2.654593	-1.947980	2.063621
H	-4.138715	-0.985949	2.248350
H	-4.234959	-2.750057	2.099461

2'Mn-a Gsolv= -2821.089984

C	0.058225	0.283623	1.333277
O	0.143481	1.442252	1.997794
H	-0.723497	1.848163	2.154587

C	-1.135909	-0.401687	0.932752
C	-0.634904	-1.585182	0.285142
C	0.770105	-1.544196	0.209668
C	1.246692	-0.336595	0.827700
Si	-2.951399	0.085672	1.193491
C	-3.244309	0.220791	3.037625
H	-3.101621	-0.744902	3.537737
H	-4.268223	0.560251	3.239293
H	-2.556729	0.943676	3.496661
C	-4.003460	-1.240941	0.402185
H	-3.812634	-2.232508	0.831229
H	-3.835049	-1.289608	-0.681906
H	-5.064209	-1.008607	0.562961
C	-3.251280	1.739249	0.363019
H	-3.129072	1.663521	-0.726059
H	-2.571165	2.522032	0.725089
H	-4.277740	2.073405	0.563910
Si	3.031096	0.236550	1.103487
C	3.359689	0.168677	2.946264
H	4.405612	0.427050	3.156612
H	3.176393	-0.838856	3.340310
H	2.721529	0.870564	3.497043
C	4.139987	-0.970135	0.197696
H	5.190757	-0.702212	0.369167
H	3.967799	-0.960710	-0.886000
H	3.998847	-1.996052	0.561949
C	3.248317	1.976530	0.447133
H	4.275280	2.317468	0.632978
H	2.567073	2.682279	0.937981
H	3.070394	2.025538	-0.634984
O	-2.026123	-0.713520	-2.678192
C	1.365689	-0.002606	-2.059383
O	2.227276	-0.119544	-2.811963
C	-1.099322	-2.887890	-0.275123
O	0.061593	-3.386897	-0.956754
C	1.253606	-2.824287	-0.384557
H	-1.924107	-2.842464	-0.994241
H	-1.388363	-3.563570	0.546021
H	1.651245	-3.484005	0.403456
H	2.003563	-2.733984	-1.177612
H	-0.573032	2.259744	-2.768298
C	-0.410822	2.780686	-1.801252
O	-0.072460	2.047881	-0.806354
O	-0.560558	4.008655	-1.735680
N	-1.186187	-0.301066	-1.978732
Mn	-0.030999	0.052532	-0.873526

2Mn-a Gsolv= -2821.063843

C	-0.064311	-0.622027	-1.096650
O	-0.032523	-1.937466	-1.375197
H	0.367068	-2.465932	-0.630554
C	-1.293828	0.082896	-0.869098
C	-0.875649	1.426331	-0.609318
C	0.534782	1.503149	-0.603229
C	1.090744	0.209447	-0.886670
Si	-3.042623	-0.643455	-0.930836
C	-3.349761	-1.212200	-2.687510
H	-3.258065	-0.377846	-3.393959
H	-4.359640	-1.629729	-2.788414
H	-2.632409	-1.988085	-2.982586
C	-4.209596	0.735699	-0.440772
H	-4.132579	1.591281	-1.124049
H	-4.010576	1.088778	0.579853
H	-5.246884	0.378255	-0.471027
C	-3.146167	-2.067851	0.278872
H	-3.021261	-1.714718	1.311249
H	-2.380400	-2.827171	0.077953
H	-4.128109	-2.553246	0.205442
Si	2.915559	-0.219889	-1.192628
C	3.062564	-0.556539	-3.028024
H	4.100870	-0.793495	-3.293235
H	2.755314	0.319045	-3.613540
H	2.435131	-1.405394	-3.327847
C	3.914841	1.286146	-0.705652
H	4.978781	1.092060	-0.894595
H	3.806978	1.528035	0.359428
H	3.631835	2.169008	-1.293229
C	3.436940	-1.712702	-0.195033
H	4.509157	-1.891531	-0.350612
H	2.898147	-2.616371	-0.504811
H	3.272370	-1.564665	0.880585
C	1.392056	0.633689	1.928077
O	2.301734	0.960349	2.546892
H	-0.182601	-1.442843	1.485841
C	0.493172	-2.373172	1.822075
O	0.768136	-2.376740	3.017965
O	0.693734	-3.162281	0.886894
C	-1.422810	2.794957	-0.389699

O	-0.285151	3.536793	0.073786
C	0.928709	2.927201	-0.394128
H	-2.221248	2.883435	0.354746
H	-1.790910	3.201598	-1.345468
H	1.243640	3.377552	-1.349318
H	1.710709	3.103247	0.351767
Mn	-0.085718	0.206176	0.910462
N	-1.214656	0.746949	1.971700
O	-2.054807	1.218390	2.622409

2'Mn-b Gsolv= -2963.846172

C	-0.517846	-1.615175	-0.914224
O	-0.739731	-2.925821	-1.002226
H	-1.674806	-3.136463	-0.834809
C	-1.503812	-0.590209	-0.736384
C	-0.764088	0.637000	-0.702477
C	0.614518	0.358937	-0.778645
C	0.803379	-1.066311	-0.864012
C	1.468887	-0.318782	1.764099
O	2.531703	-0.157943	2.174709
C	-2.963571	-0.771184	-0.767368
C	-3.804201	-0.059687	0.099826
C	-3.547778	-1.625486	-1.710539
C	-5.182270	-0.207325	0.026973
H	-3.376046	0.614699	0.839238
C	-4.931356	-1.773808	-1.771178
H	-2.924134	-2.155825	-2.429261
C	-5.771702	-1.072879	-0.903761
H	-5.819011	0.356017	0.708254
H	-5.366070	-2.439283	-2.515792
C	2.081193	-1.786426	-0.984918
C	3.190533	-1.140180	-1.542136
C	2.238838	-3.105123	-0.531669
C	4.416040	-1.791930	-1.647717
H	3.099597	-0.121658	-1.913812
C	3.465142	-3.747326	-0.640895
H	1.399251	-3.631331	-0.083812
C	4.576414	-3.105902	-1.202221
H	5.264130	-1.269085	-2.087999
H	3.567098	-4.769589	-0.277824
C	-7.258398	-1.242990	-0.951126
H	-7.610923	-1.852479	-0.108962
H	-7.772169	-0.277163	-0.881228
H	-7.575845	-1.738810	-1.874367
C	5.885525	-3.820642	-1.332333
H	5.839727	-4.588110	-2.115756
H	6.695331	-3.130228	-1.590497
H	6.154628	-4.333377	-0.401253
C	-1.027831	2.103484	-0.762514
C	1.406968	1.616229	-0.925358
H	-1.777988	2.478976	-0.059955
H	-1.366522	2.362440	-1.774099
H	1.671366	1.745467	-1.985777
H	2.333375	1.664588	-0.347154
C	0.378473	2.714780	-0.511691
C	0.488072	3.160844	0.947409
C	0.626540	3.946519	-1.372881
O	-0.356766	3.870686	1.463879
O	0.000852	4.234806	-2.372627
O	1.570337	2.726596	1.570669
O	1.668571	4.634639	-0.917842
H	1.154883	-2.707203	2.505556
C	0.114576	-3.054425	2.331151
O	-0.680754	-2.223834	1.760829
O	-0.215506	-4.191163	2.691118
C	1.696314	3.068253	2.961801
H	2.656964	2.662103	3.278271
H	1.680206	4.153593	3.089673
H	0.882185	2.608457	3.531235
C	2.057348	5.795075	-1.675847
H	1.237693	6.517738	-1.700218
H	2.916318	6.212332	-1.151400
H	2.334974	5.503198	-2.691881
Mn	-0.180537	-0.465960	0.984149
N	-0.962813	0.520716	2.036942
O	-1.502025	1.312409	2.706880

2Mn-b Gsolv= -2963.826086

C	0.252105	-1.665816	-0.902724
O	0.419991	-2.990778	-0.933056
H	-0.082949	-3.420468	-0.185671
C	-0.999119	-0.957182	-0.858570
C	-0.637255	0.430320	-0.781001
C	0.768825	0.552404	-0.782777
C	1.357920	-0.750835	-0.806368
O	-2.010400	0.330389	2.541029
C	1.560196	0.174502	1.870042
O	2.470767	0.638223	2.394000

C	-2.345740	-1.535391	-0.964037
C	-2.556569	-2.736618	-1.653321
C	-3.458213	-0.874660	-0.422746
C	-3.838554	-3.259499	-1.788158
H	-1.715966	-3.259807	-2.102400
C	-4.734020	-1.404228	-0.562457
H	-3.331201	0.061032	0.117907
C	-4.948679	-2.608701	-1.243193
H	-3.981506	-4.190854	-2.334698
H	-5.583920	-0.873667	-0.134803
C	2.793041	-1.077521	-0.835473
C	3.663404	-0.283581	-1.587787
C	3.319803	-2.161207	-0.118470
C	5.026264	-0.569236	-1.627954
H	3.274035	0.556500	-2.160660
C	4.678751	-2.439752	-0.166213
H	2.660428	-2.776768	0.491334
C	5.556959	-1.649963	-0.920981
H	5.688781	0.058355	-2.222649
H	5.074425	-3.283219	0.398896
C	-6.324986	-3.183995	-1.366461
H	-7.066400	-2.404243	-1.575157
H	-6.374616	-3.932254	-2.164521
H	-6.630866	-3.675294	-0.433570
C	7.021672	-1.960176	-0.952144
H	7.468647	-1.858467	0.044772
H	7.202621	-2.992043	-1.276970
H	7.558031	-1.289954	-1.631759
C	-1.284452	1.775884	-0.851210
C	1.192573	1.975829	-0.889259
H	-2.139836	1.931593	-0.189514
H	-1.631987	1.941284	-1.881617
H	1.461961	2.186745	-1.932873
H	2.045190	2.259760	-0.264274
C	-0.102829	2.745769	-0.527501
C	-0.026871	3.192212	0.934559
C	-0.272108	4.005454	-1.368219
O	0.965514	3.737895	1.384532
O	0.315429	4.234101	-2.405754
O	-1.119155	2.953967	1.639120
O	-1.197836	4.799719	-0.841111
C	-1.503111	6.005502	-1.566216
H	-1.875658	5.757581	-2.563416
H	-2.275076	6.509290	-0.985518
H	-0.611244	6.632836	-1.640837
C	-1.059765	3.295757	3.035203
H	-0.862809	4.364069	3.155549
H	-2.037335	3.039885	3.443399
H	-0.273564	2.709612	3.522656
C	-0.242711	-2.867554	2.214499
O	-0.397912	-2.726971	3.423967
H	0.493384	-2.039443	1.744252
O	-0.601747	-3.727753	1.395359
N	-1.092892	-0.022715	1.923200
Mn	0.132052	-0.513988	0.937947

2'Mn-c Gsolv= -2465.774747

C	0.130732	0.653430	-1.096859
O	0.039986	1.942480	-1.411102
H	0.917591	2.357749	-1.459860
C	1.328675	-0.070351	-0.797306
C	0.901480	-1.420593	-0.588327
C	-0.498813	-1.494789	-0.656917
C	-1.025557	-0.183294	-0.927590
C	-1.419430	-0.893344	1.846944
O	-2.329905	-1.392900	2.341785
C	2.712819	0.426076	-0.820684
C	3.710772	-0.356363	-1.415166
C	3.057484	1.661450	-0.255045
C	5.027564	0.092496	-1.450591
H	3.451434	-1.313912	-1.864049
C	4.374189	2.109718	-0.300739
H	2.301253	2.258908	0.254172
C	5.361736	1.327662	-0.897899
H	5.793661	-0.523921	-1.915035
H	4.631051	3.067816	0.144824
H	6.390779	1.677849	-0.927591
C	-2.440570	0.184814	-1.086734
C	-3.385050	-0.819524	-1.341112
C	-2.883403	1.510704	-0.964125
C	-4.734493	-0.508867	-1.473003
H	-3.065992	-1.853628	-1.455394
C	-4.234441	1.816421	-1.095966
H	-2.172602	2.306972	-0.759463
C	-5.165262	0.810737	-1.350820
H	-5.450172	-1.302314	-1.675183
H	-4.560769	2.849081	-0.995938
H	-6.220112	1.054002	-1.454135

C	1.445498	-2.795003	-0.396139
O	0.289805	-3.544607	0.001712
C	-0.892714	-2.931992	-0.531832
H	1.845819	-3.175545	-1.349559
H	-1.127633	-3.344388	-1.526758
H	-1.725910	-3.148457	0.144598
H	-2.070986	1.516869	2.098592
C	-1.207141	2.189359	1.911019
O	-0.129921	1.635008	1.485050
O	-1.323751	3.402319	2.123874
H	2.217013	-2.901947	0.373944
O	2.013914	-1.401905	2.574826
N	1.170635	-0.837400	1.996044
Mn	0.047426	-0.265559	0.943949

2Mn-c Gsolv= -2465.746370

C	-0.064168	-0.811771	-0.900683
O	-0.050767	-2.145166	-0.875664
H	0.545204	-2.480221	-0.148198
C	-1.281012	-0.050802	-0.855980
C	-0.865949	1.315927	-0.872854
C	0.541423	1.388243	-0.869467
C	1.085111	0.064462	-0.888502
O	-2.326944	1.517702	2.203644
C	1.243432	1.203342	1.872178
O	2.063391	1.740555	2.468168
C	-2.660214	-0.558274	-0.824035
C	-3.663391	0.144589	-1.501421
C	-2.997895	-1.715596	-0.108971
C	-4.980671	-0.306315	-1.473370
H	-3.410679	1.039614	-2.067823
C	-4.314010	-2.163356	-0.086267
H	-2.229274	-2.253041	0.442768
C	-5.308593	-1.462056	-0.768805
H	-5.750504	0.247203	-2.005904
H	-4.566835	-3.060207	0.474549
H	-6.337302	-1.814003	-0.746101
C	2.502030	-0.318888	-1.011960
C	3.517573	0.556037	-0.601102
C	2.862779	-1.533925	-1.610660
C	4.855602	0.218424	-0.770358
H	3.271245	1.510136	-0.139890
C	4.203481	-1.867868	-1.779430
H	2.094301	-2.217393	-1.961577
C	5.204985	-0.996844	-1.357298
H	5.627905	0.909610	-0.441211
H	4.463574	-2.813236	-2.249970
H	6.251871	-1.259802	-1.489133
C	-1.413758	2.698576	-0.963578
O	-0.279439	3.520218	-0.662696
C	0.933606	2.824592	-0.981266
H	-2.218510	2.937686	-0.259989
H	-1.774033	2.889332	-1.987274
H	1.254145	3.043080	-2.012677
H	1.710389	3.168790	-0.292194
C	0.777093	-1.840824	2.214402
O	1.195128	-2.685733	1.406681
H	-0.051858	-1.119871	1.722140
O	0.962891	-1.634720	3.409022
Mn	-0.114960	0.431558	0.884728
N	-1.369207	1.036355	1.755372

2'Mn Gsolv= -2824.436386

C	0.032783	-0.643944	1.207942
O	-0.144292	-1.896258	1.651618
H	0.677093	-2.411277	1.648156
C	1.261056	-0.012093	0.853333
C	0.877962	1.341592	0.491879
C	1.759997	2.498254	0.142565
H	2.586701	2.185950	-0.505836
H	2.223016	2.860978	1.073896
C	0.956548	3.625286	-0.498499
H	1.593198	4.511542	-0.601466
H	0.649146	3.331650	-1.515495
C	-0.274710	3.942407	0.338842
H	-0.785034	4.836838	-0.036346
H	0.048672	4.169322	1.366296
C	-1.255618	2.770663	0.363542
H	-1.965974	2.892979	1.191435
H	-1.862434	2.765691	-0.552109
C	-0.537213	1.463464	0.547255
C	-1.095605	0.182425	0.926855
Si	2.995487	-0.780561	0.978466
C	3.246578	-1.297735	2.764704
H	3.187455	-0.431979	3.436206
H	4.240906	-1.748153	2.883746
H	2.505971	-2.034352	3.101960
C	4.330198	0.428191	0.475515

H	4.329216	1.346440	1.073872
H	4.267198	0.698491	-0.586118
H	5.298304	-0.068352	0.630242
C	3.080187	-2.271347	-0.155860
H	2.977904	-1.965983	-1.205824
H	2.310842	-3.025629	0.054401
H	4.058749	-2.757023	-0.042195
Si	-2.894942	-0.356815	1.197504
C	-3.098709	-0.746417	3.019620
H	-4.141457	-1.017449	3.231538
H	-2.845848	0.122580	3.640380
H	-2.462409	-1.583848	3.330661
C	-4.083827	1.009234	0.714257
H	-5.105011	0.614281	0.807523
H	-3.952889	1.340357	-0.323340
H	-4.007109	1.884734	1.369916
C	-3.267662	-1.869225	0.153560
H	-4.273680	-2.235077	0.400281
H	-2.558841	-2.688222	0.326493
H	-3.257335	-1.626737	-0.918042
C	-1.405161	0.529661	-1.936355
H	-1.161296	-1.810900	-2.979107
C	-0.745074	-2.494762	-2.209216
O	-0.169978	-1.947631	-1.204169
O	-0.853468	-3.718677	-2.365718
O	-2.269760	0.952016	-2.570017
Mn	0.017032	0.016949	-0.905419
N	1.166254	0.409937	-2.004234
O	2.029670	0.827949	-2.674118

2Mn Gsolv= -2824.412769

C	0.014687	-0.724764	-1.063639
O	-0.038148	-2.041977	-1.355175
H	-0.299215	-2.586841	-0.562459
C	-1.117482	0.124532	-0.884412
C	-0.561644	1.431243	-0.608056
C	-1.278946	2.723594	-0.381050
H	-2.179492	2.572345	0.225402
H	-1.627221	3.091127	-1.359585
C	-0.352873	3.756798	0.252217
H	-0.858046	4.728884	0.281002
H	-0.141334	3.474132	1.296708
C	0.948868	3.848788	-0.532084
H	1.567978	4.677489	-0.170519
H	0.708996	4.067593	-1.583660
C	1.749217	2.548614	-0.452939
H	2.499081	2.517261	-1.254170
H	2.315469	2.510398	0.487304
C	0.862694	1.344838	-0.595440
C	1.244034	-0.029206	-0.821120
Si	-2.926782	-0.393835	-1.148825
C	-3.103027	-0.730234	-2.983244
H	-2.867484	0.163211	-3.575123
H	-4.133458	-1.027721	-3.217556
H	-2.435433	-1.538582	-3.306850
C	-4.107232	0.961840	-0.619744
H	-3.983589	1.892809	-1.184710
H	-4.022455	1.186507	0.451674
H	-5.128415	0.596529	-0.796829
C	-3.338263	-1.923300	-0.150961
H	-3.185640	-1.756021	0.923995
H	-2.754537	-2.799651	-0.453719
H	-4.401002	-2.156850	-0.302796
Si	2.951953	-0.847679	-0.964147
C	3.170347	-1.330470	-2.762011
H	4.158851	-1.780409	-2.921196
H	3.094836	-0.448196	-3.410583
H	2.411469	-2.053965	-3.083755
C	4.302663	0.347548	-0.460295
H	5.261543	-0.186661	-0.507547
H	4.179537	0.711741	0.567255
H	4.374045	1.213244	-1.129370
C	3.011784	-2.339176	0.167680
H	3.978124	-2.848523	0.054048
H	2.219460	-3.063514	-0.057445
H	2.915638	-2.037042	1.219450
O	-2.038620	1.123694	2.517939
C	1.434366	0.548819	2.027431
O	2.295537	0.897913	2.703756
H	0.209271	-1.522079	1.563208
C	-0.461884	-2.465941	1.865503
O	-0.820324	-2.449520	3.039397
O	-0.570631	-3.288579	0.943964
Mn	0.030580	0.109347	0.926909
N	-1.160033	0.650988	1.918665

3'Co-a Gsolv= -3015.724157

C	0.049982	0.367730	1.359620

O	-0.028635	1.498320	1.880622
H	-0.207194	2.437988	0.073328
C	-1.101871	-0.445010	0.883180
C	-0.536171	-1.639204	0.384722
C	0.888953	-1.528049	0.356612
C	1.288760	-0.259605	0.837051
Si	-2.921387	-0.000172	1.156868
C	-3.169690	0.156146	3.008302
H	-2.870532	-0.762329	3.528709
H	-4.227288	0.343972	3.234674
H	-2.583788	0.986894	3.420621
C	-3.957876	-1.400877	0.472560
H	-3.696015	-2.357317	0.943910
H	-3.836564	-1.506096	-0.612896
H	-5.020154	-1.211929	0.674999
C	-3.299070	1.624759	0.306588
H	-3.203873	1.541065	-0.783441
H	-2.628050	2.420880	0.655041
H	-4.328514	1.933115	0.531433
Si	3.028265	0.464004	1.011720
C	3.386468	0.632668	2.841930
H	4.403752	1.013879	2.998751
H	3.303294	-0.332497	3.356524
H	2.687754	1.333344	3.315732
C	4.211251	-0.729962	0.186250
H	5.241055	-0.364139	0.290178
H	4.002082	-0.825651	-0.887488
H	4.165590	-1.729573	0.637063
C	3.092707	2.132361	0.163803
H	4.095062	2.566637	0.274415
H	2.373199	2.838817	0.596169
H	2.883527	2.042611	-0.910331
C	-1.377620	-0.392877	-2.070002
C	1.260318	-0.276777	-2.149029
O	2.033846	-0.432091	-2.974977
C	-0.902909	-2.995694	-0.105072
O	0.301351	-3.468485	-0.725934
C	1.439817	-2.816082	-0.149130
H	-1.710385	-3.030180	-0.842566
H	-1.174482	-3.632945	0.752229
H	1.837392	-3.395277	0.700465
H	2.220439	-2.739487	-0.912733
H	-0.622112	2.348825	-2.763154
C	-0.660492	2.840271	-1.780604
O	-0.148357	2.044008	-0.830937
O	-1.084954	3.948321	-1.561786
Co	0.029884	-0.104051	-0.824354
N	-2.238384	-0.563461	-2.850130

3Co-a Gsolv= -2826.456620

C	0.019482	1.289496	0.071743
O	0.129074	2.374727	-0.661237
H	-0.720574	2.772831	-0.917941
C	-1.198189	0.564055	0.393456
C	-0.717238	-0.552082	1.130417
C	0.712839	-0.553894	1.148370
C	1.212319	0.563399	0.429979
Si	-3.025632	1.060164	0.090734
C	-3.226283	2.699532	0.969512
H	-3.029155	2.602319	2.044036
H	-4.249832	3.075030	0.845032
H	-2.541266	3.457686	0.567210
C	-4.093363	-0.278349	0.827745
H	-3.884299	-0.426770	1.894585
H	-3.963798	-1.234463	0.305762
H	-5.147937	0.011428	0.735574
C	-3.269652	1.250443	-1.752498
H	-3.220542	0.280691	-2.261802
H	-2.511302	1.906200	-2.200145
H	-4.252595	1.692975	-1.957671
Si	3.013859	1.090718	0.078287
C	3.272146	2.721714	0.952356
H	4.307645	3.060408	0.820865
H	3.079878	2.633181	2.028397
H	2.610792	3.498242	0.548974
C	4.087304	-0.269581	0.774960
H	5.145979	-0.006091	0.656523
H	3.924341	-1.220013	0.250307
H	3.900683	-0.427263	1.844941
C	3.217303	1.255523	-1.772850
H	4.221104	1.634283	-2.004088
H	2.489371	1.956181	-2.199521
H	3.101321	0.288590	-2.279077
C	-1.385130	-1.775841	-1.396115
C	1.273980	-1.869568	-1.332565
O	2.035659	-2.651045	-1.649282
C	-1.186446	-1.731234	1.903299
O	-0.014872	-2.548694	2.009341

C	1.159647	-1.734559	1.931499
H	-1.984324	-2.318376	1.440344
H	-1.521822	-1.392114	2.897623
H	1.474979	-1.392525	2.931533
H	1.970257	-2.324411	1.492598
Co	0.005049	-0.657335	-0.762134
N	-2.234519	-2.480938	-1.791310

3'Co-b Gsolv= -3158.487201

C	-0.503958	-1.576912	-1.172000
O	-0.777025	-2.782346	-1.302019
H	-0.970245	-3.063490	0.653058
C	-1.466804	-0.462465	-0.907822
C	-0.698038	0.722108	-0.845924
C	0.689467	0.391641	-0.877031
C	0.843717	-1.015572	-0.957828
C	-1.257381	0.448665	2.037658
C	1.310352	-0.372898	1.789364
O	2.280977	-0.340676	2.390281
C	-2.927687	-0.597324	-0.890252
C	-3.735627	0.373729	-0.274503
C	-3.560117	-1.677508	-1.520985
C	-5.117529	0.261465	-0.288075
H	-3.280719	1.219256	0.235462
C	-4.948458	-1.779504	-1.532322
H	-2.963822	-2.436516	-2.017888
C	-5.752263	-0.818935	-0.915395
H	-5.722562	1.025567	0.199076
H	-5.417223	-2.624204	-2.035658
C	2.097031	-1.780160	-1.001053
C	3.208456	-1.276626	-1.688608
C	2.213979	-3.012450	-0.345974
C	4.399915	-1.992405	-1.724849
H	3.136007	-0.323112	-2.209590
C	3.409464	-3.721824	-0.388333
H	1.370672	-3.407631	0.218819
C	4.520818	-3.228239	-1.079870
H	5.254950	-1.586383	-2.264454
H	3.486831	-4.674669	0.133865
C	-7.244730	-0.930089	-0.912651
H	-7.627846	-1.062726	0.107169
H	-7.711382	-0.019958	-1.308856
H	-7.584855	-1.779875	-1.513371
C	5.802919	-3.999464	-1.144230
H	5.938783	-4.454800	-2.133800
H	6.668014	-3.348564	-0.971799
H	5.823600	-4.805353	-0.403147
C	-0.878745	2.200832	-0.834889
C	1.529176	1.619572	-0.891530
H	-1.655821	2.582749	-0.168544
H	-1.130433	2.522469	-1.855067
H	1.850930	1.798360	-1.928781
H	2.430631	1.577600	-0.273751
C	0.527771	2.731524	-0.458058
C	0.558899	3.076627	1.032096
C	0.871460	4.013051	-1.208949
O	-0.294235	3.781445	1.540620
O	0.292463	4.417511	-2.196167
O	1.594753	2.578995	1.685876
O	1.933118	4.600877	-0.669091
H	-0.398992	-2.327733	3.362040
C	-0.552723	-3.054212	2.550534
O	-0.883498	-2.429851	1.408201
O	-0.455262	-4.252646	2.649540
C	2.403977	5.797709	-1.315815
H	1.621183	6.560412	-1.306691
H	3.264478	6.127230	-0.734468
H	2.701440	5.574217	-2.343510
C	1.670805	2.879348	3.091169
H	0.827695	2.418038	3.615692
H	2.612590	2.450852	3.433173
H	1.665710	3.961164	3.246220
N	-1.908130	0.979840	2.858435
Co	-0.179553	-0.469124	0.750170

3Co-b Gsolv= -2969.220910

C	0.312732	-1.964479	-0.562101
O	0.456849	-3.252357	-0.393146
H	1.396019	-3.520256	-0.375896
C	-0.985349	-1.317671	-0.522625
C	-0.691437	0.070914	-0.655808
C	0.722380	0.256225	-0.719670
C	1.378204	-0.988888	-0.566518
C	-1.257265	-0.231009	2.270175
C	1.382237	0.376935	2.077765
O	2.134768	0.994498	2.664562
C	-2.297260	-1.971255	-0.496663
C	-2.457300	-3.299671	-0.911549

C	-3.438407	-1.250534	-0.108218
C	-3.719409	-3.884509	-0.932456
H	-1.601029	-3.880138	-1.241134
C	-4.690056	-1.844168	-0.128432
H	-3.348345	-0.220368	0.227414
C	-4.855414	-3.173641	-0.540030
H	-3.823487	-4.915563	-1.266847
H	-5.562176	-1.269074	0.180361
C	2.821805	-1.257731	-0.516216
C	3.673263	-0.666612	-1.455699
C	3.363236	-2.095761	0.467010
C	5.039437	-0.918996	-1.412683
H	3.260116	-0.020199	-2.228666
C	4.730355	-2.341563	0.499808
H	2.712662	-2.535924	1.223865
C	5.590508	-1.756344	-0.436011
H	5.693976	-0.460544	-2.152480
H	5.142104	-2.992260	1.269875
C	-6.214242	-3.798531	-0.555580
H	-6.911487	-3.211961	-1.166125
H	-6.182530	-4.817616	-0.953847
H	-6.637771	-3.842033	0.455670
C	7.065990	-1.998031	-0.372757
H	7.549227	-1.273771	0.296051
H	7.290134	-2.996812	0.017096
H	7.532563	-1.892870	-1.357874
C	-1.389824	1.367658	-0.858728
C	1.071634	1.675018	-0.955734
H	-2.252005	1.553357	-0.216152
H	-1.745626	1.387733	-1.900584
H	1.324751	1.784406	-2.020247
H	1.924857	2.043783	-0.376768
C	-0.253721	2.421066	-0.659480
C	-0.200701	3.020647	0.748156
C	-0.480256	3.562032	-1.647441
O	0.782155	3.613853	1.154659
O	0.001056	3.603871	-2.760928
O	-1.304628	2.845968	1.450455
O	-1.318912	4.462555	-1.154953
C	-1.660561	5.563348	-2.019548
H	-2.337822	6.190724	-1.441383
H	-0.758715	6.119472	-2.287499
H	-2.157107	5.189414	-2.918466
C	-1.298158	3.365748	2.792064
H	-2.281028	3.133484	3.201434
H	-0.514033	2.873398	3.376033
H	-1.134682	4.446373	2.774859
N	-2.114672	-0.056409	3.051243
Co	0.171826	-0.598006	1.070786

3'Co-c Gsolv= -2660.411700

C	0.101205	-0.454648	-1.360119
O	0.057476	-1.599180	-1.830869
H	-0.055726	-2.417731	0.140636
C	-1.062954	0.377282	-0.943870
C	-0.538545	1.625725	-0.534326
C	0.881085	1.550595	-0.483177
C	1.308119	0.255041	-0.854238
C	-1.451550	0.532788	1.945364
C	1.233688	0.527593	2.135270
O	1.997574	0.775987	2.946684
C	-2.477636	0.017793	-1.079050
C	-3.432456	1.024620	-1.274025
C	-2.906532	-1.312528	-0.963068
C	-4.785415	0.711208	-1.352349
H	-3.116284	2.060979	-1.379081
C	-4.260841	-1.621298	-1.038814
H	-2.180217	-2.105210	-0.800846
C	-5.204124	-0.612772	-1.232724
H	-5.513512	1.504061	-1.506804
H	-4.581724	-2.655824	-0.940913
H	-6.262095	-0.858066	-1.289518
C	2.686535	-0.241971	-0.906967
C	3.751267	0.664411	-1.010577
C	2.968002	-1.614549	-0.843014
C	5.065397	0.210144	-1.054823
H	3.553675	1.732722	-1.080217
C	4.283718	-2.064187	-0.887658
H	2.155019	-2.330029	-0.753345
C	5.336124	-1.155754	-0.993177
H	5.879418	0.926049	-1.141668
H	4.487666	-3.131234	-0.835734
H	6.363234	-1.511245	-1.029045
C	-0.941124	3.006235	-0.147076
O	0.238538	3.534301	0.472162
C	1.396026	2.884235	-0.063525
H	-1.197694	3.582941	-1.050921
H	1.774239	3.422201	-0.948628

H	2.179945	2.871014	0.701056
H	-0.777248	-2.034391	2.879816
C	-0.756557	-2.597004	1.936309
O	-0.058139	-1.931145	0.997806
O	-1.264084	-3.673365	1.742819
H	-1.770575	3.069872	0.564017
Co	0.034923	0.211014	0.800327
N	-2.401796	0.720855	2.609622

3Co-c Gsolv= -2471.140857

C	-0.085690	-1.232564	0.127000
O	-0.037393	-2.341873	-0.561296
H	-0.919261	-2.656740	-0.835165
C	1.125670	-0.521211	0.486039
C	0.670715	0.653067	1.141448
C	-0.751495	0.709233	1.083331
C	-1.256794	-0.439516	0.423942
C	1.583166	1.660788	-1.381130
C	-1.042342	2.022468	-1.494820
O	-1.665972	2.885702	-1.890577
C	2.511781	-0.951389	0.276024
C	3.483291	-0.604928	1.221912
C	2.887557	-1.649317	-0.879312
C	4.812940	-0.961875	1.020900
H	3.197751	-0.068918	2.125297
C	4.218299	-1.998145	-1.076869
H	2.143753	-1.891919	-1.634608
C	5.183001	-1.656322	-0.128993
H	5.560457	-0.693695	1.763317
H	4.506084	-2.531395	-1.979660
H	6.223326	-1.929395	-0.288823
C	-2.655169	-0.845631	0.220622
C	-3.628568	0.071406	-0.195729
C	-3.032452	-2.162924	0.513264
C	-4.951993	-0.329478	-0.332705
H	-3.352157	1.100949	-0.415789
C	-4.359203	-2.559710	0.370160
H	-2.302273	-2.872722	0.899462
C	-5.319323	-1.646666	-0.056911
H	-5.699454	0.388699	-0.660233
H	-4.641101	-3.583009	0.605012
H	-6.355097	-1.957732	-0.168789
C	1.146723	1.846365	1.888995
O	0.004631	2.709701	1.893645
C	-1.195846	1.936693	1.793051
H	1.992846	2.374745	1.439464
H	1.415624	1.544283	2.914570
H	-1.574833	1.652144	2.788323
H	-1.958229	2.532493	1.282734
Co	0.054544	0.701532	-0.788375
N	2.544876	2.225794	-1.743499

3'Co Gsolv= -3019.074160

C	0.012970	-0.546488	1.339163
O	0.073386	-1.712230	1.790877
H	0.129475	-2.513297	-0.050521
C	1.161187	0.262659	0.882120
C	0.634072	1.527877	0.490491
C	1.348824	2.776146	0.095170
H	2.257549	2.539460	-0.468546
H	1.678737	3.271053	1.023325
C	0.429845	3.715594	-0.678783
H	0.944067	4.667601	-0.852184
H	0.207673	3.284180	-1.668673
C	-0.863722	3.938001	0.093151
H	-1.480927	4.706267	-0.385671
H	-0.612167	4.313561	1.096329
C	-1.673814	2.648506	0.220540
H	-2.412475	2.734749	1.029006
H	-2.259978	2.472623	-0.691763
C	-0.808568	1.462511	0.519516
C	-1.207209	0.145267	0.889169
Si	2.945302	-0.347110	1.085657
C	3.216686	-0.610595	2.923875
H	3.090503	0.327603	3.479216
H	4.238147	-0.971352	3.103725
H	2.519576	-1.348623	3.338773
C	4.184723	0.912808	0.463525
H	4.110148	1.868811	0.996256
H	4.086699	1.102056	-0.612735
H	5.193192	0.513326	0.639259
C	3.179902	-1.960629	0.154769
H	3.043434	-1.827585	-0.926635
H	2.488877	-2.741268	0.497178
H	4.203941	-2.322035	0.320721
Si	-2.930784	-0.630937	1.022832
C	-3.296171	-0.873712	2.845056
H	-4.303769	-1.286421	2.984609

H	-3.244671	0.080971	3.384042
H	-2.580108	-1.564247	3.307373
C	-4.225704	0.476797	0.241262
H	-5.188506	-0.051507	0.272445
H	-4.005993	0.695241	-0.811768
H	-4.350810	1.426778	0.774049
C	-2.936992	-2.267658	0.104007
H	-3.930053	-2.728064	0.195470
H	-2.200146	-2.978044	0.498070
H	-2.733655	-2.121156	-0.965934
C	1.380167	0.377837	-2.070795
C	-1.257701	0.339083	-2.088076
O	-2.034686	0.532068	-2.904398
H	0.247068	-2.301135	-2.911814
C	0.250506	-2.865243	-1.967522
O	0.119381	-2.044560	-0.921816
O	0.354840	-4.063889	-1.860697
N	2.224188	0.544409	-2.870672
Co	-0.006881	0.081058	-0.799604

3Co Gsolv= -2829.812669

C	-0.009532	-1.310752	-0.326482
O	0.060491	-2.544026	0.130116
H	-0.809037	-2.945578	0.300521
C	-1.194532	-0.503082	-0.478931
C	-0.698054	0.763140	-0.932227
C	-1.450211	1.987105	-1.313352
H	-2.338215	2.107977	-0.684973
H	-1.814995	1.826430	-2.341947
C	-0.554000	3.221077	-1.274644
H	-1.104450	4.076978	-1.679367
H	-0.305540	3.462636	-0.228474
C	0.720119	2.975403	-2.070245
H	1.317266	3.889892	-2.148335
H	0.447383	2.684572	-3.095217
C	1.572204	1.876018	-1.438678
H	2.307484	1.485130	-2.155407
H	2.166735	2.279213	-0.606551
C	0.749378	0.722698	-0.970811
C	1.193812	-0.547893	-0.499323
Si	-2.998326	-1.120641	-0.287707
C	-3.256841	-2.280968	-1.732410
H	-3.171454	-1.750514	-2.688762
H	-4.255550	-2.732993	-1.682254
H	-2.518899	-3.093785	-1.725894
C	-4.220826	0.287261	-0.321820
H	-4.213165	0.828484	-1.274866
H	-4.060593	0.999770	0.496243
H	-5.222607	-0.145512	-0.194722
C	-3.097772	-2.048020	1.340541
H	-2.534521	-1.542899	2.135464
H	-2.745404	-3.085907	1.271724
H	-4.147645	-2.095209	1.658257
Si	2.955265	-1.228533	-0.206467
C	3.262936	-2.468763	-1.570167
H	4.260002	-2.915528	-1.470504
H	3.202523	-1.989541	-2.555267
H	2.523207	-3.278531	-1.539853
C	4.188588	0.175260	-0.252436
H	5.169696	-0.226938	0.033868
H	3.938945	0.970903	0.460893
H	4.291506	0.620100	-1.248959
C	2.973448	-2.006972	1.494784
H	4.001794	-2.285681	1.759048
H	2.353245	-2.908391	1.551567
H	2.616673	-1.294635	2.251353
C	-1.391695	1.252121	1.872759
C	1.257312	1.407617	1.806728
O	2.009766	2.084950	2.325220
Co	0.003976	0.373165	0.938701
N	-2.240992	1.791090	2.476213

3'Fe-Casey Gsolv= -2917.183738

Fe	-0.022478	-0.124001	0.858783
C	-0.052949	0.488523	-1.267022
O	0.014427	1.704273	-1.636458
H	0.119541	2.340461	0.048155
C	1.099504	-0.351703	-0.910803
C	0.544639	-1.588869	-0.465032
C	-0.867167	-1.493601	-0.413391
C	-1.280033	-0.191298	-0.827577
Si	2.908444	0.106387	-1.164718
C	3.182284	0.424398	-2.992332
H	2.922868	-0.457029	-3.592314
H	4.235427	0.665861	-3.187005
H	2.573072	1.266046	-3.345108
C	3.948378	-1.345163	-0.590760
H	3.702183	-2.262624	-1.141009

H	3.820744	-1.541262	0.481807
H	5.011313	-1.131270	-0.764234
C	3.343679	1.636977	-0.171656
H	3.202276	1.472793	0.905297
H	2.741265	2.503227	-0.473267
H	4.399084	1.894155	-0.333473
Si	-3.023894	0.501785	-0.990792
C	-3.353004	0.802276	-2.812786
H	-4.368967	1.189418	-2.964721
H	-3.257865	-0.129188	-3.385317
H	-2.648242	1.530919	-3.232636
C	-4.213676	-0.782862	-0.319573
H	-5.246730	-0.429985	-0.437378
H	-4.048873	-0.970192	0.749368
H	-4.125115	-1.737593	-0.854240
C	-3.190009	2.097042	-0.018101
H	-4.196189	2.515197	-0.154577
H	-2.465838	2.852181	-0.348024
H	-3.042771	1.924766	1.056453
C	1.276313	-0.587059	1.995544
O	2.109839	-0.959362	2.700768
C	-1.306978	-0.359005	2.079787
O	-2.144299	-0.562597	2.845949
C	0.931446	-2.986829	-0.117499
O	-0.262458	-3.529501	0.467442
C	-1.412930	-2.827913	-0.030438
H	1.747487	-3.098705	0.603935
H	1.198196	-3.537260	-1.034722
H	-1.818899	-3.335993	-0.920501
H	-2.178989	-2.828767	0.752110
H	0.771655	2.206165	2.862627
C	0.691623	2.734103	1.900820
O	0.126434	1.952380	0.972733
O	1.044479	3.869080	1.689874

3Fe-Casey Gsolv= -2917.180358

Fe	0.034984	-0.385275	0.871589
C	-0.007400	0.511644	-1.171570
O	-0.031312	1.742748	-1.467288
H	-0.068657	2.986469	-0.438474
C	1.204506	-0.264090	-0.869475
C	0.747407	-1.589122	-0.615748
C	1.238474	-2.984565	-0.434484
H	2.049032	-3.121887	0.288703
H	1.562264	-3.391761	-1.406359
C	-1.112880	-3.022542	-0.391575
H	-1.461690	-3.445621	-1.347784
H	-1.888434	-3.181754	0.364929
C	-0.673195	-1.612423	-0.591980
C	-1.182743	-0.303670	-0.841660
Si	2.953925	0.432544	-0.923669
C	3.312757	1.018450	-2.667947
H	3.244800	0.193520	-3.388177
H	4.325206	1.437977	-2.732762
H	2.604505	1.797879	-2.975721
C	4.138080	-0.937351	-0.437119
H	4.045589	-1.801424	-1.108009
H	3.972871	-1.281608	0.591868
H	5.172333	-0.574803	-0.503014
C	3.073481	1.873903	0.273230
H	2.792710	1.582735	1.294820
H	2.423877	2.702503	-0.036888
H	4.103949	2.252280	0.305219
Si	-2.965406	0.297252	-0.940912
C	-3.292181	0.855265	-2.701037
H	-4.325125	1.210807	-2.809261
H	-3.139210	0.036797	-3.415526
H	-2.622326	1.678834	-2.979015
C	-4.079363	-1.139475	-0.482482
H	-5.131542	-0.853611	-0.610721
H	-3.944746	-1.445819	0.562896
H	-3.891292	-2.011937	-1.122084
C	-3.231312	1.736038	0.233436
H	-4.281582	2.055001	0.194171
H	-2.614375	2.600621	-0.044138
H	-3.004512	1.469060	1.274113
C	1.341793	-0.899504	1.984649
O	2.182502	-1.306095	2.660109
C	-1.260861	-0.878269	2.008049
O	-2.097394	-1.269691	2.697285
H	-0.298624	2.047517	1.441791
C	-0.173119	3.149542	1.455373
O	-0.156735	3.791028	2.488345
O	-0.059060	3.701080	0.267068
O	0.082682	-3.687166	0.047518

3'Fe Gsolv= -2920.528972

Fe	-0.002092	0.071552	0.840068

C	0.007768	-0.608100	-1.258143
O	-0.029202	-1.839510	-1.595342
H	-0.080438	-2.412544	0.086659
C	-1.152494	0.202392	-0.897372
C	-0.647095	1.494150	-0.510560
C	-1.401941	2.748533	-0.200671
H	-2.316408	2.531555	0.363761
H	-1.731126	3.184595	-1.157840
C	-0.519790	3.752669	0.532975
H	-1.051756	4.706438	0.629098
H	-0.319070	3.392062	1.555528
C	0.793123	3.943424	-0.215447
H	1.381674	4.756989	0.224273
H	0.564057	4.242086	-1.250039
C	1.627479	2.663212	-0.229323
H	2.403621	2.726431	-1.003530
H	2.165544	2.555186	0.722595
C	0.782064	1.450833	-0.503588
C	1.208784	0.125287	-0.866257
Si	-2.917380	-0.435312	-1.101071
C	-3.180457	-0.834568	-2.916060
H	-3.042132	0.058027	-3.539391
H	-4.200410	-1.206134	-3.081879
H	-2.479611	-1.602875	-3.265331
C	-4.186258	0.840078	-0.565376
H	-4.119567	1.773312	-1.137649
H	-4.110297	1.080317	0.503144
H	-5.186072	0.416517	-0.735461
C	-3.174139	-1.976140	-0.055196
H	-3.052202	-1.759065	1.015348
H	-2.479124	-2.781945	-0.322147
H	-4.196489	-2.350167	-0.203782
Si	2.939319	-0.614254	-1.012971
C	3.262913	-0.963628	-2.828766
H	4.270513	-1.376451	-2.970197
H	3.191364	-0.041543	-3.420146
H	2.542467	-1.683424	-3.236971
C	4.244458	0.571895	-0.369337
H	5.216521	0.060398	-0.393282
H	4.056597	0.877944	0.667614
H	4.329260	1.475974	-0.984505
C	3.051729	-2.199488	-0.008395
H	4.042033	-2.653077	-0.151316
H	2.296630	-2.938375	-0.304083
H	2.930759	-1.997441	1.064833
C	-1.308489	0.494345	1.978691
O	-2.159119	0.837720	2.680165
C	1.290990	0.362314	2.038411
O	2.131676	0.591782	2.795441
H	-0.266158	-2.276321	2.977669
C	-0.237963	-2.824970	2.024298
O	-0.084996	-1.988777	0.998118
O	-0.330489	-4.023507	1.896938

3Fe Gsolv= -2920.522537

Fe	0.007395	0.181229	0.881247
C	-0.012558	-0.594230	-1.163203
O	-0.032068	-1.829268	-1.476000
H	-0.073878	-2.984690	-0.387200
C	-1.181138	0.212623	-0.829534
C	-0.690315	1.523708	-0.506456
C	-1.454647	2.773548	-0.208108
H	-2.355701	2.554466	0.376368
H	-1.805430	3.188099	-1.167270
C	-0.572432	3.801571	0.492407
H	-1.119657	4.746134	0.591768
H	-0.339915	3.456656	1.513549
C	0.715909	4.007735	-0.293040
H	1.304409	4.831678	0.126591
H	0.453126	4.298585	-1.321506
C	1.570667	2.741043	-0.324509
H	2.307542	2.800666	-1.136795
H	2.158114	2.658829	0.600090
C	0.743704	1.506054	-0.535174
C	1.185561	0.176009	-0.840098
Si	-2.943682	-0.432204	-1.024994
C	-3.217111	-0.784193	-2.848001
H	-3.107872	0.133012	-3.441020
H	-4.230209	-1.173133	-3.015353
H	-2.503293	-1.522791	-3.233090
C	-4.215139	0.825446	-0.456356
H	-4.168011	1.762887	-1.023636
H	-4.128088	1.059856	0.612340
H	-5.212299	0.391623	-0.616142
C	-3.170427	-1.994818	-0.009931
H	-2.938687	-1.822285	1.050636
H	-2.538684	-2.815231	-0.371012
H	-4.216595	-2.323957	-0.072650

Si	2.928779	-0.532107	-0.993661
C	3.236796	-0.889575	-2.809870
H	4.244882	-1.297294	-2.960959
H	3.155573	0.032519	-3.400300
H	2.515303	-1.611847	-3.211491
C	4.218067	0.685615	-0.379277
H	5.204647	0.209378	-0.465652
H	4.072957	0.953213	0.675113
H	4.245541	1.609375	-0.969666
C	3.074087	-2.093255	0.039979
H	4.100575	-2.478868	-0.027267
H	2.394970	-2.884955	-0.298296
H	2.865871	-1.887047	1.099329
C	-1.303745	0.602534	2.027697
O	-2.153227	0.954553	2.724171
C	1.309948	0.593733	2.043938
O	2.145364	0.939504	2.760062
H	0.003456	-2.098231	1.562402
C	-0.043737	-3.208660	1.517264
O	-0.048499	-3.887486	2.526345
O	-0.090724	-3.715750	0.309606

3'Fe-Renaud Gsolv= -2675.818358

Fe	0.045312	-0.074447	0.962623
C	0.035246	-0.758583	-1.130817
O	-0.069648	-1.979220	-1.473184
H	-0.358923	-2.551451	0.198600
C	-1.081028	0.117697	-0.788010
C	-0.543201	1.416872	-0.500654
C	-0.350406	3.602399	0.368292
H	-0.844989	4.576312	0.300714
H	-0.277601	3.329403	1.437693
C	1.019291	3.680953	-0.262191
H	1.634677	4.404767	0.280354
H	0.918252	4.042956	-1.294280
C	0.890159	1.293134	-0.415625
C	1.248064	-0.069742	-0.734186
C	-1.083533	0.543772	2.189753
O	-1.771351	0.966487	3.021240
C	1.384665	-0.102200	2.135414
O	2.242621	-0.194935	2.905738
H	-1.077312	-2.289653	2.984429
C	-1.081243	-2.809716	2.014913
O	-0.328949	-2.160130	1.121212
O	-1.670082	-3.836930	1.773217
C	2.603501	-0.609933	-0.955638
C	3.044896	-1.765976	-0.301837
C	3.458091	0.015311	-1.872789
C	4.314829	-2.280491	-0.551738
H	2.388693	-2.258464	0.414568
C	4.730239	-0.494989	-2.117402
H	3.118564	0.906085	-2.398506
C	5.163191	-1.643923	-1.456489
H	4.644209	-3.178388	-0.033266
H	5.383683	0.003942	-2.829820
H	6.157150	-2.042601	-1.646955
C	-2.481711	-0.268349	-1.071282
C	-2.947610	-0.155437	-2.387049
C	-3.345774	-0.754994	-0.086667
C	-4.259956	-0.493638	-2.705853
H	-2.273479	0.215539	-3.158724
C	-4.659307	-1.094462	-0.404558
H	-2.991923	-0.853956	0.938788
C	-5.120796	-0.960328	-1.712742
H	-4.611847	-0.392033	-3.730160
H	-5.323688	-1.464669	0.373160
H	-6.147226	-1.222978	-1.958786
N	1.718881	2.389698	-0.262540
N	-1.169709	2.621592	-0.342256
C	2.813445	2.294152	0.691828
H	3.325695	1.331788	0.604674
H	3.545145	3.081330	0.484870
H	2.449574	2.415825	1.726859
C	-2.587455	2.681126	-0.019996
H	-3.178746	2.116681	-0.744472
H	-2.801131	2.301234	0.990762
H	-2.903386	3.726827	-0.068977

3Fe-Renaud Gsolv= -3031.116409

Fe	0.009718	0.090256	0.986507
C	0.091597	0.588152	-1.139378
O	0.292803	1.747813	-1.623526
H	0.723915	3.040277	-0.761066
C	1.126946	-0.332623	-0.695808
C	0.422960	-1.486431	-0.198244
C	-0.017652	-3.502560	0.913926
H	0.391252	-4.495563	1.127361
H	-0.170333	-2.993307	1.875235

C	-1.343136	-3.648565	0.192432
H	-2.090867	-4.054151	0.886149
H	-1.273998	-4.349374	-0.652260
C	-1.003441	-1.322731	-0.434637
C	-1.227466	0.067946	-0.740451
Si	2.971840	-0.027076	-0.963752
C	3.289935	-0.133347	-2.811990
H	3.028653	-1.124285	-3.205820
H	4.349680	0.049515	-3.033622
H	2.696229	0.612547	-3.356092
C	4.062212	-1.265472	-0.065798
H	3.926231	-2.301851	-0.395337
H	3.917622	-1.231084	1.021231
H	5.106567	-0.988465	-0.267629
C	3.471307	1.670532	-0.336359
H	3.209191	1.812551	0.721566
H	3.022323	2.483688	-0.917220
H	4.563371	1.760990	-0.420087
Si	-2.753602	1.191486	-0.880017
C	-3.242428	1.325914	-2.687052
H	-4.090938	2.012057	-2.808512
H	-3.538877	0.349880	-3.093195
H	-2.409938	1.705531	-3.293143
C	-4.236702	0.631676	0.137553
H	-4.835782	1.529556	0.343088
H	-3.956936	0.199665	1.106199
H	-4.885028	-0.080800	-0.382736
C	-2.333751	2.888797	-0.191680
H	-3.256182	3.485666	-0.173300
H	-1.591570	3.430414	-0.785628
H	-1.971372	2.817479	0.844000
C	1.315105	-0.219680	2.143648
O	2.158739	-0.501151	2.885551
C	-1.270178	-0.231163	2.176402
O	-2.092942	-0.581540	2.914981
H	0.561985	2.543062	1.310356
C	0.836770	3.591172	1.068429
O	1.027583	4.426762	1.933084
O	0.936860	3.858658	-0.213826
N	-1.840530	-2.355652	-0.293809
N	0.971012	-2.737083	0.151574
C	-3.258075	-2.305242	-0.586326
H	-3.467000	-1.539577	-1.337130
H	-3.555768	-3.272021	-1.006438
H	-3.854895	-2.121128	0.315912
C	1.458271	-3.466859	-1.024387
H	0.654728	-3.717093	-1.736498
H	2.201019	-2.869171	-1.560847
H	1.937341	-4.395657	-0.697070

3'Fe-williams-1 Gsolv= -2870.978516

Fe	0.004930	-0.654188	1.014078
C	-0.025077	-1.394510	-1.099134
O	-0.056500	-2.630977	-1.379856
H	-0.084799	-3.163048	0.316035
C	-1.176076	-0.576458	-0.729664
C	-0.704649	0.726331	-0.350852
C	0.728569	0.702492	-0.355519
C	1.158084	-0.614730	-0.750970
C	-1.233296	-0.279931	2.256583
O	-2.004796	-0.022348	3.072344
C	1.324593	-0.400558	2.204930
O	2.155833	-0.235786	2.984339
C	-2.578185	-0.985171	-0.938313
C	-3.607505	-0.636367	-0.052984
C	-2.911934	-1.693056	-2.101768
C	-4.926634	-0.989003	-0.320134
H	-3.385947	-0.077119	0.853220
C	-4.232240	-2.046706	-2.368075
H	-2.130835	-1.955672	-2.811433
C	-5.245194	-1.698328	-1.477258
H	-5.708946	-0.708384	0.381555
H	-4.468797	-2.592830	-3.278636
H	-6.276694	-1.974561	-1.683658
C	2.547841	-1.066077	-0.952446
C	3.610644	-0.586667	-0.170562
C	2.841265	-1.964232	-1.988959
C	4.916603	-0.999671	-0.411071
H	3.425464	0.124002	0.632219
C	4.149628	-2.377966	-2.227704
H	2.037443	-2.334699	-2.619115
C	5.193237	-1.900815	-1.438730
H	5.722256	-0.614863	0.210301
H	4.351477	-3.074181	-3.038850
H	6.214867	-2.225212	-1.622950
C	-1.539644	1.937416	-0.212745
C	-1.560412	2.729425	0.938942
C	-2.312594	2.321266	-1.316579

C	-2.339942	3.882617	0.986756
H	-0.975379	2.438601	1.809052
C	-3.088270	3.475783	-1.268193
H	-2.299942	1.710479	-2.218585
C	-3.105055	4.259108	-0.115248
H	-2.350396	4.486019	1.891581
H	-3.680635	3.763245	-2.133848
H	-3.713768	5.159515	-0.075592
C	1.597573	1.893509	-0.240142
C	1.777474	2.607509	0.947149
C	2.251130	2.326111	-1.401009
C	2.600774	3.730802	0.975289
H	1.283944	2.277004	1.859227
C	3.072006	3.449517	-1.372238
H	2.114748	1.771687	-2.328916
C	3.249878	4.154546	-0.182669
H	2.737066	4.273466	1.907943
H	3.574201	3.773520	-2.280933
H	3.894638	5.030066	-0.158121
H	-0.155216	-2.976625	3.209599
C	-0.168658	-3.541137	2.265778
O	-0.059462	-2.717971	1.214824
O	-0.264643	-4.739397	2.160740

3Fe-williams-1 Gsolv= -2870.971114

Fe	-0.028600	0.643544	0.941967
C	-0.027257	1.280718	-1.153006
O	-0.076603	2.498327	-1.497754
H	0.058629	3.628146	-0.285280
C	1.159384	0.546800	-0.758950
C	0.752893	-0.767487	-0.335060
C	-0.685234	-0.829614	-0.383090
C	-1.176813	0.441064	-0.802344
C	1.328910	0.787690	2.113918
O	2.190720	0.906012	2.866795
C	-1.146504	0.125457	2.255062
O	-1.816826	-0.250196	3.112772
H	-1.306183	2.882673	1.166786
C	-0.700692	3.768708	1.461295
O	-0.786783	4.285631	2.558357
O	0.106882	4.218401	0.521951
C	-2.577503	0.859904	-0.996694
C	-2.930110	1.507894	-2.188323
C	-3.579488	0.604907	-0.050686
C	-4.248233	1.889706	-2.426808
H	-2.167783	1.701254	-2.939742
C	-4.895758	0.984929	-0.290688
H	-3.337048	0.099941	0.881647
C	-5.235874	1.630140	-1.479217
H	-4.502637	2.388928	-3.359135
H	-5.658223	0.779072	0.457125
H	-6.264904	1.929825	-1.663857
C	2.540154	1.017800	-0.977253
C	2.988808	2.229126	-0.438286
C	3.414799	0.266252	-1.773367
C	4.285601	2.674693	-0.681467
H	2.319975	2.820374	0.186186
C	4.712347	0.711145	-2.013059
H	3.072588	-0.670067	-2.212727
C	5.152088	1.915824	-1.466456
H	4.620915	3.615482	-0.250622
H	5.380009	0.115500	-2.631675
H	6.166241	2.262427	-1.651818
C	-1.487739	-2.037071	-0.112069
C	-1.247088	-2.849300	1.002345
C	-2.467901	-2.417277	-1.036001
C	-1.980166	-4.016179	1.191913
H	-0.484411	-2.564303	1.726444
C	-3.195316	-3.589470	-0.847700
H	-2.650338	-1.799654	-1.914113
C	-2.955625	-4.389834	0.267536
H	-1.789210	-4.636081	2.064739
H	-3.950249	-3.876514	-1.575891
H	-3.527191	-5.302990	0.416307
C	1.634046	-1.938907	-0.144226
C	1.455301	-3.039783	-0.993318
C	2.669394	-1.970597	0.793881
C	2.288851	-4.150125	-0.898547
H	0.661354	-3.019957	-1.739097
C	3.499296	-3.084361	0.892446
H	2.835827	-1.125376	1.456454
C	3.310859	-4.177578	0.049201
H	2.139036	-4.994854	-1.566998
H	4.295655	-3.095776	1.632949
H	3.959847	-5.046625	0.128328

3'Fe-williams-2 Gsolv= -3059.946332

Fe	-0.186297	-0.497488	0.839161

C	-0.505077	-1.619089	-1.055648
O	-0.770188	-2.857542	-1.090406
H	-0.866860	-2.997510	0.673043
C	-1.472686	-0.527330	-0.838310
C	-0.718052	0.681275	-0.776984
C	0.662699	0.375660	-0.820692
C	0.832787	-1.039519	-0.908087
C	-1.173345	0.417820	2.025797
O	-1.791144	1.026418	2.785521
C	1.333481	-0.334412	1.771332
O	2.357283	-0.225470	2.289412
C	-2.936744	-0.671739	-0.856027
C	-3.770483	0.263490	-0.221375
C	-3.545138	-1.725239	-1.550070
C	-5.152060	0.142036	-0.276936
H	-3.338904	1.098134	0.327947
C	-4.932622	-1.841328	-1.599670
H	-2.926793	-2.455159	-2.065011
C	-5.761893	-0.915927	-0.963565
H	-5.775633	0.881798	0.224759
H	-5.379854	-2.668816	-2.149616
C	2.105870	-1.772591	-0.988712
C	3.175711	-1.238187	-1.718658
C	2.292954	-2.999046	-0.337873
C	4.389085	-1.912775	-1.800185
H	3.053735	-0.288744	-2.238128
C	3.508605	-3.670255	-0.427848
H	1.486688	-3.422538	0.259311
C	4.576564	-3.143200	-1.161156
H	5.208457	-1.478195	-2.372282
H	3.635729	-4.619957	0.090835
C	-7.253973	-1.039590	-1.003354
H	-7.665077	-1.199925	0.001488
H	-7.719183	-0.125346	-1.392160
H	-7.569815	-1.877553	-1.633571
C	5.880568	-3.871885	-1.274937
H	6.009479	-4.296589	-2.278946
H	6.729293	-3.199330	-1.102772
H	5.943870	-4.695832	-0.556324
C	-0.931828	2.158328	-0.822657
C	1.485674	1.617066	-0.901272
H	-1.705799	2.550952	-0.157497
H	-1.201508	2.442886	-1.848518
H	1.780302	1.774524	-1.949771
H	2.398934	1.619873	-0.299903
C	0.471084	2.724429	-0.479373
C	0.522971	3.091365	1.004091
C	0.788078	3.985058	-1.273037
O	-0.369287	3.724316	1.541697
O	0.271150	4.285486	-2.330227
O	1.619326	2.692420	1.627541
O	1.759706	4.681586	-0.693012
H	-0.181409	-2.377432	3.410610
C	-0.376666	-3.072412	2.580702
O	-0.760315	-2.408629	1.479461
O	-0.281801	-4.274306	2.630636
C	2.211107	5.859687	-1.385923
H	1.387753	6.571065	-1.489458
H	3.001463	6.280165	-0.764925
H	2.601753	5.587043	-2.369650
C	1.702174	2.994439	3.030806
H	0.882264	2.505304	3.566353
H	2.662554	2.599307	3.361360
H	1.661347	4.075570	3.187400

3Fe-williams-2 Gsolv= -3059.937318

Fe	-0.226894	0.423550	0.741792
C	-0.660605	1.375257	-1.179397
O	-1.140134	2.535957	-1.313519
H	-1.523709	3.480450	-0.032492
C	0.756998	1.043215	-0.983715
C	0.826925	-0.373116	-0.835983
C	1.842871	-1.463524	-0.772974
H	2.706842	-1.259677	-0.134325
H	2.222241	-1.651885	-1.788191
C	-0.455608	-2.394930	-0.750768
H	-0.614333	-2.799345	-1.759442
H	-1.204924	-2.848956	-0.094043
C	-0.485747	-0.907838	-0.818689
C	-1.430653	0.146742	-0.936690
C	1.240323	0.556939	1.775902
O	2.233925	0.657537	2.349016
C	-1.237065	-0.548274	1.872192
O	-1.913369	-1.212827	2.526351
H	-1.125500	2.499101	1.851742
C	-1.527313	3.533215	1.891701
O	-1.738397	4.100164	2.946378
O	-1.759915	4.094065	0.724805

C	-2.894943	0.030836	-0.951562
C	-3.708216	0.991183	-0.331407
C	-3.510067	-1.053847	-1.585099
C	-5.091092	0.866590	-0.355265
H	-3.248742	1.833071	0.184393
C	-4.898012	-1.172706	-1.602855
H	-2.899884	-1.806149	-2.082983
C	-5.712046	-0.215904	-0.992406
H	-5.707943	1.620201	0.134021
H	-5.357506	-2.023273	-2.105089
C	1.877073	1.993033	-1.040408
C	1.788728	3.255665	-0.436234
C	3.071060	1.643688	-1.681269
C	2.860952	4.138159	-0.483033
H	0.878813	3.537891	0.091806
C	4.141985	2.532906	-1.721150
H	3.162120	0.671341	-2.163428
C	4.055476	3.795559	-1.128537
H	2.776907	5.111506	-0.000382
H	5.063973	2.241193	-2.223185
C	-7.205248	-0.333528	-1.009138
H	-7.611331	-0.374763	0.009235
H	-7.666884	0.532344	-1.500064
H	-7.529464	-1.235040	-1.539488
C	5.195536	4.764355	-1.196620
H	5.068481	5.464795	-2.032579
H	5.264028	5.365193	-0.282640
H	6.150993	4.249433	-1.344826
C	0.999274	-2.687366	-0.302561
C	1.023544	-2.928561	1.210037
C	1.530381	-3.973850	-0.924128
O	0.198922	-3.637381	1.759384
O	2.790266	-4.186001	-0.558731
O	2.027825	-2.342749	1.839336
O	0.898221	-4.708892	-1.655413
C	2.063092	-2.504087	3.268626
H	2.123629	-3.564138	3.527620
H	2.957351	-1.978377	3.602519
H	1.166705	-2.057175	3.711639
C	3.424824	-5.359883	-1.097754
H	4.440655	-5.351911	-0.703995
H	2.894631	-6.257380	-0.768595
H	3.438776	-5.309283	-2.189572

3'Fe-wills-1 Gsolv= -2561.870042

Fe	-0.050639	-0.160759	0.849541
C	-0.052107	0.479186	-1.283128
O	-0.003421	1.680897	-1.667918
H	0.019536	2.326482	0.076173
C	1.100462	-0.350051	-0.892079
C	0.577098	-1.606473	-0.468378
C	-0.832413	-1.547724	-0.445663
C	-1.261908	-0.251927	-0.861421
C	1.278247	-0.582679	1.973415
O	2.165903	-0.929854	2.621790
C	-1.380805	-0.443534	2.018365
O	-2.277725	-0.688797	2.698838
C	2.521395	-0.000668	-1.030571
C	3.451961	-0.999208	-1.347617
C	2.981733	1.308857	-0.826418
C	4.806529	-0.699056	-1.463149
H	3.112091	-2.018766	-1.523202
C	4.335952	1.606250	-0.945281
H	2.278187	2.096349	-0.566849
C	5.253808	0.605401	-1.263387
H	5.512583	-1.487861	-1.712900
H	4.677223	2.626197	-0.782218
H	6.311672	0.841226	-1.353874
C	-2.650925	0.218296	-0.955909
C	-3.694459	-0.708886	-1.088874
C	-2.970588	1.582713	-0.885039
C	-5.019350	-0.285876	-1.151317
H	-3.471446	-1.772179	-1.162303
C	-4.295744	2.002022	-0.950793
H	-2.177105	2.316748	-0.773751
C	-5.326001	1.071768	-1.082242
H	-5.813719	-1.021407	-1.257283
H	-4.524571	3.063938	-0.892004
H	-6.360668	1.403247	-1.130679
C	0.992775	-2.992778	-0.105906
O	-0.191036	-3.546775	0.483713
C	-1.346905	-2.895899	-0.062213
H	1.267982	-3.549937	-1.016793
H	-1.704020	-3.429846	-0.958408
H	-2.139526	-2.907600	0.693422
H	0.751146	2.145518	2.856626
C	0.690188	2.664449	1.889236
O	0.016188	1.926134	0.991406

O	1.141411	3.755389	1.643561
H	1.813038	-3.073413	0.615069

3Fe-wills-1 Gsolv= -2561.862504

Fe	-0.009245	-0.282667	0.889418
C	-0.002985	0.353601	-1.222923
O	-0.007080	1.542848	-1.641728
H	-0.019054	2.860413	-0.651478
C	1.179847	-0.422355	-0.820629
C	0.703583	-1.698895	-0.407232
C	1.166423	-3.065083	-0.028481
H	1.969410	-3.107241	0.714983
H	1.490486	-3.611421	-0.929611
C	-1.176734	-3.067229	-0.044427
H	-1.487411	-3.612521	-0.950764
H	-1.990866	-3.110866	0.686583
C	-0.710386	-1.701633	-0.416275
C	-1.185802	-0.426299	-0.824141
C	1.335585	-0.585732	2.045251
O	2.235486	-0.862515	2.708089
C	-1.335977	-0.626235	2.054193
O	-2.218373	-0.931881	2.727792
H	0.270394	2.180101	1.361627
C	0.079615	3.264228	1.218548
O	0.021977	4.038577	2.153622
O	-0.064392	3.646013	-0.032797
O	-0.008545	-3.669132	0.530687
C	2.581863	0.000819	-0.937353
C	2.958807	1.337040	-0.738364
C	3.575070	-0.944337	-1.226391
C	4.294075	1.714732	-0.835084
H	2.202223	2.080307	-0.497721
C	4.911195	-0.563365	-1.320666
H	3.299517	-1.984048	-1.396865
C	5.275466	0.767451	-1.126628
H	4.570362	2.754553	-0.674844
H	5.668564	-1.309852	-1.548913
H	6.318700	1.065921	-1.199611
C	-2.586210	0.003297	-0.933464
C	-2.964592	1.314269	-0.611369
C	-3.571037	-0.908007	-1.334330
C	-4.297084	1.703785	-0.699693
H	-2.211614	2.023288	-0.271387
C	-4.904933	-0.515915	-1.418773
H	-3.289046	-1.927371	-1.595102
C	-5.271592	0.790951	-1.103722
H	-4.577565	2.722802	-0.442514
H	-5.658489	-1.234127	-1.733908
H	-6.312986	1.097590	-1.168950

3'Fe-wills-2 Gsolv= -2601.132855

Fe	0.034641	0.159600	0.849069
C	0.004729	-0.702769	-1.204165
O	0.111993	-1.933999	-1.463436
H	0.401582	-2.365747	0.323965
C	-1.231751	-0.015632	-0.813344
C	-0.887340	1.344753	-0.545984
C	0.512371	1.496944	-0.655608
C	1.114007	0.241764	-0.952925
C	-1.300218	0.190844	2.048607
O	-2.190473	0.161270	2.778535
C	1.247573	0.947734	1.903932
O	2.029360	1.535472	2.514852
C	-2.581140	-0.597274	-0.891057
C	-3.607647	0.112808	-1.526458
C	-2.861883	-1.862733	-0.359570
C	-4.886576	-0.429116	-1.627708
H	-3.398040	1.092587	-1.954489
C	-4.139310	-2.404839	-0.465383
H	-2.076857	-2.415574	0.153347
C	-5.155677	-1.690244	-1.099057
H	-5.673147	0.134839	-2.124217
H	-4.343794	-3.386883	-0.044555
H	-6.154214	-2.113994	-1.179011
C	2.551531	-0.034646	-1.085637
C	3.454569	1.021596	-1.280399
C	3.061260	-1.339712	-0.998344
C	4.821906	0.783094	-1.380031
H	3.090131	2.042746	-1.373759
C	4.429583	-1.574348	-1.096054
H	2.381765	-2.174070	-0.850738
C	5.316896	-0.516307	-1.286100
H	5.502025	1.617857	-1.534278
H	4.803569	-2.593227	-1.020715
H	6.385659	-0.702921	-1.362225
C	-1.502378	2.697256	-0.348332
O	-0.365372	3.507028	0.023281
C	0.837985	2.945510	-0.505075

H	-1.877122	3.035901	-1.331812
H	1.068356	3.371441	-1.496124
H	1.662261	3.186310	0.175394
C	-2.573310	2.864528	0.696296
H	-2.967514	3.885617	0.673603
H	-3.402823	2.171109	0.514136
H	-2.163097	2.674402	1.694485
H	1.531387	-1.779636	2.905216
C	1.394807	-2.401896	2.009516
O	0.483773	-1.862206	1.182245
O	1.956879	-3.444345	1.781180

3Fe-wills-2 Gsolv= -2601.123261

Fe	-0.103666	-0.035493	0.972982
C	-0.087637	0.513133	-1.165547
O	-0.106024	1.705195	-1.582071
H	-0.167326	2.918001	-0.422430
C	1.110092	-0.242840	-0.744730
C	0.648626	-1.493896	-0.254120
C	1.140377	-2.853388	0.139807
H	1.895468	-2.849628	0.934882
C	-1.222342	-2.871831	0.145234
H	-1.566411	-3.437869	-0.735825
H	-2.015486	-2.891871	0.901154
C	-0.765659	-1.514271	-0.265095
C	-1.258528	-0.270481	-0.755756
C	1.075935	-0.386983	2.288751
O	1.806265	-0.688806	3.125956
C	-1.530103	-0.212583	2.048185
O	-2.484133	-0.405239	2.662989
H	1.237559	2.236445	1.011587
C	0.618225	3.111054	1.304502
O	0.705025	3.647989	2.391596
O	-0.212542	3.528196	0.367534
O	-0.042346	-3.463040	0.704313
C	2.504959	0.180652	-0.944228
C	2.836236	1.069698	-1.976774
C	3.539158	-0.334492	-0.147753
C	4.161740	1.432833	-2.202378
H	2.051420	1.466155	-2.614763
C	4.861536	0.030422	-0.375092
H	3.314507	-1.026743	0.662100
C	5.179457	0.918274	-1.402894
H	4.398255	2.118397	-3.013181
H	5.647130	-0.380556	0.255054
H	6.214055	1.202826	-1.580164
C	-2.670134	0.096353	-0.939150
C	-3.116112	1.416577	-0.783550
C	-3.603938	-0.897918	-1.259635
C	-4.460726	1.730587	-0.955284
H	-2.408215	2.196050	-0.511206
C	-4.949532	-0.581602	-1.425945
H	-3.273363	-1.926482	-1.396907
C	-5.382530	0.734393	-1.276829
H	-4.792438	2.758784	-0.828634
H	-5.659530	-1.366804	-1.675765
H	-6.433327	0.982678	-1.407303
C	1.640242	-3.615970	-1.070802
H	2.537942	-3.133730	-1.475999
H	1.893884	-4.643493	-0.791313
H	0.875191	-3.640037	-1.856855

3'Fe-wills-3 Gsolv= -2778.790368

Fe	0.214804	0.073740	0.830897
C	0.084130	-0.593241	-1.275265
O	0.124091	-1.810339	-1.628706
H	0.415578	-2.418664	0.070546
C	-1.107675	0.122407	-0.791793
C	-0.676959	1.435399	-0.427887
C	0.727707	1.505461	-0.564927
C	1.253398	0.251791	-0.989022
Si	3.051848	-0.221792	-1.295676
C	3.265698	-0.576572	-3.123921
H	4.312226	-0.823333	-3.345726
H	2.989202	0.294278	-3.731597
H	2.645524	-1.423756	-3.442368
C	4.115484	1.233161	-0.777724
H	5.173493	1.000961	-0.957578
H	4.002455	1.454787	0.291890
H	3.875663	2.140312	-1.347258
C	3.509649	-1.727212	-0.275890
H	4.532090	-2.046258	-0.517973
H	2.839212	-2.574474	-0.468474
H	3.477331	-1.497414	0.798235
C	-1.085248	0.129914	2.061967
O	-1.958547	0.125054	2.813156
C	1.504083	0.632973	1.940776
O	2.326682	1.062066	2.625909

C	-2.490225	-0.376780	-0.862669
C	-3.495965	0.433570	-1.404678
C	-2.823981	-1.662648	-0.417266
C	-4.805421	-0.030712	-1.500790
H	-3.245965	1.431649	-1.763140
C	-4.132228	-2.126791	-0.517709
H	-2.054351	-2.293194	0.024141
C	-5.126949	-1.313414	-1.060237
H	-5.574883	0.610882	-1.924582
H	-4.377194	-3.126130	-0.164596
H	-6.149072	-1.677485	-1.136224
C	-1.195921	2.805379	-0.110131
O	0.000226	3.509825	0.290688
C	1.155801	2.910244	-0.305249
H	-1.565463	3.240158	-1.057327
H	1.401725	3.401328	-1.261267
H	2.003070	3.037393	0.376852
C	-2.234860	2.966949	0.967602
H	-3.114250	2.349027	0.751088
H	-1.825556	2.673125	1.940646
H	-2.557208	4.011388	1.029349
H	1.129120	-2.189152	2.864492
C	1.028340	-2.749862	1.923409
O	0.471859	-1.988789	0.972518
O	1.353603	-3.898777	1.748367

3Fe-wills-3 Gsolv= -2778.782408

Fe	-0.356661	-0.029223	0.937686
C	-0.155100	0.584362	-1.155047
O	-0.017681	1.801290	-1.485171
H	0.896962	2.682554	-0.457140
C	0.920121	-0.323665	-0.720859
C	0.275059	-1.525095	-0.303329
C	0.568286	-2.947424	0.063969
H	1.250404	-3.058769	0.916223
C	-1.776749	-2.664903	-0.085659
H	-2.134198	-3.142328	-1.012628
H	-2.611905	-2.620726	0.621694
C	-1.128849	-1.362886	-0.408955
C	-1.442288	-0.047560	-0.851000
Si	-3.121030	0.768299	-1.118812
C	-3.303252	1.126702	-2.949621
H	-4.284841	1.569747	-3.161723
H	-3.213002	0.207276	-3.541753
H	-2.534151	1.829037	-3.294975
C	-4.435272	-0.441636	-0.552003
H	-5.432289	-0.027326	-0.750968
H	-4.371484	-0.643030	0.525140
H	-4.360574	-1.397387	-1.086878
C	-3.207634	2.359739	-0.128456
H	-4.156906	2.876033	-0.323688
H	-2.392821	3.043302	-0.399009
H	-3.150034	2.167563	0.951188
C	0.832157	-0.436977	2.223095
O	1.583196	-0.760284	3.033629
C	-1.747986	-0.225085	2.056803
O	-2.641683	-0.420233	2.756578
H	-0.214399	2.466383	1.355165
C	0.758696	3.000565	1.427196
O	1.189526	3.425591	2.482326
O	1.386099	3.160610	0.281710
O	-0.719884	-3.428495	0.511147
C	2.366945	-0.080221	-0.834499
C	2.864161	0.864256	-1.744397
C	3.285334	-0.822321	-0.076042
C	4.234908	1.067209	-1.879984
H	2.170787	1.439956	-2.351443
C	4.653924	-0.616804	-0.212232
H	2.933165	-1.570031	0.632498
C	5.136185	0.332214	-1.113061
H	4.599317	1.802639	-2.593949
H	5.345961	-1.202247	0.389027
H	6.206576	0.493451	-1.218462
C	1.067751	-3.732621	-1.132223
H	2.040894	-3.348364	-1.460964
H	1.182814	-4.788955	-0.869046
H	0.362367	-3.650095	-1.968709

3'Fe-wills-4 Gsolv= -2739.528575

Fe	0.149705	0.114106	0.848877
C	-0.013500	-0.421684	-1.298938
O	-0.048206	-1.612880	-1.728630
H	0.122169	-2.355327	-0.038468
C	-1.162256	0.340678	-0.775747
C	-0.646050	1.595206	-0.336614
C	0.762917	1.581350	-0.447335
C	1.205633	0.324863	-0.957928
Si	2.964595	-0.265370	-1.282949

C	3.182823	-0.517063	-3.128374
H	4.197815	-0.874982	-3.345306
H	3.033203	0.421797	-3.676299
H	2.474492	-1.256450	-3.522196
C	4.132560	1.067433	-0.669870
H	5.170069	0.778799	-0.884162
H	4.048494	1.218744	0.414185
H	3.948282	2.028533	-1.167640
C	3.279433	-1.870306	-0.364501
H	4.279039	-2.252880	-0.609761
H	2.547582	-2.642075	-0.635770
H	3.236586	-1.719072	0.722925
C	-1.127636	0.375631	2.074663
O	-1.990536	0.609254	2.802242
C	1.495221	0.468554	1.978101
O	2.356185	0.772947	2.682280
C	-2.576587	-0.055126	-0.829127
C	-3.563820	0.914077	-1.053054
C	-2.970337	-1.389041	-0.648525
C	-4.909424	0.559442	-1.104227
H	-3.275951	1.953119	-1.207364
C	-4.315479	-1.740724	-0.701549
H	-2.217675	-2.149762	-0.456285
C	-5.290095	-0.769745	-0.931236
H	-5.661174	1.325004	-1.283028
H	-4.604680	-2.779370	-0.556693
H	-6.340710	-1.048091	-0.971424
C	-1.071153	2.948278	0.123726
O	0.148658	3.530646	0.606154
C	1.269648	2.931025	-0.061535
H	-1.810193	2.966681	0.932270
H	-1.465434	3.528615	-0.726624
H	1.531358	3.501605	-0.967713
H	2.125558	2.949045	0.620730
H	0.797180	-2.347182	2.771116
C	0.663058	-2.842855	1.798255
O	0.194637	-1.982439	0.885747
O	0.888964	-4.004814	1.562314

3Fe-wills-4 Gsolv= -2739.519973

Fe	-0.161594	-0.257041	0.880256
C	-0.040004	0.362838	-1.222376
O	0.038719	1.558707	-1.627801
H	0.090544	2.859095	-0.643743
C	1.090196	-0.466693	-0.772908
C	0.534759	-1.716480	-0.384876
C	0.915215	-3.101737	0.005928
H	1.678156	-3.183675	0.787737
H	1.260262	-3.657314	-0.881358
C	-1.429347	-2.977651	-0.094506
H	-1.754225	-3.497649	-1.010549
H	-2.256539	-2.982945	0.622593
C	-0.878067	-1.637679	-0.447470
C	-1.280914	-0.342983	-0.885059
Si	-3.018158	0.341534	-1.140155
C	-3.271647	0.640724	-2.973286
H	-4.277085	1.039716	-3.160538
H	-3.166482	-0.290041	-3.544734
H	-2.544630	1.363423	-3.364547
C	-4.230904	-0.943267	-0.514466
H	-5.258179	-0.594915	-0.683918
H	-4.117516	-1.126491	0.561704
H	-4.113583	-1.899628	-1.040670
C	-3.215875	1.949773	-0.193874
H	-4.241808	2.324820	-0.307581
H	-2.535897	2.722311	-0.575695
H	-3.024620	1.819096	0.879838
C	1.140193	-0.614579	2.061956
O	2.013155	-0.925087	2.746066
C	-1.497095	-0.534001	2.053059
O	-2.349863	-0.779064	2.787565
H	-0.424511	2.211373	1.332074
C	-0.205712	3.291619	1.197466
O	-0.259857	4.079312	2.122220
O	0.109509	3.650409	-0.027833
O	-0.312253	-3.654922	0.502089
C	2.513519	-0.104565	-0.820703
C	2.944540	1.169106	-0.424129
C	3.464317	-1.043207	-1.239975
C	4.295899	1.497512	-0.460372
H	2.215829	1.894553	-0.064755
C	4.817099	-0.712858	-1.271807
H	3.141040	-2.034702	-1.555148
C	5.236253	0.558633	-0.885323
H	4.618194	2.487661	-0.145728
H	5.544291	-1.451326	-1.601871
H	6.292580	0.816369	-0.909726

3'Fe-wills-5 Gsolv= -2896.558433

Fe	0.452370	-0.200003	1.086303
C	-0.023279	0.702794	-0.874116
O	-0.148749	1.952341	-1.049115
H	0.048892	2.348262	0.706310
C	1.253773	-0.028236	-0.843546
C	0.942436	-1.386583	-0.526456
C	-0.443017	-1.482070	-0.267649
C	-1.066627	-0.207367	-0.371464
Si	-2.896704	0.174663	-0.114557
C	-3.671081	-1.263534	0.815394
H	-4.708687	-1.007015	1.068762
H	-3.150545	-1.469487	1.759199
H	-3.693490	-2.189267	0.225932
C	-3.098976	1.725764	0.922347
H	-4.158841	2.008921	0.977137
H	-2.540830	2.582530	0.526048
H	-2.755473	1.532876	1.948756
C	-3.728183	0.342252	-1.823608
C	2.062452	-0.331006	1.859513
O	3.119227	-0.373687	2.315893
C	-0.417779	-0.927613	2.473438
O	-0.958775	-1.456822	3.343817
C	2.560028	0.526478	-1.233549
C	3.401430	-0.197113	-2.088372
C	2.980881	1.782367	-0.775222
C	4.634636	0.321771	-2.476069
H	3.081827	-1.170108	-2.459940
C	4.211682	2.300693	-1.166277
H	2.344567	2.346202	-0.095697
C	5.042710	1.572926	-2.017801
H	5.276274	-0.253223	-3.140180
H	4.526434	3.274769	-0.798190
H	6.005448	1.978879	-2.319991
C	1.524905	-2.767693	-0.534931
O	0.482287	-3.555493	0.081894
C	-0.789779	-2.918801	-0.075402
H	1.624714	-3.073795	-1.592616
H	-1.307661	-3.290758	-0.975902
H	-1.404947	-3.154727	0.799297
C	2.815133	-3.023115	0.198647
H	3.608836	-2.366601	-0.176865
H	2.683775	-2.845723	1.272164
H	3.132576	-4.061122	0.055415
C	-5.247434	0.343775	-1.639461
H	-5.585744	1.155494	-0.979148
H	-5.744498	0.486567	-2.612569
H	-5.614639	-0.604017	-1.222825
H	0.102855	1.810031	3.549651
C	-0.039783	2.468797	2.680500
O	0.226857	1.821182	1.539861
O	-0.377818	3.626796	2.722939
C	-3.329832	-0.843780	-2.703507
H	-2.249913	-0.856571	-2.909814
H	-3.597338	-1.807797	-2.247102
H	-3.848559	-0.787292	-3.674185
C	-3.308772	1.641573	-2.510256
H	-3.811156	1.731084	-3.487242
H	-3.582719	2.527315	-1.919487
H	-2.226296	1.681154	-2.692204

3Fe-wills-5 Gsolv=

Fe	0.056903	0.951555	0.725610
C	-0.220737	0.069205	-1.224452
O	-0.617290	-1.049850	-0.482031
H	-1.088142	-1.786807	0.579419
C	-1.404208	0.961390	-1.132546
C	-0.896328	2.282975	-0.657646
C	-1.040508	3.264897	0.523535
H	-0.834796	2.445372	1.242291
C	1.060578	3.520529	-0.482270
H	1.069622	4.443752	-1.089077
H	2.124113	3.381987	-0.226841
C	0.360290	2.381937	-1.309988
C	1.003423	0.982327	-0.894532
Si	2.501376	-0.459715	-0.159404
C	4.262224	0.172500	-1.111945
H	5.029987	-0.248099	-0.448651
H	5.104002	0.978447	-1.665379
H	4.235294	-0.575392	-1.943960
C	2.789404	0.167554	1.687992
H	3.582565	-0.573377	1.915352
H	2.085160	0.216584	2.523442
H	3.431448	1.146397	1.617432
C	3.299614	-2.231340	-0.287956
C	-1.404211	0.383410	2.039122
O	-2.158549	-0.116083	2.485977
C	1.356820	1.303789	0.896147

O	2.147582	1.109099	0.205987
H	-0.237606	-0.599435	4.780727
C	-1.570280	-2.742291	2.820168
O	-4.364923	-4.864203	1.499830
O	-1.473401	-2.281869	1.628842
O	0.030051	4.170821	0.299694
C	-2.652886	0.422799	-1.676148
C	-2.629000	-0.264827	-2.856164
C	-3.711203	0.129680	-0.792622
C	-3.287301	-1.499149	-2.924057
H	-1.722645	-0.218958	-3.447989
C	-4.197290	-1.150526	-0.755965
H	-3.942262	0.831524	-0.018273
C	-3.815891	-2.012019	-1.785291
H	-2.909150	-2.195855	-3.669903
H	-4.657339	-1.519467	0.152338
H	-3.958445	-3.078821	-1.710182
C	-2.255947	3.822459	1.165559
H	-3.071808	3.561619	0.450260
H	-2.499087	3.389460	2.159240
H	-2.192233	4.923537	1.256282
C	4.744329	-1.603229	-0.448512
H	5.173033	-1.018304	0.393715
H	5.385024	-2.462094	-0.372330
H	4.995439	-1.081233	-1.381022
C	3.459507	-3.207053	0.852870
H	2.546879	-3.688150	1.079906
H	4.262028	-3.816525	0.594466
H	3.791216	-2.665775	1.773407
C	3.287464	-2.713806	-1.680312
H	2.468267	-3.259120	-1.904798
H	3.481639	-1.887333	-2.372813
H	4.114106	-3.338937	-1.797581

3'Mn-a Gsolv= -2821.072903

C	-0.038782	-0.542876	1.253097
O	0.001482	-1.772767	1.580489
H	0.083024	-2.341704	-0.097746
C	1.127414	0.287826	0.940819
C	0.598824	1.551872	0.546059
C	-0.813003	1.488745	0.469026
C	-1.249900	0.176648	0.830327
Si	2.930404	-0.232328	1.114676
C	3.240811	-0.741624	2.892210
H	2.986968	0.069840	3.585870
H	4.299815	-0.990494	3.040109
H	2.646795	-1.621764	3.167765
C	3.984980	1.248718	0.655689
H	3.767264	2.115972	1.292617
H	3.828667	1.543699	-0.390730
H	5.048875	1.006356	0.776609
C	3.290850	-1.659329	-0.048616
H	3.197072	-1.347147	-1.097939
H	2.611603	-2.504867	0.120650
H	4.317279	-2.019599	0.101576
Si	-3.006412	-0.485788	1.010227
C	-3.278248	-0.857915	2.827936
H	-4.299795	-1.222688	2.997249
H	-3.135695	0.042392	3.438913
H	-2.582148	-1.625413	3.188634
C	-4.189842	0.853702	0.443227
H	-5.224547	0.530677	0.618164
H	-4.087339	1.066020	-0.628578
H	-4.036795	1.789666	0.996242
C	-3.248098	-2.037437	-0.014378
H	-4.264652	-2.424308	0.137630
H	-2.543062	-2.827880	0.271493
H	-3.125015	-1.838663	-1.087204
O	1.989247	1.257191	-2.566655
C	-1.389351	0.418543	-2.052170
O	-2.260415	0.678638	-2.760042
C	1.021919	2.951218	0.255071
O	-0.156508	3.550322	-0.305214
C	-1.327050	2.853119	0.152855
H	1.841601	3.069861	-0.461765
H	1.305344	3.455015	1.193736
H	-1.724067	3.328694	1.064517
H	-2.087579	2.911038	-0.632758
H	0.523412	-2.173655	-2.956532
C	0.508678	-2.716960	-2.000440
O	0.051465	-1.932571	-1.015444
O	0.842776	-3.864353	-1.833204
Mn	0.015992	0.162518	-0.901621
N	1.162526	0.717493	-1.935764

3Mn-a Gsolv= -2821.065048

Mn	0.063850	-0.395475	0.928126
N	1.177319	-1.057267	1.934063

O	1.964604	-1.695692	2.521984
C	0.004724	0.554920	-1.149138
O	-0.045284	1.788858	-1.433018
H	-0.147165	3.023713	-0.404799
C	1.227347	-0.201381	-0.865762
C	0.795235	-1.540892	-0.642650
C	1.320605	-2.927952	-0.505001
H	2.136874	-3.067999	0.211864
H	1.655647	-3.291059	-1.490390
C	-1.030215	-3.023226	-0.457265
H	-1.371654	-3.419402	-1.427479
H	-1.798035	-3.229308	0.295857
C	-0.621537	-1.596654	-0.602383
C	-1.153918	-0.287950	-0.825531
Si	2.970569	0.513172	-0.873923
C	3.388161	1.081415	-2.610644
H	3.349986	0.246744	-3.321854
H	4.401106	1.503451	-2.643624
H	2.689858	1.853862	-2.956214
C	4.138519	-0.846973	-0.325187
H	4.090677	-1.713164	-0.998064
H	3.913727	-1.190219	0.693423
H	5.173024	-0.479557	-0.331354
C	3.035814	1.960760	0.318661
H	2.726731	1.661343	1.329495
H	2.384207	2.780240	-0.010970
H	4.059511	2.352745	0.383378
Si	-2.949996	0.269768	-0.973184
C	-3.229179	0.815939	-2.745313
H	-4.269737	1.133253	-2.892236
H	-3.021912	-0.000316	-3.448734
H	-2.578531	1.660852	-3.003581
C	-4.041102	-1.198353	-0.564261
H	-5.094419	-0.937768	-0.731737
H	-3.940824	-1.513865	0.481899
H	-3.807584	-2.058158	-1.206144
C	-3.283925	1.700635	0.192321
H	-4.333553	2.012692	0.109201
H	-2.661009	2.569945	-0.056118
H	-3.098186	1.435304	1.241352
C	-1.377650	-0.862650	1.980880
O	-2.255116	-1.266804	2.606401
H	-0.217305	2.088921	1.488255
C	-0.197094	3.197362	1.490034
O	-0.204563	3.848739	2.517000
O	-0.170989	3.744707	0.294708
O	0.183642	-3.675515	-0.047837

3'Mn-b Gsolv= -2963.834875

C	-0.495893	-1.635233	-1.054610
O	-0.737061	-2.878655	-1.101823
H	-0.808537	-3.019939	0.643777
C	-1.482430	-0.570525	-0.826313
C	-0.755182	0.654730	-0.758290
C	0.632579	0.385161	-0.809538
C	0.830695	-1.027137	-0.906678
O	-1.596255	1.178889	2.683561
C	1.441422	-0.348347	1.734306
O	2.495229	-0.197803	2.174302
C	-2.941585	-0.747327	-0.828654
C	-3.783672	0.135144	-0.132592
C	-3.535800	-1.781954	-1.562047
C	-5.162645	-0.018125	-0.170106
H	-3.359452	0.948863	0.453038
C	-4.920638	-1.928916	-1.594213
H	-2.908677	-2.470945	-2.121482
C	-5.759145	-1.055102	-0.899450
H	-5.794906	0.677926	0.380779
H	-5.358797	-2.739639	-2.175411
C	2.119848	-1.731460	-0.999014
C	3.202773	-1.128156	-1.652135
C	2.313491	-2.994959	-0.424057
C	4.434670	-1.768764	-1.730496
H	3.079740	-0.150946	-2.116182
C	3.548078	-3.630586	-0.509561
H	1.496278	-3.479007	0.107358
C	4.629854	-3.032854	-1.164389
H	5.262758	-1.279738	-2.242961
H	3.678762	-4.609425	-0.049219
C	-7.248572	-1.209496	-0.924129
H	-7.644926	-1.392137	0.082693
H	-7.736367	-0.299414	-1.294757
H	-7.554307	-2.043982	-1.563795
C	5.953190	-3.725505	-1.275721
H	6.091810	-4.152422	-2.277670
H	6.783397	-3.029476	-1.108040
H	6.039418	-4.545176	-0.554485
C	-1.010616	2.125021	-0.798630

C	1.420673	1.647927	-0.914604
H	-1.782400	2.494271	-0.117118
H	-1.311858	2.401355	-1.817864
H	1.693457	1.804939	-1.969272
H	2.342704	1.681442	-0.328045
C	0.383663	2.730884	-0.485229
C	0.449923	3.112197	0.994044
C	0.651978	3.993179	-1.293780
O	-0.431150	3.762558	1.528572
O	0.092645	4.284105	-2.331760
O	1.541486	2.699172	1.616940
O	1.634148	4.704682	-0.750264
H	0.053310	-2.483240	3.350199
C	-0.200393	-3.151650	2.514658
O	-0.657798	-2.451888	1.460597
O	-0.108827	-4.353732	2.516410
C	2.039413	5.891090	-1.457466
H	1.199783	6.586910	-1.532151
H	2.842373	6.326131	-0.863344
H	2.401448	5.626478	-2.454281
C	1.627904	2.988668	3.022745
H	0.812284	2.489371	3.556163
H	2.591074	2.593714	3.345780
H	1.583456	4.067865	3.190863
Mn	-0.188118	-0.483259	0.905483
N	-1.021385	0.433095	1.985963

3Mn-b Gsolv= -3158.485587

Co	-0.212484	0.323310	0.696525
N	2.111755	0.764555	2.656965
C	-0.647384	1.356819	-1.213881
O	-1.115387	2.486368	-1.411160
H	-1.584555	3.610460	-0.162491
C	0.791309	1.022676	-0.979656
C	0.860881	-0.377556	-0.904182
C	1.875496	-1.455877	-0.787888
H	2.731400	-1.205749	-0.154815
H	2.262037	-1.675982	-1.792848
C	-0.412851	-2.407269	-0.764734
H	-0.549503	-2.850699	-1.761168
H	-1.172274	-2.837135	-0.104006
C	-0.465458	-0.926725	-0.887698
C	-1.414251	0.111694	-0.974752
C	1.206442	0.578929	1.931407
C	-1.377423	-0.441156	1.869636
O	-2.154695	-0.935811	2.543970
H	-1.055829	2.533648	1.597463
C	-1.506079	3.537807	1.740341
O	-1.699127	4.026324	2.834635
O	-1.817210	4.168542	0.620331
C	-2.875473	-0.003781	-0.977136
C	-3.683088	0.988490	-0.402171
C	-3.489742	-1.131036	-1.534631
C	-5.064426	0.849523	-0.390274
H	-3.222994	1.861426	0.056795
C	-4.875012	-1.260106	-1.520150
H	-2.882418	-1.907081	-1.997502
C	-5.685573	-0.274283	-0.950271
H	-5.678637	1.623004	0.069555
H	-5.336920	-2.143317	-1.959406
C	1.892869	1.984475	-0.997599
C	1.732319	3.281793	-0.488486
C	3.139549	1.618952	-1.521014
C	2.787028	4.183289	-0.514673
H	0.781409	3.579287	-0.053189
C	4.189392	2.530911	-1.547282
H	3.285659	0.621106	-1.931186
C	4.031351	3.828450	-1.051224
H	2.648521	5.184585	-0.108406
H	5.150091	2.232032	-1.964313
C	-7.177076	-0.400877	-0.948742
H	-7.602532	-0.083540	0.010281
H	-7.626183	0.235082	-1.722744
H	-7.492210	-1.431132	-1.144285
C	5.147302	4.823591	-1.110378
H	5.001824	5.523699	-1.943531
H	5.196146	5.423664	-0.194567
H	6.115560	4.333534	-1.257028
C	1.037492	-2.660613	-0.274289
C	1.062112	-2.776939	1.259823
C	1.531735	-4.018114	-0.757462
O	0.092059	-3.069723	1.930895
O	2.823389	-4.024028	-1.046255
O	2.275626	-2.584428	1.751947
O	0.805790	-4.992548	-0.823632
C	2.407779	-2.686875	3.181811
H	2.192443	-3.709296	3.503531
H	3.443431	-2.426946	3.399611

H	1.727128	-1.984631	3.671219
C	3.375918	-5.283870	-1.473458
H	4.428159	-5.087361	-1.676490
H	3.271984	-6.026213	-0.677876
H	2.868663	-5.625188	-2.379299

3'Mn-c Gsolv= -2465.759371

C	0.022776	-0.523881	-1.265388
O	-0.016495	-1.734504	-1.626589
H	-0.036940	-2.337372	0.106879
C	-1.130779	0.308082	-0.895538
C	-0.612524	1.575319	-0.503876
C	0.796868	1.526852	-0.470929
C	1.227825	0.223541	-0.864049
O	-1.899430	1.309865	2.601143
C	1.513593	0.396701	1.969853
O	2.467479	0.628577	2.571068
C	-2.549318	-0.051869	-1.017053
C	-3.491656	0.940578	-1.320604
C	-2.995973	-1.367577	-0.820034
C	-4.843599	0.628172	-1.430552
H	-3.163017	1.964515	-1.491310
C	-4.347981	-1.676370	-0.931936
H	-2.282826	-2.149389	-0.568879
C	-5.276915	-0.682146	-1.238491
H	-5.558528	1.411806	-1.671002
H	-4.678900	-2.700461	-0.773863
H	-6.332846	-0.927595	-1.325653
C	2.620773	-0.235854	-0.972179
C	3.642453	0.693622	-1.211707
C	2.964758	-1.586434	-0.813028
C	4.971025	0.285278	-1.294073
H	3.396970	1.745077	-1.353481
C	4.293172	-1.991380	-0.897506
H	2.189211	-2.321059	-0.614708
C	5.301976	-1.059263	-1.137970
H	5.748859	1.021608	-1.483471
H	4.541620	-3.042493	-0.767798
H	6.339427	-1.379351	-1.201139
C	-1.040028	2.964980	-0.171823
O	0.142698	3.550442	0.388885
C	1.303113	2.891907	-0.140312
H	-1.335361	3.492717	-1.093682
H	1.649391	3.400195	-1.055352
H	2.099799	2.935662	0.609814
H	-0.658068	-2.127189	2.914109
C	-0.648570	-2.652458	1.948719
O	0.006396	-1.931957	1.020496
O	-1.133672	-3.732691	1.723491
H	-1.853440	3.054277	0.556755
N	-1.086161	0.740111	1.979492
Mn	0.027041	0.176545	0.911969

3Mn-c Gsolv= -2660.405297

Co	-0.000858	-0.355135	0.865110
N	2.328357	-0.436303	2.869084
C	0.001317	0.285421	-1.263205
O	0.013172	1.426050	-1.742654
H	0.015974	2.928376	-0.827854
C	1.191789	-0.500642	-0.819150
C	0.706613	-1.759279	-0.429887
C	1.153449	-3.100011	0.028920
H	1.951343	-3.086230	0.778932
H	1.486956	-3.694585	-0.837170
C	-1.193001	-3.083299	0.021546
H	-1.527159	-3.668584	-0.850572
H	-1.997944	-3.066408	0.764590
C	-0.724221	-1.745909	-0.428561
C	-1.194213	-0.480823	-0.825920
C	1.420034	-0.402626	2.124743
C	-1.306348	-0.489041	2.126024
O	-2.148710	-0.631890	2.882786
H	0.048232	2.146520	1.153629
C	0.031025	3.250277	1.050185
O	0.029564	4.000515	2.003940
O	0.012963	3.689586	-0.197086
O	-0.026127	-3.667088	0.612420
C	2.586592	-0.065493	-0.918508
C	2.941391	1.273943	-0.705036
C	3.590179	-1.001279	-1.201221
C	4.273365	1.665396	-0.777475
H	2.176035	2.006361	-0.460696
C	4.921809	-0.604208	-1.276613
H	3.326641	-2.041957	-1.382683
C	5.266674	0.729346	-1.064436
H	4.537679	2.705628	-0.602616
H	5.691110	-1.338702	-1.502381
H	6.307463	1.039480	-1.120347

C	-2.586785	-0.032193	-0.921377
C	-2.929777	1.306364	-0.684639
C	-3.597686	-0.953003	-1.226149
C	-4.257526	1.712837	-0.760308
H	-2.157730	2.026845	-0.425269
C	-4.924916	-0.541164	-1.302287
H	-3.342939	-1.992983	-1.423747
C	-5.258094	0.791990	-1.069709
H	-4.512496	2.752671	-0.569777
H	-5.700068	-1.264074	-1.544988
H	-6.295347	1.113397	-1.127473

3'Mn Gsolv= -2824.421314

C	-0.014779	-0.654860	-1.226081
O	0.036642	-1.896111	-1.530661
H	0.084880	-2.409016	0.123394
C	-1.221708	0.079388	-0.873603
C	-0.804441	1.414967	-0.532587
C	-1.644726	2.615716	-0.233344
H	-2.511114	2.347910	0.383026
H	-2.051762	2.983467	-1.188906
C	-0.820757	3.718831	0.423259
H	-1.422872	4.632429	0.490511
H	-0.563963	3.428402	1.454959
C	0.454277	3.971471	-0.369987
H	0.987860	4.849203	0.012813
H	0.180189	4.196999	-1.412120
C	1.383491	2.758888	-0.339846
H	2.138870	2.842742	-1.132204
H	1.942773	2.737637	0.605847
C	0.623381	1.477426	-0.539990
C	1.135786	0.174061	-0.875115
Si	-2.942808	-0.690816	-1.003004
C	-3.208087	-1.238652	-2.778890
H	-3.145855	-0.388941	-3.470586
H	-4.202982	-1.689913	-2.890985
H	-2.462102	-1.981575	-3.086100
C	-4.286744	0.529049	-0.529711
H	-4.282297	1.433906	-1.149375
H	-4.224969	0.828857	0.524473
H	-5.258341	0.035433	-0.672691
C	-3.072584	-2.164314	0.155120
H	-2.954392	-1.856290	1.203010
H	-2.324046	-2.936592	-0.061484
H	-4.066156	-2.621628	0.051756
Si	2.912448	-0.437949	-1.084923
C	3.159822	-0.838359	-2.901368
H	4.185910	-1.185947	-3.080384
H	2.991731	0.049269	-3.524730
H	2.472537	-1.624295	-3.238083
C	4.162620	0.865016	-0.572976
H	5.166885	0.429366	-0.670347
H	4.042646	1.186056	0.469140
H	4.126861	1.754565	-1.213596
C	3.198017	-1.971579	-0.037714
H	4.219990	-2.338669	-0.204748
H	2.503804	-2.782040	-0.292172
H	3.094439	-1.755959	1.034909
C	1.388430	0.490527	1.986975
O	2.262239	0.840040	2.653727
H	0.384514	-2.260510	3.009576
C	0.320246	-2.811956	2.059927
O	0.102047	-1.981176	1.037723
O	0.422539	-4.008571	1.929515
N	-1.195148	0.530805	1.976822
O	-2.060289	0.973579	2.634684
Mn	-0.035234	0.090656	0.905361

3Mn Gsolv= -2824.412030

Mn	-0.052628	0.234803	0.971051
N	-1.172732	0.802229	2.027127
O	-1.970326	1.358946	2.683122
C	-0.004869	-0.632733	-1.120921
O	0.052318	-1.859427	-1.452144
H	0.148827	-3.097946	-0.445505
C	-1.218170	0.108994	-0.802347
C	-0.809520	1.462554	-0.536143
C	-1.653741	2.676445	-0.317197
H	-2.527751	2.443057	0.301871
H	-2.049026	2.984646	-1.298826
C	-0.838299	3.817166	0.285080
H	-1.442582	4.731617	0.294549
H	-0.592854	3.585431	1.334153
C	0.446193	4.028332	-0.504981
H	0.974648	4.925115	-0.161519
H	0.186047	4.198634	-1.560828
C	1.375613	2.820072	-0.398696
H	2.136222	2.857938	-1.190300

H	1.929677	2.852201	0.549875
C	0.620246	1.528813	-0.530545
C	1.139703	0.210775	-0.785904
Si	-2.939129	-0.654324	-0.935667
C	-3.286938	-0.921872	-2.761058
H	-3.248826	0.030972	-3.305169
H	-4.283758	-1.356464	-2.911653
H	-2.549629	-1.597962	-3.212220
C	-4.257824	0.462006	-0.204129
H	-4.352197	1.414645	-0.739232
H	-4.080128	0.673914	0.858324
H	-5.223075	-0.057668	-0.279726
C	-2.976768	-2.282945	-0.004466
H	-2.702858	-2.143787	1.050601
H	-2.301219	-3.027828	-0.440692
H	-3.995438	-2.693162	-0.031243
Si	2.924669	-0.374626	-0.994745
C	3.209442	-0.627896	-2.832273
H	4.227645	-0.993886	-3.018514
H	3.089665	0.320793	-3.372336
H	2.505018	-1.352451	-3.259208
C	4.159918	0.889869	-0.363968
H	5.165765	0.462813	-0.481769
H	4.026511	1.124293	0.699113
H	4.132807	1.827832	-0.931312
C	3.192127	-1.972651	-0.046758
H	4.244643	-2.275136	-0.132809
H	2.575212	-2.792791	-0.432740
H	2.970227	-1.846502	1.022330
C	1.388700	0.645678	2.040889
O	2.264796	1.003418	2.697853
H	0.267437	-2.247141	1.500121
C	0.232646	-3.354749	1.445114
O	0.252065	-4.053906	2.440756
O	0.174335	-3.846369	0.228420

4Co-a Gsolv= -2826.047425

C	-0.021061	1.369723	0.071541
O	-0.041176	2.422356	-0.579784
C	-1.214494	0.533362	0.407970
C	-0.714709	-0.528028	1.176742
C	0.723631	-0.500719	1.181830
C	1.194230	0.583700	0.421697
Si	-3.001987	1.045123	0.051705
C	-3.287249	2.629056	1.014896
H	-3.110259	2.475444	2.086836
H	-4.322080	2.973099	0.889633
H	-2.620710	3.429391	0.670155
C	-4.130027	-0.313857	0.671315
H	-3.958600	-0.520134	1.736034
H	-3.990418	-1.246652	0.110885
H	-5.178264	-0.008170	0.558217
C	-3.204246	1.338072	-1.785984
H	-3.076746	0.409334	-2.355917
H	-2.474411	2.069639	-2.154408
H	-4.207858	1.729420	-1.996868
Si	2.967266	1.114119	0.030781
C	3.279743	2.719446	0.943361
H	4.312436	3.056456	0.787019
H	3.123324	2.597352	2.022290
H	2.608171	3.511221	0.588774
C	4.100819	-0.248715	0.633727
H	5.148371	0.028208	0.458308
H	3.916688	-1.192307	0.103362
H	3.980436	-0.428877	1.709814
C	3.117983	1.344530	-1.821610
H	4.107644	1.745718	-2.075425
H	2.363780	2.045560	-2.200253
H	2.997059	0.392129	-2.354214
C	-1.357078	-1.795690	-1.440212
C	1.295934	-1.834165	-1.318594
O	2.094095	-2.582203	-1.649363
C	-1.154091	-1.704407	1.971010
O	0.038893	-2.489658	2.110658
C	1.198879	-1.655524	1.989472
H	-1.924552	-2.323309	1.500542
H	-1.519644	-1.369455	2.955349
H	1.531776	-1.298327	2.977625
H	2.005866	-2.243591	1.539942
N	-2.195726	-2.487059	-1.885403
Co	0.016300	-0.706548	-0.713694

4Co-b Gsolv= -2968.811271

C	-0.417541	-2.007030	-0.651296
O	-0.594566	-3.222210	-0.537427
C	-1.466758	-0.937304	-0.572783
C	-0.800209	0.284008	-0.745898
C	0.618471	0.063134	-0.777340

C	0.893816	-1.308305	-0.624745
C	-1.300983	0.209685	2.284602
C	1.342220	-0.289444	2.025409
O	2.312915	-0.120422	2.604571
C	-2.909325	-1.187488	-0.493163
C	-3.784828	-0.232910	0.050226
C	-3.456016	-2.369165	-1.011576
C	-5.152652	-0.458539	0.074211
H	-3.392120	0.688049	0.474833
C	-4.831049	-2.584334	-0.987710
H	-2.803852	-3.117577	-1.452633
C	-5.703063	-1.639024	-0.443447
H	-5.813237	0.293568	0.504569
H	-5.235413	-3.505551	-1.405125
C	2.203147	-1.967455	-0.579517
C	3.265933	-1.481447	-1.350510
C	2.425923	-3.072975	0.253388
C	4.515116	-2.090706	-1.294252
H	3.111793	-0.628995	-2.010219
C	3.678012	-3.672841	0.305314
H	1.619323	-3.444655	0.882596
C	4.742584	-3.197001	-0.469624
H	5.331406	-1.700731	-1.901099
H	3.839972	-4.523672	0.966163
C	-7.181685	-1.866690	-0.407146
H	-7.545880	-1.932460	0.625956
H	-7.721861	-1.037695	-0.880480
H	-7.458570	-2.792838	-0.921318
C	6.080096	-3.868432	-0.431219
H	6.127070	-4.689193	-1.159110
H	6.886789	-3.169576	-0.677675
H	6.282261	-4.300397	0.555119
C	-1.102097	1.727507	-0.933475
C	1.344444	1.346002	-0.976047
H	-1.906339	2.127784	-0.311124
H	-1.383934	1.887480	-1.983894
H	1.632296	1.422127	-2.035641
H	2.255991	1.456048	-0.381353
C	0.257592	2.415811	-0.653986
C	0.271152	2.929492	0.786704
C	0.479915	3.616723	-1.565254
O	-0.644400	3.597655	1.232576
O	-0.107585	3.808102	-2.610341
O	1.358718	2.614808	1.470176
O	1.449822	4.393744	-1.096939
C	1.411964	3.074770	2.833096
H	2.393614	2.781630	3.204847
H	1.299835	4.161207	2.868246
H	0.621161	2.592656	3.417607
C	1.804542	5.533748	-1.902112
H	0.937735	6.187740	-2.025835
H	2.593788	6.047126	-1.354085
H	2.171123	5.201970	-2.876926
Co	-0.127504	-0.563175	1.007490
N	-1.995988	0.687072	3.103189

4Co-c Gsolv= -2470.736078

C	-0.008192	-1.239139	-0.623982
O	-0.018042	-2.454975	-0.438578
C	-1.198121	-0.326932	-0.651004
C	-0.714097	0.943617	-0.995746
C	0.717738	0.932838	-0.994338
C	1.187260	-0.346335	-0.651607
C	-1.407190	1.170298	1.902752
C	1.309632	1.264714	1.808615
O	2.162573	1.806780	2.341683
C	-2.589826	-0.748469	-0.483847
C	-3.610844	-0.107157	-1.197160
C	-2.921184	-1.773147	0.414158
C	-4.937625	-0.487893	-1.021097
H	-3.366663	0.680290	-1.908326
C	-4.248498	-2.148586	0.588618
H	-2.136732	-2.258597	0.990325
C	-5.259622	-1.508610	-0.128126
H	-5.721330	0.013227	-1.584348
H	-4.495945	-2.940087	1.292097
H	-6.296879	-1.804602	0.010297
C	2.576359	-0.778620	-0.475113
C	3.600161	-0.184360	-1.223711
C	2.900125	-1.765599	0.466908
C	4.923023	-0.575778	-1.039701
H	3.358630	0.574868	-1.965972
C	4.223573	-2.152368	0.648101
H	2.113640	-2.214146	1.069954
C	5.237845	-1.560181	-0.104352
H	5.709377	-0.110787	-1.629606
H	4.465211	-2.914463	1.385273
H	6.271901	-1.864335	0.040135

C	-1.160596	2.325380	-1.315130
O	0.019876	3.113649	-1.116685
C	1.183285	2.305990	-1.329568
H	-1.492705	2.375978	-2.364812
H	1.498770	2.340603	-2.384991
H	1.999331	2.687143	-0.706157
H	-1.957994	2.711413	-0.671436
N	-2.306769	1.598240	2.525860
Co	0.002381	0.458304	0.847673

4Co Gsolv= -2829.396602

C	-0.028824	-1.380363	-0.405568
O	-0.058781	-2.578919	-0.082704
C	-1.200912	-0.476253	-0.507276
C	-0.706614	0.767631	-0.960918
C	-1.451068	1.999504	-1.342682
H	-2.343848	2.116257	-0.718424
H	-1.811905	1.853306	-2.374494
C	-0.554009	3.231882	-1.288727
H	-1.097060	4.093797	-1.692133
H	-0.312222	3.465500	-0.238908
C	0.726213	2.985367	-2.075439
H	1.322955	3.900770	-2.153870
H	0.458774	2.692393	-3.101806
C	1.573508	1.887388	-1.435157
H	2.330308	1.515674	-2.138978
H	2.139154	2.294809	-0.584724
C	0.748818	0.723510	-0.983200
C	1.181729	-0.538476	-0.516848
Si	-2.966477	-1.121859	-0.265734
C	-3.276978	-2.333712	-1.663745
H	-3.182878	-1.844178	-2.641390
H	-4.291758	-2.746292	-1.589568
H	-2.567775	-3.170115	-1.632897
C	-4.233667	0.255006	-0.340730
H	-4.227034	0.777298	-1.305242
H	-4.096200	0.993083	0.459349
H	-5.230243	-0.190059	-0.213271
C	-3.073631	-1.989295	1.392140
H	-2.868463	-1.298498	2.219913
H	-2.368134	-2.825615	1.460617
H	-4.086411	-2.390021	1.533169
Si	2.918181	-1.225854	-0.197344
C	3.282240	-2.480715	-1.539273
H	4.284682	-2.907756	-1.406911
H	3.241094	-2.016892	-2.532889
H	2.557138	-3.303786	-1.519314
C	4.193765	0.145754	-0.221454
H	5.163033	-0.280473	0.071361
H	3.959454	0.948254	0.489236
H	4.315592	0.589925	-1.216670
C	2.915792	-2.023360	1.499813
H	3.910899	-2.431705	1.720506
H	2.190921	-2.843011	1.567368
H	2.676166	-1.291375	2.282985
C	-1.371314	1.194595	1.946916
C	1.266347	1.306347	1.836537
Co	0.007804	0.393882	0.918581
N	-2.205195	1.713400	2.592114
O	2.044682	1.940073	2.386110

4Fe-Casey Gsolv= -2727.498499

Fe	-0.000047	-0.641966	-0.828682
C	-0.000011	1.378723	0.111316
O	-0.000039	2.468859	-0.514604
C	-1.194724	0.564623	0.411736
C	-0.710080	-0.587173	1.090861
C	0.710171	-0.587136	1.090797
C	1.194735	0.564646	0.411616
Si	-2.969430	1.096897	0.080392
C	-3.273296	2.727496	0.956088
H	-3.085703	2.644304	2.033965
H	-4.313289	3.051031	0.818135
H	-2.620425	3.514656	0.558381
C	-4.098961	-0.238873	0.756891
H	-3.925193	-0.410976	1.827194
H	-3.959299	-1.191652	0.229244
H	-5.148943	0.057141	0.633468
C	-3.233845	1.300280	-1.765768
H	-3.148268	0.340278	-2.291408
H	-2.501218	1.991688	-2.201034
H	-4.235207	1.703709	-1.965899
Si	2.969416	1.096973	0.080174
C	3.273347	2.727407	0.956142
H	4.313250	3.051110	0.817903
H	3.086204	2.643793	2.034067
H	2.620216	3.514621	0.558984
C	4.099061	-0.238789	0.756502

H	5.149012	0.057267	0.632916
H	3.959357	-1.191594	0.228912
H	3.925453	-0.410852	1.826838
C	3.233728	1.300431	-1.765987
H	4.235316	1.703291	-1.966148
H	2.501473	1.992288	-2.201153
H	3.147593	0.340505	-2.291675
C	-1.298384	-1.758808	-1.341872
O	-2.135971	-2.518214	-1.573486
C	1.298211	-1.758963	-1.341647
O	2.135716	-2.518595	-1.572832
C	-1.175768	-1.757606	1.886946
O	0.000181	-2.573357	2.009110
C	1.176044	-1.757497	1.886857
H	-1.967485	-2.363951	1.434437
H	-1.517348	-1.419119	2.879047
H	1.517649	-1.418939	2.878927
H	1.967801	-2.363768	1.434321

4Fe Gsolv= -2730.846525

Fe	-0.013910	0.340418	0.982459
C	-0.007861	-1.388581	-0.368242
O	-0.013467	-2.587951	0.024008
C	-1.189308	-0.527399	-0.499602
C	-0.714722	0.761718	-0.909055
C	-1.492251	1.970869	-1.320884
H	-2.396331	2.085019	-0.711327
H	-1.839484	1.806227	-2.353928
C	-0.627072	3.226239	-1.275789
H	-1.183061	4.068611	-1.703636
H	-0.404370	3.486890	-0.227893
C	0.671505	2.997093	-2.037988
H	1.245693	3.926724	-2.125326
H	0.423843	2.681375	-3.063083
C	1.535064	1.928017	-1.370210
H	2.301729	1.566247	-2.068437
H	2.086768	2.363157	-0.525280
C	0.720266	0.752209	-0.913998
C	1.178856	-0.536014	-0.489178
Si	-2.932205	-1.202576	-0.247861
C	-3.194882	-2.617876	-1.453733
H	-3.063227	-2.283343	-2.490753
H	-4.214731	-3.013653	-1.356620
H	-2.493540	-3.441220	-1.271008
C	-4.240852	0.107578	-0.556613
H	-4.186652	0.524688	-1.569715
H	-4.183240	0.933637	0.163754
H	-5.229146	-0.359075	-0.441838
C	-3.110594	-1.825130	1.515303
H	-3.050925	-1.002501	2.240483
H	-2.333474	-2.557116	1.767299
H	-4.087102	-2.311573	1.643848
Si	2.926493	-1.191540	-0.227478
C	3.282777	-2.460744	-1.563643
H	4.300122	-2.860152	-1.458843
H	3.197755	-2.013084	-2.562311
H	2.580920	-3.302731	-1.511222
C	4.203740	0.180653	-0.328491
H	5.182834	-0.245615	-0.069063
H	4.005097	1.000760	0.372686
H	4.285487	0.602707	-1.337726
C	3.046141	-1.978745	1.472773
H	4.053671	-2.390364	1.621879
H	2.325908	-2.795663	1.600941
H	2.867668	-1.240609	2.266717
C	-1.298947	1.322546	1.738332
O	-2.122872	2.022977	2.145796
C	1.288727	1.244023	1.806032
O	2.129576	1.877312	2.281589

4Fe-Renaud Gsolv= -2486.130060

Fe	-0.048552	0.320812	1.241737
C	0.021786	-1.433789	-0.071488
O	0.079119	-2.610949	0.373280
C	-1.166544	-0.604595	-0.240971
C	-0.704403	0.709214	-0.625271
C	-0.664835	3.018260	-1.012172
H	-1.244969	3.845907	-1.433388
H	-0.476955	3.247151	0.046163
C	0.655235	2.901098	-1.753255
H	1.275476	3.773664	-1.517575
H	0.502300	2.893612	-2.841561
C	0.736058	0.673493	-0.805420
C	1.186529	-0.550933	-0.217286
C	-1.412581	1.082471	2.083099
O	-2.298765	1.633790	2.584065
C	1.096611	1.527070	1.872734
O	1.791796	2.402786	2.180762

C	2.562638	-1.090499	-0.131075
C	3.386154	-0.889311	0.979321
C	3.048534	-1.846334	-1.205995
C	4.682547	-1.401238	1.000769
H	3.011505	-0.324711	1.831576
C	4.342842	-2.357584	-1.186531
H	2.404680	-2.016390	-2.068607
C	5.166544	-2.129653	-0.083952
H	5.315214	-1.230291	1.868992
H	4.709919	-2.933399	-2.033369
H	6.179555	-2.525417	-0.067753
C	-2.556999	-1.090283	-0.192770
C	-3.634767	-0.228786	0.068747
C	-2.839186	-2.439011	-0.459112
C	-4.942378	-0.701870	0.077117
H	-3.447029	0.825633	0.255270
C	-4.149656	-2.911066	-0.448381
H	-2.023403	-3.120854	-0.683066
C	-5.208161	-2.047502	-0.176766
H	-5.759292	-0.013301	0.282873
H	-4.341782	-3.960983	-0.659810
H	-6.231354	-2.416363	-0.167897
N	1.404056	1.697131	-1.357443
N	-1.472515	1.799494	-1.071428
C	2.849926	1.844319	-1.280154
H	3.150788	2.316715	-0.333584
H	3.351865	0.880071	-1.378888
H	3.176348	2.480386	-2.108016
C	-2.068317	1.559379	-2.388854
H	-2.664608	2.432407	-2.673830
H	-1.315038	1.375188	-3.172809
H	-2.734319	0.691376	-2.346642

4Fe-williams-1 Gsolv= -2681.294965

Fe	0.003751	-0.618837	1.389886
C	-0.000040	-1.920809	-0.377215
O	-0.000954	-3.168508	-0.234345
C	-1.172077	-1.044142	-0.293984
C	-0.719722	0.313405	-0.305245
C	0.717767	0.314052	-0.296881
C	1.171256	-1.045644	-0.300234
C	-1.261327	0.029223	2.490201
O	-2.054806	0.480815	3.192916
C	1.308632	-0.052499	2.486578
O	2.133135	0.341441	3.188099
C	-2.566718	-1.517740	-0.352904
C	-3.616049	-0.854493	0.301960
C	-2.875051	-2.640596	-1.134557
C	-4.926459	-1.305715	0.184701
H	-3.415674	0.027663	0.907107
C	-4.187624	-3.091046	-1.251084
H	-2.079666	-3.157541	-1.665533
C	-5.218687	-2.427635	-0.590367
H	-5.723503	-0.777401	0.703185
H	-4.403584	-3.961730	-1.866396
H	-6.243775	-2.780085	-0.679295
C	2.564814	-1.518514	-0.390007
C	3.628068	-0.867347	0.253783
C	2.856519	-2.627184	-1.198116
C	4.935878	-1.315795	0.099592
H	3.441650	0.002037	0.880946
C	4.166010	-3.075095	-1.351437
H	2.049903	-3.134730	-1.721302
C	5.211429	-2.423014	-0.701931
H	5.743806	-0.796473	0.610241
H	4.368276	-3.934405	-1.987073
H	6.234379	-2.773139	-0.819925
C	-1.571201	1.501772	-0.520581
C	-1.670739	2.558790	0.388391
C	-2.299016	1.560329	-1.716107
C	-2.490233	3.650245	0.110207
H	-1.121058	2.524486	1.326508
C	-3.113606	2.653550	-1.994483
H	-2.225841	0.738730	-2.427576
C	-3.213773	3.700750	-1.079544
H	-2.565111	4.461941	0.830269
H	-3.673456	2.685172	-2.926315
H	-3.855272	4.552812	-1.292359
C	1.563934	1.511570	-0.481108
C	1.677011	2.520115	0.480042
C	2.267825	1.634212	-1.685301
C	2.483261	3.630583	0.242576
H	1.145345	2.429453	1.425610
C	3.071907	2.745532	-1.921966
H	2.184590	0.848758	-2.435614
C	3.182433	3.746065	-0.957343
H	2.567638	4.405225	1.001377
H	3.614146	2.828943	-2.861010

H	3.814151	4.612510	-1.139053

4Fe-williams-2 Gsolv= -2870.260799

Fe	-0.159409	-0.622109	1.120810
C	-0.434898	-2.041973	-0.555772
O	-0.616519	-3.271292	-0.398900
C	-1.466137	-0.982337	-0.495151
C	-0.786069	0.258858	-0.637461
C	0.613526	0.030687	-0.670273
C	0.871949	-1.359964	-0.531119
C	-1.232131	0.355849	2.177727
O	-1.912839	1.022388	2.828220
C	1.343733	-0.224083	2.010450
O	2.359012	0.029672	2.494473
C	-2.919113	-1.211417	-0.460982
C	-3.802619	-0.232534	0.023206
C	-3.470789	-2.400667	-0.955406
C	-5.174754	-0.442336	0.019350
H	-3.418632	0.706697	0.416444
C	-4.848981	-2.604130	-0.955483
H	-2.815206	-3.170037	-1.353879
C	-5.726354	-1.635329	-0.464816
H	-5.836419	0.333718	0.403848
H	-5.250982	-3.536890	-1.349938
C	2.184359	-2.021157	-0.517717
C	3.217337	-1.557660	-1.341396
C	2.443659	-3.110471	0.325504
C	4.467783	-2.169064	-1.326374
H	3.038890	-0.716425	-2.009901
C	3.694326	-3.717746	0.333102
H	1.663757	-3.466856	0.996269
C	4.727305	-3.262446	-0.494785
H	5.258514	-1.791365	-1.973985
H	3.880181	-4.558181	1.001456
C	-7.207773	-1.853771	-0.446374
H	-7.584625	-1.930092	0.581722
H	-7.740197	-1.018583	-0.917492
H	-7.484088	-2.774127	-0.971697
C	6.062815	-3.940749	-0.504940
H	6.082647	-4.758814	-1.237173
H	6.863894	-3.244300	-0.776196
H	6.298344	-4.376522	0.472374
C	-1.086361	1.697909	-0.896790
C	1.355921	1.292305	-0.950935
H	-1.873171	2.141944	-0.280957
H	-1.383939	1.810410	-1.948108
H	1.622135	1.309001	-2.018425
H	2.277606	1.435734	-0.380049
C	0.283332	2.388876	-0.669023
C	0.336045	2.960571	0.748311
C	0.505010	3.538191	-1.644277
O	-0.596406	3.578906	1.231306
O	-0.011279	3.615984	-2.741090
O	1.482937	2.753709	1.375643
O	1.387679	4.411477	-1.171864
C	1.575267	3.259453	2.718119
H	2.588539	3.034271	3.050099
H	1.401790	4.338566	2.728342
H	0.843679	2.753450	3.356503
C	1.726509	5.513688	-2.033620
H	0.833702	6.105492	-2.251142
H	2.451124	6.108999	-1.479113
H	2.169018	5.140678	-2.960815

4Fe-wills-1 Gsolv= -2372.188767

Fe	0.002683	0.440171	0.927288
C	-0.000187	-1.278434	-0.496636
O	-0.003538	-2.493193	-0.204705
C	-1.180619	-0.391039	-0.574517
C	-0.704826	0.897286	-0.937160
C	0.710054	0.895909	-0.938729
C	1.183959	-0.393958	-0.576556
C	-1.335334	1.335324	1.715709
O	-2.230551	1.943177	2.113710
C	1.328273	1.356805	1.712959
O	2.211811	1.982851	2.109046
C	-2.582568	-0.806454	-0.432246
C	-3.559979	-0.292365	-1.293611
C	-2.970054	-1.698740	0.577307
C	-4.894534	-0.665632	-1.152759
H	-3.270268	0.393603	-2.088804
C	-4.303019	-2.072906	0.713755
H	-2.221976	-2.084269	1.267611
C	-5.269665	-1.558495	-0.150681
H	-5.641928	-0.259253	-1.830633
H	-4.590288	-2.762225	1.504694
H	-6.311575	-1.850357	-0.040436
C	2.584214	-0.812859	-0.432776

C	3.577589	-0.240094	-1.237735
C	2.956407	-1.768396	0.523937
C	4.910664	-0.616902	-1.094669
H	3.303388	0.494837	-1.993325
C	4.288491	-2.144656	0.663148
H	2.197329	-2.203177	1.170914
C	5.270453	-1.571468	-0.145227
H	5.669243	-0.164500	-1.729596
H	4.562867	-2.883374	1.413007
H	6.311288	-1.866286	-0.032875
C	-1.170296	2.246557	-1.366612
O	0.002201	3.061073	-1.218831
C	1.173917	2.246033	-1.369436
H	-1.489578	2.216055	-2.421099
H	1.489532	2.215180	-2.425095
H	1.982680	2.682636	-0.774002
H	-1.977497	2.682340	-0.768399
C	5.011260	-0.558518	-1.148180
H	3.372807	0.510484	-2.044321
C	4.433529	-2.097669	0.616076
H	2.344939	-2.209911	1.127536
C	5.397550	-1.500523	-0.196413
H	5.756859	-0.089625	-1.786428
H	4.729292	-2.827051	1.366903
H	6.446159	-1.766954	-0.085360
C	-1.140255	2.196050	-1.259410
O	0.042916	3.018653	-1.147394
C	1.214969	2.219276	-1.327512
H	-1.421912	2.119943	-2.326092
H	1.511052	2.193958	-2.389383
H	2.035926	2.656154	-0.748632
C	-2.252142	2.842992	-0.477839
H	-2.532975	3.794445	-0.940830
H	-3.137193	2.196393	-0.460142
H	-1.933223	3.038691	0.552064

4Fe-wills-2 Gsolv= -2411.451808

Fe	0.116432	0.296593	0.973950
C	0.117778	-1.339154	-0.550465
O	0.153093	-2.568342	-0.328520
C	-1.079270	-0.479205	-0.549069
C	-0.639945	0.846525	-0.839224
C	0.774878	0.860634	-0.906488
C	1.283633	-0.423184	-0.605688
C	-1.255981	0.887255	1.969866
O	-2.167384	1.241315	2.579711
C	1.344509	1.353101	1.737323
O	2.142646	2.089959	2.126018
C	-2.463169	-0.967197	-0.443786
C	-3.428604	-0.549611	-1.367954
C	-2.837533	-1.859399	0.569915
C	-4.739131	-1.014138	-1.281646
H	-3.144796	0.136997	-2.164936
C	-4.145884	-2.325737	0.653028
H	-2.099568	-2.170425	1.308061
C	-5.100793	-1.905399	-0.272832
H	-5.478178	-0.680423	-2.006707
H	-4.423222	-3.013391	1.448958
H	-6.123809	-2.268550	-0.205171
C	2.693991	-0.811229	-0.477708
C	3.668861	-0.215668	-1.288381
C	3.091826	-1.756675	0.478601

4Fe-wills-3 Gsolv= -2589.107143

Fe	0.272063	0.364659	0.952466
C	0.154764	-1.409660	-0.347760
O	0.108617	-2.590896	0.072292
C	-0.991319	-0.485711	-0.473291
C	-0.463472	0.762249	-0.916248
C	0.949695	0.663779	-0.975692
C	1.381980	-0.610548	-0.534119
Si	3.136294	-1.253854	-0.302741
C	3.428287	-2.649684	-1.519894
H	4.452625	-3.033614	-1.427875
H	3.290148	-2.304327	-2.552333
H	2.737981	-3.484407	-1.345728
C	4.312650	0.165650	-0.643710
H	5.349347	-0.185688	-0.556313
H	4.180399	0.986897	0.072836
H	4.184800	0.567408	-1.657326
C	3.340863	-1.856437	1.461030
H	4.346429	-2.270450	1.612079
H	2.613476	-2.642156	1.700593
H	3.202880	-1.035103	2.177323
C	-1.065202	1.160781	1.843151
O	-1.962347	1.642031	2.383346
C	1.546897	1.427958	1.628945
O	2.352641	2.171963	1.987703

C	-2.405061	-0.861863	-0.329670
C	-3.342820	-0.435779	-1.279088
C	-2.839367	-1.656004	0.740420
C	-4.683801	-0.792251	-1.160940
H	-3.015060	0.170441	-2.122882
C	-4.179089	-2.015404	0.854439
H	-2.122325	-1.976856	1.494102
C	-5.105913	-1.585079	-0.095121
H	-5.399483	-0.451860	-1.906114
H	-4.502276	-2.628958	1.692588
H	-6.152966	-1.864646	-0.002864
C	-0.872138	2.085988	-1.487742
O	0.370811	2.823514	-1.502634
C	1.485216	1.927172	-1.554770
H	-1.192768	1.906257	-2.530435
H	1.793850	1.745971	-2.597612
H	2.325205	2.383517	-1.020098
C	-1.906643	2.908250	-0.765020
H	-2.832613	2.336124	-0.634261
H	-1.532216	3.208764	0.220073
H	-2.140130	3.812184	-1.336686
O	2.012177	2.320647	-1.738631
C	-1.485332	1.531740	-1.573355
O	-2.336978	2.222010	-1.932331
C	2.495737	-0.719489	0.328770
C	3.441558	-0.194221	1.219223
C	2.941946	-1.497092	-0.749842
C	4.799721	-0.444930	1.040180
H	3.112065	0.404264	2.067618
C	4.299248	-1.748394	-0.924541
H	2.219504	-1.889533	-1.462317
C	5.233280	-1.223939	-0.030882
H	5.520579	-0.030696	1.741654
H	4.630306	-2.349531	-1.768624
H	6.293965	-1.419323	-0.171355
C	0.872990	2.061197	1.679710
O	-0.351549	2.808342	1.639470
C	-1.467749	1.904474	1.628846
H	1.651621	2.640311	1.171537
H	1.186039	1.889226	2.722616
H	-1.801453	1.690153	2.657347
H	-2.290325	2.381710	1.086546

4Fe-wills-4 Gsolv= -2549.843692

Fe	-0.161154	0.535106	-0.884882
C	-0.060520	-1.355505	0.279410
O	0.021241	-2.506651	-0.211210
C	1.068700	-0.424983	0.510153
C	0.505669	0.765614	1.042227
C	-0.907848	0.667279	1.011660
C	-1.303873	-0.588094	0.471121
Si	-3.037733	-1.268503	0.202520
C	-3.276654	-2.728960	1.352806
H	-4.297945	-3.123139	1.270013
H	-3.111505	-2.439540	2.398385
H	-2.581288	-3.543496	1.114293
C	-4.253582	0.097445	0.616891
H	-5.281101	-0.277764	0.521860
H	-4.148496	0.952298	-0.063945
H	-4.126668	0.458268	1.645935
C	-3.238317	-1.800056	-1.584275
H	-4.228706	-2.246297	-1.743551
H	-2.483385	-2.545223	-1.864658
H	-3.141097	-0.943954	-2.265166
C	1.141197	1.611876	-1.475587

4Fe-wills-5 Gsolv= -2706.874085

Fe	0.448758	0.867003	-0.962731
C	-0.025079	-1.134997	-0.227194
O	-0.146316	-2.126610	-0.986267
C	1.250674	-0.596014	0.286964
C	0.931748	0.587695	1.012217
C	-0.459149	0.834125	0.893667
C	-1.076948	-0.138820	0.069304
Si	-2.890616	-0.250145	-0.437214
C	-3.680771	1.437206	-0.191321
H	-4.757377	1.366996	-0.398646
H	-3.265883	2.180542	-0.883876
H	-3.566990	1.819120	0.831020
C	-3.015167	-0.711338	-2.252299
H	-4.037162	-0.534821	-2.613461
H	-2.763309	-1.760774	-2.446138
H	-2.339486	-0.083511	-2.849805
C	-3.759085	-1.528471	0.681043
C	2.062652	1.483278	-1.445717
O	3.123392	1.830955	-1.732053
C	-0.425189	2.346810	-1.472514
O	-0.965804	3.337593	-1.712026

C	2.558261	-1.258941	0.174138
C	3.401993	-1.339195	1.289632
C	2.980204	-1.829968	-1.034611
C	4.638577	-1.973576	1.199139
H	3.081643	-0.907409	2.237297
C	4.214567	-2.466431	-1.122356
H	2.342460	-1.754757	-1.913481
C	5.047014	-2.542689	-0.005840
H	5.282287	-2.026487	2.074467
H	4.530479	-2.899754	-2.068832
H	6.012203	-3.038978	-0.077260
C	1.511207	1.577078	1.976053
O	0.468151	2.572088	2.078700
C	-0.803587	2.008805	1.741851
H	1.612908	1.063177	2.949676
H	-1.334682	1.666217	2.645975
H	-1.407184	2.784996	1.258982
C	2.800123	2.272538	1.624695
H	3.598097	1.542616	1.445327
H	2.667735	2.886276	0.726426
H	3.111369	2.925418	2.446621
C	-5.208084	-1.692535	0.218180
H	-5.270382	-2.089791	-0.804799
H	-5.736145	-2.401364	0.876417
H	-5.765609	-0.745732	0.245886
C	-3.061072	-2.886425	0.614894
H	-3.600709	-3.615679	1.240758
H	-3.033447	-3.289602	-0.407103
H	-2.028229	-2.837642	0.986248
C	-3.740588	-1.027973	2.126070
H	-2.715520	-0.870339	2.493530
H	-4.289805	-0.083626	2.243914
H	-4.215525	-1.768306	2.790045

4Mn-a Gsolv= -2631.389061

C	-0.005421	1.400460	0.123811
O	0.013067	2.506344	-0.473849
C	-1.207738	0.597777	0.408017
C	-0.739136	-0.568216	1.074797
C	0.678477	-0.603435	1.062688
C	1.176410	0.557464	0.400444
Si	-2.980405	1.114421	0.039463
C	-3.321051	2.751503	0.887227
H	-3.152582	2.685865	1.969366
H	-4.362145	3.059518	0.724719
H	-2.670830	3.541583	0.490872
C	-4.107970	-0.232334	0.696531
H	-3.958664	-0.403590	1.770517
H	-3.940953	-1.182140	0.170520
H	-5.158782	0.047663	0.545902
C	-3.201864	1.280497	-1.815726
H	-3.105936	0.303901	-2.308962
H	-2.456266	1.956976	-2.252565
H	-4.196890	1.680117	-2.051319
Si	2.960352	1.101119	0.128127
C	3.220932	2.728476	1.024063
H	4.264278	3.055321	0.922900
H	2.999704	2.636001	2.094803
H	2.579765	3.516885	0.611141
C	4.077678	-0.219023	0.852677
H	5.126673	0.095316	0.773487
H	3.978177	-1.178520	0.329256
H	3.861112	-0.384776	1.916269
C	3.288993	1.325120	-1.705087
H	4.287688	1.752739	-1.864255
H	2.557033	2.007375	-2.156187
H	3.244217	0.372169	-2.247725
O	-1.933869	-2.670308	-1.284260
C	1.408094	-1.665661	-1.409569
O	2.290805	-2.374052	-1.627305
C	-1.227138	-1.741800	1.852374
O	-0.067579	-2.581655	1.962331
C	1.124496	-1.786543	1.852233
H	-2.031032	-2.325914	1.391935
H	-1.563038	-1.408908	2.848141
H	1.467835	-1.466369	2.849698
H	1.905007	-2.403331	1.394514
N	-1.141548	-1.804925	-1.239524
Mn	-0.032431	-0.653173	-0.881393

4Mn-b Gsolv= -2774.151651

C	-0.401681	-2.078292	-0.503938
O	-0.554570	-3.313796	-0.363030
C	-1.450344	-1.046224	-0.442104
C	-0.800966	0.213284	-0.592079
C	0.602013	0.025654	-0.624865
C	0.890234	-1.361559	-0.476461
O	-1.703267	1.233467	2.671128

C	1.467650	-0.196024	2.003854
O	2.504184	0.111720	2.398785
C	-2.898482	-1.298918	-0.415329
C	-3.787830	-0.385435	0.173454
C	-3.436235	-2.439083	-1.025243
C	-5.157875	-0.607961	0.148815
H	-3.407062	0.507666	0.666286
C	-4.812299	-2.656319	-1.043960
H	-2.773019	-3.156243	-1.502289
C	-5.697681	-1.749124	-0.458596
H	-5.827214	0.115436	0.614243
H	-5.206330	-3.548378	-1.529817
C	2.216768	-1.994690	-0.484492
C	3.232696	-1.491324	-1.306308
C	2.504660	-3.100133	0.328000
C	4.493803	-2.079750	-1.320100
H	3.032648	-0.637879	-1.952667
C	3.765620	-3.685277	0.305513
H	1.738174	-3.489922	0.995571
C	4.781174	-3.190608	-0.521389
H	5.270075	-1.671250	-1.966435
H	3.973028	-4.540078	0.948766
C	-7.177950	-1.976211	-0.472079
H	-7.577235	-2.050277	0.547341
H	-7.703773	-1.145106	-0.958382
H	-7.437796	-2.897903	-1.003327
C	6.126607	-3.847328	-0.566730
H	6.146001	-4.650711	-1.315056
H	6.912091	-3.133372	-0.837815
H	6.385235	-4.298387	0.397697
C	-1.148844	1.637325	-0.874964
C	1.306535	1.301101	-0.943380
H	-1.942479	2.067447	-0.257291
H	-1.467105	1.718293	-1.923138
H	1.567293	1.298557	-2.012619
H	2.226201	1.489514	-0.382313
C	0.203787	2.372769	-0.684406
C	0.247839	2.998976	0.709375
C	0.388244	3.501415	-1.690003
O	-0.672966	3.671446	1.139343
O	-0.193829	3.586417	-2.752471
O	1.366892	2.770346	1.376816
O	1.325363	4.350613	-1.281287
C	1.434387	3.295285	2.713681
H	2.432364	3.050570	3.077015
H	1.287284	4.378235	2.704309
H	0.672195	2.815585	3.336882
C	1.641499	5.440257	-2.166359
H	0.753513	6.054981	-2.334241
H	2.412950	6.017621	-1.657748
H	2.019882	5.053785	-3.116111
N	-1.066216	0.408206	2.130963
Mn	-0.151914	-0.603926	1.216428

4Mn-c Gsolv= -2276.079171

C	-0.034020	-1.316771	-0.488383
O	-0.018796	-2.539088	-0.233818
C	-1.219716	-0.436069	-0.540713
C	-0.755649	0.852047	-0.921610
C	0.657705	0.872006	-0.920722
C	1.138996	-0.418902	-0.557803
O	-1.822538	2.447563	1.836295
C	1.496704	1.245086	1.690254
O	2.459040	1.799312	1.994497
C	-2.616936	-0.852926	-0.376868
C	-3.634763	-0.209979	-1.095160
C	-2.964873	-1.879246	0.514062
C	-4.965679	-0.582903	-0.928214
H	-3.383539	0.577904	-1.803666
C	-4.295452	-2.250846	0.677128
H	-2.186964	-2.374138	1.090705
C	-5.300974	-1.605230	-0.042413
H	-5.742195	-0.074839	-1.495778
H	-4.549587	-3.044986	1.375762
H	-6.340563	-1.896693	0.088550
C	2.544135	-0.833939	-0.437509
C	3.513659	-0.297381	-1.293818
C	2.942316	-1.747129	0.549284
C	4.850468	-0.669059	-1.170694
H	3.217204	0.404602	-2.072220
C	4.277360	-2.119175	0.668425
H	2.200696	-2.150937	1.236098
C	5.236104	-1.581944	-0.191019
H	5.591571	-0.245661	-1.844999
H	4.572567	-2.824411	1.442212
H	6.279813	-1.872132	-0.094407
C	-1.236551	2.183506	-1.389676
O	-0.073103	3.014933	-1.282463

C	1.107515	2.207896	-1.408209
H	-1.564864	2.107715	-2.439443
H	1.417198	2.141625	-2.464002
H	1.913147	2.677634	-0.834408
H	-2.043916	2.635845	-0.804089
Mn	-0.024850	0.473526	0.992027
N	-1.079749	1.566331	1.612123

4Mn Gsolv= -2634.737116

C	-0.009829	-1.407957	-0.382433
O	-0.002454	-2.621580	-0.038593
C	-1.193137	-0.554648	-0.498021
C	-0.729844	0.744216	-0.898217
C	-1.522213	1.942050	-1.313621
H	-2.414740	2.063112	-0.688353
H	-1.890861	1.753968	-2.335004
C	-0.665109	3.204155	-1.310610
H	-1.229839	4.028940	-1.760658
H	-0.438863	3.499338	-0.273203
C	0.633714	2.965303	-2.069206
H	1.196276	3.898554	-2.188023
H	0.388956	2.612121	-3.082746
C	1.509737	1.929396	-1.366376
H	2.284979	1.559306	-2.050718
H	2.048919	2.398120	-0.531465
C	0.702139	0.756944	-0.887559
C	1.167804	-0.533769	-0.465445
Si	-2.935155	-1.217994	-0.215195
C	-3.262488	-2.592300	-1.451779
H	-3.182050	-2.223500	-2.482361
H	-4.275895	-2.993113	-1.316857
H	-2.551860	-3.419176	-1.330718
C	-4.233124	0.122636	-0.425045
H	-4.230279	0.560619	-1.430634
H	-4.114920	0.931711	0.307796
H	-5.222312	-0.327681	-0.262169
C	-3.057669	-1.872563	1.540539
H	-2.970969	-1.052679	2.266718
H	-2.277856	-2.610561	1.764397
H	-4.033117	-2.352888	1.696686
Si	2.923983	-1.188985	-0.248648
C	3.256088	-2.407889	-1.636632
H	4.273334	-2.813876	-1.559359
H	3.160849	-1.920979	-2.615892
H	2.551811	-3.248783	-1.607387
C	4.198775	0.186774	-0.325238
H	5.179063	-0.246230	-0.081859
H	4.006464	0.992387	0.394019
H	4.274447	0.628884	-1.326302
C	3.068731	-2.038055	1.419589
H	4.080700	-2.446642	1.544172
H	2.356181	-2.865106	1.523243
H	2.891148	-1.332474	2.242817
O	-2.009801	2.119408	1.957735
C	1.386473	1.202781	1.830622
O	2.256402	1.825662	2.261349
Mn	-0.036818	0.351038	1.038085
N	-1.176594	1.339717	1.674028

5Co-a Gsolv= -2827.215401

C	-0.010028	1.439587	0.141250
O	-0.023661	2.579346	-0.335715
C	-1.196642	0.561519	0.382549
C	-0.703624	-0.534165	1.128337
C	0.725049	-0.507267	1.140524
C	1.195865	0.597023	0.392346
Si	-2.991626	1.068292	0.052874
C	-3.282426	2.684623	0.956947
H	-3.067471	2.586470	2.028447
H	-4.330969	2.992521	0.852044
H	-2.653139	3.487708	0.554797
C	-4.102866	-0.272341	0.740649
H	-3.916985	-0.435125	1.810490
H	-3.964707	-1.226573	0.216678
H	-5.154503	0.022137	0.628771
C	-3.222943	1.290408	-1.791598
H	-3.116026	0.336226	-2.323214
H	-2.487408	1.996392	-2.198788
H	-4.223333	1.687833	-2.006072
Si	2.978219	1.118318	0.025835
C	3.293903	2.742575	0.901586
H	4.335729	3.057365	0.759704
H	3.110893	2.656818	1.979815
H	2.645252	3.534825	0.508192
C	4.089842	-0.242971	0.671501
H	5.142401	0.012922	0.494016
H	3.892114	-1.195326	0.161348
H	3.961354	-0.396260	1.750736

C	3.159001	1.294943	-1.829907
H	4.148194	1.695180	-2.086510
H	2.402749	1.974820	-2.243462
H	3.051013	0.319315	-2.323105
C	-1.366268	-1.880440	-1.309850
C	1.244600	-1.944658	-1.203077
O	2.008377	-2.757086	-1.450385
C	-1.150394	-1.692031	1.950571
O	0.038700	-2.483238	2.090823
C	1.196604	-1.646140	1.977798
H	-1.932159	-2.315680	1.507382
H	-1.495548	-1.330671	2.933031
H	1.500802	-1.259682	2.964541
H	2.018902	-2.240687	1.568051
H	0.401025	0.181849	-2.211462
H	-0.404692	0.176017	-2.197151
N	-2.203526	-2.631700	-1.645155
Co	0.012724	-0.687600	-0.764802

5Co-b Gsolv= -2969.976148

C	-0.354364	-2.044318	-0.724645
O	-0.487791	-3.258822	-0.875262
C	-1.421639	-1.008398	-0.522610
C	-0.779061	0.250459	-0.651236
C	0.632142	0.064797	-0.660298
C	0.926806	-1.316687	-0.522459
C	-1.318476	0.434338	2.184914
C	1.311618	-0.128461	2.074924
O	2.265638	0.121482	2.650998
C	-2.866633	-1.267051	-0.481157
C	-3.761865	-0.267459	-0.063425
C	-3.398740	-2.500344	-0.882082
C	-5.129311	-0.496846	-0.047422
H	-3.387878	0.697460	0.269146
C	-4.773621	-2.718911	-0.868523
H	-2.734575	-3.289945	-1.218655
C	-5.663515	-1.728012	-0.449399
H	-5.801951	0.294032	0.283248
H	-5.163420	-3.682628	-1.194124
C	2.250616	-1.951779	-0.499958
C	3.304697	-1.426190	-1.253432
C	2.483115	-3.097117	0.275254
C	4.558851	-2.032159	-1.234182
H	3.143078	-0.547314	-1.875554
C	3.735223	-3.695599	0.287808
H	1.678236	-3.504844	0.885475
C	4.795599	-3.174597	-0.466679
H	5.368114	-1.610483	-1.828854
H	3.903689	-4.581498	0.899592
C	-7.140983	-1.963445	-0.417826
H	-7.507829	-2.029865	0.614625
H	-7.684916	-1.139466	-0.894861
H	-7.410493	-2.894395	-0.927434
C	6.139516	-3.834256	-0.441593
H	6.084775	-4.857823	-0.833172
H	6.869030	-3.281420	-1.042381
H	6.526574	-3.908288	0.582119
C	-1.117650	1.681465	-0.895769
C	1.341716	1.352274	-0.895505
H	-1.924030	2.096661	-0.287061
H	-1.414009	1.784889	-1.948880
H	1.659915	1.376333	-1.948625
H	2.233318	1.514361	-0.283368
C	0.227211	2.416257	-0.660058
C	0.221697	3.043651	0.734705
C	0.434570	3.549414	-1.658388
O	-0.698230	3.746000	1.113563
O	-0.135831	3.643907	-2.725882
O	1.298236	2.781009	1.455892
O	1.375927	4.384890	-1.234599
H	-0.065877	-2.132723	1.867601
H	-0.840524	-1.906862	1.959298
C	1.712006	5.476295	-2.111244
H	0.831872	6.101049	-2.283101
H	2.485497	6.042330	-1.593291
H	2.093773	5.090220	-3.059783
C	1.330624	3.331106	2.785333
H	0.542342	2.874101	3.392608
H	2.313081	3.079250	3.183991
H	1.200022	4.415402	2.749271
Co	-0.141183	-0.610306	1.100612
N	-2.030051	1.063064	2.875382

5Co-c Gsolv= -2471.904048

C	0.027396	-1.315158	-0.552540
O	0.033563	-2.538883	-0.443634
C	-1.160113	-0.406049	-0.563623
C	-0.691640	0.857566	-0.998982

C	0.730606	0.859670	-0.991052
C	1.205131	-0.392926	-0.535676
C	-1.473250	1.470405	1.654008
C	1.192736	1.652944	1.668528
O	1.950147	2.371377	2.130549
C	-2.553558	-0.835388	-0.410810
C	-3.565963	-0.228652	-1.164266
C	-2.893049	-1.839236	0.506452
C	-4.892255	-0.621657	-1.007857
H	-3.316536	0.543393	-1.890268
C	-4.218616	-2.229714	0.659698
H	-2.116821	-2.298395	1.115436
C	-5.221860	-1.622679	-0.096324
H	-5.668888	-0.144330	-1.600827
H	-4.471509	-3.005605	1.378502
H	-6.258232	-1.927936	0.027969
C	2.600213	-0.814128	-0.365253
C	3.614149	-0.238344	-1.140886
C	2.934277	-1.802367	0.570928
C	4.936394	-0.646367	-0.986261
H	3.368708	0.517188	-1.885404
C	4.255220	-2.209030	0.720804
H	2.155520	-2.239672	1.193016
C	5.260036	-1.632690	-0.056948
H	5.714023	-0.194105	-1.597316
H	4.503154	-2.974265	1.452628
H	6.292754	-1.951676	0.063193
C	-1.151528	2.184573	-1.496051
O	0.018473	3.004291	-1.378974
C	1.189689	2.188352	-1.486792
H	-1.459973	2.096072	-2.550556
H	1.504542	2.091602	-2.538862
H	2.001149	2.654916	-0.919579
H	0.410593	-0.702400	1.992712
H	-0.391632	-0.630058	2.080380
H	-1.962726	2.644444	-0.923880
N	-2.403826	2.027919	2.103218
Co	-0.008849	0.531717	0.883490

5Co Gsolv= -2830.565968

C	-0.009022	-1.447701	-0.413899
O	-0.026449	-2.675937	-0.258730
H	0.377536	-0.781493	2.103261
C	-1.177204	-0.530928	-0.441594
C	-0.693608	0.716493	-0.938833
C	-1.452792	1.908214	-1.417450
H	-2.344874	2.072091	-0.803396
H	-1.813821	1.676274	-2.433032
C	-0.563596	3.146194	-1.464112
H	-1.108418	3.968074	-1.942249
H	-0.327805	3.470686	-0.437375
C	0.722841	2.845794	-2.222216
H	1.312949	3.756861	-2.370919
H	0.460773	2.471414	-3.223202
C	1.577323	1.804997	-1.499304
H	2.319593	1.372310	-2.184153
H	2.159461	2.277387	-0.696560
C	0.749109	0.680983	-0.954971
C	1.185371	-0.568584	-0.425515
Si	-2.944575	-1.178483	-0.215516
C	-3.257032	-2.384680	-1.618283
H	-3.143851	-1.890999	-2.592159
H	-4.280939	-2.776621	-1.557997
H	-2.565076	-3.234746	-1.585940
C	-4.221625	0.189108	-0.293018
H	-4.229657	0.698577	-1.264428
H	-4.079941	0.938308	0.495707
H	-5.213117	-0.262790	-0.149969
C	-3.043249	-2.033719	1.449567
H	-2.920051	-1.311387	2.267692
H	-2.276826	-2.811173	1.558518
H	-4.025682	-2.509252	1.569789
Si	2.934583	-1.232519	-0.132919
C	3.315561	-2.416987	-1.533572
H	4.330826	-2.822085	-1.433801
H	3.251438	-1.903110	-2.501672
H	2.612382	-3.258668	-1.549047
C	4.184539	0.163316	-0.101231
H	5.161165	-0.253520	0.180422
H	3.929155	0.929881	0.641589
H	4.301126	0.650417	-1.076610
C	2.958145	-2.092131	1.532881
H	3.929720	-2.578689	1.690580
H	2.177547	-2.858053	1.617689
H	2.815786	-1.363702	2.343187
C	-1.401162	1.435505	1.759114
C	1.195683	1.554737	1.721976
O	1.918093	2.301691	2.199160

H	-0.433046	-0.726581	2.131220
N	-2.251807	2.066946	2.265348
Co	-0.000839	0.426530	0.957883

5Fe-Casey Gsolv= -2728.678440

Fe	0.000142	-0.700123	-0.808937
C	-0.000031	1.410353	0.110964
O	-0.000183	2.548132	-0.410236
C	-1.190295	0.570569	0.380167
C	-0.708209	-0.558779	1.106579
C	0.708577	-0.558455	1.106652
C	1.190385	0.570932	0.380194
Si	-2.970587	1.100847	0.068391
C	-3.273132	2.713430	0.978155
H	-3.078037	2.604986	2.052593
H	-4.315541	3.035360	0.855876
H	-2.625837	3.511926	0.594792
C	-4.096302	-0.243458	0.734209
H	-3.925851	-0.418733	1.804590
H	-3.955443	-1.194414	0.203999
H	-5.146282	0.052355	0.609652
C	-3.238040	1.325248	-1.773954
H	-3.144894	0.368059	-2.304210
H	-2.508303	2.025278	-2.201082
H	-4.241518	1.724227	-1.971869
Si	2.970522	1.101283	0.067916
C	3.273233	2.714253	0.976931
H	4.315503	3.036383	0.854015
H	3.078663	2.606190	2.051503
H	2.625566	3.512459	0.593586
C	4.096428	-0.242815	0.733854
H	5.146392	0.052845	0.608808
H	3.955268	-1.193920	0.203981
H	3.926354	-0.417737	1.804351
C	3.237435	1.324778	-1.774617
H	4.240756	1.723840	-1.973137
H	2.507380	2.024356	-2.201939
H	3.144253	0.367190	-2.304167
C	-1.298824	-1.836960	-1.265821
O	-2.148288	-2.572954	-1.520954
C	1.298190	-1.838586	-1.264541
O	2.147035	-2.575468	-1.519164
C	-1.174938	-1.693155	1.955473
O	0.000586	-2.504410	2.106294
C	1.175718	-1.692572	1.955647
H	-1.969883	-2.317672	1.535161
H	-1.509018	-1.310816	2.934034
H	1.509409	-1.309933	2.934225
H	1.971096	-2.316689	1.535570
H	0.416523	0.124563	-2.193481
H	-0.413709	0.132194	-2.189676

5Fe Gsolv= -2732.025933

Fe	-0.006256	0.414461	1.004156
C	-0.004687	-1.427602	-0.387342
O	-0.003520	-2.665037	-0.182059
H	0.358541	-0.770381	2.107565
C	-1.182559	-0.545544	-0.437472
C	-0.719972	0.734481	-0.901674
C	-1.514605	1.908247	-1.381599
H	-2.409723	2.061104	-0.767156
H	-1.879110	1.667381	-2.393715
C	-0.655916	3.167083	-1.439845
H	-1.217807	3.971782	-1.928298
H	-0.428904	3.509073	-0.416683
C	0.640882	2.888019	-2.188932
H	1.205425	3.812924	-2.354496
H	0.390631	2.487874	-3.183582
C	1.519163	1.882847	-1.444367
H	2.289531	1.482124	-2.117142
H	2.062519	2.387178	-0.633430
C	0.710596	0.732530	-0.912134
C	1.172100	-0.544241	-0.438439
Si	-2.930328	-1.217383	-0.221428
C	-3.259382	-2.433124	-1.613756
H	-3.168180	-1.942756	-2.591670
H	-4.275714	-2.841313	-1.535288
H	-2.553172	-3.272166	-1.590108
C	-4.225416	0.139300	-0.281843
H	-4.256255	0.652813	-1.250607
H	-4.085048	0.890990	0.505573
H	-5.209814	-0.322828	-0.122039
C	-3.058395	-2.062627	1.450095
H	-2.985321	-1.321768	2.258420
H	-2.272222	-2.812402	1.602223
H	-4.029758	-2.565992	1.546694
Si	2.927096	-1.194552	-0.210856
C	3.287079	-2.380614	-1.619887

H	4.303557	-2.787074	-1.536034
H	3.208505	-1.867923	-2.587714
H	2.583022	-3.222022	-1.625664
C	4.196658	0.188048	-0.227062
H	5.187435	-0.256870	-0.058915
H	4.027175	0.920879	0.572070
H	4.233846	0.723219	-1.183453
C	3.046220	-2.063054	1.449258
H	4.035793	-2.526168	1.561924
H	2.290074	-2.849013	1.566991
H	2.921440	-1.342389	2.269423
C	-1.273921	1.453642	1.702683
O	-2.096173	2.146534	2.122001
C	1.303422	1.365555	1.751455
O	2.157474	1.992171	2.209173
H	-0.468406	-0.682185	2.161276

5Fe-Renaud Gsolv= -2487.306555

Fe	0.019679	0.395612	1.216543
C	-0.008495	-1.464823	-0.125535
O	0.024121	-2.687120	0.142550
H	0.379675	-0.757599	2.364119
C	-1.186694	-0.589647	-0.159194
C	-0.762418	0.682317	-0.686078
C	-0.754804	2.958626	-1.271106
H	-1.373714	3.724720	-1.748475
H	-0.457134	3.335220	-0.280481
C	0.482807	2.681010	-2.103695
H	1.068881	3.595342	-2.234056
H	0.189711	2.332294	-3.103804
C	0.669207	0.670017	-0.826119
C	1.143692	-0.567735	-0.256384
C	-1.143659	1.533520	1.938324
O	-1.870902	2.321166	2.369322
C	1.396398	1.285605	1.930718
O	2.285109	1.817301	2.443067
H	-0.450963	-0.693252	2.376849
C	2.529845	-1.081741	-0.239031
C	3.160567	-1.438576	0.957573
C	3.211902	-1.278386	-1.446553
C	4.452506	-1.959695	0.950534
H	2.632292	-1.300364	1.900836
C	4.506445	-1.791388	-1.453830
H	2.720033	-1.031337	-2.386098
C	5.131869	-2.130049	-0.254510
H	4.930770	-2.228723	1.889830
H	5.025618	-1.931616	-2.399456
H	6.143832	-2.528775	-0.259725
C	-2.570785	-1.100109	-0.070612
C	-2.948184	-2.142684	-0.928830
C	-3.528907	-0.567519	0.797713
C	-4.250803	-2.633474	-0.923029
H	-2.214261	-2.559572	-1.616676
C	-4.834507	-1.053354	0.799413
H	-3.256349	0.233593	1.480882
C	-5.199952	-2.087562	-0.060012
H	-4.525144	-3.441820	-1.597331
H	-5.566508	-0.624797	1.480464
H	-6.218671	-2.468603	-0.055119
N	1.345269	1.670978	-1.470458
N	-1.568398	1.752625	-1.087642
C	2.582762	2.187590	-0.903088
H	3.166533	1.386422	-0.442617
H	3.189867	2.641116	-1.692637
H	2.369649	2.956448	-0.142677
C	-2.440061	1.450077	-2.224648
H	-3.072949	0.586244	-1.996640
H	-3.092729	2.309651	-2.405483
H	-1.877197	1.231382	-3.146755

5Fe-williams-1 Gsolv= -2682.473411

Fe	0.002070	-0.564214	1.464255
C	-0.016439	-1.943986	-0.421686
O	-0.035033	-3.185710	-0.535214
C	-1.175520	-1.061238	-0.210093
C	-0.730714	0.301854	-0.262371
C	0.703540	0.300373	-0.254979
C	1.151080	-1.071736	-0.237221
C	-1.183566	0.249874	2.531012
O	-1.914618	0.786195	3.241268
C	1.331663	0.004816	2.520955
O	2.168761	0.367727	3.222977
C	-2.575793	-1.520674	-0.301211
C	-3.582163	-1.049689	0.550192
C	-2.929296	-2.405685	-1.329280
C	-4.903874	-1.451310	0.381040
H	-3.337473	-0.357740	1.352734
C	-4.251390	-2.809566	-1.497126

H	-2.164802	-2.766650	-2.013597
C	-5.243970	-2.334694	-0.642497
H	-5.669878	-1.072891	1.054262
H	-4.505748	-3.493523	-2.303837
H	-6.276653	-2.650027	-0.772924
C	2.552805	-1.520186	-0.358790
C	3.611370	-0.857298	0.281372
C	2.860095	-2.602285	-1.196732
C	4.927042	-1.269987	0.099380
H	3.417135	-0.001717	0.924448
C	4.178353	-3.014199	-1.378355
H	2.059393	-3.118385	-1.718951
C	5.217719	-2.353447	-0.728983
H	5.729284	-0.740964	0.609088
H	4.390939	-3.854242	-2.036095
H	6.246833	-2.676437	-0.868696
C	-1.597230	1.473905	-0.504272
C	-1.597665	2.616594	0.301615
C	-2.426892	1.438902	-1.633490
C	-2.416164	3.699149	-0.011959
H	-0.966876	2.659072	1.186734
C	-3.240080	2.523347	-1.947564
H	-2.428155	0.556502	-2.272103
C	-3.238666	3.656375	-1.135929
H	-2.411011	4.578212	0.628461
H	-3.875619	2.482045	-2.829148
H	-3.877737	4.502566	-1.377450
C	1.563163	1.475480	-0.516939
C	1.771194	2.505748	0.403295
C	2.189318	1.542928	-1.768058
C	2.598250	3.579911	0.082487
H	1.297429	2.462954	1.382336
C	3.012145	2.618334	-2.088887
H	2.031719	0.740505	-2.487976
C	3.221628	3.638872	-1.162393
H	2.757402	4.371505	0.811191
H	3.492630	2.656984	-3.063800
H	3.869937	4.476319	-1.409634
H	0.282744	-2.037299	2.163156
H	-0.547844	-1.955826	2.163704

5Fe-williams-2 Gsolv= -2871.439481

Fe	-0.118383	-0.591119	1.169242
C	-0.371017	-2.068954	-0.603096
O	-0.512490	-3.306058	-0.651949
C	-1.427004	-1.037679	-0.442123
C	-0.791442	0.229731	-0.602464
C	0.611371	0.051087	-0.640835
C	0.909134	-1.337180	-0.493033
C	-1.161784	0.410710	2.229500
O	-1.823280	1.047363	2.926407
C	1.390287	-0.126471	2.004888
O	2.405448	0.139355	2.480361
C	-2.877885	-1.291954	-0.430083
C	-3.773803	-0.360677	0.119874
C	-3.412914	-2.446967	-1.013870
C	-5.143613	-0.581780	0.089395
H	-3.400467	0.549326	0.586094
C	-4.789712	-2.662199	-1.040295
H	-2.747055	-3.179771	-1.460601
C	-5.680012	-1.739517	-0.489044
H	-5.815622	0.157020	0.525904
H	-5.179398	-3.567535	-1.504744
C	2.241795	-1.960466	-0.504274
C	3.255627	-1.452952	-1.322894
C	2.532486	-3.067822	0.306147
C	4.521869	-2.035396	-1.333089
H	3.052910	-0.601428	-1.970984
C	3.794435	-3.646601	0.287197
H	1.765141	-3.461843	0.971069
C	4.812943	-3.141607	-0.532544
H	5.297355	-1.623144	-1.977739
H	4.003990	-4.502794	0.928302
C	-7.160109	-1.966928	-0.506609
H	-7.562486	-2.037673	0.511903
H	-7.684762	-1.137858	-0.997460
H	-7.417849	-2.891140	-1.034547
C	6.167899	-3.780073	-0.541659
H	6.121673	-4.801909	-0.939321
H	6.874389	-3.211990	-1.155871
H	6.579597	-3.854560	0.472295
C	-1.151923	1.648345	-0.897645
C	1.305502	1.333562	-0.957740
H	-1.953140	2.076577	-0.289224
H	-1.457839	1.720657	-1.950021
H	1.563631	1.335102	-2.027419
H	2.223744	1.529457	-0.397182
C	0.191869	2.393600	-0.694392

C	0.225030	2.995264	0.710249
C	0.371451	3.530862	-1.691051
O	-0.724454	3.600101	1.176828
O	-0.177126	3.592506	-2.772950
O	1.373712	2.827805	1.346012
O	1.262505	4.414514	-1.254504
H	0.053615	-2.025609	1.978750
H	-0.765395	-1.870172	2.001960
C	1.573441	5.507198	-2.138011
H	0.674102	6.096434	-2.334549
H	2.314557	6.108531	-1.612420
H	1.988105	5.124945	-3.074262
C	1.448336	3.353507	2.681977
H	0.714429	2.850770	3.319993
H	2.460000	3.139816	3.026581
H	1.266670	4.431322	2.674694
H	3.300374	0.524699	-1.912907
C	4.290565	-2.208098	0.644245
H	2.205667	-2.267876	1.173288
C	5.269114	-1.613982	-0.153622
H	5.662946	-0.155183	-1.691242
H	4.566457	-2.975619	1.363978
H	6.308621	-1.920433	-0.062141
C	-1.167336	2.186382	-1.463493
O	0.006197	3.007256	-1.377875
C	1.178400	2.184837	-1.465438
H	-1.491232	2.084589	-2.512263
H	1.499496	2.080255	-2.514804
H	1.983060	2.664121	-0.897940
H	0.453276	-0.571866	2.114677
H	-0.370119	-0.666549	2.047386
H	-1.969853	2.665950	-0.893276

5Fe-wills-1 Gsolv= -2373.366991

Fe	0.001228	0.520379	0.944282
C	0.006074	-1.312564	-0.486927
O	0.006637	-2.545397	-0.319127
C	-1.171311	-0.411301	-0.520398
C	-0.700668	0.866991	-0.944536
C	0.711367	0.865866	-0.945974
C	1.182717	-0.409568	-0.518567
C	-1.344635	1.463201	1.650067
O	-2.249979	2.065684	2.029753
C	1.304274	1.533116	1.632226
O	2.178351	2.184652	2.004279
C	-2.575241	-0.829169	-0.397763
C	-3.558821	-0.233097	-1.197058
C	-2.957887	-1.815305	0.522293
C	-4.893343	-0.616056	-1.084155
H	-3.277494	0.525210	-1.926286
C	-4.290053	-2.200620	0.629286
H	-2.207116	-2.268463	1.167047
C	-5.262905	-1.602565	-0.172692
H	-5.644310	-0.143561	-1.713422
H	-4.572521	-2.965551	1.349197
H	-6.304349	-1.903202	-0.084039
C	2.585667	-0.827657	-0.388034
C	3.575131	-0.235118	-1.182760
C	2.960707	-1.816496	0.532518
C	4.907437	-0.624453	-1.065019

5Fe-wills-2 Gsolv= -2412.630152

Fe	0.092978	0.380460	1.000569
C	0.128946	-1.364639	-0.522006
O	0.159300	-2.603745	-0.408849
C	-1.067800	-0.493747	-0.499978
C	-0.637339	0.822781	-0.857442
C	0.774613	0.843232	-0.893226
C	1.283845	-0.431311	-0.526534
C	-1.300931	1.041614	1.908261
O	-2.226909	1.399202	2.492570
C	1.302961	1.494467	1.704299
O	2.108279	2.220926	2.093109
C	-2.450225	-0.991778	-0.412826
C	-3.404901	-0.593167	-1.356009
C	-2.828031	-1.886440	0.596950
C	-4.709913	-1.076668	-1.290188
H	-3.118584	0.092668	-2.152485
C	-4.129601	-2.373939	0.658138
H	-2.096868	-2.183430	1.347930
C	-5.075093	-1.969860	-0.284809
H	-5.441283	-0.755930	-2.028722
H	-4.410018	-3.064481	1.450398
H	-6.093858	-2.347181	-0.232713
C	2.699601	-0.814731	-0.427360
C	3.662438	-0.164116	-1.209232
C	3.112862	-1.829345	0.447458
C	5.006499	-0.519152	-1.120834

H	3.358502	0.615223	-1.906544
C	4.454564	-2.185927	0.530625
H	2.378274	-2.327648	1.076994
C	5.406613	-1.532113	-0.252345
H	5.741025	-0.004429	-1.736163
H	4.760257	-2.973018	1.216391
H	6.455677	-1.810513	-0.182967
C	-1.140817	2.144503	-1.359836
O	0.037489	2.977817	-1.285994
C	1.218660	2.178440	-1.385292
H	-1.413529	2.005682	-2.422220
H	1.545236	2.092296	-2.435053
H	2.019033	2.657541	-0.810734
C	-2.259644	2.833343	-0.625197
H	-2.551688	3.746935	-1.153072
H	-3.137708	2.180690	-0.556868
H	-1.938777	3.105424	0.386867
H	0.716418	-0.747246	2.046424
H	-0.098634	-0.916850	2.015343

5Fe-wills-3 Gsolv= -2590.287484

Fe	0.264376	0.447052	0.962289
C	0.145670	-1.445468	-0.354339
O	0.080192	-2.662660	-0.086029
C	-0.986755	-0.491862	-0.428258
C	-0.459258	0.738983	-0.929560
C	0.951276	0.636580	-0.969837
C	1.374143	-0.627727	-0.474668
Si	3.132051	-1.279964	-0.283472
C	3.400738	-2.656003	-1.529231
H	4.434516	-3.021681	-1.475851
H	3.221124	-2.303130	-2.552611
H	2.732919	-3.505456	-1.340536
C	4.306432	0.142125	-0.619260
H	5.343344	-0.205028	-0.518662
H	4.162424	0.965972	0.092269
H	4.188822	0.538753	-1.636136
C	3.373209	-1.914936	1.463746
H	4.350615	-2.405105	1.562601
H	2.600836	-2.645705	1.736393
H	3.336002	-1.089992	2.187959
C	-1.082279	1.289869	1.777487
O	-1.989112	1.775061	2.296673
C	1.519306	1.572281	1.561676
O	2.331438	2.308150	1.918023
C	-2.403438	-0.866606	-0.289860
C	-3.323113	-0.513296	-1.284921
C	-2.852073	-1.598843	0.817176
C	-4.662090	-0.881320	-1.175033
H	-2.983172	0.044829	-2.156607
C	-4.189021	-1.969347	0.924248
H	-2.148087	-1.858909	1.606794
C	-5.098782	-1.610877	-0.070898
H	-5.364529	-0.598553	-1.955969
H	-4.524250	-2.532614	1.792369
H	-6.144509	-1.896917	0.016267
C	-0.862961	2.029008	-1.578160
O	0.379304	2.766434	-1.610489
C	1.493578	1.868176	-1.612948
H	-1.163071	1.790711	-2.615345
H	1.803311	1.632732	-2.644609
H	2.331507	2.352956	-1.101128
C	-1.913633	2.884953	-0.922237
H	-2.840299	2.316365	-0.780661
H	-1.562177	3.240366	0.053338
H	-2.138107	3.755292	-1.547222
H	0.830912	-0.576106	2.134316
H	0.009105	-0.712661	2.115976

5Fe-wills-4 Gsolv= -2551.023460

Fe	0.178050	0.595832	0.872084
C	0.033581	-1.379847	-0.321332
O	-0.068121	-2.575172	0.021161
C	-1.073749	-0.404771	-0.480977
C	-0.501782	0.768232	-1.055336
C	0.907382	0.647549	-1.037121
C	1.284534	-0.601553	-0.460025
Si	3.013179	-1.300047	-0.186597
C	3.233982	-2.791209	-1.299903
H	4.258870	-3.177360	-1.223284
H	3.047513	-2.536891	-2.350863
H	2.547460	-3.600291	-1.021138
C	4.246357	0.039870	-0.632794
H	5.269075	-0.341520	-0.514018
H	4.142766	0.919917	0.015238
H	4.133030	0.364980	-1.675241
C	3.203066	-1.792968	1.612750
H	4.165630	-2.295449	1.775051

H	2.406587	-2.482139	1.922555
H	3.168174	-0.912641	2.268490
C	-1.110214	1.689118	1.451476
O	-1.986567	2.371035	1.759022
C	1.514056	1.618297	1.485319
O	2.381200	2.288000	1.842091
C	-2.504512	-0.693540	-0.307815
C	-3.446471	-0.167559	-1.200811
C	-2.952867	-1.486712	0.757794
C	-4.804597	-0.430542	-1.034878
H	-3.115666	0.439737	-2.042396
C	-4.308709	-1.751558	0.919350
H	-2.232227	-1.881230	1.471880
C	-5.240040	-1.224042	0.024012
H	-5.523013	-0.015250	-1.738180
H	-4.641435	-2.364443	1.754240
H	-6.300300	-1.428219	0.154900
C	-0.856288	2.042802	-1.743156
O	0.379721	2.771373	-1.741931
C	1.481983	1.851480	-1.707993
H	-1.622662	2.654958	-1.256278
H	-1.177764	1.831652	-2.776451
H	1.799006	1.590948	-2.731136
H	2.317853	2.337376	-1.194926
H	-0.285590	-0.395564	2.122999
H	0.544763	-0.439720	2.122641

5Fe-wills-5 Gsolv= -2708.055503

Fe	0.456566	0.924291	-0.971233
C	-0.034774	-1.198455	-0.205893
O	-0.172012	-2.297202	-0.780978
C	1.238742	-0.595007	0.244937
C	0.903116	0.580573	0.989583
C	-0.489784	0.803159	0.862826
C	-1.077534	-0.160972	0.004956
Si	-2.891470	-0.287636	-0.501927
C	-3.661185	1.419713	-0.367763
H	-4.694437	1.383903	-0.738312
H	-3.121424	2.150324	-0.983760
H	-3.689318	1.794249	0.663691
C	-2.998804	-0.866627	-2.283554
H	-4.031926	-1.133720	-2.543292
H	-2.360221	-1.736260	-2.480403
H	-2.689314	-0.057096	-2.958412
C	-3.772881	-1.485915	0.692978
C	2.091224	1.468579	-1.437471
O	3.165617	1.762084	-1.732196
C	-0.269004	2.531792	-1.274286
O	-0.693208	3.593675	-1.419240
C	2.546571	-1.266008	0.172646
C	3.363113	-1.336382	1.308323
C	2.986025	-1.869565	-1.013378
C	4.589837	-1.994901	1.260312
H	3.029324	-0.882738	2.240841
C	4.209612	-2.530431	-1.059317
H	2.369271	-1.802272	-1.908503
C	5.015202	-2.596511	0.077620
H	5.211964	-2.040298	2.151499
H	4.538809	-2.990529	-1.988411
H	5.972384	-3.111547	0.039362
C	1.453760	1.554395	1.987980
O	0.386698	2.523459	2.106756
C	-0.869560	1.936194	1.753745
H	1.559558	1.022072	2.950882
H	-1.382241	1.537807	2.645576
H	-1.503079	2.710560	1.308013
C	2.727514	2.286081	1.658035
H	3.543813	1.577515	1.475451
H	2.586982	2.906532	0.764909
H	3.017127	2.936024	2.490253
C	-5.283928	-1.374327	0.478706
H	-5.573966	-1.587380	-0.560430
H	-5.808865	-2.101192	1.119364
H	-5.664417	-0.376765	0.737280
H	-0.241489	0.453643	-2.395707
H	0.502381	0.075775	-2.396717
C	-3.338531	-2.928788	0.437027
H	-3.879212	-3.609886	1.114222
H	-3.556158	-3.248810	-0.591932
H	-2.264007	-3.073903	0.612447
C	-3.441219	-1.109384	2.137638
H	-2.369623	-1.226065	2.355210
H	-3.722748	-0.072484	2.371852
H	-3.991140	-1.761549	2.835420

5Mn-a Gsolv= -2632.563957

C	-0.005430	1.421274	0.123021
O	0.002729	2.568862	-0.376233

C	-1.200650	0.587959	0.383830
C	-0.726409	-0.546987	1.104393
C	0.689245	-0.566952	1.097209
C	1.177312	0.567546	0.377292
Si	-2.978980	1.108206	0.045747
C	-3.311039	2.716732	0.951690
H	-3.132413	2.610809	2.029135
H	-4.353786	3.029992	0.811518
H	-2.664063	3.520252	0.578100
C	-4.102013	-0.253048	0.679905
H	-3.959184	-0.430336	1.753844
H	-3.929543	-1.199174	0.149720
H	-5.153036	0.024431	0.525675
C	-3.213242	1.332242	-1.801053
H	-3.111400	0.372916	-2.326161
H	-2.477114	2.031239	-2.218810
H	-4.213660	1.729759	-2.016743
Si	2.957474	1.116404	0.091972
C	3.239459	2.707699	1.045785
H	4.281593	3.037015	0.941029
H	3.036467	2.568778	2.115256
H	2.591929	3.513168	0.678218
C	4.094436	-0.225894	0.742817
H	5.139798	0.096829	0.649673
H	3.986477	-1.166889	0.188448
H	3.904937	-0.428952	1.805202
C	3.240966	1.394818	-1.740823
H	4.242938	1.808696	-1.914817
H	2.510277	2.101606	-2.154773
H	3.163515	0.455452	-2.303957
O	-2.016505	-2.638051	-1.384234
C	1.411463	-1.785319	-1.282948
O	2.307157	-2.472341	-1.507634
C	-1.209278	-1.689310	1.931928
O	-0.038038	-2.503718	2.099981
C	1.145814	-1.703676	1.949154
H	-1.994931	-2.307566	1.484107
H	-1.567002	-1.318916	2.906421
H	1.483208	-1.325183	2.927949
H	1.933928	-2.337622	1.529507
H	0.408568	0.021986	-2.316701
H	-0.319362	0.358163	-2.108930
Mn	-0.029202	-0.734961	-0.842638
N	-1.171937	-1.845355	-1.229038

5Mn-b Gsolv= -2775.325284

C	-0.379201	-2.079716	-0.613531
O	-0.524504	-3.315351	-0.678639
C	-1.433807	-1.049879	-0.454519
C	-0.798326	0.217863	-0.613001
C	0.605025	0.041888	-0.637770
C	0.900287	-1.348803	-0.488886
O	-1.697760	1.198116	2.773789
C	1.471893	-0.161082	1.977393
O	2.513445	0.090467	2.395959
C	-2.883154	-1.303401	-0.430508
C	-3.763689	-0.409038	0.199456
C	-3.429094	-2.422176	-1.070897
C	-5.133975	-0.628985	0.184693
H	-3.374191	0.466255	0.717321
C	-4.806114	-2.636608	-1.079834
H	-2.771985	-3.125173	-1.575180
C	-5.682906	-1.748864	-0.454122
H	-5.796442	0.078573	0.683050
H	-5.207120	-3.512768	-1.588398
C	2.232361	-1.972290	-0.502477
C	3.273329	-1.407183	-1.246340
C	2.497922	-3.135707	0.235600
C	4.540999	-1.985996	-1.253159
H	3.092534	-0.511947	-1.839294
C	3.762143	-3.709597	0.220425
H	1.708289	-3.581438	0.838081
C	4.807972	-3.145842	-0.523218
H	5.336789	-1.528483	-1.839865
H	3.950861	-4.610497	0.804111
C	-7.163781	-1.972537	-0.459627
H	-7.559627	-2.035074	0.561761
H	-7.689133	-1.145043	-0.952794
H	-7.427651	-2.898339	-0.981659
C	6.166227	-3.777272	-0.524792
H	6.129224	-4.797549	-0.926830
H	6.874892	-3.201518	-1.129250
H	6.570549	-3.853479	0.492254
C	-1.160930	1.637530	-0.901536
C	1.297590	1.323379	-0.965126
H	-1.962460	2.059561	-0.288372
H	-1.472306	1.714345	-1.951888
H	1.550727	1.320653	-2.036186

H	2.217371	1.524721	-0.409092
C	0.184462	2.383576	-0.702153
C	0.222392	2.992372	0.700120
C	0.361429	3.520180	-1.699687
O	-0.712973	3.631300	1.149065
O	-0.215809	3.603034	-2.765056
O	1.354465	2.786759	1.354146
O	1.286502	4.378588	-1.283067
H	0.058117	-1.968801	2.139622
H	-0.716892	-2.011429	1.843165
C	1.597894	5.470914	-2.166750
H	0.705834	6.078501	-2.338949
H	2.362481	6.054442	-1.654881
H	1.983471	5.087162	-3.114746
C	1.420316	3.294694	2.697603
H	0.666772	2.797907	3.318226
H	2.422656	3.056415	3.053423
H	1.260225	4.375878	2.702568
N	-1.059228	0.439905	2.153001
Mn	-0.150756	-0.552801	1.210763
C	2.919875	-1.852981	0.480448
C	4.853724	-0.636359	-1.113888
H	3.239357	0.520401	-1.936942
C	4.251577	-2.241548	0.580497
H	2.169510	-2.311892	1.121201
C	5.223762	-1.635128	-0.215841
H	5.604449	-0.157064	-1.738264
H	4.533959	-3.015683	1.290582
H	6.264888	-1.938544	-0.133183
C	-1.229811	2.159538	-1.463743
O	-0.056931	2.983128	-1.415164
C	1.115814	2.161176	-1.510095
H	-1.577536	2.041727	-2.503197
H	1.413626	2.036914	-2.564276
H	1.929716	2.656270	-0.970416
H	0.322046	-0.507793	2.276560
H	-0.389894	-0.773634	1.946583
H	-2.022118	2.645647	-0.883983
Mn	-0.018740	0.573101	0.986213
N	-1.082377	1.660271	1.601328

5Mn-c Gsolv= -2277.255021

C	-0.042026	-1.324649	-0.469862
O	-0.044147	-2.557690	-0.302708
C	-1.218347	-0.419613	-0.490587
C	-0.751368	0.846700	-0.941443
C	0.660469	0.853317	-0.950898
C	1.133874	-0.428286	-0.529890
O	-1.859619	2.483662	1.890791
C	1.522967	1.347133	1.621920
O	2.512048	1.837185	1.945153
C	-2.618914	-0.838697	-0.346443
C	-3.616227	-0.246676	-1.132468
C	-2.983782	-1.834304	0.571034
C	-4.945915	-0.641756	-1.007548
H	-3.349820	0.516204	-1.862420
C	-4.311330	-2.230967	0.690307
H	-2.222368	-2.286012	1.203964
C	-5.297427	-1.636883	-0.098220
H	-5.707147	-0.173174	-1.627282
H	-4.579487	-3.003099	1.407955
H	-6.335118	-1.947752	-0.001293
C	2.536668	-0.854615	-0.426511
C	3.519800	-0.249108	-1.219237

5Mn Gsolv= -2635.912506

C	-0.009102	-1.436993	-0.373844
O	-0.001525	-2.675258	-0.174291
H	0.367209	-0.643499	2.289061
C	-1.191055	-0.562007	-0.435734
C	-0.731902	0.716830	-0.907563
C	-1.530899	1.888584	-1.383525
H	-2.407175	2.055094	-0.745703
H	-1.925267	1.637068	-2.381629
C	-0.667916	3.143133	-1.478107
H	-1.233001	3.939153	-1.976858
H	-0.427996	3.506062	-0.465364
C	0.621709	2.845860	-2.231956
H	1.183244	3.766630	-2.427898
H	0.364217	2.416950	-3.212714
C	1.506049	1.862981	-1.465561
H	2.272385	1.444588	-2.132322
H	2.054107	2.388671	-0.671410
C	0.697618	0.726310	-0.903850
C	1.161769	-0.546718	-0.416369
Si	-2.940187	-1.227422	-0.202684
C	-3.293307	-2.429766	-1.599782
H	-3.218604	-1.931757	-2.575147

H	-4.307397	-2.840627	-1.507893
H	-2.585177	-3.267729	-1.593720
C	-4.222147	0.142202	-0.218136
H	-4.268020	0.675168	-1.175505
H	-4.052382	0.875720	0.581183
H	-5.208433	-0.310421	-0.043951
C	-3.047377	-2.091450	1.460806
H	-2.946231	-1.364538	2.278446
H	-2.273209	-2.858307	1.587165
H	-4.026113	-2.578104	1.568995
Si	2.917918	-1.208576	-0.220105
C	3.239915	-2.401411	-1.633223
H	4.258252	-2.807223	-1.570462
H	3.140755	-1.890197	-2.600043
H	2.536079	-3.242575	-1.621771
C	4.206657	0.154872	-0.286815
H	5.192693	-0.305629	-0.132522
H	4.074319	0.912445	0.495245
H	4.230925	0.663773	-1.258102
C	3.058453	-2.069782	1.441789
H	4.043458	-2.545292	1.540778
H	2.293662	-2.844884	1.574885
H	2.954756	-1.344893	2.261046
O	-1.971201	2.243849	2.025656
C	1.402648	1.341369	1.744527
O	2.294415	1.939918	2.161606
H	-0.376119	-0.888844	2.015326
Mn	-0.041854	0.455993	1.044644
N	-1.161857	1.473596	1.674875

6Co-a Gsolv= -2942.854404

C	0.003016	0.533628	-0.983384
O	0.068636	1.839285	-1.338884
C	1.154593	-0.303468	-0.779546
C	0.608305	-1.615634	-0.549085
C	-0.791413	-1.552965	-0.551040
C	-1.220785	-0.195241	-0.775233
Si	2.963563	0.216245	-0.976327
C	3.214769	0.570614	-2.799895
H	2.992941	-0.314337	-3.409583
H	4.254713	0.863327	-2.994077
H	2.564200	1.388072	-3.135719
C	4.037122	-1.216601	-0.431133
H	3.823881	-2.121772	-1.014743
H	3.895790	-1.447333	0.632347
H	5.094814	-0.965473	-0.584205
C	3.291268	1.754395	0.035615
H	3.132373	1.575417	1.106491
H	2.636797	2.576141	-0.282325
H	4.330502	2.079987	-0.104035
Si	-2.986023	0.473069	-0.910771
C	-3.310031	0.831114	-2.719879
H	-4.327934	1.217748	-2.857800
H	-3.206711	-0.076197	-3.327923
H	-2.607823	1.581746	-3.104247
C	-4.130539	-0.863590	-0.271658
H	-5.170690	-0.517303	-0.329623
H	-3.921248	-1.113691	0.776573
H	-4.053078	-1.781662	-0.868438
C	-3.154132	2.035232	0.107662
H	-4.197626	2.376215	0.090667
H	-2.535089	2.843823	-0.301908
H	-2.872903	1.869470	1.156443
C	1.345827	-0.656701	2.126417
C	-1.272575	-0.514151	2.146012
O	-2.070785	-0.613760	2.964681
H	0.034479	1.080568	1.437527
C	-1.336530	-2.919828	-0.313525
O	-0.185431	-3.666644	0.114399
C	1.029282	-3.024517	-0.311076
H	-1.745599	-3.340719	-1.246005
H	-2.102040	-2.989124	0.467309
H	1.782508	-3.161068	0.472733
H	1.401226	-3.482633	-1.241481
H	0.053684	2.449968	-0.557774
O	-0.113987	3.585364	0.733647
H	-0.909510	3.277101	1.191131
N	2.205153	-0.874209	2.898134
Co	-0.032895	-0.298375	0.915612
C	0.910413	3.793639	1.704228
H	1.784236	4.189471	1.180679
H	0.588117	4.522556	2.456459
H	1.187514	2.855386	2.204798

6Co-b Gsolv= -2942.854591

C	0.001807	0.540337	-0.973844
O	0.070390	1.848430	-1.319373
C	1.152652	-0.299692	-0.778113

C	0.605347	-1.612918	-0.556701
C	-0.794394	-1.548446	-0.556118
C	-1.222602	-0.188744	-0.769912
Si	2.961162	0.220530	-0.976513
C	3.205912	0.580431	-2.799738
H	2.980826	-0.301038	-3.413234
H	4.245514	0.871612	-2.998133
H	2.556988	1.400727	-3.131686
C	4.034503	-1.216319	-0.440331
H	3.812644	-2.120148	-1.022968
H	3.900645	-1.446962	0.624090
H	5.092477	-0.972267	-0.602126
C	3.288452	1.756383	0.039448
H	3.102861	1.583183	1.107079
H	2.653513	2.586572	-0.295696
H	4.334632	2.068792	-0.076805
Si	-2.984644	0.486367	-0.912609
C	-3.281317	0.844819	-2.726269
H	-4.290666	1.245582	-2.884160
H	-3.181787	-0.067829	-3.327072
H	-2.561599	1.581043	-3.106125
C	-4.139901	-0.846094	-0.284286
H	-5.179425	-0.501508	-0.359834
H	-3.946158	-1.083512	0.769956
H	-4.053474	-1.771221	-0.868553
C	-3.152914	2.042506	0.115240
H	-4.192423	2.394710	0.086666
H	-2.520001	2.849216	-0.275922
H	-2.890581	1.861970	1.166630
C	1.349692	-0.673894	2.122856
C	-1.273773	-0.534196	2.146437
O	-2.076855	-0.647438	2.958513
H	0.035401	1.068415	1.452459
C	-1.340712	-2.915822	-0.324194
O	-0.190234	-3.665491	0.099885
C	1.024836	-3.023534	-0.325782
H	-1.750397	-3.333341	-1.257829
H	-2.105672	-2.987476	0.456907
H	1.779482	-3.165351	0.455810
H	1.392497	-3.480114	-1.258554
H	0.039265	2.454461	-0.534871
O	-0.122971	3.578232	0.765252
H	-0.901990	3.257758	1.242515
N	2.210430	-0.892203	2.892766
Co	-0.032545	-0.306065	0.918892
C	0.927078	3.788202	1.707519
H	1.790372	4.171299	1.157760
H	0.629672	4.526766	2.460575
H	1.211209	2.853304	2.209916

6Co-c Gsolv= -2587.539023

C	-0.068506	0.510709	-0.976628
O	-0.049360	1.792952	-1.385669
C	1.080409	-0.343860	-0.792445
C	0.548705	-1.654867	-0.519037
C	-0.846490	-1.596074	-0.500423
C	-1.272399	-0.244511	-0.734075
C	1.389913	-0.601349	2.075403
C	-1.297112	-0.520441	2.170492
O	-2.119549	-0.629395	2.962536
H	-0.002785	1.080603	1.430739
C	-1.383428	-2.952829	-0.194055
O	-0.231119	-3.649936	0.302080
C	0.969008	-3.053937	-0.215081
H	-1.760792	-3.435315	-1.109758
H	-2.168796	-2.980426	0.568985
H	1.290714	-3.573710	-1.132195
C	-2.656998	0.240507	-0.813413
C	-3.018441	1.501689	-0.323357
C	-3.636614	-0.576315	-1.389705
C	-4.334409	1.940323	-0.421777
H	-2.268035	2.128861	0.153912
C	-4.953952	-0.134789	-1.484849
H	-3.363102	-1.555190	-1.781139
C	-5.305432	1.124263	-1.002850
H	-4.605773	2.919538	-0.034085
H	-5.705914	-0.777064	-1.937278
H	-6.334339	1.468992	-1.075226
C	2.500626	-0.001520	-0.934483
C	2.964901	1.312308	-0.788895
C	3.427160	-1.017508	-1.204194
C	4.320535	1.599645	-0.903589
H	2.266973	2.115518	-0.576401
C	4.782959	-0.727205	-1.322347
H	3.089953	-2.043111	-1.341670
C	5.235704	0.581663	-1.169158
H	4.662478	2.625084	-0.779771
H	5.486723	-1.528449	-1.535231

H	6.295899	0.807432	-1.256484
H	0.103791	2.435850	-0.643767
O	0.248292	3.590109	0.616141
H	-0.516090	3.390424	1.174873
H	1.757482	-3.146957	0.539871
N	2.330087	-0.764734	2.761918
Co	-0.061589	-0.304770	0.930686
C	1.413674	3.607481	1.440721
H	2.250455	3.944901	0.822530
H	1.287662	4.307039	2.274314
H	1.640825	2.607760	1.837623

6Co Gsolv= -2946.205799

Co	0.041550	0.171929	0.937476
C	-0.035415	-0.637089	-0.965089
O	-0.169403	-1.933452	-1.349604
H	0.579229	-3.565260	1.111354
C	-1.121586	0.270555	-0.757502
C	-0.507317	1.563662	-0.513242
C	-1.170896	2.879240	-0.257817
H	-2.062113	2.747114	0.366978
H	-1.523358	3.285280	-1.219937
C	-0.190404	3.855914	0.383520
H	-0.642678	4.853045	0.436963
H	0.014010	3.537902	1.419435
C	1.112907	3.898919	-0.404839
H	1.770760	4.692942	-0.033130
H	0.881377	4.143655	-1.452928
C	1.849033	2.560927	-0.348164
H	2.611212	2.512871	-1.138346
H	2.392834	2.466156	0.602604
C	0.899225	1.412834	-0.526506
C	1.221166	0.013942	-0.742920
Si	-2.939998	-0.192638	-1.019885
C	-3.137766	-0.430158	-2.870654
H	-2.871443	0.485090	-3.415087
H	-4.178089	-0.678448	-3.118219
H	-2.498677	-1.241859	-3.240647
C	-4.100385	1.158357	-0.438565
H	-3.962016	2.095635	-0.990935
H	-3.995780	1.365138	0.633899
H	-5.130985	0.819793	-0.613053
C	-3.317676	-1.784423	-0.109984
H	-3.165186	-1.673333	0.971087
H	-2.690880	-2.610540	-0.467822
H	-4.367372	-2.062220	-0.274958
Si	2.911344	-0.829896	-0.888231
C	3.230445	-1.058227	-2.720905
H	4.214962	-1.510166	-2.896499
H	3.205204	-0.090601	-3.239258
H	2.471948	-1.706065	-3.178453
C	4.257281	0.222746	-0.118086
H	5.197281	-0.344771	-0.155757
H	4.053592	0.448868	0.936448
H	4.418246	1.167442	-0.650208
C	2.871189	-2.472321	0.013245
H	3.867013	-2.933456	-0.028452
H	2.159710	-3.176234	-0.435148
H	2.614380	-2.330205	1.072574
C	-1.335041	0.572215	2.141956
C	1.276260	0.319004	2.179217
O	2.066445	0.386016	3.010589
H	-0.097266	-1.213454	1.429599
O	-0.284234	-3.735396	0.708180
H	-0.317617	-2.542104	-0.584656
N	-2.188504	0.807647	2.915738
C	-1.251752	-3.847806	1.748955
H	-2.203317	-4.122686	1.287089
H	-0.966336	-4.629757	2.461853
H	-1.377881	-2.896991	2.286170

6Fe-Casey Gsolv= -2844.318654

Fe	0.037720	-0.382098	0.967615
C	0.005158	0.641024	-0.866526
O	0.044265	1.980953	-1.084070
C	1.200549	-0.149455	-0.768111
C	0.721944	-1.500046	-0.647125
C	-0.680831	-1.506617	-0.620605
C	-1.180870	-0.160366	-0.733391
Si	2.983727	0.448000	-0.901769
C	3.252346	1.042202	-2.660086
H	3.065080	0.237484	-3.382209
H	4.282565	1.392971	-2.802511
H	2.576786	1.873989	-2.897933
C	4.088065	-1.018360	-0.521887
H	3.926412	-1.846221	-1.224368
H	3.929968	-1.394789	0.497333
H	5.140884	-0.717122	-0.602485

C	3.323848	1.837675	0.307565
H	3.092648	1.543414	1.339705
H	2.746161	2.738303	0.065273
H	4.388401	2.105118	0.266294
Si	-2.990283	0.348066	-0.900668
C	-3.254981	0.848592	-2.688034
H	-4.301430	1.128778	-2.864675
H	-3.007309	0.023484	-3.367965
H	-2.626276	1.707840	-2.955226
C	-4.025980	-1.152944	-0.469002
H	-5.091627	-0.904919	-0.559742
H	-3.848980	-1.482667	0.563285
H	-3.825443	-1.997711	-1.140585
C	-3.415225	1.768824	0.240043
H	-4.495232	1.962764	0.195816
H	-2.898628	2.691196	-0.052698
H	-3.157507	1.541537	1.283305
C	1.320849	-0.833630	2.068975
O	2.181185	-1.132732	2.787054
C	-1.246274	-0.746786	2.102052
O	-2.107398	-0.974476	2.845013
H	0.084584	0.993410	1.604635
C	-1.153984	-2.919091	-0.536677
O	0.039901	-3.652304	-0.211194
C	1.211880	-2.906930	-0.584479
H	-1.556366	-3.256228	-1.505951
H	-1.900288	-3.121424	0.239926
H	1.992643	-3.103267	0.159126
H	1.576000	-3.237198	-1.570920
H	-0.430268	2.488642	-0.380129
O	-0.813192	3.560049	0.958070
H	-1.223241	3.007183	1.638733
C	0.436477	4.033803	1.454256
H	0.935602	4.556800	0.633750
H	0.288530	4.735045	2.283936
H	1.071457	3.203928	1.791628

6Fe Gsolv= -2847.666701

Fe	0.030667	0.190818	0.963348
C	-0.037470	-0.627841	-0.954734
O	-0.188224	-1.931340	-1.338498
H	0.568311	-3.636734	1.092329
C	-1.117348	0.291654	-0.781437
C	-0.491989	1.572651	-0.516931
C	-1.143367	2.902135	-0.286286
H	-2.038592	2.794137	0.338485
H	-1.488191	3.299314	-1.255172
C	-0.157461	3.881945	0.342339
H	-0.598185	4.885712	0.367903
H	0.033986	3.586810	1.387362
C	1.153963	3.891094	-0.433498
H	1.815455	4.689784	-0.077566
H	0.934129	4.109659	-1.490264
C	1.875684	2.547939	-0.333258
H	2.656249	2.481886	-1.103997
H	2.396467	2.472693	0.632291
C	0.916439	1.404261	-0.510966
C	1.225958	0.008308	-0.741298
Si	-2.932111	-0.163841	-1.031860
C	-3.187080	-0.406578	-2.875211
H	-2.949830	0.509820	-3.430928
H	-4.230587	-0.670671	-3.091284
H	-2.547602	-1.210409	-3.261842
C	-4.078766	1.184142	-0.410672
H	-3.959815	2.126663	-0.958558
H	-3.940535	1.383591	0.659851
H	-5.114288	0.845025	-0.552232
C	-3.314415	-1.748975	-0.106994
H	-3.160847	-1.623363	0.973004
H	-2.687105	-2.580250	-0.451851
H	-4.364475	-2.028575	-0.267347
Si	2.901060	-0.849656	-0.881352
C	3.240651	-1.102734	-2.709645
H	4.218014	-1.576737	-2.867933
H	3.242608	-0.140811	-3.239314
H	2.475368	-1.739737	-3.171529
C	4.266294	0.187646	-0.119568
H	5.199974	-0.390097	-0.162148
H	4.069548	0.417268	0.935488
H	4.434911	1.130511	-0.652868
C	2.864637	-2.495965	0.018009
H	3.859916	-2.957996	-0.033019
H	2.150210	-3.197688	-0.429509
H	2.613333	-2.360044	1.079308
C	-1.263213	0.534877	2.087202
O	-2.133153	0.735713	2.830285
C	1.299350	0.361190	2.152479
O	2.150280	0.466141	2.935984

H	-0.087309	-1.238341	1.436623
O	-0.287261	-3.819690	0.678024
H	-0.310192	-2.536015	-0.569577
C	-1.266174	-3.936648	1.706682
H	-2.213023	-4.207269	1.232169
H	-0.991857	-4.723287	2.419160
H	-1.395948	-2.988363	2.247225

6Fe-Renaud Gsolv= -2602.945728

Fe	-0.156524	-0.115672	1.134812
C	-0.028634	0.910362	-0.685248
O	0.064224	2.239640	-0.892845
H	1.119423	3.800684	1.421088
C	1.039926	-0.030644	-0.566233
C	0.413292	-1.338651	-0.489707
C	0.102464	-3.608043	0.016198
H	0.569415	-4.591399	-0.102456
H	-0.104219	-3.459444	1.086791
C	-1.193007	-3.539891	-0.775843
H	-1.875271	-4.335517	-0.461287
H	-0.980739	-3.699974	-1.842273
C	-0.999761	-1.179706	-0.544894
C	-1.285363	0.240189	-0.583472
C	0.967625	-0.755812	2.315877
O	1.711734	-1.159797	3.110968
C	-1.500936	-0.127996	2.259262
O	-2.370461	-0.039676	3.025805
H	0.117156	1.242775	1.744066
O	1.786856	3.535026	0.773201
H	0.806174	2.634419	-0.369990
C	2.847585	2.882878	1.467999
H	3.592268	2.585902	0.723923
H	3.316730	3.562575	2.188939
H	2.490271	1.987344	1.995675
C	-2.597565	0.903192	-0.730727
C	-2.986843	1.949531	0.114064
C	-3.459831	0.510239	-1.761395
C	-4.213443	2.583240	-0.063117
H	-2.324130	2.259791	0.920905
C	-4.689685	1.140875	-1.934432
H	-3.161768	-0.290824	-2.435028
C	-5.070873	2.178219	-1.085326
H	-4.501802	3.392505	0.604174
H	-5.350021	0.822784	-2.738172
H	-6.031879	2.669864	-1.218740
C	2.473259	0.269141	-0.758874
C	3.473743	-0.259451	0.065752
C	2.853126	1.072141	-1.842784
C	4.816286	0.002016	-0.190672
H	3.205648	-0.871685	0.923158
C	4.196404	1.343388	-2.092982
H	2.089066	1.477956	-2.503376
C	5.183565	0.806847	-1.268952
H	5.578823	-0.418963	0.461053
H	4.470584	1.969278	-2.939392
H	6.233238	1.013641	-1.465105
N	-1.885072	-2.251484	-0.611587
N	1.060632	-2.583385	-0.414960
C	-2.948408	-2.278623	0.384781
H	-2.555458	-2.523592	1.387365
H	-3.457208	-1.311263	0.436239
H	-3.690390	-3.033124	0.104953
C	1.756023	-2.932743	-1.656728
H	2.464929	-2.142355	-1.925245
H	2.320066	-3.858624	-1.503285
H	1.067290	-3.076913	-2.505573

6Fe-williams-1 Gsolv= -2798.124294

Fe	-0.005921	-0.586337	1.159483
C	-0.186997	-1.431885	-0.774250
O	-0.408382	-2.715749	-1.111588
H	-1.210601	-3.075583	-0.654581
C	-1.151684	-0.393616	-0.591020
C	-0.408358	0.822904	-0.331487
C	0.979806	0.515129	-0.329232
C	1.121468	-0.906196	-0.566211
C	-1.122280	0.004560	2.376412
O	-1.862703	0.359935	3.194643
C	1.269113	-0.845365	2.331467
O	2.090279	-1.078163	3.116662
H	-0.442760	-1.959511	1.605353
C	-2.606662	-0.510543	-0.810845
C	-3.540551	0.135701	0.009951
C	-3.073152	-1.239320	-1.912475
C	-4.902005	0.049602	-0.261103
H	-3.204169	0.712458	0.869609
C	-4.437305	-1.328750	-2.181230
H	-2.361316	-1.730590	-2.573205

C	-5.356988	-0.685229	-1.356244
H	-5.611651	0.557237	0.388442
H	-4.779077	-1.897372	-3.043259
H	-6.422227	-0.752393	-1.565314
C	2.382339	-1.654289	-0.738440
C	2.630101	-2.843471	-0.042663
C	3.343849	-1.183883	-1.641525
C	3.815717	-3.544802	-0.243329
H	1.892290	-3.211930	0.668989
C	4.531795	-1.883742	-1.837426
H	3.156217	-0.266318	-2.197955
C	4.771075	-3.065778	-1.138946
H	3.995984	-4.465467	0.307153
H	5.270495	-1.505309	-2.540428
H	5.699399	-3.611976	-1.290162
C	2.071680	1.510532	-0.262819
C	3.097298	1.459934	0.685991
C	2.094057	2.525670	-1.228172
C	4.117020	2.408949	0.675667
H	3.099563	0.679222	1.443755
C	3.112717	3.474326	-1.238614
H	1.305868	2.565982	-1.979244
C	4.127271	3.419747	-0.284177
H	4.904448	2.359353	1.424428
H	3.113912	4.255788	-1.995205
H	4.922821	4.161353	-0.288055
C	-0.973667	2.181176	-0.195914
C	-1.765980	2.696839	-1.227598
C	-0.679918	2.990476	0.906592
C	-2.256179	3.998442	-1.156905
H	-1.989374	2.075629	-2.094298
C	-1.168439	4.292222	0.975514
H	-0.064988	2.591991	1.713696
C	-1.958540	4.799645	-0.055572
H	-2.869000	4.388018	-1.966725
H	-0.933982	4.910851	1.838906
H	-2.341785	5.816009	-0.000230
O	-2.303568	-3.941218	0.399988
H	-1.679137	-4.312446	1.038777
C	-3.317775	-3.244613	1.120990
H	-4.027907	-2.850669	0.388102
H	-3.848932	-3.923318	1.798255
H	-2.898084	-2.410935	1.700665

6Fe-williams-2 Gsolv= -2987.084745

Fe	0.054685	-0.410517	0.960150
C	-0.221168	-1.646068	-0.735390
O	-0.387532	-2.982903	-0.775200
C	-1.253412	-0.647770	-0.686341
C	-0.570617	0.614637	-0.742561
C	-0.886616	2.069186	-0.868011
H	-1.693727	2.436162	-0.228766
H	-1.149834	2.300667	-1.909446
C	0.482103	2.713340	-0.512040
C	1.559466	1.680169	-0.937456
H	1.819749	1.848686	-1.991670
H	2.482265	1.751135	-0.354664
C	0.815768	0.392965	-0.800720
C	1.071781	-1.021106	-0.760319
C	-1.025633	0.276890	2.161146
O	-1.734207	0.687280	2.982779
C	1.503515	-0.186095	1.918212
O	2.493181	-0.082837	2.513514
H	-0.121543	-1.692322	1.743822
C	0.512540	3.017050	0.995304
O	-0.474505	3.293414	1.649698
O	1.744878	3.018388	1.487135
C	0.709030	4.056052	-1.189573
O	1.774961	4.411059	-1.656086
O	-0.384819	4.808620	-1.174908
C	1.861459	3.283922	2.895845
H	2.922920	3.193656	3.125825
H	1.505640	4.293397	3.118488
H	1.283529	2.546922	3.463207
C	-0.265435	6.119364	-1.756652
H	-1.239639	6.589575	-1.626225
H	0.507789	6.691924	-1.237723
H	-0.022867	6.036077	-2.819323
C	2.382961	-1.686442	-0.833964
C	2.670732	-2.848230	-0.103176
C	3.384621	-1.147660	-1.647605
C	3.919035	-3.449126	-0.196813
H	1.915935	-3.269793	0.558515
C	4.636167	-1.754152	-1.733495
H	3.182048	-0.250161	-2.230342
C	4.924543	-2.915593	-1.014086
H	4.127409	-4.347195	0.384383
H	5.402513	-1.316538	-2.372304

C	-2.708249	-0.872362	-0.749550
C	-3.234912	-1.865507	-1.586573
C	-3.600895	-0.070852	-0.029535
C	-4.608465	-2.057437	-1.682403
H	-2.563249	-2.486621	-2.176637
C	-4.974898	-0.266148	-0.132838
H	-3.220700	0.716934	0.619086
C	-5.503879	-1.265993	-0.954500
H	-4.997486	-2.832657	-2.342250
H	-5.651192	0.369817	0.437312
C	6.260557	-3.585352	-1.113135
H	6.639367	-3.867434	-0.123625
H	6.197120	-4.508417	-1.704005
H	7.000797	-2.935735	-1.591961
C	-6.980981	-1.492491	-1.056823
H	-7.543874	-0.679739	-0.585888
H	-7.299927	-1.570452	-2.103089
H	-7.273505	-2.428964	-0.564614
H	-1.143963	-3.245716	-0.194836
O	-2.190078	-3.498742	1.227627
H	-2.115638	-2.595630	1.577027
C	-1.427736	-4.362424	2.068539
H	-1.520311	-5.373771	1.664864
H	-0.366029	-4.078501	2.075486
H	-1.808716	-4.352710	3.096055

6Fe-wills-1 Gsolv= -2489.003426

Fe	-0.072872	-0.312254	0.949589
C	-0.059529	0.508791	-0.969533
O	-0.012599	1.799330	-1.378327
C	1.077143	-0.360675	-0.802590
C	0.528619	-1.658093	-0.518480
C	-0.870294	-1.578713	-0.499252
C	-1.278877	-0.227827	-0.749563
C	1.289021	-0.499069	2.036742
O	2.229237	-0.583937	2.709672
C	-1.329711	-0.595847	2.138265
O	-2.195744	-0.761241	2.890506
H	-0.101440	1.114959	1.433007
C	-1.422464	-2.933797	-0.208352
O	-0.278976	-3.653727	0.279828
C	0.929513	-3.067283	-0.231323
H	-1.805919	-3.406370	-1.127267
H	-2.207028	-2.964209	0.556295
H	1.243907	-3.586267	-1.151805
C	-2.657271	0.275903	-0.833642
C	-2.987043	1.588047	-0.465855
C	-3.674340	-0.576562	-1.281063
C	-4.301106	2.034849	-0.556634
H	-2.212973	2.256651	-0.094374
C	-4.990181	-0.127848	-1.365706
H	-3.433513	-1.595518	-1.581167
C	-5.307875	1.179723	-1.005788
H	-4.542109	3.054970	-0.265857
H	-5.767130	-0.803113	-1.716987
H	-6.334824	1.531702	-1.071339
C	2.503427	-0.033272	-0.944707
C	2.987332	1.272200	-0.781354
C	3.417871	-1.054997	-1.234060
C	4.345530	1.545374	-0.903569
H	2.300841	2.080543	-0.550336
C	4.777169	-0.779537	-1.356420
H	3.066279	-2.074315	-1.383795
C	5.247702	0.521244	-1.190074
H	4.699936	2.565281	-0.768011
H	5.469515	-1.586788	-1.584397
H	6.309775	0.735973	-1.282893
H	0.140923	2.428264	-0.629577
O	0.298982	3.608279	0.654779
H	-0.461629	3.377018	1.207168
H	1.715715	-3.181806	0.523882
C	1.466380	3.588741	1.474859
H	1.675596	2.577643	1.853562
H	2.307479	3.920857	0.859520
H	1.357982	4.275372	2.321989

6Fe-wills-2 Gsolv= -2528.270408

Fe	0.120766	0.250266	0.952884
C	0.133473	-0.632041	-0.937016
O	0.118712	-1.934592	-1.308622
C	-1.038259	0.190268	-0.797199
C	-0.558828	1.521537	-0.558688
C	0.843943	1.504292	-0.555928
C	1.319842	0.170182	-0.756130
C	-1.245184	0.197618	2.049385
O	-2.161461	0.108844	2.754753
C	1.281100	0.800868	2.145799
O	2.082006	1.154864	2.905038

H	0.404472	-1.135426	1.476242
C	1.339950	2.897201	-0.363041
O	0.173989	3.602982	0.078508
C	-1.032399	2.929053	-0.355229
H	1.700905	3.311711	-1.318682
H	2.130251	3.016408	0.387444
H	-1.338612	3.347411	-1.330984
C	-2.110178	3.166156	0.670167
H	-1.764831	2.844827	1.660258
H	-2.368932	4.229373	0.714586
H	-3.015603	2.603175	0.413390
C	-2.433204	-0.243018	-0.970571
C	-2.877188	-1.486346	-0.503674
C	-3.337743	0.591806	-1.638191
C	-4.194544	-1.886024	-0.701922
H	-2.188241	-2.135150	0.032559
C	-4.657608	0.191835	-1.832825
H	-3.002417	1.555982	-2.018396
C	-5.090063	-1.047926	-1.366126
H	-4.524243	-2.853371	-0.328616
H	-5.348598	0.851190	-2.353235
H	-6.120991	-1.359702	-1.517077
C	2.722773	-0.259479	-0.848221
C	3.130506	-1.546126	-0.469681
C	3.685625	0.637761	-1.328429
C	4.464986	-1.923479	-0.576846
H	2.402974	-2.250960	-0.074223
C	5.022297	0.259723	-1.428459
H	3.385746	1.636427	-1.642782
C	5.416857	-1.022839	-1.054686
H	4.764816	-2.925041	-0.276284
H	5.755126	0.970082	-1.804529
H	6.460137	-1.319909	-1.132509
H	0.102926	-2.551493	-0.534116
O	0.184289	-3.713531	0.754019
H	0.933890	-3.410753	1.285828
C	-0.943986	-3.846503	1.615349
H	-1.221766	-2.883208	2.065858
H	-1.777988	-4.213649	1.010683
H	-0.742210	-4.570484	2.412988

6Fe-wills-3 Gsolv= -2705.927961

Fe	0.305571	0.224999	0.924477
C	0.154926	-0.650541	-0.965014
O	0.042027	-1.959703	-1.311088
C	-0.952345	0.245061	-0.761978
C	-0.364025	1.539319	-0.557972
C	1.032475	1.414151	-0.623411
C	1.407066	0.046783	-0.845688
Si	3.129576	-0.696418	-1.026786
C	3.365899	-1.184927	-2.821675
H	2.624510	-1.936000	-3.122894
H	4.364302	-1.612629	-2.980148
H	3.259275	-0.318395	-3.486158
C	4.363347	0.624119	-0.530113
H	5.383833	0.227872	-0.614809
H	4.218017	0.946351	0.509374
H	4.297513	1.507774	-1.177883
C	3.310251	-2.200735	0.074992
H	4.326516	-2.607005	-0.017150
H	2.609229	-2.994252	-0.213952
H	3.141659	-1.952844	1.131148
C	-0.999473	0.329601	2.086097
O	-1.889354	0.336643	2.830438
C	1.574887	0.612495	2.069470
O	2.430245	0.836965	2.819539
H	0.432194	-1.187033	1.438841
C	1.640672	2.768286	-0.477789
O	0.545575	3.582469	-0.034635
C	-0.728115	2.978634	-0.366760
H	2.018706	3.126870	-1.448910
H	2.448782	2.846250	0.258617
H	-1.072513	3.390254	-1.332553
C	-2.381948	-0.088596	-0.859957
C	-2.891598	-1.284130	-0.338405
C	-3.254988	0.791747	-1.510949
C	-4.241782	-1.592770	-0.466854
H	-2.226933	-1.965900	0.187770
C	-4.607461	0.483507	-1.635602
H	-2.869692	1.718690	-1.933666
C	-5.105006	-0.709826	-1.115316
H	-4.621734	-2.523868	-0.051385
H	-5.273055	1.177771	-2.143607
H	-6.161454	-0.949691	-1.211584
C	-1.720611	3.313314	0.716934
H	-1.333550	2.998414	1.693582
H	-1.910255	4.391630	0.744721
H	-2.673726	2.801911	0.534302

H	-0.041598	-2.555508	-0.525979
O	0.023389	-3.731310	0.760386
H	0.823692	-3.474069	1.240760
C	-1.053093	-3.801590	1.691406
H	-1.950946	-4.086260	1.135504
H	-0.857726	-4.561408	2.456969
H	-1.223476	-2.832941	2.182066

6Fe-wills-4 Gsolv= -2666.660198

Fe	-0.257280	-0.291435	0.932302
C	-0.097637	0.534548	-0.982011
O	0.062163	1.830006	-1.360789
C	0.966152	-0.413972	-0.775228
C	0.306869	-1.667294	-0.530092
C	-1.082165	-1.470621	-0.565220
C	-1.382266	-0.089540	-0.820447
Si	-3.057575	0.759096	-0.981936
C	-3.294595	1.247365	-2.776713
H	-2.520447	1.956927	-3.095647
H	-4.271938	1.725265	-2.922792
H	-3.244900	0.372309	-3.436803
C	-4.356180	-0.483597	-0.453538
H	-5.356857	-0.040516	-0.540994
H	-4.219960	-0.793306	0.591017
H	-4.337674	-1.381996	-1.084216
C	-3.111733	2.281940	0.109432
H	-4.076560	2.793433	-0.006355
H	-2.322052	2.993582	-0.165319
H	-2.991622	2.024417	1.169726
C	1.064565	-0.560829	2.047658
O	1.982331	-0.710907	2.740536
C	-1.533610	-0.532873	2.110356
O	-2.387819	-0.668896	2.882572
H	-0.230279	1.132514	1.428543
C	-1.752886	-2.784848	-0.340996
O	-0.689676	-3.623980	0.141955
C	0.585998	-3.110345	-0.276707
H	-2.154520	-3.182907	-1.286806
H	-2.553643	-2.784970	0.406628
H	1.316540	-3.311405	0.515681
H	0.915855	-3.619107	-1.197487
C	2.417632	-0.189793	-0.850311
C	2.985435	1.067107	-0.600304
C	3.267838	-1.259984	-1.158280
C	4.363190	1.246360	-0.656569
H	2.347543	1.908250	-0.346768
C	4.647521	-1.078788	-1.214290
H	2.849608	-2.242294	-1.370938
C	5.201521	0.174348	-0.961936
H	4.783230	2.229348	-0.452724
H	5.290216	-1.922120	-1.456765
H	6.279136	0.315485	-1.001496
H	0.211327	2.435468	-0.593319
O	0.357029	3.614884	0.694389
H	-0.427318	3.412592	1.224999
C	1.501619	3.552509	1.541917
H	1.652336	2.539647	1.942812
H	2.372066	3.831986	0.941353
H	1.409407	4.258340	2.375279

6Fe-wills-5 Gsolv= -2823.695314

Fe	0.395756	-0.470580	1.132847
C	-0.002422	0.706294	-0.545478
O	-0.051347	2.057165	-0.667224
C	1.178426	-0.080221	-0.782823
C	0.756269	-1.447894	-0.682343
C	-0.616577	-1.471559	-0.388165
C	-1.133747	-0.139979	-0.260894
Si	-2.910303	0.380564	0.100902
C	-3.750767	-1.021990	1.023893
H	-4.808561	-0.774257	1.186870
H	-3.294986	-1.176389	2.010652
H	-3.714502	-1.972632	0.477416
C	-2.941954	1.914326	1.180097
H	-3.977278	2.145082	1.464743
H	-2.523534	2.797346	0.681806
H	-2.378284	1.735835	2.106454
C	-3.781024	0.677004	-1.568694
C	1.967260	-0.536778	1.898883
O	3.016111	-0.527307	2.394420
C	-0.430400	-1.279153	2.450997
O	-0.981329	-1.806086	3.324614
H	0.224172	0.800644	1.928366
C	-1.074548	-2.890737	-0.357254
O	0.147670	-3.641875	-0.368261
C	1.258401	-2.847037	-0.850823
H	-1.677949	-3.118919	-1.251546
H	-1.648868	-3.183037	0.529655

H	1.396641	-3.051493	-1.927516
C	-5.194903	1.203261	-1.318550
H	-5.726055	1.331973	-2.275600
H	-5.793332	0.515517	-0.704068
H	-5.184110	2.180647	-0.816100
C	2.511322	0.427740	-1.144879
C	3.031385	1.591085	-0.563126
C	3.275258	-0.247272	-2.104911
C	4.284221	2.067977	-0.933207
H	2.456292	2.114031	0.197879
C	4.530991	0.230423	-2.473377
H	2.878994	-1.145877	-2.576020
C	5.039281	1.388977	-1.889261
H	4.674549	2.969833	-0.466319
H	5.112285	-0.304370	-3.221181
H	6.020491	1.760721	-2.175453
C	2.498910	-3.237681	-0.088506
H	2.325816	-3.128702	0.989334
H	2.769487	-4.277654	-0.300020
H	3.342659	-2.598130	-0.375596
H	0.097733	2.524442	0.192311
O	0.224817	3.495182	1.622394
H	-0.432124	3.099004	2.212703
C	1.479344	3.522745	2.298199
H	1.818886	2.510176	2.557447
H	2.205994	3.981078	1.621473
H	1.418593	4.126442	3.210996
C	-3.008643	1.696692	-2.405276
H	-2.922650	2.668534	-1.899021
H	-1.993404	1.349313	-2.642998
H	-3.527744	1.870271	-3.361933
C	-3.857400	-0.643655	-2.335866
H	-2.859811	-1.069844	-2.520174
H	-4.452398	-1.398320	-1.802558
H	-4.331880	-0.486116	-3.318007

6Mn-a Gsolv= -2748.205489

C	0.018184	0.667590	-0.839010
O	0.066999	2.008221	-1.036349
C	1.204571	-0.131938	-0.780329
C	0.720655	-1.478321	-0.688090
C	-0.682992	-1.483429	-0.651149
C	-1.173863	-0.133264	-0.717314
Si	2.998292	0.446190	-0.885972
C	3.285854	1.051534	-2.636538
H	3.104456	0.252563	-3.366416
H	4.317518	1.402597	-2.766601
H	2.612812	1.885560	-2.873862
C	4.068622	-1.043207	-0.501822
H	3.885502	-1.871683	-1.198341
H	3.897559	-1.408313	0.519828
H	5.129217	-0.771285	-0.582240
C	3.339791	1.816986	0.342446
H	3.093885	1.509003	1.367253
H	2.773100	2.726268	0.106736
H	4.407491	2.072873	0.316763
Si	-2.979250	0.393281	-0.894461
C	-3.198392	0.979014	-2.661988
H	-4.233083	1.297953	-2.841810
H	-2.962432	0.176985	-3.372873
H	-2.539174	1.829123	-2.879825
C	-4.035797	-1.119523	-0.571108
H	-5.092858	-0.862586	-0.720691
H	-3.928596	-1.489106	0.456784
H	-3.797508	-1.940407	-1.259806
C	-3.422481	1.764402	0.299718
H	-4.503667	1.951565	0.253330
H	-2.913313	2.701133	0.041039
H	-3.171400	1.503987	1.336478
O	2.122680	-1.144558	2.771024
C	-1.344368	-0.872722	2.055303
O	-2.247426	-1.175606	2.714959
H	-0.172604	1.010584	1.538861
C	-1.157829	-2.897729	-0.623521
O	0.032725	-3.641052	-0.309772
C	1.209138	-2.886569	-0.647680
H	-1.546876	-3.198587	-1.609916
H	-1.914207	-3.128508	0.134934
H	1.977544	-3.095279	0.105942
H	1.592746	-3.194832	-1.633778
H	-0.427269	2.513470	-0.344304
O	-0.806102	3.626035	0.966603
H	-1.249143	3.112002	1.656792
N	1.232046	-0.825060	2.066832
Mn	0.051946	-0.423682	1.016558
C	0.459308	4.054511	1.465239
H	0.980009	4.555064	0.644195
H	0.335962	4.764067	2.291703

H	1.061346	3.202318	1.807444

6Mn-b Gsolv= -2890.969156

C	-0.224212	-1.656956	-0.735273
O	-0.386532	-2.991627	-0.791984
C	-1.256395	-0.662216	-0.709230
C	-0.576901	0.597644	-0.752744
C	-0.899365	2.051376	-0.873168
H	-1.706509	2.411951	-0.229928
H	-1.171552	2.280708	-1.912552
C	0.467348	2.705922	-0.523913
C	1.550229	1.674115	-0.937641
H	1.810453	1.833720	-1.993340
H	2.471933	1.755782	-0.354799
C	0.813606	0.383768	-0.789885
C	1.068951	-1.027871	-0.743163
O	-1.596097	0.852447	2.952190
C	1.593956	-0.198755	1.878636
O	2.624859	-0.086180	2.394351
H	-0.021843	-1.785864	1.646676
C	0.494766	3.037714	0.978644
O	-0.488380	3.374056	1.610441
O	1.719424	2.998490	1.487442
C	0.688034	4.041999	-1.217975
O	1.757534	4.401417	-1.673055
O	-0.413184	4.782868	-1.228978
C	1.830352	3.293332	2.890462
H	2.881122	3.147257	3.140011
H	1.531950	4.327587	3.081968
H	1.201816	2.608233	3.468845
C	-0.298854	6.089605	-1.820584
H	-1.278478	6.552169	-1.704277
H	0.463589	6.673277	-1.298093
H	-0.044138	5.999787	-2.879838
C	2.381041	-1.692377	-0.817183
C	2.663963	-2.870700	-0.111368
C	3.389167	-1.133683	-1.609323
C	3.913920	-3.467611	-0.208439
H	1.904959	-3.309278	0.533755
C	4.642241	-1.736240	-1.698198
H	3.191110	-0.223975	-2.174206
C	4.926049	-2.913753	-1.003716
H	4.118112	-4.379246	0.352721
H	5.413169	-1.282731	-2.320123
C	-2.709819	-0.889993	-0.757554
C	-3.245387	-1.874816	-1.598397
C	-3.591274	-0.103590	-0.007238
C	-4.619558	-2.071610	-1.671488
H	-2.580695	-2.484541	-2.207936
C	-4.965624	-0.305444	-0.086832
H	-3.200117	0.672903	0.648862
C	-5.504345	-1.295726	-0.914177
H	-5.017761	-2.838908	-2.334970
H	-5.634613	0.316383	0.506966
C	6.264148	-3.578595	-1.105987
H	6.640323	-3.871187	-0.118507
H	6.205275	-4.494921	-1.707656
H	7.004144	-2.921137	-1.574350
C	-6.981508	-1.531410	-0.987194
H	-7.540978	-0.710692	-0.526134
H	-7.317306	-1.637360	-2.025533
H	-7.260709	-2.456854	-0.466911
H	-1.145078	-3.264771	-0.217986
O	-2.183144	-3.532779	1.193919
H	-2.087592	-2.638376	1.559891
Mn	0.028970	-0.380957	1.016122
N	-0.915924	0.322777	2.147187
C	-1.431667	-4.427627	2.011643
H	-1.540543	-5.427645	1.584529
H	-0.365833	-4.159743	2.022555
H	-1.810001	-4.436586	3.040131

6Mn-c Gsolv= -2392.891458

C	-0.031442	0.534358	-0.953510
O	0.014603	1.826521	-1.352922
C	1.103867	-0.338768	-0.817681
C	0.556796	-1.636433	-0.560478
C	-0.844194	-1.566157	-0.534180
C	-1.251269	-0.212165	-0.756080
O	2.100646	-0.814969	2.739976
C	-1.476469	-0.596298	2.065143
O	-2.427051	-0.755347	2.706537
H	-0.254121	1.143837	1.342616
C	-1.386757	-2.935866	-0.296469
O	-0.241051	-3.659692	0.180153
C	0.965753	-3.049117	-0.302874
H	-1.753945	-3.380657	-1.235770
H	-2.178668	-3.003017	0.457937

H	1.294663	-3.538365	-1.234448
C	-2.632065	0.287046	-0.840400
C	-2.969992	1.602219	-0.491729
C	-3.645976	-0.579918	-1.267236
C	-4.288493	2.036619	-0.579653
H	-2.200628	2.283747	-0.135521
C	-4.965971	-0.143605	-1.348944
H	-3.399823	-1.601563	-1.552949
C	-5.291840	1.166692	-1.006891
H	-4.535277	3.059278	-0.303097
H	-5.739619	-0.830835	-1.683790
H	-6.322075	1.509319	-1.069694
C	2.529130	-0.001709	-0.931288
C	2.999123	1.307817	-0.755715
C	3.456864	-1.014641	-1.211562
C	4.356680	1.592563	-0.854209
H	2.301226	2.109400	-0.535691
C	4.814960	-0.726675	-1.311989
H	3.117725	-2.036211	-1.372833
C	5.271383	0.577386	-1.132081
H	4.700385	2.614721	-0.709118
H	5.517648	-1.526546	-1.533868
H	6.332852	0.801450	-1.207850
H	0.131033	2.458523	-0.599116
O	0.255337	3.651211	0.664462
H	-0.514289	3.431261	1.208732
H	1.746798	-3.177545	0.455729
N	1.158667	-0.601984	2.063175
Mn	-0.049676	-0.338831	0.999324
C	1.412620	3.618833	1.498175
H	2.263364	3.949377	0.895474
H	1.298471	4.299849	2.348869
H	1.609394	2.603755	1.871340

6Mn Gsolv= -2751.551705

C	-0.029105	-0.652681	-0.926144
O	-0.137324	-1.962200	-1.295489
H	0.894586	-3.718170	1.086759
C	-1.144656	0.227024	-0.802212
C	-0.578788	1.534245	-0.559431
C	-1.289878	2.836385	-0.353873
H	-2.181715	2.698620	0.269851
H	-1.650109	3.196152	-1.331476
C	-0.352402	3.873852	0.256399
H	-0.840203	4.855767	0.256535
H	-0.151854	3.613074	1.308602
C	0.960340	3.925222	-0.514818
H	1.582484	4.761878	-0.175897
H	0.735363	4.108579	-1.577118
C	1.743695	2.619469	-0.380480
H	2.519561	2.568149	-1.157243
H	2.275379	2.595456	0.581458
C	0.836651	1.428577	-0.519290
C	1.204884	0.042441	-0.707642
Si	-2.941369	-0.325991	-1.000428
C	-3.215440	-0.682626	-2.821785
H	-3.053733	0.217812	-3.428066
H	-4.243683	-1.025588	-2.996445
H	-2.533304	-1.461501	-3.185250
C	-4.139329	1.000465	-0.433273
H	-4.063476	1.923775	-1.019919
H	-4.004702	1.249367	0.627416
H	-5.160094	0.611736	-0.553650
C	-3.232840	-1.868862	0.023492
H	-3.042312	-1.678654	1.088401
H	-2.590221	-2.695518	-0.302818
H	-4.277559	-2.192235	-0.079429
Si	2.924646	-0.720707	-0.888340
C	3.221658	-0.910018	-2.730947
H	4.216470	-1.329463	-2.929085
H	3.158978	0.064785	-3.232950
H	2.476219	-1.573212	-3.188499
C	4.255928	0.376995	-0.152254
H	5.212673	-0.158046	-0.228482
H	4.084403	0.595038	0.908935
H	4.365023	1.326927	-0.688458
C	3.002741	-2.385837	-0.030742
H	4.026785	-2.777484	-0.098287
H	2.335148	-3.120331	-0.497682
H	2.750572	-2.297336	1.035385
O	-2.118326	0.867614	2.788442
C	1.361253	0.416566	2.139655
O	2.254282	0.544219	2.868837
H	0.051081	-1.272128	1.369978
O	0.044543	-3.901811	0.662395
H	-0.071576	-2.581703	-0.530424
N	-1.217581	0.580653	2.079206
Mn	-0.030564	0.224329	1.021733

C	-0.940624	-4.051114	1.681208
H	-1.087991	-3.114729	2.236305
H	-1.879659	-4.326821	1.193992
H	-0.661179	-4.846404	2.381888

CH3OH Gsolv= -115.639784

C	0.666053	-0.019773	0.000008
H	1.096669	0.985296	-0.001170
H	1.017863	-0.552457	-0.892785
H	1.018056	-0.550566	0.893858
O	-0.748352	0.124214	0.000013
H	-1.142089	-0.757345	-0.000057

CO2 Gsolv= -188.511562

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.164851
O	0.000000	0.000000	-1.164851

H2O Gsolv= -76.407718

O	0.000000	0.000000	0.118252
H	0.000000	0.762582	-0.473009
H	0.000000	-0.762582	-0.473009

H2 Gsolv= -1.168442

H	0.000000	0.000000	0.371621
H	0.000000	0.000000	-0.371621

HCOOH Gsolv= -189.679971

H	-0.102755	1.502708	0.000031
C	-0.124446	0.404199	-0.000001
O	1.109572	-0.092248	-0.000008
O	-1.136722	-0.265364	0.000008
H	1.066636	-1.067000	-0.000024

HCOO Gsolv= -189.240472

H	-0.003691	1.457792	0.000022
C	-0.000467	0.339719	0.000021
O	1.128329	-0.218077	-0.000017
O	-1.127517	-0.218936	-0.000001

TS1,2-Co-a Gsolv= -3019.059494

C	-0.013347	-0.530489	1.240204
O	-0.102282	-1.761883	1.734946
H	0.758356	-2.200970	1.824503
C	1.173803	0.195662	0.876226
C	0.694135	1.503477	0.480699
C	1.476651	2.711689	0.087086
H	2.368186	2.431713	-0.483273
H	1.836241	3.189330	1.013015
C	0.604984	3.693872	-0.688824
H	1.161194	4.623933	-0.851033
H	0.378542	3.275314	-1.683216
C	-0.688738	3.968242	0.065871
H	-1.265435	4.763231	-0.419778
H	-0.436940	4.329102	1.074425
C	-1.553736	2.713685	0.176771
H	-2.310960	2.835900	0.962876
H	-2.114469	2.552072	-0.754367
C	-0.732272	1.504211	0.502770
C	-1.196855	0.193031	0.889744
Si	2.966705	-0.420808	1.090681
C	3.197479	-0.671987	2.934153
H	3.083056	0.274122	3.477944
H	4.205663	-1.056876	3.135558
H	2.478129	-1.389731	3.349141
C	4.214535	0.815329	0.455427
H	4.156535	1.778870	0.974869
H	4.126310	0.986949	-0.624194
H	5.212719	0.396141	0.643518
C	3.172112	-2.047868	0.181544
H	2.917960	-1.951694	-0.882374
H	2.574751	-2.865536	0.604455
H	4.225758	-2.351611	0.248047
Si	-2.961711	-0.497738	1.068128
C	-3.300478	-0.655359	2.902323
H	-4.315027	-1.038134	3.071935
H	-3.218325	0.317697	3.402808
H	-2.594611	-1.345513	3.380708
C	-4.195901	0.655660	0.261674
H	-5.187384	0.186794	0.325065
H	-3.978846	0.822417	-0.800996
H	-4.258464	1.629402	0.761239
C	-3.040272	-2.160875	0.209742
H	-4.060367	-2.559650	0.291861
H	-2.356022	-2.894012	0.652405
H	-2.804094	-2.070249	-0.859673
C	1.370709	0.302643	-2.053967
C	-1.260207	0.255276	-2.064566

O	-2.043043	0.367615	-2.889716
H	0.035927	-1.495443	-1.130114
C	0.067964	-2.781190	-1.679500
O	0.053850	-2.664144	-2.878373
O	0.098206	-3.538459	-0.744071
Co	-0.008294	0.049411	-0.793027
N	2.219772	0.448130	-2.851929

TS1,2-Co-b Gsolv= -3158.471073

C	0.500115	-1.494751	-1.138697
O	0.774274	-2.762742	-1.365816
H	1.733154	-2.926505	-1.417562
C	-0.855195	-1.019545	-0.977351
C	-0.742767	0.404305	-0.875592
C	0.623525	0.761583	-0.846311
C	1.431083	-0.418457	-0.920142
C	-1.345185	-0.456978	1.834846
C	1.285614	0.243343	1.953214
O	2.005031	0.667282	2.730680
C	-2.082998	-1.820703	-1.044304
C	-2.155109	-3.095070	-0.470180
C	-3.219007	-1.297171	-1.674056
C	-3.334778	-3.827302	-0.535122
H	-1.292497	-3.507149	0.050419
C	-4.392966	-2.038202	-1.735703
H	-3.180809	-0.310616	-2.132788
C	-4.471739	-3.315572	-1.169675
H	-3.378890	-4.814513	-0.077412
H	-5.267135	-1.619834	-2.233292
C	2.899671	-0.498851	-0.936985
C	3.631028	0.402876	-1.720808
C	3.587255	-1.461441	-0.189757
C	5.017459	0.332838	-1.758357
H	3.107554	1.153184	-2.311344
C	4.976360	-1.526672	-0.238954
H	3.033927	-2.147360	0.452559
C	5.713586	-0.633928	-1.022229
H	5.575296	1.038406	-2.373105
H	5.499438	-2.278408	0.350235
C	-5.740537	-4.105787	-1.251884
H	-5.971573	-4.371835	-2.291110
H	-5.674801	-5.033354	-0.673985
H	-6.593182	-3.527369	-0.876273
C	7.208254	-0.695976	-1.076946
H	7.656583	0.235287	-0.709179
H	7.597429	-1.521662	-0.472715
H	7.560332	-0.830913	-2.107014
C	-1.610431	1.612336	-0.821298
C	0.794527	2.237088	-0.791719
H	-2.491642	1.520728	-0.181790
H	-1.962661	1.833958	-1.838615
H	1.019521	2.598952	-1.804119
H	1.591870	2.588966	-0.130349
C	-0.615082	2.719328	-0.361165
C	-0.626820	2.959464	1.157865
C	-0.940564	4.079162	-0.969149
O	0.344385	3.379330	1.759308
O	-0.105938	4.839483	-1.418621
O	-1.796832	2.716605	1.719702
O	-2.238726	4.339728	-0.905908
C	-2.664241	5.616160	-1.417826
H	-2.431727	5.686981	-2.483509
H	-3.741756	5.649471	-1.260289
H	-2.172492	6.423101	-0.868538
C	-1.858514	2.884125	3.147965
H	-1.650486	3.923906	3.413387
H	-2.874570	2.612628	3.432934
H	-1.134780	2.218288	3.628882
C	0.766581	-2.967506	2.174740
O	0.613818	-2.655766	3.336328
H	0.463875	-1.941026	1.401353
O	1.092784	-3.887281	1.455094
Co	0.182618	-0.506784	0.723031
N	-2.305115	-0.505062	2.508389

TS1,2-Co-c Gsolv= -3158.471092

C	0.502111	-1.492484	-1.144108
O	0.776847	-2.760022	-1.373125
H	1.735847	-2.923689	-1.422638
C	-0.853528	-1.017259	-0.985146
C	-0.740870	0.406354	-0.880009
C	0.625470	0.763239	-0.846936
C	1.432900	-0.416874	-0.921124
C	-1.349719	-0.460052	1.827495
C	1.281029	0.239734	1.952772
O	1.999119	0.662082	2.732333
C	-2.081573	-1.817834	-1.053440
C	-2.150640	-3.096754	-0.485770

C	-3.217829	-1.293983	-1.679589
C	-3.328132	-3.829383	-0.552224
H	-1.284783	-3.511960	0.026708
C	-4.392332	-2.037008	-1.742897
H	-3.180537	-0.307390	-2.138332
C	-4.469483	-3.313788	-1.178934
H	-3.368583	-4.821787	-0.105113
H	-5.265906	-1.620016	-2.242278
C	2.901537	-0.497607	-0.934024
C	3.635542	0.406438	-1.712669
C	3.586664	-1.462745	-0.187786
C	5.022084	0.336088	-1.746248
H	3.114088	1.158763	-2.302418
C	4.975856	-1.528358	-0.233081
H	3.031196	-2.150640	0.450589
C	5.715713	-0.633296	-1.011202
H	5.581984	1.043447	-2.357052
H	5.496893	-2.282249	0.355157
C	-5.743798	-4.097899	-1.217628
H	-6.344780	-3.842803	-2.097175
H	-5.550048	-5.176045	-1.227682
H	-6.358597	-3.887901	-0.332451
C	7.210521	-0.695797	-1.061631
H	7.597370	-1.524649	-0.460250
H	7.565658	-0.825893	-2.091274
H	7.658206	0.233417	-0.687940
C	-1.608356	1.614497	-0.824854
C	0.796705	2.238593	-0.788807
H	-2.490844	1.521643	-0.187285
H	-1.958530	1.838468	-1.842362
H	1.023864	2.602586	-1.799960
H	1.592768	2.588966	-0.125113
C	-0.613662	2.720232	-0.360144
C	-0.628528	2.957175	1.159369
C	-0.937549	4.081516	-0.965706
O	0.341361	3.376171	1.763551
O	-0.102110	4.841816	-1.413683
O	-1.799486	2.712689	1.718505
O	-2.235434	4.343415	-0.901941
C	-2.659298	5.621730	-1.410504
H	-2.426406	5.695274	-2.475915
H	-3.736807	5.655925	-1.253129
H	-2.166716	6.426552	-0.858841
C	-1.863957	2.877433	3.146974
H	-1.656499	3.916696	3.414850
H	-2.880550	2.605315	3.429433
H	-1.141112	2.210764	3.628055
C	0.761361	-2.971124	2.168138
O	0.607717	-2.661105	3.330093
H	0.460043	-1.943220	1.396232
O	1.087817	-3.889956	1.447386
Co	0.180630	-0.507926	0.718946
N	-2.311475	-0.510142	2.498282

TS1,2-Co Gsolv= -3019.059494

C	-0.013347	-0.530489	1.240204
O	-0.102282	-1.761883	1.734946
H	0.758356	-2.200970	1.824503
C	1.173803	0.195662	0.876226
C	0.694135	1.503477	0.480699
C	1.476651	2.711689	0.087086
H	2.368186	2.431713	-0.483273
H	1.836241	3.189330	1.013015
C	0.604984	3.693872	-0.688824
H	1.161194	4.623933	-0.851033
H	0.378542	3.275314	-1.683216
C	-0.688738	3.968242	0.065871
H	-1.265435	4.763231	-0.419778
H	-0.436940	4.329102	1.074425
C	-1.553736	2.713685	0.176771
H	-2.310960	2.835900	0.962876
H	-2.114469	2.552072	-0.754367
C	-0.732272	1.504211	0.502770
C	-1.196855	0.193031	0.889744
Si	2.966705	-0.420808	1.090681
C	3.197479	-0.671987	2.934153
H	3.083056	0.274122	3.477944
H	4.205663	-1.056876	3.135558
H	2.478129	-1.389731	3.349141
C	4.214535	0.815329	0.455427
H	4.156535	1.778870	0.974869
H	4.126310	0.986949	-0.624194
H	5.212719	0.396141	0.643518
C	3.172112	-2.047868	0.181544
H	2.917960	-1.951694	-0.882374
H	2.574751	-2.865536	0.604455
H	4.225758	-2.351611	0.248047
Si	-2.961711	-0.497738	1.068128

C	-3.300478	-0.655359	2.902323
H	-4.315027	-1.038134	3.071935
H	-3.218325	0.317697	3.402808
H	-2.594611	-1.345513	3.380708
C	-4.195901	0.655660	0.261674
H	-5.187384	0.186794	0.325065
H	-3.978846	0.822417	-0.800996
H	-4.258464	1.629402	0.761239
C	-3.040272	-2.160875	0.209742
H	-4.060367	-2.559650	0.291861
H	-2.356022	-2.894012	0.652405
H	-2.804094	-2.070249	-0.859673
C	1.370709	0.302643	-2.053967
C	-1.260207	0.255276	-2.064566
O	-2.043043	0.367615	-2.889716
H	0.035927	-1.495443	-1.130114
C	0.067964	-2.781190	-1.679500
O	0.053850	-2.664144	-2.878373
O	0.098206	-3.538459	-0.744071
Co	-0.008294	0.049411	-0.793027
N	2.219772	0.448130	-2.851929

TS1,2-Fe-Casey Gsolv= -2917.175952

Fe	0.011560	0.027894	-0.823017
C	0.000126	0.123858	1.302055
O	0.095846	1.231376	2.057780
H	-0.767032	1.645423	2.213033
C	-1.201255	-0.492380	0.811615
C	-0.719844	-1.655133	0.109760
C	0.687122	-1.676136	0.121301
C	1.186210	-0.526947	0.825207
Si	-3.000039	0.025971	1.093989
C	-3.337404	-0.110604	2.931998
H	-3.171662	-1.134629	3.289312
H	-4.376656	0.161949	3.156019
H	-2.684008	0.557163	3.508990
C	-4.082890	-1.144079	0.117107
H	-3.942834	-2.184540	0.436712
H	-3.891261	-1.082651	-0.961518
H	-5.137437	-0.887766	0.282695
C	-3.235761	1.798646	0.529737
H	-2.994078	1.928021	-0.533479
H	-2.622455	2.505798	1.103765
H	-4.284920	2.089828	0.673790
Si	2.970583	0.010610	1.142867
C	3.299813	-0.125112	2.982353
H	4.345766	0.123870	3.203548
H	3.113546	-1.144683	3.342501
H	2.661954	0.558974	3.555872
C	4.072298	-1.165821	0.189137
H	5.126552	-0.922967	0.375230
H	3.902565	-1.103653	-0.893250
H	3.911881	-2.205551	0.502849
C	3.200076	1.779508	0.565999
H	4.228154	2.108239	0.767810
H	2.522070	2.461199	1.095061
H	3.018904	1.885239	-0.511987
C	-1.269604	0.128405	-2.042933
O	-2.108524	0.200993	-2.832874
C	1.302196	0.062291	-2.033948
O	2.146227	0.092013	-2.821017
H	0.061246	1.600304	-0.773538
C	0.059626	3.060054	-1.060899
O	0.259070	3.170033	-2.235795
O	-0.139420	3.554034	0.010382
C	-1.207847	-2.880339	-0.587494
O	-0.029682	-3.375255	-1.245508
C	1.152004	-2.911828	-0.570924
H	-1.981821	-2.721528	-1.346013
H	-1.577295	-3.617084	0.144201
H	1.492727	-3.658165	0.164850
H	1.940591	-2.771992	-1.318198

TS1,2-Fe Gsolv= -2920.523590

Fe	0.010834	0.040299	0.826636
C	0.020019	-0.508937	-1.222889
O	0.098167	-1.751911	-1.737194
H	-0.761245	-2.198431	-1.758109
C	-1.159151	0.231633	-0.894425
C	-0.664447	1.525278	-0.451187
C	-1.444331	2.738380	-0.048635
H	-2.337269	2.461587	0.523843
H	-1.806195	3.235045	-0.963373
C	-0.567432	3.705507	0.740505
H	-1.113154	4.641366	0.908485
H	-0.349679	3.276437	1.732706
C	0.734237	3.971203	-0.004629
H	1.311982	4.763841	0.484836

H	0.489252	4.335542	-1.014271
C	1.591334	2.710591	-0.114009
H	2.357423	2.841647	-0.890094
H	2.140203	2.543824	0.823577
C	0.756594	1.510092	-0.458550
C	1.209240	0.201732	-0.880559
Si	-2.944068	-0.357833	-1.151643
C	-3.172956	-0.627154	-2.993916
H	-3.043117	0.309484	-3.550545
H	-4.184308	-1.003135	-3.196989
H	-2.458836	-1.358675	-3.394128
C	-4.191645	0.892743	-0.535294
H	-4.100997	1.864099	-1.035354
H	-4.133824	1.048813	0.549052
H	-5.192084	0.495954	-0.756889
C	-3.221312	-1.976301	-0.239349
H	-3.045246	-1.868358	0.839391
H	-2.600140	-2.804978	-0.603416
H	-4.269238	-2.277055	-0.376892
Si	2.955562	-0.503753	-1.076593
C	3.295177	-0.685423	-2.911835
H	4.307690	-1.075984	-3.077846
H	3.218258	0.281623	-3.425064
H	2.585974	-1.377233	-3.383305
C	4.227386	0.638324	-0.307080
H	5.211228	0.155923	-0.387699
H	4.036743	0.824087	0.757330
H	4.289810	1.604496	-0.821939
C	3.051692	-2.173722	-0.227358
H	4.065046	-2.582063	-0.342423
H	2.348054	-2.896079	-0.658308
H	2.844567	-2.093935	0.848695
C	-1.279963	0.267677	2.013566
O	-2.127015	0.419413	2.785537
C	1.295631	0.200096	2.030131
O	2.137616	0.309202	2.814786
H	-0.017093	-1.506468	1.109459
C	-0.161712	-2.897893	1.689520
O	-0.221895	-2.752587	2.874300
O	-0.155193	-3.595354	0.719819

TS1,2-Fe-Renaud Gsolv= -2487.262428

Fe	0.011620	0.239004	1.205953
C	-0.021593	-1.336333	-0.121872
O	0.003567	-2.506701	0.517119
C	-1.206349	-0.531953	-0.275658
C	-0.758848	0.783023	-0.684638
C	-0.723254	3.110222	-0.984993
H	-1.328320	3.936292	-1.371372
H	-0.438380	3.352939	0.050687
C	0.523665	2.920702	-1.831699
H	1.119339	3.837959	-1.850915
H	0.240368	2.693327	-2.868733
C	0.668713	0.772562	-0.804611
C	1.141433	-0.526460	-0.362733
C	-1.174876	1.233143	2.090398
O	-1.928652	1.917077	2.634738
C	1.395412	0.967422	2.072581
O	2.288851	1.375576	2.680353
H	-0.052198	-1.034298	2.294584
H	-0.027134	-1.746669	1.614307
C	2.525879	-1.042894	-0.384600
C	3.157318	-1.527943	0.765605
C	3.214191	-1.084201	-1.603907
C	4.453934	-2.032547	0.700557
H	2.630406	-1.502739	1.718118
C	4.512435	-1.583135	-1.666963
H	2.724981	-0.725161	-2.508041
C	5.137416	-2.055905	-0.513858
H	4.933089	-2.402867	1.604123
H	5.036319	-1.604209	-2.619969
H	6.152620	-2.443192	-0.562194
C	-2.582950	-1.061579	-0.224105
C	-3.620152	-0.437165	0.478045
C	-2.870160	-2.219272	-0.959602
C	-4.912602	-0.953092	0.437327
H	-3.423440	0.457721	1.063078
C	-4.161461	-2.738239	-0.995754
H	-2.072349	-2.709026	-1.515803
C	-5.188343	-2.104485	-0.298771
H	-5.707007	-0.454387	0.988114
H	-4.365371	-3.636994	-1.573558
H	-6.198748	-2.505966	-0.327699
N	1.371521	1.836617	-1.312557
N	-1.549413	1.899687	-0.964592
C	2.565073	2.285067	-0.608726
H	3.164086	1.434270	-0.271798
H	3.181310	2.889002	-1.281695

H	2.294489	2.900232	0.266171
C	-2.397907	1.744724	-2.148662
H	-1.815898	1.709297	-3.083912
H	-2.981812	0.821844	-2.075667
H	-3.095200	2.586814	-2.200412

TS1,2-Fe-williams-1 Gsolv= -2870.973472

Fe	0.023078	-0.626234	1.035387
C	0.041273	-1.326958	-0.997648
O	0.172230	-2.591360	-1.411432
H	-0.689605	-3.039441	-1.450104
C	-1.164799	-0.640994	-0.692582
C	-0.797710	0.715689	-0.333111
C	0.627355	0.805619	-0.357327
C	1.163444	-0.485701	-0.720550
C	-1.312723	-0.758261	2.203168
O	-2.159794	-0.896808	2.971880
C	1.147646	-0.089371	2.306441
O	1.860257	0.238412	3.150362
C	-2.530196	-1.158447	-0.916739
C	-2.999400	-2.305564	-0.267171
C	-3.366499	-0.498085	-1.826395
C	-4.282531	-2.784434	-0.522340
H	-2.357277	-2.819780	0.448579
C	-4.650356	-0.973927	-2.073463
H	-3.005278	0.391128	-2.341367
C	-5.111472	-2.117491	-1.421692
H	-4.635854	-3.675792	-0.009288
H	-5.291861	-0.451688	-2.779471
H	-6.115715	-2.487602	-1.614751
C	2.574766	-0.852237	-0.952303
C	3.584915	-0.557282	-0.028918
C	2.923238	-1.476462	-2.156492
C	4.910169	-0.876888	-0.304676
H	3.340532	-0.074553	0.914646
C	4.250224	-1.799556	-2.429889
H	2.151845	-1.697378	-2.891285
C	5.248290	-1.500211	-1.505410
H	5.681559	-0.641970	0.425050
H	4.502710	-2.282355	-3.371243
H	6.284809	-1.751858	-1.717690
C	-1.741183	1.842191	-0.179290
C	-2.863951	1.772842	0.652438
C	-1.552522	2.987064	-0.965016
C	-3.772270	2.825995	0.704639
H	-3.041317	0.889395	1.261633
C	-2.462003	4.039808	-0.912859
H	-0.694919	3.046469	-1.633735
C	-3.574365	3.963070	-0.076926
H	-4.637638	2.756041	1.359567
H	-2.302489	4.919541	-1.532054
H	-4.285010	4.785270	-0.035127
C	1.418244	2.032845	-0.139620
C	1.217093	2.857076	0.972822
C	2.344481	2.415478	-1.116331
C	1.934174	4.041929	1.106868
H	0.495194	2.567802	1.736241
C	3.059533	3.602521	-0.981307
H	2.494295	1.786697	-1.992806
C	2.857368	4.417347	0.131019
H	1.772991	4.673016	1.977720
H	3.773856	3.891178	-1.748811
H	3.417768	5.343196	0.238222
C	0.845885	-3.410004	1.429986
O	-0.127408	-4.122746	1.468143
H	0.378179	-2.118866	1.487181
O	2.050524	-3.373996	1.392656

TS1,2-Fe-williams-2 Gsolv= -3059.934370

Fe	0.199191	-0.446945	0.816415
C	0.476720	-1.566575	-0.975252
O	0.795783	-2.862101	-1.066310
H	1.759275	-2.985328	-1.013588
C	-0.876944	-1.097530	-0.880652
C	-0.771087	0.339063	-0.835924
C	0.587480	0.707163	-0.863925
C	1.401485	-0.471029	-0.884061
C	-1.161576	-0.331303	1.956520
O	-2.044140	-0.286040	2.697483
C	1.355824	0.417302	1.850556
O	2.149378	0.954451	2.492597
C	-2.107427	-1.902447	-0.964938
C	-2.127448	-3.125604	-1.644866
C	-3.310577	-1.432998	-0.414325
C	-3.307962	-3.855760	-1.761495
H	-1.219503	-3.507656	-2.103104
C	-4.482275	-2.166598	-0.535393
H	-3.333756	-0.485907	0.122057

C	-4.504090	-3.394345	-1.209616
H	-3.298889	-4.802234	-2.300709
H	-5.403421	-1.782922	-0.097303
C	2.871123	-0.550013	-0.942687
C	3.572440	0.265106	-1.838964
C	3.593887	-1.431102	-0.128474
C	4.959018	0.194874	-1.919417
H	3.024271	0.950602	-2.483912
C	4.979771	-1.503512	-0.224273
H	3.070170	-2.044048	0.606694
C	5.686068	-0.691460	-1.117523
H	5.490333	0.834727	-2.623163
H	5.526895	-2.195448	0.414909
C	-5.775330	-4.176435	-1.328277
H	-6.574342	-3.570610	-1.772909
H	-5.638753	-5.068656	-1.948117
H	-6.134456	-4.501202	-0.343487
C	7.180454	-0.746271	-1.193203
H	7.634768	0.002350	-0.530815
H	7.561417	-1.725997	-0.885345
H	7.536709	-0.537296	-2.207955
C	-1.644015	1.550190	-0.894808
C	0.750737	2.185889	-0.940031
H	-2.532409	1.532635	-0.260591
H	-1.981123	1.698591	-1.930899
H	0.936220	2.476047	-1.982774
H	1.560071	2.600734	-0.331011
C	-0.651646	2.683531	-0.505378
C	-0.627799	2.993086	0.998707
C	-1.005703	4.007894	-1.168261
O	0.305704	3.573763	1.522747
O	-0.211534	4.720942	-1.749295
O	-1.721963	2.625084	1.645185
O	-2.290763	4.298930	-1.003004
C	-2.744946	5.542215	-1.568150
H	-2.584151	5.542141	-2.649317
H	-3.809515	5.595874	-1.342599
H	-2.213753	6.379092	-1.107297
C	-1.737091	2.886703	3.060482
H	-1.662374	3.961625	3.244286
H	-2.691760	2.503893	3.420854
H	-0.905943	2.362300	3.543514
C	0.897707	-2.825507	2.516838
O	0.963479	-2.308353	3.597492
H	0.635263	-1.779904	1.549772
O	0.955180	-3.824178	1.853948

TS1,2-Fe-wills-1 Gsolv= -2561.858933

Fe	-0.097766	0.561282	0.747242
C	-0.123447	-0.928450	-0.761205
O	-0.101275	-2.256812	-0.572843
H	0.645656	-2.508263	0.007073
C	-1.341854	-0.176628	-0.782832
C	-0.945604	1.179052	-1.033906
C	0.456562	1.243289	-1.130149
C	1.015302	-0.055923	-0.931812
C	-1.484429	0.970280	1.768369
O	-2.423011	1.234684	2.384276
C	0.981818	1.691358	1.590452
O	1.668079	2.442463	2.132737
C	-2.714352	-0.689451	-0.638796
C	-3.737273	-0.132178	-1.414204
C	-3.024386	-1.713111	0.266730
C	-5.045181	-0.597023	-1.295592
H	-3.508095	0.659482	-2.125918
C	-4.330253	-2.176601	0.380177
H	-2.241700	-2.128420	0.898511
C	-5.344519	-1.621917	-0.401316
H	-5.830076	-0.156680	-1.906139
H	-4.559557	-2.968426	1.089605
H	-6.365400	-1.985046	-0.307886
C	2.430976	-0.456515	-1.011956
C	3.437851	0.341398	-0.453847
C	2.788947	-1.637242	-1.673659
C	4.772306	-0.038138	-0.549413
H	3.176051	1.261681	0.066179
C	4.125854	-2.017770	-1.762821
H	2.019637	-2.255766	-2.131511
C	5.120801	-1.222557	-1.198723
H	5.542617	0.590040	-0.107975
H	4.389059	-2.938131	-2.279190
H	6.164137	-1.521847	-1.265936
C	-1.504831	2.535544	-1.299374
O	-0.352504	3.387637	-1.193054
C	0.842513	2.641978	-1.473245
H	-2.258422	2.876577	-0.580754
H	-1.928807	2.591469	-2.314731
H	1.099971	2.705618	-2.542550

H	1.662169	3.072632	-0.890146
C	1.456255	-1.355450	2.359676
O	1.521142	-2.358996	1.705401
H	0.259322	-0.594814	1.782116
O	1.847196	-0.698615	3.276688

TS1,2-Fe-wills-2 Gsolv= -2601.124496

Fe	0.056704	0.008176	0.848745
C	0.109486	-0.360958	-1.249948
O	0.122058	-1.540919	-1.874898
H	1.030015	-1.850968	-2.028833
C	-1.112677	0.281462	-0.862831
C	-0.716311	1.545471	-0.303986
C	0.684644	1.623499	-0.296378
C	1.243136	0.414269	-0.819551
C	-1.304123	-0.168885	1.982469
O	-2.197714	-0.350622	2.688083
C	1.297671	0.255706	2.098038
O	2.135312	0.415562	2.873798
C	-2.479042	-0.210096	-1.114138
C	-2.843551	-1.528883	-0.815570
C	-3.432410	0.654845	-1.662711
C	-4.136399	-1.974304	-1.071058
H	-2.114667	-2.199218	-0.361510
C	-4.727614	0.207361	-1.913425
H	-3.153450	1.681059	-1.899267
C	-5.081411	-1.108163	-1.621114
H	-4.409656	-2.999318	-0.831084
H	-5.460335	0.889090	-2.339190
H	-6.092770	-1.457671	-1.815549
C	2.668940	0.100429	-1.012911
C	3.526019	1.090523	-1.508131
C	3.187644	-1.167243	-0.718282
C	4.875517	0.815996	-1.711433
H	3.128819	2.076661	-1.744355
C	4.535503	-1.441125	-0.932513
H	2.539312	-1.935089	-0.295425
C	5.382438	-0.451124	-1.428677
H	5.531386	1.593676	-2.095870
H	4.927442	-2.428202	-0.698690
H	6.436467	-0.665168	-1.589456
C	-1.272629	2.852498	0.173936
O	-0.117460	3.474591	0.782906
C	1.091697	2.964220	0.209824
H	-1.563039	3.435836	-0.718780
H	1.423161	3.600112	-0.626861
H	1.874599	2.959014	0.976595
C	-2.400629	2.839648	1.170497
H	-2.731968	3.861186	1.382723
H	-3.254358	2.276753	0.774894
H	-2.074965	2.378187	2.109604
C	0.352112	-2.916453	1.449543
O	0.392767	-2.903328	2.650115
H	0.273283	-1.559378	1.003531
O	0.356080	-3.567946	0.440026

TS1,2-Fe-wills-3 Gsolv= -2778.774213

Fe	0.272124	0.170684	0.802998
C	0.010432	-0.741752	-1.096067
O	-0.133651	-2.056903	-1.326907
H	0.712778	-2.527738	-1.288841
C	-1.120503	0.088415	-0.801259
C	-0.575964	1.413015	-0.634221
C	0.815152	1.350105	-0.822283
C	1.245040	-0.001762	-1.034421
Si	3.024164	-0.618612	-1.260510
C	3.182472	-1.283706	-3.003693
H	4.196110	-1.665277	-3.180548
H	2.977962	-0.503125	-3.746717
H	2.479011	-2.108677	-3.178264
C	4.157796	0.838176	-0.965939
H	5.200334	0.499647	-1.028496
H	4.013611	1.275043	0.030508
H	4.021393	1.627507	-1.715441
C	3.372777	-1.974568	-0.011152
H	4.395801	-2.347922	-0.153852
H	2.696480	-2.833842	-0.112594
H	3.293562	-1.597800	1.017387
C	-0.912707	0.340102	2.114432
O	-1.662005	0.415489	2.988614
C	1.605034	0.742342	1.826095
O	2.477488	1.098152	2.490855
C	-2.538384	-0.315842	-0.846012
C	-3.498642	0.303300	-0.034448
C	-2.963394	-1.287678	-1.762728
C	-4.841631	-0.045554	-0.127836
H	-3.197454	1.062293	0.683312
C	-4.308266	-1.635782	-1.854571

H	-2.242063	-1.763250	-2.421642
C	-5.252276	-1.019771	-1.036388
H	-5.569401	0.445356	0.514168
H	-4.617920	-2.389397	-2.575059
H	-6.302337	-1.293400	-1.108441
C	-0.997115	2.850353	-0.511907
O	0.197718	3.563153	-0.922024
C	1.367859	2.736881	-0.843691
H	-1.781739	3.085135	-1.245246
H	1.981390	2.920474	-1.734065
H	1.964713	2.993222	0.044373
C	-1.401578	3.331799	0.864589
H	-1.591504	4.409934	0.834060
H	-2.314211	2.838091	1.214394
H	-0.595432	3.134820	1.583891
C	0.435750	-2.445588	2.169045
O	1.008507	-2.189131	3.191880
H	0.613609	-1.288827	1.300862
O	-0.192975	-3.231309	1.516356

TS1,2-Fe-wills-4 Gsolv= -2739.515970

Fe	-0.176352	0.016625	0.833921
C	0.025161	0.161011	-1.278539
O	0.211925	1.270055	-2.008358
H	-0.620569	1.718639	-2.221426
C	1.145299	-0.525565	-0.700381
C	0.583613	-1.683666	-0.069876
C	-0.814665	-1.645062	-0.198230
C	-1.220227	-0.462408	-0.914676
Si	-2.990640	0.061491	-1.348115
C	-3.138755	-0.003960	-3.214311
H	-4.147308	0.280032	-3.540183
H	-2.929998	-1.012174	-3.593005
H	-2.427517	0.687184	-3.686349
C	-4.148308	-1.140600	-0.505547
H	-5.186525	-0.875444	-0.743892
H	-4.040673	-1.108489	0.586397
H	-3.984674	-2.171838	-0.842847
C	-3.284265	1.808655	-0.734231
H	-4.283630	2.146228	-1.039881
H	-2.558651	2.524370	-1.143132
H	-3.233460	1.861942	0.361567
C	1.090405	0.082671	2.069655
O	1.962095	0.103998	2.825422
C	-1.525478	0.005310	1.988377
O	-2.409515	-0.002719	2.729594
C	2.572242	-0.180412	-0.813118
C	3.505138	-1.199630	-1.034576
C	3.021225	1.141011	-0.685497
C	4.862192	-0.903611	-1.139336
H	3.164868	-2.228834	-1.140444
C	4.376672	1.433359	-0.793609
H	2.306161	1.936788	-0.481208
C	5.300742	0.413288	-1.022963
H	5.576332	-1.705089	-1.313860
H	4.715213	2.461748	-0.689830
H	6.360184	0.645269	-1.104181
C	0.973174	-2.928676	0.648519
O	-0.270264	-3.378283	1.209541
C	-1.373621	-2.876248	0.437430
H	1.696047	-2.795931	1.461222
H	1.368860	-3.676118	-0.057870
H	-1.665981	-3.605141	-0.335552
H	-2.220285	-2.722622	1.114311
C	-0.381066	3.040485	1.078349
O	-0.115549	3.548689	0.026909
H	-0.222001	1.596364	0.827427
O	-0.707336	3.150046	2.225613

TS1,2-Fe-wills-5 Gsolv= -2818.036272

Fe	0.066480	0.174999	0.818506
C	0.009053	-0.434078	-1.219515
O	0.199243	-1.669781	-1.702727
H	-0.634624	-2.166584	-1.752569
C	-1.235953	0.162422	-0.829254
C	-0.897694	1.505512	-0.442702
C	0.493313	1.671134	-0.550259
C	1.115093	0.449065	-0.969825
Si	2.950240	0.076082	-1.219892
C	3.245890	-0.252093	-3.041509
H	4.321442	-0.315611	-3.251963
H	2.829248	0.550938	-3.662031
H	2.782841	-1.197226	-3.353064
C	3.896182	1.588905	-0.646546
H	4.972808	1.429274	-0.791563
H	3.728996	1.789016	0.420090
H	3.617784	2.485018	-1.215858
C	3.439313	-1.427899	-0.198447

H	2.715665	-2.236239	-0.379541
H	3.350136	-1.166608	0.868001
C	-1.220938	-0.031311	2.024520
O	-2.066634	-0.210398	2.789078
C	1.270929	0.736510	1.993446
O	2.067056	1.095125	2.747226
C	-2.579470	-0.431882	-0.943063
C	-3.606203	0.306378	-1.544036
C	-2.847517	-1.727628	-0.482657
C	-4.877027	-0.243436	-1.685628
H	-3.401893	1.312704	-1.907708
C	-4.117295	-2.277855	-0.634998
H	-2.065128	-2.295211	0.022854
C	-5.134333	-1.537659	-1.235647
H	-5.667399	0.339766	-2.152477
H	-4.314929	-3.283719	-0.271853
H	-6.127402	-1.966380	-1.348433
C	-1.525494	2.814369	-0.079341
O	-0.383421	3.599348	0.335445
C	0.826864	3.091156	-0.239873
H	-1.947825	3.257443	-0.999247
H	1.072779	3.629810	-1.169400
H	1.642021	3.245373	0.475549
C	-2.552781	2.829638	1.021981
H	-3.384785	2.157754	0.778634
H	-2.099536	2.504836	1.966165
H	-2.954882	3.839052	1.156655
C	4.854459	-1.908849	-0.514588
H	5.598607	-1.115236	-0.361353
H	5.150268	-2.754735	0.118457
H	4.940785	-2.239858	-1.557822
C	0.557830	-2.605576	1.766046
O	0.155408	-3.361584	0.927614
H	0.568353	-1.293777	1.105386
O	0.977037	-2.425942	2.874837

TS1,2-Mn-a Gsolv= -2821.063189

C	0.014046	-0.308595	1.284335
O	-0.091343	-1.505879	1.874327
H	0.757874	-1.972192	1.931932
C	1.215497	0.352523	0.867482
C	0.735848	1.580945	0.295307
C	-0.673982	1.610398	0.307225
C	-1.173408	0.395036	0.881366
Si	3.026884	-0.181544	1.079422
C	3.362643	-0.273642	2.917981
H	3.244498	0.704958	3.398770
H	4.386364	-0.622859	3.103034
H	2.675444	-0.977211	3.406247
C	4.086366	1.100406	0.228070
H	3.946120	2.103227	0.650274
H	3.881906	1.141350	-0.849700
H	5.143990	0.834213	0.353740
C	3.265454	-1.860783	0.286328
H	2.988028	-1.845643	-0.776162
H	2.684795	-2.649982	0.781580
H	4.323815	-2.146480	0.351629
Si	-2.962849	-0.151634	1.194938
C	-3.210258	-0.222414	3.049352
H	-4.237513	-0.529896	3.283714
H	-3.039263	0.758777	3.509280
H	-2.528471	-0.943023	3.517675
C	-4.070661	1.144837	0.424369
H	-5.119707	0.912699	0.649790
H	-3.968101	1.181425	-0.667393
H	-3.859205	2.144526	0.825547
C	-3.241990	-1.832902	0.419344
H	-4.270893	-2.163911	0.612634
H	-2.564926	-2.587482	0.838628
H	-3.098527	-1.810528	-0.669043
C	-1.435569	0.220272	-2.020584
O	-2.306731	0.390847	-2.750063
H	-0.224437	-1.697529	-0.973476
C	-0.091585	-2.814455	-1.400573
O	-0.409600	-2.921980	-2.583749
O	0.304709	-3.573815	-0.519212
C	1.231222	2.878836	-0.247643
O	0.056126	3.465588	-0.826919
C	-1.125553	2.935311	-0.206203
H	2.000138	2.811438	-1.024961
H	1.615442	3.505518	0.573198
H	-1.443248	3.575234	0.632600
H	-1.925246	2.914670	-0.953897
O	2.013762	0.460538	-2.771018
N	1.150277	0.217514	-2.028786
Mn	-0.007245	0.021742	-0.881961

TS1,2-Mn-b Gsolv= -2963.822587

C	0.332372	-1.623909	-0.988209
O	0.508667	-2.944618	-1.111022
H	1.454943	-3.166146	-1.104025
C	-0.958131	-1.006260	-0.928796
C	-0.691295	0.408674	-0.860495
C	0.699552	0.623609	-0.857583
C	1.372878	-0.638010	-0.857438
O	-2.057803	-0.014755	2.566860
C	1.452017	0.283391	1.857604
O	2.311438	0.754087	2.465572
C	-2.268284	-1.670610	-1.002815
C	-2.424489	-2.909998	-1.636799
C	-3.410032	-1.052248	-0.470216
C	-3.678227	-3.507593	-1.727227
H	-1.565769	-3.406572	-2.079335
C	-4.656664	-1.656031	-0.565137
H	-3.327280	-0.090287	0.031827
C	-4.815173	-2.898305	-1.190968
H	-3.775977	-4.467985	-2.232184
H	-5.527561	-1.154764	-0.144162
C	2.828235	-0.875669	-0.879533
C	3.632471	-0.127941	-1.745267
C	3.438089	-1.829212	-0.050965
C	5.009424	-0.331668	-1.784373
H	3.175652	0.614423	-2.398236
C	4.810972	-2.033759	-0.104867
H	2.833645	-2.393722	0.660298
C	5.621275	-1.288256	-0.970424
H	5.621106	0.262717	-2.461855
H	5.269924	-2.775254	0.548410
C	-6.158183	-3.556010	-1.264780
H	-6.410014	-4.044375	-0.314248
H	-6.950411	-2.826573	-1.468655
H	-6.183944	-4.323536	-2.045569
C	7.100864	-1.516287	-1.009855
H	7.547887	-1.390336	-0.016118
H	7.335281	-2.537397	-1.335613
H	7.594128	-0.820654	-1.696465
C	-1.421699	1.712860	-0.923621
C	1.031899	2.072728	-0.947610
H	-2.300359	1.805242	-0.281196
H	-1.747330	1.890437	-1.959209
H	1.261158	2.325956	-1.991021
H	1.874183	2.399787	-0.330091
C	-0.306174	2.737005	-0.537508
C	-0.260531	3.065791	0.957085
C	-0.560006	4.032836	-1.296228
O	0.722881	3.564409	1.476582
O	-0.071521	4.308546	-2.373706
O	-1.378001	2.796189	1.612293
O	-1.438328	4.798638	-0.658308
C	-1.813782	6.026574	-1.308180
H	-2.276703	5.811881	-2.274877
H	-2.530821	6.503677	-0.640927
H	-0.935250	6.662471	-1.443384
C	-1.362728	3.060623	3.025675
H	-1.163757	4.119787	3.209153
H	-2.355103	2.792365	3.387635
H	-0.597559	2.444086	3.509050
C	0.212284	-2.935323	2.369022
O	0.817272	-2.694835	3.374819
H	0.652823	-1.874454	1.411093
O	-0.528180	-3.644314	1.751078
Mn	0.129418	-0.466296	0.862637
N	-1.120197	-0.213164	1.893926

TS1,2-Mn-c Gsolv= -2963.822587

C	0.332372	-1.623909	-0.988209
O	0.508667	-2.944618	-1.111022
H	1.454943	-3.166146	-1.104025
C	-0.958131	-1.006260	-0.928796
C	-0.691295	0.408674	-0.860495
C	0.699552	0.623609	-0.857583
C	1.372878	-0.638010	-0.857438
O	-2.057803	-0.014755	2.566860
C	1.452017	0.283391	1.857604
O	2.311438	0.754087	2.465572
C	-2.268284	-1.670610	-1.002815
C	-2.424489	-2.909998	-1.636799
C	-3.410032	-1.052248	-0.470216
C	-3.678227	-3.507593	-1.727227
H	-1.565769	-3.406572	-2.079335
C	-4.656664	-1.656031	-0.565137
H	-3.327280	-0.090287	0.031827
C	-4.815173	-2.898305	-1.190968
H	-3.775977	-4.467985	-2.232184
H	-5.527561	-1.154764	-0.144162
C	2.828235	-0.875669	-0.879533

C	3.632471	-0.127941	-1.745267
C	3.438089	-1.829212	-0.050965
C	5.009424	-0.331668	-1.784373
H	3.175652	0.614423	-2.398236
C	4.810972	-2.033759	-0.104867
H	2.833645	-2.393722	0.660298
C	5.621275	-1.288256	-0.970424
H	5.621106	0.262717	-2.461855
H	5.269924	-2.775254	0.548410
C	-6.158183	-3.556010	-1.264780
H	-6.410014	-4.044375	-0.314248
H	-6.950411	-2.826573	-1.468655
H	-6.183944	-4.323536	-2.045569
C	7.100864	-1.516287	-1.009855
H	7.547887	-1.390336	-0.016118
H	7.335281	-2.537397	-1.335613
H	7.594128	-0.820654	-1.696465
C	-1.421699	1.712860	-0.923621
C	1.031899	2.072728	-0.947610
H	-2.300359	1.805242	-0.281196
H	-1.747330	1.890437	-1.959209
H	1.261158	2.325956	-1.991021
H	1.874183	2.399787	-0.330091
C	-0.306174	2.737005	-0.537508
C	-0.260531	3.065791	0.957085
C	-0.560006	4.032836	-1.296228
O	0.722881	3.564409	1.476582
O	-0.071521	4.308546	-2.373706
O	-1.378001	2.796189	1.612293
O	-1.438328	4.798638	-0.658308
C	-1.813782	6.026574	-1.308180
H	-2.276703	5.811881	-2.274877
H	-2.530821	6.503677	-0.640927
H	-0.935250	6.662471	-1.443384
C	-1.362728	3.060623	3.025675
H	-1.163757	4.119787	3.209153
H	-2.355103	2.792365	3.387635
H	-0.597559	2.444086	3.509050
C	0.212284	-2.935323	2.369022
O	0.817272	-2.694835	3.374819
H	0.652823	-1.874454	1.411093
O	-0.528180	-3.644314	1.751078
Mn	0.129418	-0.466296	0.862637
N	-1.120197	-0.213164	1.893926

TS1,2-Mn Gsolv= -2824.409694

C	-0.004332	-0.528883	-1.217725
O	0.121146	-1.769918	-1.724889
H	-0.728771	-2.232449	-1.779198
C	-1.208858	0.165507	-0.897621
C	-0.770536	1.483223	-0.477042
C	-1.605988	2.661566	-0.084970
H	-2.469985	2.350028	0.513491
H	-2.014927	3.112349	-1.003524
C	-0.767954	3.694952	0.661296
H	-1.357618	4.607492	0.806744
H	-0.517670	3.309990	1.663503
C	0.511512	3.999359	-0.106757
H	1.052762	4.836360	0.349461
H	0.240747	4.314722	-1.126250
C	1.430027	2.779959	-0.179073
H	2.185076	2.923656	-0.963684
H	1.987829	2.672695	0.761832
C	0.650451	1.531070	-0.479697
C	1.154584	0.236192	-0.884635
Si	-2.965289	-0.530608	-1.076509
C	-3.265267	-0.789702	-2.909278
H	-3.197346	0.158223	-3.457679
H	-4.265585	-1.208787	-3.078701
H	-2.533491	-1.483305	-3.344197
C	-4.254451	0.615914	-0.354099
H	-4.295227	1.587644	-0.859565
H	-4.105650	0.782633	0.720279
H	-5.233568	0.133519	-0.480931
C	-3.066636	-2.169027	-0.163855
H	-2.838521	-2.039486	0.903136
H	-2.403273	-2.949184	-0.559002
H	-4.093744	-2.551294	-0.242044
Si	2.931100	-0.378456	-1.129866
C	3.220467	-0.522701	-2.976452
H	4.236796	-0.886690	-3.176026
H	3.108627	0.451431	-3.469685
H	2.514731	-1.222389	-3.441362
C	4.162915	0.827081	-0.393498
H	5.167115	0.393538	-0.497591
H	3.991039	1.010761	0.674212
H	4.164251	1.791377	-0.915567
C	3.144932	-2.047467	-0.302330

H	4.179472	-2.388877	-0.443670
H	2.479372	-2.808807	-0.726711
H	2.957547	-1.993146	0.778889
O	-2.064338	0.551953	2.752272
C	1.389412	0.250483	1.994282
O	2.280062	0.390927	2.715578
H	0.109634	-1.534754	1.056522
C	0.184014	-2.910084	1.679405
O	0.341023	-2.745044	2.852951
O	0.058301	-3.633129	0.736439
N	-1.191536	0.305504	2.006601
Mn	-0.032622	0.057126	0.882954

TS2,3-Co-a Gsolv= -3015.708173

Co	-0.051802	0.249694	0.819120
N	-2.231971	0.901744	2.869808
C	-0.027654	-0.566056	-1.125515
O	-0.032387	-1.849105	-1.383095
H	0.247504	-2.470970	-0.563405
C	-1.250777	0.185178	-0.865594
C	-0.802861	1.505112	-0.612278
C	0.624927	1.537690	-0.609759
C	1.151026	0.240091	-0.879351
Si	-3.021364	-0.506819	-0.971101
C	-3.266164	-1.029867	-2.751379
H	-3.103582	-0.190775	-3.438875
H	-4.289250	-1.397537	-2.901587
H	-2.574312	-1.836212	-3.024444
C	-4.176244	0.887074	-0.503129
H	-4.016663	1.770328	-1.135161
H	-4.050949	1.183856	0.545686
H	-5.217173	0.565790	-0.636729
C	-3.181179	-1.966694	0.185451
H	-2.935877	-1.697842	1.220882
H	-2.531305	-2.794490	-0.124050
H	-4.216377	-2.332197	0.170620
Si	2.974289	-0.278236	-1.078754
C	3.177507	-0.755946	-2.875327
H	4.215631	-1.049795	-3.075828
H	2.929069	0.080293	-3.540259
H	2.531085	-1.603554	-3.134626
C	3.999274	1.220770	-0.635429
H	5.064300	0.985994	-0.759225
H	3.847371	1.525115	0.408303
H	3.772016	2.076714	-1.283639
C	3.360614	-1.715639	0.051046
H	4.435679	-1.932891	-0.001489
H	2.819709	-2.621080	-0.248060
H	3.115763	-1.498334	1.099403
C	-1.405964	0.653330	2.074985
C	1.234656	0.668712	2.049557
O	2.024218	0.953453	2.818381
H	-0.208068	-1.412315	1.381292
C	0.253782	-2.466089	1.634995
O	0.400059	-2.669606	2.832291
O	0.461947	-3.172248	0.621850
C	-1.298341	2.878627	-0.335803
O	-0.140120	3.556823	0.167305
C	1.050353	2.936808	-0.332946
H	-2.098642	2.953815	0.406102
H	-1.641667	3.335121	-1.278643
H	1.375213	3.408559	-1.275119
H	1.844561	3.056092	0.410930

TS2,3-Co-b Gsolv= -3158.469496

Co	0.154224	-0.492776	0.829936
C	0.278028	-1.604809	-0.973122
O	0.458326	-2.893072	-1.012033
H	-0.022533	-3.405571	-0.224781
C	-0.999071	-0.900406	-0.861161
C	-0.654083	0.478800	-0.793622
C	0.763832	0.614718	-0.809807
C	1.371928	-0.668144	-0.854128
C	-1.265562	-0.120468	2.036142
C	1.425290	0.165393	1.966471
O	2.243657	0.576255	2.643755
C	-2.333434	-1.501983	-0.945579
C	-2.529848	-2.724870	-1.602113
C	-3.453787	-0.835041	-0.426964
C	-3.806536	-3.260781	-1.728322
H	-1.685578	-3.254175	-2.035853
C	-4.722635	-1.379637	-0.555240
H	-3.334580	0.110962	0.095194
C	-4.923782	-2.603945	-1.205331
H	-3.939957	-4.207093	-2.250605
H	-5.578805	-0.845745	-0.145061
C	2.804944	-0.989515	-0.849586
C	3.693547	-0.200719	-1.585750

C	3.307561	-2.067647	-0.106782
C	5.055459	-0.490286	-1.587158
H	3.319503	0.634899	-2.174926
C	4.666859	-2.345309	-0.112421
H	2.631578	-2.673621	0.494444
C	5.564214	-1.564859	-0.854237
H	5.735742	0.130133	-2.168763
H	5.047772	-3.179523	0.475746
C	-6.294656	-3.191540	-1.319994
H	-6.598319	-3.663017	-0.376226
H	-7.040511	-2.421269	-1.546811
H	-6.336514	-3.958320	-2.100502
C	7.025801	-1.887289	-0.856682
H	7.216352	-2.846166	-1.355254
H	7.605343	-1.116946	-1.375597
H	7.413387	-1.979958	0.164947
C	-1.303178	1.818870	-0.821514
C	1.170847	2.038343	-0.849888
H	-2.161189	1.948982	-0.159475
H	-1.651154	1.998100	-1.850237
H	1.452449	2.280430	-1.884659
H	2.022237	2.296528	-0.211931
C	-0.129447	2.790461	-0.477721
C	-0.069217	3.208392	0.993024
C	-0.296618	4.061310	-1.305109
O	0.929851	3.715437	1.472224
O	0.295504	4.294166	-2.338814
O	-1.184255	2.991872	1.664187
O	-1.219318	4.852621	-0.773112
C	-1.517518	6.066062	-1.489781
H	-1.885130	5.827056	-2.490928
H	-2.290944	6.566876	-0.908694
H	-0.622927	6.690590	-1.554077
C	-1.161750	3.327102	3.062504
H	-0.956684	4.393290	3.189984
H	-2.153586	3.081421	3.440862
H	-0.398769	2.731251	3.573436
C	-0.197727	-3.116014	1.986884
O	-0.367172	-3.196508	3.196236
H	0.300194	-2.107071	1.629848
O	-0.424813	-3.917404	1.048956
N	-2.131778	0.026976	2.813195

TS2,3-Co-c Gsolv= -2660.390896

Co	-0.107188	0.543194	0.729803
N	-2.531265	1.290026	2.441972
C	-0.080129	-0.886938	-0.854424
O	-0.037078	-2.166719	-0.646446
H	0.618310	-2.418831	0.158610
C	-1.309501	-0.118270	-0.827190
C	-0.909968	1.235433	-1.000281
C	0.511093	1.307722	-1.078083
C	1.068067	0.016095	-0.940832
C	-1.589917	1.002348	1.803615
C	0.949083	1.648319	1.738931
O	1.560229	2.375790	2.365426
C	-2.672348	-0.648961	-0.706984
C	-3.708622	-0.040655	-1.423934
C	-2.955621	-1.737935	0.127913
C	-5.010095	-0.523740	-1.318576
H	-3.496077	0.801322	-2.080681
C	-4.257217	-2.213787	0.231584
H	-2.158997	-2.193867	0.712202
C	-5.286342	-1.610402	-0.492076
H	-5.808143	-0.048661	-1.883888
H	-4.471786	-3.054242	0.887291
H	-6.303468	-1.985776	-0.407277
C	2.482587	-0.383312	-0.978452
C	3.472499	0.417736	-0.394236
C	2.853585	-1.568146	-1.627046
C	4.807493	0.035037	-0.451544
H	3.202309	1.341782	0.114565
C	4.191811	-1.944942	-1.684122
H	2.096523	-2.190838	-2.097855
C	5.170578	-1.149000	-1.092790
H	5.566345	0.661443	0.010940
H	4.469182	-2.864835	-2.193193
H	6.215044	-1.448831	-1.132197
C	-1.453619	2.607402	-1.178213
O	-0.308200	3.444099	-0.976256
C	0.884419	2.728493	-1.316261
H	-2.234951	2.891788	-0.466426
H	-1.843214	2.718820	-2.203165
H	1.133235	2.852554	-2.382935
H	1.711695	3.115237	-0.714755
C	1.054429	-1.553610	2.161801
O	1.301107	-2.505503	1.379362
H	0.147042	-0.883660	1.815642

O	1.545979	-1.235562	3.236892

TS2,3-Co Gsolv= -3019.059464

Co	-0.024106	0.130793	0.838419
C	-0.009259	-0.615382	-1.126623
O	-0.038322	-1.888738	-1.441010
H	0.048397	-2.569756	-0.616505
C	-1.196866	0.171295	-0.848882
C	-0.722101	1.483540	-0.547239
C	-1.490362	2.719882	-0.235619
H	-2.394900	2.481304	0.333488
H	-1.829123	3.135151	-1.199233
C	-0.619109	3.745880	0.480973
H	-1.173724	4.685202	0.580608
H	-0.395750	3.392586	1.500687
C	0.676382	3.964276	-0.287766
H	1.257869	4.784385	0.146879
H	0.430392	4.259457	-1.318500
C	1.534682	2.701008	-0.310920
H	2.295672	2.762078	-1.100948
H	2.094178	2.602294	0.629863
C	0.722243	1.470383	-0.553495
C	1.182322	0.141790	-0.842594
Si	-2.963328	-0.519186	-1.047558
C	-3.136249	-0.914544	-2.870406
H	-2.999820	-0.014615	-3.482952
H	-4.137700	-1.313753	-3.076657
H	-2.400351	-1.661413	-3.192210
C	-4.240163	0.751186	-0.543808
H	-4.171524	1.676799	-1.127490
H	-4.180794	1.001153	0.522918
H	-5.233544	0.317927	-0.724938
C	-3.158482	-2.057435	0.001065
H	-2.956928	-1.855475	1.061423
H	-2.499432	-2.867784	-0.331791
H	-4.194574	-2.412859	-0.079748
Si	2.958047	-0.525129	-1.029532
C	3.231530	-0.696561	-2.872486
H	4.236169	-1.086945	-3.078627
H	3.136478	0.275440	-3.373278
H	2.502168	-1.383702	-3.319630
C	4.188144	0.668149	-0.275888
H	5.181735	0.202328	-0.326523
H	3.976558	0.876246	0.780569
H	4.243095	1.620989	-0.814843
C	3.108227	-2.168885	-0.149751
H	4.151443	-2.506299	-0.215335
H	2.473418	-2.944909	-0.591544
H	2.855135	-2.080697	0.915786
C	-1.390952	0.495385	2.095538
C	1.268758	0.399154	2.097331
O	2.067660	0.571388	2.891435
H	-0.297698	-1.552279	1.345685
C	-0.048835	-2.674957	1.561015
O	-0.011186	-2.963415	2.749996
O	0.099272	-3.357271	0.518954
N	-2.232983	0.695062	2.888164

TS2,3-Fe Gsolv= -2920.523287

Fe	0.149101	0.121480	0.912069
C	0.023976	-0.731275	-1.044666
O	-0.132428	-2.026145	-1.214366
H	-0.866731	-2.477321	-0.524272
C	-1.028152	0.230154	-0.826415
C	-0.348129	1.475413	-0.570112
C	-0.939867	2.832136	-0.368726
H	-1.873885	2.777701	0.206378
H	-1.215172	3.221738	-1.361794
C	0.070424	3.777626	0.273022
H	-0.340563	4.793121	0.292955
H	0.248408	3.480951	1.319461
C	1.379452	3.744091	-0.505275
H	2.071859	4.512765	-0.143723
H	1.165196	3.980591	-1.558446
C	2.054698	2.375941	-0.420014
H	2.810166	2.274347	-1.210370
H	2.603640	2.284051	0.526950
C	1.065318	1.257924	-0.571802
C	1.315364	-0.140401	-0.804669
Si	-2.890314	-0.000747	-1.143256
C	-3.162953	-1.522014	-2.203998
H	-2.563587	-1.482929	-3.123346
H	-4.220516	-1.545531	-2.499912
H	-2.939261	-2.459884	-1.684843
C	-3.500320	1.481316	-2.122059
H	-2.866264	1.682141	-2.994243
H	-3.554847	2.395424	-1.519600
H	-4.512255	1.263602	-2.489566

C	-3.858452	-0.120670	0.456843
H	-3.819863	0.819404	1.022419
H	-3.498552	-0.929066	1.104826
H	-4.913331	-0.321843	0.224390
Si	2.930720	-1.128771	-0.861502
C	3.202664	-1.674051	-2.634684
H	4.125481	-2.262763	-2.718814
H	3.293620	-0.806223	-3.301737
H	2.371020	-2.293143	-2.995308
C	4.371708	-0.075779	-0.282925
H	5.274491	-0.702220	-0.273489
H	4.228052	0.306114	0.736578
H	4.566584	0.774503	-0.948396
C	2.782726	-2.610000	0.282580
H	3.696759	-3.216102	0.215926
H	1.930717	-3.252562	0.027828
H	2.673618	-2.292312	1.329018
C	-1.032656	0.852852	2.064261
O	-1.756863	1.385361	2.779368
C	1.526402	0.351405	2.048514
O	2.414338	0.551397	2.751998
H	-0.310033	-2.128037	1.659981
C	-1.278103	-2.698674	1.586224
O	-1.869023	-2.965659	2.639241
O	-1.639980	-3.017167	0.405930

TS2.3-Mn-a Gsolv= -2821.074900

C	-0.052335	0.620296	1.151013
O	0.047633	1.907323	1.291602
H	0.131510	2.192437	-0.074534
C	-1.295089	-0.074914	0.851779
C	-0.908722	-1.422216	0.579791
C	0.499733	-1.540997	0.606342
C	1.080113	-0.269716	0.913430
Si	-3.029608	0.671811	0.898035
C	-3.345434	1.265897	2.646929
H	-3.283707	0.440712	3.367244
H	-4.344313	1.713070	2.731020
H	-2.609836	2.026462	2.938220
C	-4.228315	-0.682701	0.408477
H	-4.171212	-1.544085	1.086277
H	-4.040824	-1.034946	-0.614827
H	-5.256919	-0.300432	0.443358
C	-3.161927	2.100052	-0.307113
H	-2.965091	1.773859	-1.336887
H	-2.467014	2.912721	-0.063187
H	-4.180584	2.509382	-0.275402
Si	2.901218	0.174367	1.154046
C	3.127060	0.646695	2.953375
H	4.175782	0.903480	3.152210
H	2.851629	-0.181204	3.618712
H	2.511196	1.515452	3.217843
C	3.910670	-1.350679	0.745575
H	4.975487	-1.144305	0.916333
H	3.797265	-1.653892	-0.303070
H	3.633730	-2.201024	1.382275
C	3.395003	1.607771	0.052202
H	4.446654	1.863453	0.239230
H	2.793233	2.500914	0.263327
H	3.297526	1.367148	-1.014786
O	-2.051887	-1.118306	-2.648145
C	1.370248	-0.728197	-1.935267
O	2.236269	-1.145560	-2.569151
C	-1.489979	-2.774430	0.344797
O	-0.363782	-3.554734	-0.084586
C	0.854664	-2.976777	0.412083
H	-2.267785	-2.838348	-0.423991
H	-1.899496	-3.170501	1.288277
H	1.130937	-3.431511	1.377283
H	1.650862	-3.181379	-0.311332
H	0.957395	2.025048	-2.947655
C	0.798261	2.566751	-2.001947
O	0.159147	1.828493	-1.102749
O	1.141370	3.712046	-1.801401
N	-1.197504	-0.665897	-1.990095
Mn	-0.054405	-0.208113	-0.906711

TS2,3-Mn Gsolv= -2824.412751

Mn	0.119530	0.132198	0.976595
N	-0.876820	0.953637	1.992597
O	-1.559294	1.679820	2.599245
C	0.016364	-0.749738	-1.030083
O	-0.120524	-2.048966	-1.195904
H	-0.836138	-2.511195	-0.496746
C	-1.042249	0.201909	-0.834608
C	-0.377339	1.458327	-0.582768
C	-0.990836	2.809999	-0.416701
H	-1.917329	2.758081	0.170728

H	-1.285716	3.158414	-1.419343
C	0.004990	3.797476	0.184044
H	-0.419583	4.807228	0.150100
H	0.177792	3.557552	1.245378
C	1.323156	3.742897	-0.577329
H	2.000197	4.538410	-0.246074
H	1.120655	3.922202	-1.644294
C	2.013125	2.389507	-0.410850
H	2.801593	2.267970	-1.164636
H	2.519895	2.345656	0.563153
C	1.037026	1.256921	-0.552380
C	1.298656	-0.142428	-0.777080
Si	-2.908712	-0.052129	-1.108263
C	-3.195995	-1.605496	-2.115807
H	-2.605415	-1.601586	-3.040624
H	-4.256803	-1.635920	-2.399743
H	-2.969364	-2.524117	-1.564335
C	-3.555596	1.400707	-2.106391
H	-2.939959	1.593015	-2.994239
H	-3.613082	2.325493	-1.520462
H	-4.570917	1.161478	-2.451022
C	-3.814791	-0.135701	0.530025
H	-3.727483	0.807813	1.084513
H	-3.439518	-0.945649	1.168568
H	-4.882972	-0.317356	0.350827
Si	2.923325	-1.114439	-0.893782
C	3.067144	-1.742185	-2.653926
H	4.002670	-2.302449	-2.781100
H	3.071686	-0.911834	-3.371245
H	2.235947	-2.410015	-2.911326
C	4.389337	-0.021223	-0.485546
H	5.294948	-0.643336	-0.501195
H	4.315663	0.424926	0.514067
H	4.530973	0.784783	-1.215644
C	2.873947	-2.547051	0.318157
H	3.766966	-3.172275	0.184455
H	1.991594	-3.180622	0.166368
H	2.868167	-2.196101	1.358695
C	1.610469	0.299300	2.052497
O	2.534030	0.502769	2.705476
H	-0.279855	-2.155457	1.697238
C	-1.238112	-2.742052	1.619933
O	-1.825905	-3.019052	2.671976
O	-1.593990	-3.067147	0.440004

TS3',2'-Co-a Gsolv= -3015.716443

C	0.009190	0.425416	1.242078
O	-0.031314	1.689835	1.510255
H	-0.080173	2.128169	0.310287
C	-1.170773	-0.362294	0.869107
C	-0.651634	-1.614701	0.447985
C	0.770698	-1.574816	0.449535
C	1.225351	-0.293945	0.875627
Si	-2.975467	0.197009	1.069604
C	-3.231429	0.470648	2.904534
H	-3.073541	-0.456054	3.470223
H	-4.256165	0.813105	3.098127
H	-2.542918	1.230374	3.295401
C	-4.058236	-1.193438	0.442787
H	-3.857828	-2.129177	0.980885
H	-3.913946	-1.371778	-0.630059
H	-5.114897	-0.941944	0.601583
C	-3.266733	1.785491	0.121258
H	-3.094632	1.658287	-0.955138
H	-2.619623	2.594690	0.482916
H	-4.308543	2.103536	0.260254
Si	2.996186	0.369614	1.046839
C	3.290670	0.642786	2.874210
H	4.300211	1.036152	3.048051
H	3.191462	-0.295482	3.433881
H	2.571866	1.362746	3.285437
C	4.128345	-0.943433	0.343716
H	5.174357	-0.625336	0.440353
H	3.932202	-1.113720	-0.723083
H	4.019639	-1.899324	0.872105
C	3.165203	1.969369	0.085740
H	4.193919	2.341520	0.181731
H	2.491513	2.748246	0.463451
H	2.962442	1.826338	-0.983936
C	-1.346987	-0.446589	-2.097308
C	1.286908	-0.397341	-2.094334
O	2.071760	-0.582079	-2.900057
C	-1.079608	-2.973963	0.020301
O	0.114186	-3.543227	-0.535103
C	1.271563	-2.912724	0.028445
H	-1.866650	-3.003697	-0.739327
H	-1.412543	-3.545192	0.901966
H	1.626881	-3.460553	0.916454

H	2.067257	-2.910281	-0.723270
H	-0.268236	2.345305	-2.775571
C	-0.242442	2.790642	-1.766741
O	-0.093728	1.890902	-0.820911
O	-0.339322	3.984847	-1.550337
N	-2.181142	-0.619216	-2.904285
Co	0.017878	-0.140112	-0.812050

TS3',2'-Co-b Gsolv= -3080.003095

C	-0.088322	-1.365112	-1.005220
O	-0.125354	-2.650837	-0.906712
H	-0.266750	-2.730906	0.346108
C	-1.260406	-0.481872	-0.848713
C	-0.749547	0.840080	-0.782071
C	0.669473	0.796993	-0.799193
C	1.112620	-0.558427	-0.893997
C	-1.225143	0.478259	2.087416
C	1.414557	0.109442	1.882725
O	2.333518	0.330747	2.519162
C	-2.658656	-0.922759	-0.868052
C	-3.662681	-0.189671	-0.215860
C	-3.028423	-2.063899	-1.591418
C	-4.987738	-0.594102	-0.283669
H	-3.405796	0.696439	0.360659
C	-4.361058	-2.458078	-1.657793
H	-2.272452	-2.638152	-2.120161
C	-5.362268	-1.736752	-1.003180
H	-5.753002	-0.014876	0.231998
H	-4.629595	-3.343206	-2.232860
C	2.501688	-1.038236	-0.933775
C	3.447167	-0.349260	-1.701662
C	2.910859	-2.163706	-0.206655
C	4.768276	-0.782391	-1.746975
H	3.145318	0.524738	-2.277054
C	4.233196	-2.587567	-0.257763
H	2.196272	-2.690424	0.424317
C	5.183284	-1.908629	-1.029869
H	5.493454	-0.235542	-2.348417
H	4.540979	-3.456579	0.322503
C	-6.794968	-2.165666	-1.055051
H	-7.138600	-2.507482	-0.070288
H	-7.448046	-1.334472	-1.346907
H	-6.943288	-2.985999	-1.764799
C	6.600837	-2.384770	-1.099893
H	6.733871	-3.098708	-1.923437
H	7.292885	-1.554296	-1.277153
H	6.898057	-2.895857	-0.177661
C	-1.232864	2.247992	-0.761085
C	1.248749	2.167921	-0.790274
H	-2.078659	2.449361	-0.098949
H	-1.538276	2.522869	-1.779952
H	1.551610	2.421175	-1.817179
H	2.127354	2.295403	-0.151926
C	0.034990	3.049675	-0.368424
C	-0.019252	3.397250	1.121030
C	0.106844	4.386074	-1.096066
O	-0.980461	3.963934	1.605325
O	-0.634142	4.739853	-1.987371
O	1.064708	3.070835	1.808604
H	0.945018	3.338917	2.738632
O	1.126653	5.113821	-0.640727
H	1.166550	5.959400	-1.124208
H	0.050005	-2.137345	3.362641
C	-0.021298	-2.820252	2.499181
O	-0.340202	-2.196802	1.381397
O	0.158941	-4.021000	2.571128
Co	-0.020426	-0.264687	0.814686
N	-1.946310	0.906066	2.908425

TS3',2'-Co-c Gsolv= -2660.401512

C	-0.026532	-0.366746	-1.239413
O	0.008248	-1.615186	-1.572888
H	0.007713	-2.109884	-0.449857
C	-1.240332	0.348500	-0.819162
C	-0.797245	1.602429	-0.321610
C	0.617193	1.648172	-0.341987
C	1.135970	0.427939	-0.858378
C	-1.420543	0.230161	2.122352
C	1.261994	0.339724	2.107185
O	2.071060	0.528895	2.886279
C	-2.636226	-0.081799	-0.968493
C	-3.607429	0.890135	-1.244106
C	-3.031165	-1.419733	-0.829481
C	-4.944176	0.533237	-1.388608
H	-3.313360	1.930910	-1.369011
C	-4.369641	-1.770577	-0.970634
H	-2.299644	-2.187620	-0.595285
C	-5.329058	-0.798664	-1.251532

H	-5.684637	1.298327	-1.608972
H	-4.665239	-2.810573	-0.854386
H	-6.373989	-1.079179	-1.361033
C	2.554422	0.082017	-1.026105
C	3.456356	1.088127	-1.394890
C	3.029929	-1.219203	-0.813337
C	4.807744	0.798069	-1.556892
H	3.097646	2.100211	-1.575470
C	4.381736	-1.503601	-0.976773
H	2.348178	-2.007656	-0.504654
C	5.273707	-0.498297	-1.348641
H	5.496276	1.587892	-1.847820
H	4.741267	-2.515354	-0.805126
H	6.329956	-0.724961	-1.473645
C	-1.293252	2.897128	0.222585
O	-0.130032	3.456005	0.845054
C	1.043775	2.976672	0.180430
H	-1.636342	3.536837	-0.607076
H	1.310365	3.631346	-0.665514
H	1.876318	2.961871	0.891118
H	0.485444	-2.471769	2.622018
C	0.437807	-2.847038	1.585725
O	-0.043639	-1.962710	0.738421
O	0.779861	-3.970303	1.262859
H	-2.091288	2.819171	0.966846
N	-2.307264	0.313114	2.886537
Co	-0.029334	0.082041	0.834996

TS3',2'-Co Gsolv= -3019.069699

C	0.014220	-0.585683	1.207619
O	0.079105	-1.860858	1.423758
H	0.121677	-2.244392	0.183346
C	1.165427	0.242295	0.867658
C	0.637836	1.524888	0.511383
C	1.361267	2.777916	0.150693
H	2.271227	2.550715	-0.415030
H	1.689710	3.246063	1.092940
C	0.448973	3.740374	-0.601823
H	0.966753	4.695037	-0.746898
H	0.231430	3.336101	-1.603882
C	-0.847944	3.946005	0.169306
H	-1.461735	4.725816	-0.294733
H	-0.600874	4.297599	1.182122
C	-1.661450	2.655702	0.263235
H	-2.401898	2.723815	1.071685
H	-2.244637	2.501285	-0.654851
C	-0.798324	1.462646	0.536131
C	-1.205158	0.129704	0.875686
Si	2.953573	-0.373422	1.077398
C	3.137549	-0.768611	2.900736
H	2.962483	0.119954	3.520155
H	4.153506	-1.129161	3.108310
H	2.431376	-1.547347	3.214314
C	4.191536	0.944334	0.590560
H	4.071424	1.867999	1.169469
H	4.143918	1.191837	-0.477194
H	5.198086	0.553351	0.793546
C	3.239323	-1.911859	0.044786
H	3.104488	-1.715948	-1.026915
H	2.572125	-2.732957	0.333749
H	4.273338	-2.250805	0.195767
Si	-2.937568	-0.640023	1.022755
C	-3.233017	-0.923957	2.850066
H	-4.228339	-1.353849	3.020297
H	-3.173265	0.021106	3.404833
H	-2.489376	-1.612566	3.270570
C	-4.226388	0.517276	0.309505
H	-5.193374	-0.003671	0.310639
H	-4.003829	0.796384	-0.728361
H	-4.340992	1.434974	0.898343
C	-2.982797	-2.250314	0.062977
H	-3.985411	-2.690244	0.150093
H	-2.258463	-2.982105	0.439901
H	-2.782026	-2.085260	-1.004518
C	1.367473	0.428086	-2.073744
C	-1.283582	0.344486	-2.080962
O	-2.076346	0.518579	-2.882962
H	0.267290	-2.319461	-2.894869
C	0.253428	-2.810079	-1.907147
O	0.124193	-1.951416	-0.921020
O	0.346169	-4.013058	-1.744881
N	2.206965	0.615868	-2.872541
Co	-0.008246	0.079912	-0.809864

TS3',2'-Fe-Casey Gsolv= -2917.181905

Fe	-0.005597	0.140573	0.845967
C	-0.012339	-0.454702	-1.230651
O	0.011709	-1.725040	-1.501211

H	0.037682	-2.164016	-0.182477
C	-1.217680	0.280932	-0.865344
C	-0.753168	1.566009	-0.442803
C	0.660697	1.594854	-0.458080
C	1.168809	0.330354	-0.890144
Si	-2.984634	-0.356816	-1.043194
C	-3.292571	-0.660028	-2.867210
H	-3.184341	0.268422	-3.442034
H	-4.307734	-1.043310	-3.032427
H	-2.584301	-1.393753	-3.272547
C	-4.126899	0.979484	-0.392725
H	-3.992376	1.923056	-0.937592
H	-3.961641	1.173444	0.674864
H	-5.173243	0.670773	-0.515236
C	-3.209581	-1.943714	-0.066522
H	-3.014594	-1.794476	1.003876
H	-2.545767	-2.739481	-0.427653
H	-4.244065	-2.297243	-0.171713
Si	2.955642	-0.244433	-1.087432
C	3.254342	-0.559036	-2.910866
H	4.278578	-0.915848	-3.079803
H	3.115317	0.358074	-3.497168
H	2.564272	-1.318032	-3.300852
C	4.058133	1.136412	-0.462060
H	5.113185	0.866234	-0.600235
H	3.902377	1.329164	0.607323
H	3.881126	2.071657	-1.009227
C	3.246330	-1.813186	-0.099036
H	4.286921	-2.141545	-0.223511
H	2.595404	-2.630148	-0.436348
H	3.071361	-1.655622	0.973927
C	-1.304576	0.413332	2.046845
O	-2.143823	0.629895	2.805528
C	1.287894	0.496960	2.031199
O	2.118433	0.778436	2.778218
C	-1.247063	2.921527	-0.064898
O	-0.076573	3.570036	0.458028
C	1.106699	2.969788	-0.092134
H	-2.027034	2.949662	0.703376
H	-1.614772	3.449941	-0.959491
H	1.430656	3.509988	-0.996646
H	1.903892	3.033478	0.656026
H	0.238015	-2.356282	2.826346
C	0.197346	-2.805256	1.820540
O	0.041378	-1.895899	0.879124
O	0.284407	-3.996669	1.597332

TS3',2'-Fe Gsolv= -2920.531540

Fe	-0.000362	0.084760	-0.847492
C	-0.001847	-0.627948	1.184885
O	0.042056	-1.912320	1.391470
H	0.079681	-2.278499	0.036044
C	1.156148	0.194470	0.888942
C	0.644212	1.494355	0.532806
C	1.396201	2.753903	0.238568
H	2.310803	2.544343	-0.328717
H	1.724244	3.180445	1.200201
C	0.510261	3.762599	-0.484104
H	1.039760	4.718325	-0.573165
H	0.307653	3.410138	-1.509148
C	-0.801116	3.943567	0.269441
H	-1.393033	4.758996	-0.162046
H	-0.570233	4.234277	1.305802
C	-1.632757	2.661433	0.274875
H	-2.402656	2.714019	1.055923
H	-2.177701	2.562474	-0.674068
C	-0.783423	1.447576	0.527675
C	-1.207768	0.110971	0.860937
Si	2.924472	-0.444554	1.095664
C	3.137396	-0.937905	2.893695
H	2.952074	-0.088783	3.563733
H	4.160634	-1.293217	3.073294
H	2.446166	-1.744441	3.168309
C	4.188551	0.868793	0.653671
H	4.090608	1.775007	1.263531
H	4.140915	1.155711	-0.404621
H	5.189068	0.451931	0.834980
C	3.213613	-1.929196	-0.017464
H	3.105306	-1.666878	-1.079040
H	2.525061	-2.754706	0.201645
H	4.238301	-2.297370	0.130040
Si	-2.938530	-0.637105	1.010074
C	-3.222231	-1.037270	2.820705
H	-4.224291	-1.460170	2.970667
H	-3.143251	-0.132096	3.436398
H	-2.489462	-1.764160	3.192935
C	-4.245809	0.571916	0.418934
H	-5.219923	0.064632	0.447592

H	-4.073324	0.898597	-0.614528
H	-4.316697	1.462933	1.054198
C	-3.075285	-2.190598	-0.037141
H	-4.072723	-2.630307	0.099808
H	-2.332226	-2.949065	0.237483
H	-2.956202	-1.965566	-1.105689
C	1.298530	0.530282	-1.988220
O	2.140769	0.883757	-2.692687
C	-1.303284	0.381917	-2.034905
O	-2.152325	0.608641	-2.781433
H	0.299851	-2.286847	-2.968645
C	0.258256	-2.795793	-1.991805
O	0.084605	-1.945188	-1.000138
O	0.358638	-3.997227	-1.838140

TS3',2'-Fe-Renaud Gsolv= -2675.811283

Fe	-0.016737	-0.105028	1.014515
C	-0.037290	-0.769645	-1.034481
O	0.032157	-2.045753	-1.265096
H	-0.000235	-2.439158	0.050034
C	-1.243451	-0.061972	-0.658549
C	-0.849731	1.278714	-0.310773
C	-0.899213	3.434435	0.622830
H	-1.542736	4.314934	0.714528
H	-0.594200	3.133237	1.636448
C	0.330546	3.763335	-0.203324
H	0.898907	4.569054	0.270716
H	0.032110	4.116698	-1.199977
C	0.576170	1.396210	-0.445366
C	1.094086	0.084504	-0.758110
C	-1.182979	0.309893	2.298494
O	-1.902125	0.669855	3.127366
C	1.358173	0.195795	2.117116
O	2.241095	0.348970	2.845556
H	0.620933	-2.571522	2.983607
C	0.550356	-3.000733	1.970941
O	-0.048484	-2.185038	1.119019
O	0.959596	-4.105019	1.671383
C	2.490634	-0.298790	-1.058334
C	3.164629	-1.268915	-0.309050
C	3.144313	0.286671	-2.149832
C	4.469574	-1.633253	-0.631907
H	2.665672	-1.738494	0.537440
C	4.451125	-0.072963	-2.468707
H	2.622219	1.025265	-2.755852
C	5.118725	-1.032323	-1.708556
H	4.980051	-2.387370	-0.037063
H	4.947302	0.394796	-3.316209
H	6.139773	-1.313085	-1.956777
C	-2.603141	-0.601954	-0.859413
C	-2.940926	-1.081081	-2.132757
C	-3.574808	-0.628564	0.146409
C	-4.219047	-1.566156	-2.395013
H	-2.194431	-1.060935	-2.925285
C	-4.855604	-1.107840	-0.117342
H	-3.334143	-0.280413	1.147619
C	-5.182757	-1.577698	-1.387872
H	-4.462838	-1.932346	-3.389816
H	-5.597896	-1.119858	0.677658
H	-6.182451	-1.955166	-1.590496
N	1.220480	2.599624	-0.343864
N	-1.683906	2.346959	0.029745
C	2.462828	2.685180	0.412667
H	3.070578	1.787795	0.270033
H	3.041958	3.548353	0.070499
H	2.254148	2.808496	1.488024
C	-2.551238	2.778829	-1.070130
H	-3.134404	1.930781	-1.443757
H	-3.250116	3.533393	-0.696199
H	-1.984779	3.205991	-1.913185

TS3',2'-Fe-williams-1 Gsolv= -2870.978073

Fe	-0.004858	-0.653099	1.006345
C	-0.020488	-1.386286	-1.047963
O	-0.048984	-2.668904	-1.217886
H	-0.050630	-3.015970	0.117312
C	-1.170923	-0.557920	-0.747733
C	-0.687941	0.745376	-0.369243
C	0.742192	0.712656	-0.366155
C	1.166464	-0.610429	-0.745319
C	-1.296405	-0.335394	2.214505
O	-2.115422	-0.138738	2.998061
C	1.291481	-0.391744	2.224124
O	2.111965	-0.230392	3.013717
C	-2.575611	-0.964992	-0.935493
C	-3.615142	-0.444300	-0.150025
C	-2.901783	-1.859675	-1.964818
C	-4.935387	-0.815257	-0.381286

H	-3.399267	0.261918	0.647793
C	-4.224280	-2.230642	-2.194283
H	-2.113407	-2.261466	-2.597158
C	-5.246479	-1.712998	-1.402526
H	-5.724734	-0.400023	0.241766
H	-4.454567	-2.921600	-3.000475
H	-6.279644	-2.002526	-1.580205
C	2.550783	-1.082301	-0.933102
C	3.612764	-0.614262	-0.144865
C	2.835522	-1.987515	-1.965077
C	4.914154	-1.047010	-0.375773
H	3.430545	0.101120	0.654637
C	4.139011	-2.420784	-2.193913
H	2.030018	-2.347001	-2.600044
C	5.183577	-1.955052	-1.399080
H	5.721658	-0.672239	0.249114
H	4.336775	-3.122193	-3.001407
H	6.201641	-2.294415	-1.575786
C	-1.505717	1.970977	-0.252283
C	-1.605000	2.721784	0.921856
C	-2.181576	2.405112	-1.399856
C	-2.372358	3.884141	0.949614
H	-1.091686	2.391195	1.823211
C	-2.945131	3.568233	-1.371075
H	-2.106997	1.822458	-2.317155
C	-3.043887	4.310127	-0.194896
H	-2.446439	4.456471	1.871644
H	-3.464953	3.894242	-2.268918
H	-3.643976	5.216861	-0.170407
C	1.613614	1.898722	-0.228676
C	1.744255	2.619018	0.961471
C	2.310408	2.326599	-1.365566
C	2.562310	3.744916	1.016341
H	1.214241	2.292052	1.854287
C	3.124772	3.453993	-1.309986
H	2.211730	1.767989	-2.295633
C	3.253663	4.165626	-0.118104
H	2.659963	4.292628	1.950813
H	3.659917	3.776536	-2.200145
H	3.893154	5.044191	-0.073253
H	-0.234858	-3.036202	3.135768
C	-0.209425	-3.540614	2.156348
O	-0.030987	-2.685134	1.162885
O	-0.324923	-4.737342	1.999008

TS3',2'-Fe-williams-2 Gsolv= -3059.943393

Fe	-0.188188	-0.493118	0.850427
C	-0.519461	-1.607718	-0.974603
O	-0.799019	-2.867374	-0.868390
H	-0.835589	-2.902053	0.500167
C	-1.483456	-0.517987	-0.817660
C	-0.720419	0.688134	-0.777604
C	0.656399	0.374092	-0.830348
C	0.820191	-1.045374	-0.904230
C	-1.176586	0.417105	2.042775
O	-1.804024	1.008037	2.806252
C	1.339351	-0.338826	1.777050
O	2.363488	-0.247514	2.294839
C	-2.947380	-0.660375	-0.840781
C	-3.783507	0.277027	-0.214490
C	-3.548088	-1.711128	-1.544497
C	-5.164753	0.159100	-0.287295
H	-3.354066	1.109039	0.340846
C	-4.934637	-1.823463	-1.611738
H	-2.925101	-2.441285	-2.054411
C	-5.768286	-0.895866	-0.983903
H	-5.792912	0.899393	0.207665
H	-5.377838	-2.648147	-2.168876
C	2.091164	-1.782119	-0.991613
C	3.151850	-1.243093	-1.731710
C	2.287270	-3.009300	-0.345016
C	4.365618	-1.914316	-1.827550
H	3.022466	-0.293872	-2.249507
C	3.504292	-3.675974	-0.448646
H	1.488761	-3.439031	0.256823
C	4.563202	-3.144818	-1.191725
H	5.177374	-1.476864	-2.408111
H	3.639063	-4.626255	0.066883
C	-7.259976	-1.014880	-1.043255
H	-7.683692	-1.181637	-0.044760
H	-7.717376	-0.096161	-1.430632
H	-7.570238	-1.847080	-1.683722
C	5.868239	-3.868960	-1.319148
H	6.716041	-3.195185	-1.147227
H	5.938328	-4.698093	-0.607245
H	5.991795	-4.285283	-2.327283
C	-0.926374	2.165890	-0.827023
C	1.485935	1.610610	-0.921659

H	-1.696855	2.562564	-0.160240
H	-1.195642	2.450505	-1.852888
H	1.768232	1.766704	-1.973683
H	2.405754	1.608165	-0.330506
C	0.481252	2.721697	-0.486718
C	0.543514	3.071674	1.000854
C	0.800551	3.988274	-1.270067
O	-0.348490	3.690902	1.554193
O	0.282944	4.297715	-2.324262
O	1.648422	2.672811	1.609669
O	1.772884	4.678722	-0.684513
H	-0.123458	-2.414529	3.384182
C	-0.357189	-3.065932	2.526529
O	-0.742104	-2.374793	1.463671
O	-0.289600	-4.277501	2.550326
C	2.224511	5.863204	-1.366375
H	1.402405	6.577573	-1.458680
H	3.018194	6.275120	-0.743883
H	2.610788	5.600586	-2.354512
C	1.738486	2.954293	3.016987
H	0.938101	2.432073	3.551078
H	2.712503	2.580007	3.331425
H	1.669539	4.030962	3.192492

TS3',2'-Fe-wills-1 Gsolv= -2561.869200

Fe	-0.039675	0.144566	0.869737
C	-0.071359	-0.488472	-1.186614
O	-0.026365	-1.759688	-1.429577
H	0.032618	-2.158412	-0.137667
C	-1.279424	0.246767	-0.819254
C	-0.846830	1.547230	-0.420324
C	0.559717	1.610524	-0.458895
C	1.085187	0.352510	-0.888341
C	-1.356840	0.404260	2.062261
O	-2.245353	0.616691	2.761721
C	1.316160	0.551309	1.974742
O	2.220779	0.872460	2.609552
C	-2.672772	-0.213309	-0.921632
C	-3.676122	0.711409	-1.241411
C	-3.033433	-1.549344	-0.695520
C	-5.006073	0.311232	-1.339754
H	-3.413728	1.750751	-1.433177
C	-4.363059	-1.946221	-0.797958
H	-2.273415	-2.278025	-0.427769
C	-5.354292	-1.019655	-1.119683
H	-5.770632	1.042605	-1.591607
H	-4.626582	-2.985982	-0.617338
H	-6.392552	-1.334109	-1.196385
C	2.508085	0.015932	-1.044507
C	3.429514	1.043969	-1.286816
C	2.981167	-1.300010	-0.932324
C	4.786893	0.766835	-1.419900
H	3.082558	2.070442	-1.392201
C	4.339199	-1.573111	-1.066733
H	2.285549	-2.112312	-0.740086
C	5.247425	-0.543568	-1.310508
H	5.484695	1.578704	-1.612078
H	4.690175	-2.598665	-0.975916
H	6.307887	-0.761602	-1.413910
C	-1.365725	2.890871	-0.030272
O	-0.208344	3.541976	0.511390
C	0.972858	2.997535	-0.092215
H	-1.728214	3.426723	-0.922920
H	1.238539	3.562309	-1.001137
H	1.797836	3.076280	0.623621
H	0.909435	-2.255438	2.744207
C	0.761938	-2.695390	1.744717
O	0.051960	-1.911699	0.947851
O	1.181110	-3.785360	1.411474
H	-2.156228	2.895153	0.727579

TS3',2'-Fe-wills-2 Gsolv= -2601.132812

Fe	0.098040	0.034607	0.874182
C	0.137294	-0.558850	-1.196788
O	0.150502	-1.824125	-1.467824
H	0.184918	-2.257668	-0.176795
C	-1.054410	0.214257	-0.868904
C	-0.596473	1.493393	-0.421656
C	0.811922	1.504335	-0.418653
C	1.310199	0.235061	-0.830195
C	-1.295238	0.140136	2.004338
O	-2.219912	0.160290	2.688575
C	1.355219	0.444820	2.088939
O	2.191083	0.771175	2.809563
C	-2.449222	-0.208844	-1.081084
C	-3.342219	0.672181	-1.703858
C	-2.907585	-1.472983	-0.686719
C	-4.665054	0.299822	-1.927531

H	-2.992994	1.653068	-2.024557
C	-4.229635	-1.843765	-0.914092
H	-2.231447	-2.162831	-0.185006
C	-5.112229	-0.959941	-1.533989
H	-5.346247	0.995704	-2.411973
H	-4.573876	-2.825700	-0.597246
H	-6.145651	-1.251678	-1.706400
C	2.728369	-0.134297	-0.964118
C	3.656867	0.855293	-1.316539
C	3.188245	-1.440590	-0.743294
C	5.008422	0.550152	-1.446666
H	3.318849	1.871698	-1.510787
C	4.540115	-1.742946	-0.877098
H	2.491534	-2.222786	-0.455870
C	5.455591	-0.751065	-1.227405
H	5.711605	1.332201	-1.723034
H	4.881080	-2.760427	-0.699111
H	6.511424	-0.991207	-1.328340
C	-1.080969	2.875603	-0.097216
O	0.097790	3.494957	0.461846
C	1.274014	2.877390	-0.066140
H	-1.320285	3.366844	-1.058485
H	1.610359	3.397666	-0.978476
H	2.072370	2.935997	0.681640
C	-2.223186	3.048840	0.867545
H	-2.506128	4.104268	0.931762
H	-3.098178	2.478391	0.535054
H	-1.933614	2.707547	1.867375
H	-0.303787	-2.514811	2.790680
C	-0.229822	-2.918006	1.767900
O	0.225035	-2.022579	0.905154
O	-0.514527	-4.059221	1.462704

TS3',2'-Fe-wills-3 Gsolv= -2778.791109

Fe	0.212335	0.073519	0.837095
C	0.102186	-0.596743	-1.204224
O	0.160273	-1.872305	-1.429267
H	0.348322	-2.257438	-0.116869
C	-1.099974	0.124901	-0.795629
C	-0.670984	1.443077	-0.442006
C	0.732740	1.513222	-0.565797
C	1.265202	0.253738	-0.972548
Si	3.068217	-0.220153	-1.275574
C	3.251139	-0.670665	-3.085064
H	4.293177	-0.933650	-3.309045
H	2.969275	0.167853	-3.734116
H	2.622840	-1.530696	-3.348358
C	4.113409	1.277963	-0.857781
H	5.171954	1.053206	-1.043405
H	4.017340	1.562949	0.198204
H	3.847576	2.145803	-1.475025
C	3.555982	-1.668344	-0.191319
H	4.590425	-1.963316	-0.412182
H	2.914475	-2.540924	-0.367769
H	3.502963	-1.408084	0.874660
C	-1.093845	0.126497	2.065026
O	-1.965016	0.111024	2.816430
C	1.503941	0.612737	1.957632
O	2.332378	1.015736	2.648900
C	-2.483558	-0.373470	-0.869245
C	-3.473725	0.431694	-1.445989
C	-2.834106	-1.642800	-0.391616
C	-4.786188	-0.022736	-1.545725
H	-3.209435	1.417345	-1.827571
C	-4.145727	-2.096453	-0.495503
H	-2.077608	-2.267380	0.078818
C	-5.125409	-1.289157	-1.072761
H	-5.544180	0.613993	-1.996378
H	-4.405108	-3.082428	-0.116368
H	-6.150178	-1.645284	-1.150228
C	-1.196381	2.811398	-0.129314
O	-0.003641	3.520113	0.273828
C	1.158070	2.919345	-0.309041
H	-1.566508	3.243847	-1.077107
H	1.412667	3.407143	-1.264316
H	1.998639	3.049032	0.380859
C	-2.237466	2.965350	0.947391
H	-3.114077	2.344686	0.727295
H	-1.827558	2.669419	1.919676
H	-2.564024	4.008214	1.012674
H	1.151280	-2.255566	2.795792
C	0.994766	-2.758717	1.827311
O	0.434023	-1.958230	0.937539
O	1.287178	-3.915476	1.602763

TS3',2'-Fe-wills-4 Gsolv= -2739.528042

Fe	0.142428	0.118642	0.863561
C	-0.011716	-0.461662	-1.201976

O	-0.017173	-1.730067	-1.474470
H	0.109009	-2.171151	-0.180865
C	-1.176413	0.305060	-0.760429
C	-0.674031	1.579437	-0.355956
C	0.732446	1.582066	-0.466773
C	1.193600	0.315926	-0.944066
Si	2.964906	-0.238704	-1.288503
C	3.112154	-0.559865	-3.128752
H	4.141085	-0.839349	-3.389817
H	2.846159	0.331348	-3.710807
H	2.451278	-1.378746	-3.439937
C	4.091353	1.161581	-0.756317
H	5.135267	0.903142	-0.977364
H	4.018693	1.348720	0.323244
H	3.862328	2.095327	-1.285892
C	3.376735	-1.791644	-0.323064
H	4.406967	-2.098712	-0.548115
H	2.715833	-2.626485	-0.587431
H	3.310414	-1.624433	0.760678
C	-1.134632	0.374248	2.092581
O	-1.997472	0.586429	2.824341
C	1.500364	0.479765	1.977952
O	2.377774	0.768680	2.665558
C	-2.589681	-0.098256	-0.810928
C	-3.567302	0.866220	-1.090040
C	-2.991744	-1.421661	-0.581326
C	-4.913653	0.516631	-1.147477
H	-3.271524	1.896345	-1.283209
C	-4.338104	-1.767874	-0.641153
H	-2.247598	-2.177998	-0.345443
C	-5.303631	-0.802379	-0.925239
H	-5.658147	1.277874	-1.369138
H	-4.635229	-2.798153	-0.458303
H	-6.355006	-1.077034	-0.969749
C	-1.118498	2.934796	0.079109
O	0.093325	3.540066	0.552384
C	1.222018	2.945254	-0.106113
H	-1.858939	2.956777	0.886198
H	-1.518833	3.494479	-0.782120
H	1.475054	3.504308	-1.021775
H	2.077918	2.985836	0.575033
H	0.970988	-2.349431	2.705816
C	0.781190	-2.789442	1.712969
O	0.188984	-1.935795	0.894492
O	1.063280	-3.929901	1.406123

TS3',2'-Fe-wills-5 Gsolv= -2896.557485

Fe	-0.440071	0.332226	1.068389
C	0.021912	-0.773545	-0.719487
O	0.154811	-2.058304	-0.618716
H	-0.015184	-2.128466	0.752192
C	-1.259217	-0.079305	-0.818312
C	-0.969755	1.314526	-0.681318
C	0.411782	1.470145	-0.445261
C	1.062111	0.200998	-0.397644
Si	2.903872	-0.119893	-0.118629
C	3.669253	1.478968	0.502860
H	4.722941	1.300463	0.755301
H	3.174156	1.837438	1.414256
H	3.638180	2.281439	-0.245358
C	3.143183	-1.446335	1.186344
H	4.211815	-1.671575	1.303562
H	2.623821	-2.381421	0.945744
H	2.776581	-1.084187	2.157618
C	3.686999	-0.599190	-1.789666
C	-2.032435	0.557761	1.861651
O	-3.073654	0.649687	2.342692
C	0.479442	1.184605	2.350176
O	1.069493	1.771044	3.146718
C	-2.560997	-0.691462	-1.132162
C	-3.377779	-0.100986	-2.104738
C	-3.001375	-1.858460	-0.494068
C	-4.606939	-0.665049	-2.435652
H	-3.041586	0.801785	-2.613375
C	-4.229234	-2.422202	-0.828660
H	-2.385615	-2.314389	0.278453
C	-5.035312	-1.828963	-1.799885
H	-5.229152	-0.195068	-3.193997
H	-4.561186	-3.325914	-0.322283
H	-5.995193	-2.270957	-2.057358
C	-1.584411	2.670199	-0.851280
O	-0.563216	3.545608	-0.325406
C	0.724618	2.928010	-0.420024
H	-1.681312	2.846917	-1.938546
H	1.228095	3.213871	-1.359145
H	1.334797	3.273200	0.421411
C	-2.887203	2.979236	-0.162317
H	-3.658550	2.257364	-0.455242

H	-2.760829	2.942950	0.925615
H	-3.232149	3.981148	-0.437513
C	5.208862	-0.633179	-1.631920
H	5.529873	-1.351448	-0.863788
H	5.678453	-0.938867	-2.580713
H	5.619406	0.350395	-1.365646
H	0.019560	-1.454544	3.689389
C	0.123008	-2.156035	2.845748
O	-0.220757	-1.604809	1.693599
O	0.493015	-3.307073	2.954437
C	3.201547	-1.974566	-2.246069
H	3.432673	-2.760299	-1.512862
H	2.117717	-1.989949	-2.423377
H	3.694003	-2.252462	-3.192153
C	3.313084	0.441383	-2.846382
H	2.228000	0.477736	-3.020980
H	3.643050	1.452723	-2.568546
H	3.790891	0.194208	-3.808167

TS3',2'-Mn-a Gsolv= -2821.074900

C	-0.052335	0.620296	1.151013
O	0.047633	1.907323	1.291602
H	0.131510	2.192437	-0.074534
C	-1.295089	-0.074914	0.851779
C	-0.908722	-1.422216	0.579791
C	0.499733	-1.540997	0.606342
C	1.080113	-0.269716	0.913430
Si	-3.029608	0.671811	0.898035
C	-3.345434	1.265897	2.646929
H	-3.283707	0.440712	3.367244
H	-4.344313	1.713070	2.731020
H	-2.609836	2.026462	2.938220
C	-4.228315	-0.682701	0.408477
H	-4.171212	-1.544085	1.086277
H	-4.040824	-1.034946	-0.614827
H	-5.256919	-0.300432	0.443358
C	-3.161927	2.100052	-0.307113
H	-2.965091	1.773859	-1.336887
H	-2.467014	2.912721	-0.063187
H	-4.180584	2.509382	-0.275402
Si	2.901218	0.174367	1.154046
C	3.127060	0.646695	2.953375
H	4.175782	0.903480	3.152210
H	2.851629	-0.181204	3.618712
H	2.511196	1.515452	3.217843
C	3.910670	-1.350679	0.745575
H	4.975487	-1.144305	0.916333
H	3.797265	-1.653892	-0.303070
H	3.633730	-2.201024	1.382275
C	3.395003	1.607771	0.052202
H	4.446654	1.863453	0.239230
H	2.793233	2.500914	0.263327
H	3.297526	1.367148	-1.014786
O	-2.051887	-1.118306	-2.648145
C	1.370248	-0.728197	-1.935267
O	2.236269	-1.145560	-2.569151
C	-1.489979	-2.774430	0.344797
O	-0.363782	-3.554734	-0.084586
C	0.854664	-2.976777	0.412083
H	-2.267785	-2.838348	-0.423991
H	-1.899496	-3.170501	1.288277
H	1.130937	-3.431511	1.377283
H	1.650862	-3.181379	-0.311332
H	0.957395	2.025048	-2.947655
C	0.798261	2.566751	-2.001947
O	0.159147	1.828493	-1.102749
O	1.141370	3.712046	-1.801401
N	-1.197504	-0.665897	-1.990095
Mn	-0.054405	-0.208113	-0.906711

TS3',2'-Mn-b Gsolv= -2963.836083

C	-0.473999	-1.640841	-0.973218
O	-0.695408	-2.911789	-0.878544
H	-0.689979	-2.949280	0.501700
C	-1.484350	-0.603583	-0.806225
C	-0.781895	0.637704	-0.758098
C	0.609682	0.397400	-0.819399
C	0.839337	-1.013211	-0.904337
O	-1.645000	1.133708	2.684050
C	1.455542	-0.300076	1.737304
O	2.506310	-0.131508	2.175362
C	-2.938602	-0.815614	-0.806291
C	-3.801930	0.050144	-0.119171
C	-3.503392	-1.864768	-1.543475
C	-5.178102	-0.135153	-0.164020
H	-3.398811	0.877326	0.462483
C	-4.882640	-2.042693	-1.584377
H	-2.857440	-2.537385	-2.102159

C	-5.744909	-1.187940	-0.891873
H	-5.829679	0.549525	0.378035
H	-5.299911	-2.860357	-2.171230
C	2.145334	-1.685666	-1.004442
C	3.209622	-1.041406	-1.645008
C	2.373588	-2.957874	-0.457091
C	4.459620	-1.648431	-1.739491
H	3.061055	-0.060638	-2.093156
C	3.623130	-3.556010	-0.555986
H	1.569866	-3.479923	0.056263
C	4.690431	-2.914254	-1.197011
H	5.270767	-1.128477	-2.247853
H	3.779756	-4.542837	-0.120769
C	-7.226917	-1.400407	-0.908490
H	-7.547745	-1.999367	-0.045845
H	-7.767986	-0.448883	-0.857264
H	-7.545270	-1.933638	-1.810897
C	6.034772	-3.568958	-1.282309
H	6.724179	-2.986046	-1.902002
H	6.485574	-3.677075	-0.287505
H	5.960895	-4.577353	-1.707256
C	-1.071187	2.100815	-0.807348
C	1.368644	1.678182	-0.931165
H	-1.851613	2.455672	-0.128060
H	-1.377660	2.364362	-1.828416
H	1.632412	1.841017	-1.987192
H	2.292497	1.732267	-0.348904
C	0.309360	2.737230	-0.496967
C	0.368517	3.116751	0.983663
C	0.542882	4.011794	-1.297905
O	-0.528440	3.743889	1.519369
O	-0.053533	4.314657	-2.311355
O	1.469959	2.729931	1.605601
O	1.535345	4.723489	-0.773734
H	0.336902	-2.536503	3.279125
C	0.020483	-3.158543	2.427026
O	-0.555034	-2.441286	1.464306
O	0.154238	-4.361488	2.367295
C	1.901297	5.930976	-1.466703
H	1.050168	6.616057	-1.498912
H	2.716613	6.364483	-0.888528
H	2.235136	5.694617	-2.480277
C	1.546662	3.018030	3.012794
H	0.743572	2.495454	3.543283
H	2.519611	2.648438	3.336569
H	1.472678	4.095171	3.183318
N	-1.038530	0.407301	1.996259
Mn	-0.175570	-0.485046	0.918821

TS3',2'-Mn-c Gsolv= -2465.758831

C	-0.099575	-0.594664	-1.148081
O	-0.040155	-1.877361	-1.306514
H	0.040521	-2.175792	0.022527
C	-1.311071	0.151855	-0.832877
C	-0.890081	1.480802	-0.533208
C	0.516481	1.557954	-0.568330
C	1.048425	0.276571	-0.913057
O	-2.014029	1.242579	2.639067
C	1.441258	0.644675	1.888468
O	2.387454	1.010796	2.430786
C	-2.697111	-0.333318	-0.883657
C	-3.729171	0.566279	-1.185927
C	-3.024277	-1.673725	-0.630101
C	-5.052674	0.138039	-1.237996
H	-3.496323	1.607274	-1.403809
C	-4.348086	-2.097718	-0.683896
H	-2.241079	-2.383543	-0.380807
C	-5.367378	-1.195921	-0.987291
H	-5.838963	0.849967	-1.478217
H	-4.584418	-3.139886	-0.480826
H	-6.400969	-1.531727	-1.027404
C	2.473175	-0.059015	-1.062121
C	3.388899	0.963601	-1.346759
C	2.953650	-1.367719	-0.903664
C	4.747169	0.688385	-1.472579
H	3.037869	1.983766	-1.491632
C	4.312827	-1.638651	-1.030863
H	2.262385	-2.176063	-0.681972
C	5.215332	-0.614366	-1.313944
H	5.439897	1.495957	-1.698157
H	4.668922	-2.658535	-0.903412
H	6.276780	-0.830416	-1.411041
C	-1.426208	2.842320	-0.243723
O	-0.277383	3.552643	0.236956
C	0.913060	2.975626	-0.318208
H	-1.804098	3.299834	-1.172720
H	1.175946	3.471149	-1.267291
H	1.732860	3.120233	0.393410

H	1.025997	-2.074346	2.857531
C	0.842592	-2.576138	1.894428
O	0.089766	-1.844633	1.078475
O	1.253714	-3.680143	1.608275
H	-2.213288	2.892812	0.516713
Mn	-0.059525	0.207345	0.923505
N	-1.176038	0.717914	2.014776

TS3',2'-Mn Gsolv= -2824.421789

C	-0.019207	-0.698555	-1.142900
O	0.100463	-1.981974	-1.317568
H	0.188648	-2.300009	0.061438
C	-1.262386	-0.023177	-0.836607
C	-0.915593	1.344531	-0.543939
C	-1.819351	2.502476	-0.263546
H	-2.668277	2.199175	0.360489
H	-2.249778	2.828471	-1.224056
C	-1.051142	3.659811	0.365558
H	-1.702947	4.538808	0.429842
H	-0.762717	3.398278	1.396819
C	0.194048	3.972740	-0.452903
H	0.683056	4.884487	-0.090903
H	-0.110765	4.168501	-1.492386
C	1.192518	2.815610	-0.425740
H	1.918121	2.926363	-1.242187
H	1.779880	2.846667	0.502225
C	0.504468	1.487634	-0.578044
C	1.088198	0.205246	-0.883005
Si	-2.950444	-0.873883	-0.943008
C	-3.181431	-1.455932	-2.711835
H	-3.164714	-0.613669	-3.414932
H	-4.148418	-1.965023	-2.819212
H	-2.394188	-2.160474	-3.007205
C	-4.336689	0.298893	-0.477249
H	-4.383831	1.189423	-1.115207
H	-4.266011	0.623261	0.569529
H	-5.287592	-0.240765	-0.588783
C	-3.026547	-2.331626	0.236220
H	-2.920639	-2.002182	1.278609
H	-2.254566	-3.082165	0.029223
H	-4.005557	-2.820567	0.138890
Si	2.898694	-0.292981	-1.127658
C	3.119448	-0.700928	-2.945068
H	4.164192	-0.970632	-3.149078
H	2.866488	0.160841	-3.576006
H	2.487277	-1.543506	-3.251538
C	4.067816	1.098891	-0.662184
H	5.095283	0.720580	-0.757063
H	3.936960	1.436468	0.373412
H	3.973100	1.967931	-1.324172
C	3.321305	-1.785051	-0.071899
H	4.346685	-2.106483	-0.300655
H	2.652189	-2.632885	-0.261987
H	3.282950	-1.545543	0.999780
O	-2.090652	0.906420	2.661653
C	1.369924	0.599984	1.967085
O	2.235568	1.001746	2.613420
H	0.906158	-2.162754	2.961613
C	0.774459	-2.701468	2.009974
O	0.199632	-1.944837	1.084624
O	1.094521	-3.856114	1.824560
Mn	-0.047116	0.095292	0.922079
N	-1.213409	0.496398	2.001974

TS5,1-Co-a Gsolv= -2827.162630

C	0.001968	1.265937	0.080712
O	-0.000881	2.230961	-0.820306
C	-1.200744	0.521217	0.449706
C	-0.713444	-0.626634	1.148603
C	0.703065	-0.621649	1.156116
C	1.197937	0.536121	0.468966
Si	-2.990115	1.077531	0.146639
C	-3.179615	2.693992	1.074674
H	-2.988475	2.560953	2.146764
H	-4.196471	3.090196	0.958857
H	-2.478134	3.447617	0.694670
C	-4.099134	-0.251994	0.855936
H	-3.883610	-0.434723	1.916754
H	-3.990258	-1.199174	0.311922
H	-5.149199	0.058512	0.779947
C	-3.306052	1.324054	-1.680983
H	-3.176431	0.390453	-2.242298
H	-2.636558	2.080687	-2.107465
H	-4.338266	1.667617	-1.830109
Si	2.987628	1.090551	0.162425
C	3.204578	2.699385	1.093811
H	4.223949	3.085769	0.968432
H	3.021732	2.565848	2.167063

H	2.506589	3.459926	0.721161
C	4.084331	-0.268607	0.834253
H	5.139687	0.015661	0.734326
H	3.941592	-1.207223	0.282209
H	3.889983	-0.460883	1.897293
C	3.284928	1.336009	-1.669292
H	4.311426	1.692620	-1.827401
H	2.602391	2.080741	-2.095710
H	3.167725	0.400432	-2.230786
C	-1.369029	-1.744723	-1.403476
C	1.269112	-1.731204	-1.410465
O	2.063258	-2.448529	-1.805330
C	-1.180806	-1.834045	1.881690
O	-0.003281	-2.649015	1.967802
C	1.169416	-1.828015	1.894258
H	-1.969199	-2.411082	1.388929
H	-1.527496	-1.542269	2.886582
H	1.506298	-1.532038	2.901398
H	1.967033	-2.401796	1.411679
H	-0.032332	1.223371	-1.692848
H	-0.047555	0.336209	-2.160124
Co	-0.000218	-0.591788	-0.783538
N	-2.213649	-2.461241	-1.791000

TS5,1-Co-b Gsolv= -2969.925013

C	0.041289	-1.989219	-0.482771
O	0.101329	-3.236924	-0.067271
C	-1.183690	-1.182791	-0.488636
C	-0.758537	0.174955	-0.643983
C	0.653441	0.219027	-0.696817
C	1.188195	-1.107468	-0.577494
C	-1.246243	0.093161	2.247061
C	1.422490	0.012994	2.067725
O	2.310042	0.377574	2.684808
C	-2.552393	-1.708075	-0.450565
C	-3.620650	-0.925459	0.014142
C	-2.829466	-2.990039	-0.940386
C	-4.917336	-1.418156	-0.005076
H	-3.437558	0.072515	0.406081
C	-4.134242	-3.473444	-0.961740
H	-2.020033	-3.609971	-1.317635
C	-5.199298	-2.701329	-0.491845
H	-5.732763	-0.798032	0.366121
H	-4.329624	-4.471173	-1.352568
C	2.605910	-1.493981	-0.616393
C	3.450452	-0.887173	-1.553050
C	3.142137	-2.456209	0.249719
C	4.793419	-1.243953	-1.629505
H	3.052741	-0.140678	-2.239065
C	4.484047	-2.804893	0.166086
H	2.509602	-2.914136	1.006905
C	5.332236	-2.210981	-0.776686
H	5.435910	-0.762722	-2.365747
H	4.888919	-3.547045	0.853273
C	-6.605161	-3.214528	-0.506886
H	-6.656319	-4.232768	-0.905805
H	-7.033222	-3.222903	0.503155
H	-7.252820	-2.575601	-1.120169
C	6.770094	-2.616592	-0.873889
H	6.875469	-3.550443	-1.441503
H	7.368246	-1.853378	-1.382898
H	7.202722	-2.793335	0.117379
C	-1.333227	1.534668	-0.848629
C	1.143417	1.604651	-0.919387
H	-2.185680	1.792456	-0.215828
H	-1.661543	1.612265	-1.894032
H	1.393285	1.713670	-1.984530
H	2.033392	1.878323	-0.346752
C	-0.108282	2.460239	-0.597523
C	-0.163437	2.973220	0.851472
C	-0.109866	3.735358	-1.429502
O	-1.185698	3.407461	1.346612
O	0.911017	4.327698	-1.726435
O	1.005592	2.941771	1.468953
O	-1.330315	4.142221	-1.739193
H	0.011456	-2.075405	1.937375
H	0.040291	-2.685723	1.142207
C	1.017021	3.410143	2.830824
H	2.054943	3.344488	3.156025
H	0.666907	4.444446	2.874312
H	0.378948	2.768835	3.447549
C	-1.425117	5.376451	-2.475015
H	-0.906977	5.280597	-3.432528
H	-2.490112	5.542897	-2.633195
H	-0.992500	6.192978	-1.891185
N	-2.026372	0.525948	3.009655
Co	0.049332	-0.659025	1.079191

TS5,1-Co-c Gsolv= -2471.847169

C	0.006058	-1.180430	-0.398616
O	0.008095	-2.345863	0.208113
C	-1.189571	-0.352116	-0.578576
C	-0.713486	0.945026	-0.945644
C	0.695801	0.947352	-0.947457
C	1.186507	-0.351312	-0.591558
C	-1.402808	1.311340	1.807357
C	1.303674	1.262921	1.827909
O	2.153097	1.778953	2.386500
C	-2.593004	-0.772751	-0.482279
C	-3.522142	-0.216166	-1.370748
C	-3.031259	-1.703785	0.469210
C	-4.861826	-0.589750	-1.317208
H	-3.193072	0.497169	-2.124728
C	-4.371076	-2.073308	0.519106
H	-2.327706	-2.123444	1.183248
C	-5.289801	-1.519120	-0.371986
H	-5.570725	-0.153482	-2.016926
H	-4.701561	-2.791119	1.266221
H	-6.336926	-1.809062	-0.326339
C	2.594596	-0.761150	-0.495734
C	3.510121	-0.249802	-1.424094
C	3.044020	-1.644158	0.495056
C	4.849683	-0.624813	-1.371292
H	3.169407	0.429578	-2.204174
C	4.383201	-2.016752	0.542436
H	2.346939	-2.024027	1.237747
C	5.288913	-1.510112	-0.389427
H	5.549973	-0.224423	-2.100511
H	4.723026	-2.698904	1.318239
H	6.335570	-1.802180	-0.346590
C	-1.180074	2.311249	-1.312326
O	-0.009977	3.116706	-1.122189
C	1.160719	2.314403	-1.313718
H	-1.492719	2.323006	-2.369262
H	1.475693	2.325080	-2.370012
H	1.973306	2.715323	-0.699284
H	-0.036226	-1.607704	1.311980
H	-0.067181	-0.863888	1.994149
H	-1.991799	2.710623	-0.696924
Co	-0.007944	0.391401	0.912726
N	-2.294385	1.852955	2.345391

TS5,1-Co Gsolv= -2830.513379

C	-0.009632	-1.282954	-0.359831
O	-0.026716	-2.457515	0.249804
H	-0.066524	-1.713492	1.357290
C	-1.195441	-0.459056	-0.523043
C	-0.716656	0.844310	-0.910576
C	-1.492137	2.073205	-1.243917
H	-2.390412	2.147048	-0.621649
H	-1.843359	1.963889	-2.283055
C	-0.620708	3.318868	-1.130068
H	-1.177044	4.188026	-1.498315
H	-0.388050	3.509077	-0.069391
C	0.668416	3.132170	-1.918968
H	1.249937	4.060189	-1.949146
H	0.410932	2.884931	-2.959723
C	1.531284	2.016689	-1.331064
H	2.277231	1.679482	-2.063319
H	2.107164	2.390288	-0.473280
C	0.714201	0.828531	-0.928669
C	1.180733	-0.481833	-0.533515
Si	-2.954826	-1.157695	-0.346288
C	-3.077555	-2.543927	-1.602663
H	-2.948738	-2.166985	-2.625012
H	-4.064387	-3.021054	-1.541498
H	-2.318939	-3.315979	-1.424872
C	-4.235367	0.157481	-0.714816
H	-4.123966	0.591642	-1.715654
H	-4.215614	0.968601	0.024269
H	-5.228478	-0.309553	-0.662809
C	-3.238832	-1.820433	1.382878
H	-3.138358	-1.032142	2.139596
H	-2.543442	-2.630586	1.631266
H	-4.259920	-2.220577	1.447578
Si	2.943451	-1.168392	-0.335770
C	3.196236	-2.347856	-1.768383
H	4.185048	-2.820488	-1.712467
H	3.123062	-1.823538	-2.729446
H	2.439783	-3.142975	-1.756744
C	4.199237	0.220481	-0.364704
H	5.194895	-0.217642	-0.210341
H	4.028800	0.938909	0.447666
H	4.221711	0.768058	-1.313919
C	3.106412	-2.055415	1.306342
H	4.133458	-2.432257	1.406638

H	2.423501	-2.907526	1.393392
H	2.918396	-1.375626	2.147932
C	-1.374138	1.248691	1.854448
C	1.279034	1.159846	1.882633
O	2.093440	1.700221	2.473204
H	-0.086096	-0.983296	2.038801
N	-2.213479	1.846444	2.416987
Co	-0.010789	0.284046	0.957242

TS5,1-Fe-Casey Gsolv= -2728.634451

Fe	0.000025	-0.600932	-0.818754
C	0.000013	1.253964	0.083690
O	0.000056	2.227641	-0.827333
C	-1.196411	0.527578	0.465838
C	-0.705103	-0.645071	1.136041
C	0.705030	-0.645084	1.136078
C	1.196388	0.527566	0.465901
Si	-2.978485	1.082139	0.178743
C	-3.212879	2.688510	1.115788
H	-3.024390	2.553937	2.188213
H	-4.236595	3.065655	0.995996
H	-2.524046	3.458314	0.744467
C	-4.083587	-0.271933	0.854806
H	-3.886286	-0.465746	1.917155
H	-3.948502	-1.211639	0.302595
H	-5.137641	0.019543	0.759719
C	-3.319544	1.342860	-1.645872
H	-3.206455	0.412584	-2.217083
H	-2.649497	2.094993	-2.079599
H	-4.351030	1.695030	-1.781093
Si	2.978465	1.082111	0.178784
C	3.212894	2.688574	1.115658
H	4.236548	3.065806	0.995603
H	3.024665	2.554067	2.188137
H	2.523902	3.458281	0.744431
C	4.083542	-0.271893	0.855027
H	5.137591	0.019701	0.760266
H	3.948693	-1.211590	0.302743
H	3.885965	-0.465771	1.917314
C	3.319411	1.342714	-1.645873
H	4.350835	1.695006	-1.781232
H	2.649215	2.094740	-2.079564
H	3.206364	0.412419	-2.217058
C	-1.314113	-1.651966	-1.421607
O	-2.181096	-2.326210	-1.769257
C	1.314287	-1.651832	-1.421594
O	2.181348	-2.325971	-1.769251
C	-1.177274	-1.847872	1.879999
O	-0.000077	-2.666103	1.971350
C	1.177135	-1.847883	1.880082
H	-1.963919	-2.431928	1.390463
H	-1.526009	-1.559252	2.885040
H	1.525786	-1.559255	2.885150
H	1.963817	-2.431955	1.390627
H	0.000060	1.204321	-1.705914
H	0.000011	0.353225	-2.191983

TS5,1-Fe Gsolv= -2731.984112

Fe	-0.002691	0.307793	0.993007
C	-0.011125	-1.278338	-0.321209
O	-0.023137	-2.447266	0.327219
H	-0.027605	-1.658303	1.424507
C	-1.192805	-0.473826	-0.516706
C	-0.711737	0.838225	-0.899223
C	-1.498745	2.062953	-1.242789
H	-2.394687	2.141847	-0.615132
H	-1.858911	1.957140	-2.278809
C	-0.631066	3.311773	-1.132601
H	-1.187950	4.180523	-1.502500
H	-0.397755	3.504807	-0.072129
C	0.658095	3.124914	-1.922588
H	1.234068	4.056639	-1.962507
H	0.394991	2.871647	-2.961062
C	1.529629	2.014383	-1.335594
H	2.265306	1.681155	-2.079966
H	2.116048	2.398497	-0.489353
C	0.712397	0.826986	-0.914667
C	1.179060	-0.486679	-0.518946
Si	-2.942478	-1.175639	-0.362231
C	-3.069535	-2.597731	-1.579845
H	-2.856009	-2.266721	-2.604018
H	-4.084206	-3.017271	-1.566850
H	-2.368310	-3.403952	-1.331297
C	-4.229525	0.122636	-0.780199
H	-4.103346	0.541042	-1.786128
H	-4.233902	0.948911	-0.057716
H	-5.219276	-0.352834	-0.738390
C	-3.281305	-1.798280	1.375306

H	-3.225498	-0.991047	2.116978
H	-2.580451	-2.587138	1.672506
H	-4.296735	-2.216244	1.415465
Si	2.934096	-1.171873	-0.344154
C	3.183428	-2.378502	-1.758978
H	4.176436	-2.843177	-1.705808
H	3.095781	-1.872975	-2.729164
H	2.432964	-3.179131	-1.726758
C	4.208920	0.201861	-0.430515
H	5.203722	-0.247611	-0.303982
H	4.078091	0.937375	0.373704
H	4.205976	0.734172	-1.388920
C	3.155762	-2.045428	1.301716
H	4.190283	-2.408016	1.376999
H	2.487461	-2.906829	1.410821
H	2.978779	-1.365011	2.145234
C	-1.301795	1.213090	1.811408
O	-2.159886	1.810480	2.298540
C	1.320667	1.142117	1.850810
O	2.192408	1.683435	2.377310
H	-0.034956	-0.949078	2.098634

TS5,1-Fe-Renaud Gsolv= -2487.262428

Fe	0.011620	0.239004	1.205953
C	-0.021593	-1.336333	-0.121872
O	0.003567	-2.506701	0.517119
C	-1.206349	-0.531953	-0.275658
C	-0.758848	0.783023	-0.684638
C	-0.723254	3.110222	-0.984993
H	-1.328320	3.936292	-1.371372
H	-0.438380	3.352939	0.050687
C	0.523665	2.920702	-1.831699
H	1.119339	3.837959	-1.850915
H	0.240368	2.693327	-2.868733
C	0.668713	0.772562	-0.804611
C	1.141433	-0.526460	-0.362733
C	-1.174876	1.233143	2.090398
O	-1.928652	1.917077	2.634738
C	1.395412	0.967422	2.072581
O	2.288851	1.375576	2.680353
H	-0.052198	-1.034298	2.294584
H	-0.027134	-1.746669	1.614307
C	2.525879	-1.042894	-0.384600
C	3.157318	-1.527943	0.765605
C	3.214191	-1.084201	-1.603907
C	4.453934	-2.032547	0.700557
H	2.630406	-1.502739	1.718118
C	4.512435	-1.583135	-1.666963
H	2.724981	-0.725161	-2.508041
C	5.137416	-2.055905	-0.513858
H	4.933089	-2.402867	1.604123
H	5.036319	-1.604209	-2.619969
H	6.152620	-2.443192	-0.562194
C	-2.582950	-1.061579	-0.224105
C	-3.620152	-0.437165	0.478045
C	-2.870160	-2.219272	-0.959602
C	-4.912602	-0.953092	0.437327
H	-3.423440	0.457721	1.063078
C	-4.161461	-2.738239	-0.995754
H	-2.072349	-2.709026	-1.515803
C	-5.188343	-2.104485	-0.298771
H	-5.707007	-0.454387	0.988114
H	-4.365371	-3.636994	-1.573558
H	-6.198748	-2.505966	-0.327699
N	1.371521	1.836617	-1.312557
N	-1.549413	1.899687	-0.964592
C	2.565073	2.285067	-0.608726
H	3.164086	1.434270	-0.271798
H	3.181310	2.889002	-1.281695
H	2.294489	2.900232	0.266171
C	-2.397907	1.744724	-2.148662
H	-1.815898	1.709297	-3.083912
H	-2.981812	0.821844	-2.075667
H	-3.095200	2.586814	-2.200412

TS5,1-Fe-williams-1 Gsolv= -2682.432717

Fe	0.009567	-0.666995	1.335272
C	0.009534	-1.828006	-0.393211
O	0.017312	-3.118835	-0.071706
C	-1.160359	-0.991550	-0.372606
C	-0.704353	0.384421	-0.321493
C	0.722676	0.385802	-0.333583
C	1.180484	-0.984506	-0.364967
C	-1.334901	-0.278052	2.456271
O	-2.197580	-0.061625	3.186242
C	1.257946	-0.052602	2.464385
O	2.061355	0.326624	3.195665
C	-2.550226	-1.468784	-0.479747

C	-3.624116	-0.799686	0.125355
C	-2.820720	-2.600076	-1.261307
C	-4.927279	-1.258271	-0.038307
H	-3.447543	0.087583	0.730438
C	-4.125359	-3.057874	-1.423487
H	-2.001724	-3.119127	-1.754177
C	-5.183578	-2.390241	-0.811025
H	-5.746151	-0.727975	0.442569
H	-4.314126	-3.937103	-2.035340
H	-6.202965	-2.748242	-0.935754
C	2.568697	-1.471745	-0.452369
C	3.629240	-0.854312	0.225411
C	2.848631	-2.566178	-1.281168
C	4.930216	-1.326376	0.083734
H	3.443408	0.001734	0.871561
C	4.151016	-3.037960	-1.421368
H	2.038458	-3.046854	-1.825563
C	5.196503	-2.421462	-0.737584
H	5.739507	-0.836971	0.620898
H	4.347797	-3.888562	-2.070099
H	6.213898	-2.790879	-0.843929
C	-1.560657	1.580559	-0.463573
C	-1.746072	2.513951	0.559714
C	-2.204926	1.774658	-1.691460
C	-2.564956	3.622745	0.358656
H	-1.259080	2.364961	1.522445
C	-3.021596	2.884111	-1.891309
H	-2.065233	1.046161	-2.489554
C	-3.205405	3.809467	-0.864981
H	-2.706062	4.339577	1.164359
H	-3.516668	3.024205	-2.849508
H	-3.847185	4.674023	-1.018056
C	1.575521	1.583208	-0.472800
C	1.620965	2.600453	0.485044
C	2.348169	1.704265	-1.634619
C	2.425920	3.719023	0.284415
H	1.037244	2.511842	1.399377
C	3.150708	2.824008	-1.834073
H	2.316566	0.913806	-2.383470
C	3.192127	3.833888	-0.873879
H	2.456931	4.500613	1.040031
H	3.745491	2.906085	-2.740863
H	3.822662	4.706765	-1.026378
H	0.123835	-2.160566	2.039937
H	0.080389	-2.645786	1.197986

TS5,1-Fe-williams-2 Gsolv= -2871.398602

Fe	0.048526	-0.630119	1.120940
C	0.024568	-2.002940	-0.423799
O	0.075321	-3.243897	0.049161
C	-1.184710	-1.199846	-0.476629
C	-0.747399	0.157865	-0.650747
C	0.661390	0.191113	-0.700289
C	1.181812	-1.137290	-0.546416
C	-1.211151	0.041218	2.207189
O	-2.033914	0.443724	2.904616
C	1.448777	0.028412	2.019014
O	2.400385	0.415931	2.539464
C	-2.563555	-1.709928	-0.451708
C	-3.630270	-0.912386	-0.011221
C	-2.852129	-2.994555	-0.926577
C	-4.934116	-1.389410	-0.041663
H	-3.442245	0.090547	0.368332
C	-4.161858	-3.466029	-0.953714
H	-2.044433	-3.628647	-1.284675
C	-5.225883	-2.675632	-0.512729
H	-5.745814	-0.753486	0.310850
H	-4.362086	-4.469312	-1.328394
C	2.598363	-1.535503	-0.591805
C	3.440038	-0.950742	-1.544479
C	3.141322	-2.489661	0.280433
C	4.781983	-1.314786	-1.628821
H	3.039412	-0.215074	-2.240667
C	4.479582	-2.849855	0.187424
H	2.513223	-2.938490	1.046733
C	5.324794	-2.271020	-0.767874
H	5.418064	-0.850946	-2.381860
H	4.884455	-3.591612	0.875633
C	-6.638453	-3.171413	-0.555607
H	-6.678510	-4.246475	-0.760180
H	-7.157258	-2.982770	0.391778
H	-7.213091	-2.661863	-1.339914
C	6.768890	-2.660876	-0.843264
H	7.244890	-2.262525	-1.745454
H	7.326238	-2.282200	0.023210
H	6.887467	-3.751011	-0.844985
C	-1.313346	1.515374	-0.912976
C	1.157402	1.569165	-0.977704

H	-2.175600	1.800813	-0.305711
H	-1.610861	1.579674	-1.969181
H	1.384130	1.660052	-2.049126
H	2.055085	1.861648	-0.425811
C	-0.087115	2.431862	-0.650399
C	-0.114008	2.903975	0.812659
C	-0.115239	3.706504	-1.479993
O	-1.131497	3.034638	1.464887
O	0.852323	4.174489	-2.048507
O	1.095209	3.207319	1.264241
O	-1.319856	4.263802	-1.473744
H	0.090915	-2.025803	2.024083
H	0.086045	-2.626001	1.246974
C	1.168244	3.632111	2.636930
H	2.229186	3.763859	2.848373
H	0.631470	4.575744	2.766140
H	0.738938	2.863170	3.287282
C	-1.456475	5.503406	-2.191459
H	-1.238294	5.348354	-3.251287
H	-2.493969	5.807834	-2.057191
H	-0.781541	6.254755	-1.773008
H	-6.343037	-1.809994	-0.399710
C	2.594235	-0.765770	-0.499776
C	3.509335	-0.227682	-1.413895
C	3.052520	-1.681107	0.457960
C	4.850566	-0.600798	-1.378207
H	3.166742	0.475152	-2.172089
C	4.392153	-2.055604	0.487269
H	2.359164	-2.088490	1.189481
C	5.295987	-1.517712	-0.428899
H	5.546855	-0.174989	-2.097148
H	4.734350	-2.764658	1.237819
H	6.343132	-1.809977	-0.399573
C	-1.172152	2.322396	-1.301864
O	0.000504	3.130648	-1.124623
C	1.172848	2.322002	-1.302032
H	-1.492846	2.335602	-2.356257
H	1.493295	2.334967	-2.356505
H	1.979359	2.731801	-0.684541
H	-0.000054	-1.581308	1.351289
H	0.000833	-0.870719	2.039294
H	-1.978366	2.732399	-0.684111

TS5,1-Fe-wills-1 Gsolv= -2373.320816

Fe	0.000034	0.399486	0.957210
C	-0.000115	-1.166127	-0.378769
O	-0.000358	-2.337382	0.244250
C	-1.185323	-0.347281	-0.574956
C	-0.702241	0.958387	-0.922081
C	0.702536	0.958190	-0.922099
C	1.185324	-0.347510	-0.574865
C	-1.343796	1.221485	1.810158
O	-2.256111	1.725912	2.298223
C	1.343301	1.222265	1.810330
O	2.255142	1.726965	2.298998
C	-2.594263	-0.765414	-0.499883
C	-3.509422	-0.227263	-1.413885
C	-3.052414	-1.680969	0.457720
C	-4.850618	-0.600522	-1.378202
H	-3.166902	0.475677	-2.172008
C	-4.392011	-2.055572	0.487044
H	-2.358913	-2.088432	1.189068
C	-5.295924	-1.517617	-0.429016
H	-5.546969	-0.174705	-2.097077
H	-4.734125	-2.764772	1.237494

TS5,1-Fe-wills-2 Gsolv= -2412.584720

Fe	0.096640	0.436985	0.977012
C	0.148907	-1.261368	-0.195170
O	0.191563	-2.350967	0.562229
C	-1.061291	-0.514135	-0.468369
C	-0.631453	0.769809	-0.948474
C	0.773433	0.814339	-0.967463
C	1.306528	-0.429288	-0.498245
C	-1.311166	1.086758	1.869397
O	-2.238197	1.443121	2.451847
C	1.293137	1.555471	1.707558
O	2.082812	2.270343	2.143051
C	-2.445488	-1.007866	-0.365728
C	-3.318347	-0.791187	-1.439518
C	-2.911303	-1.700124	0.759094
C	-4.628213	-1.261035	-1.392534
H	-2.963202	-0.258305	-2.321000
C	-4.219938	-2.172353	0.801960
H	-2.250124	-1.849715	1.610199
C	-5.081861	-1.955311	-0.272571
H	-5.294306	-1.085088	-2.234188
H	-4.570494	-2.704324	1.683557

H	-6.105197	-2.321678	-0.234407
C	2.720013	-0.826608	-0.413638
C	3.735986	0.139836	-0.376997
C	3.082452	-2.180385	-0.426636
C	5.074252	-0.237540	-0.345586
H	3.484138	1.198905	-0.365183
C	4.422748	-2.555039	-0.394729
H	2.307904	-2.941374	-0.467352
C	5.424147	-1.587262	-0.352064
H	5.846806	0.527513	-0.315262
H	4.684131	-3.610853	-0.407968
H	6.470717	-1.881826	-0.326737
C	-1.170012	2.025985	-1.557582
O	-0.007865	2.882677	-1.589746
C	1.197247	2.110895	-1.570860
H	-1.472843	1.793695	-2.594812
H	1.575273	1.938597	-2.591996
H	1.951784	2.675161	-1.012715
C	-2.284322	2.741093	-0.840928
H	-2.598754	3.623392	-1.407805
H	-3.150956	2.079064	-0.725317
H	-1.948630	3.064419	0.151675
H	0.327550	-0.692897	2.177810
H	0.274324	-1.465793	1.574632

TS5,1-Fe-wills-3 Gsolv= -2590.243368

Fe	0.273361	0.347304	0.961476
C	0.156325	-1.297112	-0.272129
O	0.137884	-2.425161	0.432889
C	-1.002000	-0.449025	-0.481886
C	-0.479310	0.813607	-0.928932
C	0.924097	0.732613	-0.988266
C	1.374128	-0.557738	-0.556674
Si	3.135471	-1.227776	-0.442021
C	3.266285	-2.648664	-1.657161
H	4.283772	-3.060095	-1.665862
H	3.023503	-2.325512	-2.677163
H	2.576624	-3.458400	-1.386001
C	4.288078	0.176939	-0.901173
H	5.327269	-0.176952	-0.890483
H	4.214387	1.004960	-0.183518
H	4.081586	0.569125	-1.905140
C	3.523330	-1.824234	1.291225
H	4.544566	-2.227854	1.318424
H	2.839731	-2.619643	1.611481
H	3.467803	-1.007051	2.022044
C	-1.046916	1.085583	1.914727
O	-1.924756	1.496184	2.537077
C	1.580402	1.337683	1.681342
O	2.437723	1.977969	2.106556
C	-2.418091	-0.834065	-0.365045
C	-3.299280	-0.474309	-1.392862
C	-2.908519	-1.565315	0.724246
C	-4.640738	-0.842685	-1.337347
H	-2.925171	0.089128	-2.246871
C	-4.249426	-1.935240	0.775721
H	-2.239904	-1.827229	1.541641
C	-5.119285	-1.577137	-0.253957
H	-5.311781	-0.557203	-2.144347
H	-4.617994	-2.499606	1.629427
H	-6.166987	-1.865560	-0.209097
C	-0.915030	2.145383	-1.455985
O	0.320855	2.894819	-1.472986
C	1.447574	2.013103	-1.543646
H	-1.259637	2.000140	-2.496123
H	1.759631	1.862835	-2.590177
H	2.279623	2.467694	-0.994947
C	-1.942127	2.921359	-0.674861
H	-2.862710	2.335485	-0.565552
H	-1.553835	3.163601	0.321438
H	-2.189040	3.855410	-1.189919
H	0.414680	-0.848280	2.115546
H	0.299281	-1.591015	1.482813

TS5,1-Fe-wills-4 Gsolv= -2550.978250

Fe	0.195641	0.501698	0.891777
C	0.040601	-1.228187	-0.218063
O	-0.029435	-2.298341	0.569861
C	-1.088273	-0.360294	-0.507475
C	-0.517037	0.843878	-1.037939
C	0.885339	0.726131	-1.056050
C	1.284700	-0.552586	-0.537204
Si	3.021841	-1.266566	-0.341115
C	3.151291	-2.729516	-1.505257
H	4.143325	-3.194140	-1.438329
H	2.985229	-2.429499	-2.547269
H	2.405179	-3.493275	-1.249905
C	4.222808	0.094714	-0.806068

H	5.252646	-0.282082	-0.754890
H	4.147236	0.945369	-0.115576
H	4.053360	0.461355	-1.826677
C	3.329791	-1.823723	1.421522
H	4.349070	-2.224129	1.506341
H	2.633152	-2.615764	1.721201
H	3.234977	-0.995498	2.135382
C	-1.094062	1.492258	1.626191
O	-1.976424	2.110501	2.033315
C	1.559021	1.425357	1.595314
O	2.452532	2.020850	2.011108
C	-2.521751	-0.658054	-0.358366
C	-3.409257	-0.224297	-1.351529
C	-3.029290	-1.358052	0.744767
C	-4.772582	-0.489836	-1.249716
H	-3.027425	0.310330	-2.220287
C	-4.391209	-1.625640	0.841287
H	-2.355394	-1.675983	1.536776
C	-5.267767	-1.193160	-0.153907
H	-5.447567	-0.146785	-2.030560
H	-4.771388	-2.165795	1.705529
H	-6.332422	-1.399854	-0.071970
C	-0.894870	2.163371	-1.617970
O	0.343505	2.889229	-1.612777
C	1.447659	1.971379	-1.655936
H	-1.637462	2.733175	-1.048435
H	-1.262779	2.036944	-2.649206
H	1.751889	1.781731	-2.698273
H	2.290180	2.421671	-1.121193
H	0.083769	-1.395605	1.560736
H	0.179890	-0.604760	2.142329

TS5,1-Fe-wills-5 Gsolv= -2708.012957

Fe	0.425165	0.922338	-0.926077
C	-0.006387	-1.004573	-0.343999
O	-0.079051	-1.813818	-1.396333
C	1.243872	-0.583031	0.261544
C	0.916766	0.555988	1.073982
C	-0.461060	0.813502	0.964023
C	-1.083173	-0.117374	0.067664
Si	-2.916377	-0.231219	-0.378437
C	-3.723577	1.396581	0.098326
H	-4.798626	1.347219	-0.121666
H	-3.311943	2.235165	-0.477659
H	-3.614864	1.627582	1.165502
C	-3.146818	-0.499886	-2.219448
H	-4.215353	-0.456606	-2.469553
H	-2.753717	-1.462707	-2.565605
H	-2.641826	0.297222	-2.782068
C	-3.652276	-1.651034	0.657763
C	2.013929	1.576260	-1.417214
O	3.054995	1.933839	-1.756280
C	-0.518375	2.369105	-1.401698
O	-1.146013	3.291389	-1.686406
C	2.555624	-1.241182	0.141143
C	3.308925	-1.460858	1.301542
C	3.067829	-1.668519	-1.090740
C	4.546008	-2.096348	1.233432
H	2.916358	-1.138015	2.265186
C	4.302337	-2.307940	-1.155444
H	2.505938	-1.478364	-2.002545
C	5.045543	-2.523639	0.004660
H	5.119038	-2.259245	2.143471
H	4.690352	-2.629837	-2.119295
H	6.012001	-3.019413	-0.050396
C	1.509656	1.487981	2.083440
O	0.467887	2.476306	2.248296
C	-0.807493	1.938674	1.877881
H	1.624664	0.927758	3.029425
H	-1.341365	1.550105	2.761573
H	-1.404778	2.743322	1.435409
C	2.797095	2.189685	1.740830
H	3.584291	1.458914	1.519782
H	2.655424	2.836444	0.866884
H	3.129490	2.808139	2.580897
C	-5.138011	-1.803965	0.328017
H	-5.299539	-2.081051	-0.723215
H	-5.582683	-2.599284	0.947773
H	-5.704767	-0.882783	0.524174
H	0.270142	0.234666	-2.434469
H	0.122833	-0.672606	-2.092857
C	-2.934778	-2.966487	0.355961
H	-3.005657	-3.244782	-0.704911
H	-1.869118	-2.925566	0.622116
H	-3.385862	-3.784024	0.941370
C	-3.492674	-1.324299	2.143629
H	-2.437851	-1.187186	2.424728
H	-4.037644	-0.413593	2.428889

H	-3.890270	-2.148780	2.757207

TS5,1-Mn-a Gsolv= -2632.563994

C	-0.005416	1.421113	0.122612
O	0.002785	2.568526	-0.377053
H	-0.320044	0.356720	-2.110024
C	-1.200625	0.587877	0.383653
C	-0.726296	-0.546902	1.104370
C	-1.209325	-1.689148	1.931935
H	-1.994449	-2.307801	1.483751
H	-1.567951	-1.318535	2.906014
C	1.145985	-1.703346	1.949405
H	1.483856	-1.324240	2.927811
H	1.933751	-2.337809	1.529885
C	0.689338	-0.566959	1.097021
C	1.177347	0.567527	0.377031
Si	-2.978893	1.108504	0.045937
C	-3.310450	2.716887	0.952314
H	-3.131064	2.610823	2.029620
H	-4.353305	3.030163	0.812972
H	-2.663723	3.520426	0.578352
C	-4.101764	-0.253036	0.679697
H	-3.960884	-0.428906	1.754118
H	-3.927079	-1.199609	0.150998
H	-5.152813	0.022885	0.522881
C	-3.213238	1.332819	-1.800823
H	-3.111836	0.373492	-2.326022
H	-2.476761	2.031495	-2.218517
H	-4.213449	1.730880	-2.016467
Si	2.957473	1.116650	0.091787
C	3.239181	2.707878	1.045738
H	4.281252	3.037401	0.941055
H	3.036255	2.568629	2.115185
H	2.591468	3.513310	0.678436
C	4.094410	-0.225636	0.742640
H	5.139863	0.096632	0.649021
H	3.985855	-1.166745	0.188563
H	3.905213	-0.428397	1.805138
C	3.240789	1.394660	-1.741142
H	4.243025	1.807522	-1.915907
H	2.510459	2.101848	-2.155028
H	3.162200	0.455089	-2.303793
C	1.411336	-1.785580	-1.282435
O	2.306955	-2.472812	-1.506638
H	0.408484	0.021322	-2.317018
Mn	-0.029510	-0.735041	-0.842829
N	-1.171905	-1.845843	-1.229178
O	-2.016118	-2.638914	-1.384586
O	-0.037995	-2.503143	2.101241

TS5,1-Mn-c Gsolv= -2277.209392

C	0.024211	-1.201086	-0.188966
O	0.029859	-2.268292	0.596273
C	-1.158169	-0.440125	-0.527846
C	-0.680710	0.810564	-1.037369
C	0.725680	0.835501	-1.016850
C	1.209861	-0.407540	-0.495495
O	-2.338135	1.804634	1.897139
C	1.330044	1.658857	1.625914
O	2.157264	2.360298	2.009684
C	-2.565503	-0.838380	-0.389176
C	-3.501459	-0.348770	-1.309818
C	-3.005430	-1.680548	0.642097
C	-4.844433	-0.702153	-1.211578
H	-3.175330	0.298912	-2.122199
C	-4.347773	-2.033132	0.735099
H	-2.293214	-2.045313	1.377592
C	-5.271611	-1.548103	-0.190685
H	-5.556643	-0.316341	-1.937340
H	-4.675734	-2.684772	1.541870
H	-6.320476	-1.824815	-0.112665
C	2.610447	-0.845376	-0.376223
C	3.656640	0.088503	-0.349032
C	2.930615	-2.209677	-0.354841
C	4.981629	-0.330077	-0.289150
H	3.441401	1.155210	-0.369219
C	4.257816	-2.625871	-0.295685
H	2.134405	-2.947511	-0.392503
C	5.288854	-1.689712	-0.258877
H	5.777413	0.411025	-0.266080
H	4.484898	-3.689590	-0.283546
H	6.325084	-2.016316	-0.211719
C	-1.174818	2.077560	-1.645368
O	-0.013527	2.917743	-1.645756
C	1.176468	2.116041	-1.640504
H	-1.521234	1.895298	-2.675833
H	1.529981	1.930711	-2.667728
H	1.949877	2.669263	-1.098709

H	0.192386	-1.374748	1.586951
H	0.334610	-0.592190	2.145357
H	-1.973984	2.582806	-1.090786
N	-1.313473	1.326058	1.607604
Mn	0.000120	0.585282	0.956428

TS5,1-Mn Gsolv= -2635.873696

C	-0.018102	-1.287766	-0.329896
O	-0.027390	-2.469234	0.288592
H	0.028657	-1.713991	1.409043
C	-1.195544	-0.488368	-0.535112
C	-0.716786	0.826932	-0.903048
C	-1.508387	2.047217	-1.248111
H	-2.399074	2.128829	-0.613368
H	-1.878987	1.929961	-2.279110
C	-0.644972	3.300670	-1.156251
H	-1.205147	4.160944	-1.540469
H	-0.414239	3.512470	-0.099193
C	0.647778	3.107579	-1.938263
H	1.217622	4.042309	-1.992770
H	0.391341	2.832707	-2.972886
C	1.523447	2.014873	-1.324584
H	2.269004	1.676646	-2.056718
H	2.096935	2.420251	-0.479342
C	0.708428	0.828292	-0.894180
C	1.170847	-0.485384	-0.498261
Si	-2.947211	-1.182442	-0.347364
C	-3.105195	-2.601396	-1.564061
H	-2.966228	-2.255952	-2.596282
H	-4.102668	-3.054560	-1.492024
H	-2.363849	-3.385127	-1.365188
C	-4.235230	0.126682	-0.723370
H	-4.132588	0.555619	-1.727381
H	-4.210869	0.943377	0.010154
H	-5.227524	-0.340899	-0.659169
C	-3.235888	-1.795648	1.402110
H	-3.142165	-0.983128	2.134500
H	-2.535212	-2.591662	1.679816
H	-4.254545	-2.199851	1.480605
Si	2.928036	-1.177734	-0.359768
C	3.148998	-2.340526	-1.815143
H	4.144269	-2.803010	-1.798964
H	3.040418	-1.802680	-2.765834
H	2.400798	-3.143394	-1.793489
C	4.202829	0.196807	-0.429364
H	5.196896	-0.254103	-0.302443
H	4.069017	0.926846	0.379205
H	4.203699	0.735805	-1.384028
C	3.175497	-2.094907	1.257423
H	4.208934	-2.465813	1.299866
H	2.503867	-2.954434	1.360544
H	3.023705	-1.434177	2.121026
C	1.413205	1.116235	1.855840
O	2.320344	1.640029	2.336926
H	0.082564	-1.025809	2.081415
Mn	-0.026727	0.334684	1.044649
N	-1.214838	1.196010	1.778963
O	-2.116664	1.831501	2.169357

TS5,6-Co-a-H2O Gsolv= -2903.593411

C	-0.006577	-1.190024	-0.591699
O	-0.016348	-2.428727	-0.378696
H	-0.017643	-2.796655	1.347865
C	-1.192526	-0.305735	-0.629161
C	-0.705519	0.962370	-1.056861
C	0.711923	0.951621	-1.062744
C	1.188837	-0.325915	-0.641425
Si	-2.978059	-0.892609	-0.457194
C	-3.296116	-2.120261	-1.839318
H	-3.152499	-1.657817	-2.824080
H	-4.327441	-2.493537	-1.789782
H	-2.621234	-2.982442	-1.767047
C	-4.109226	0.588683	-0.640803
H	-3.953557	1.098352	-1.600815
H	-3.963968	1.317534	0.166445
H	-5.155437	0.256716	-0.609448
C	-3.216574	-1.723261	1.206263
H	-2.916362	-1.067887	2.034244
H	-2.639222	-2.654927	1.267191
H	-4.275161	-1.978807	1.347236
Si	2.970641	-0.919870	-0.464261
C	3.308752	-2.154948	-1.832623
H	4.342151	-2.520518	-1.772693
H	3.167948	-1.702129	-2.822066
H	2.639935	-3.021554	-1.757325
C	4.087721	0.574979	-0.635101
H	5.137170	0.259467	-0.566437
H	3.912945	1.313235	0.158297

H	3.955289	1.072224	-1.604838
C	3.198150	-1.720395	1.213995
H	4.238999	-2.047262	1.337496
H	2.555495	-2.602200	1.327752
H	2.965953	-1.019342	2.026807
C	-1.359226	1.630915	1.617541
C	1.265437	1.583857	1.621107
O	2.063745	2.206897	2.155307
H	-0.060998	-0.285399	2.136374
O	0.046847	-2.501700	2.291308
H	-0.788570	-2.753323	2.718608
H	0.000658	-1.247508	2.123236
C	1.188188	2.273413	-1.560897
O	0.017215	3.100467	-1.493726
C	-1.167326	2.290087	-1.548403
H	1.534528	2.172241	-2.602456
H	1.981079	2.750322	-0.975293
H	-1.944046	2.775606	-0.949416
H	-1.525768	2.197685	-2.586555
N	-2.200155	2.266892	2.135721
Co	0.005463	0.600614	0.810157

TS5,6-Co-a Gsolv= -2942.828032

C	0.001142	0.808474	-0.985869
O	0.024277	2.055169	-1.161048
H	-0.271348	2.881171	0.358053
C	1.184985	-0.060067	-0.784274
C	0.682271	-1.389278	-0.763883
C	-0.732628	-1.365834	-0.718521
C	-1.196788	-0.012863	-0.737657
Si	2.981299	0.515445	-0.856060
C	3.254483	1.296102	-2.539450
H	3.066126	0.578270	-3.347697
H	4.290134	1.647442	-2.635011
H	2.591203	2.157073	-2.688840
C	4.079849	-0.987163	-0.648290
H	3.909433	-1.723654	-1.444496
H	3.922307	-1.480581	0.319444
H	5.133879	-0.684053	-0.700178
C	3.287120	1.774125	0.495171
H	3.144972	1.338039	1.492292
H	2.607891	2.630144	0.387834
H	4.315453	2.153965	0.433731
Si	-2.989758	0.572024	-0.838423
C	-3.266101	1.189146	-2.586752
H	-4.301277	1.528822	-2.720031
H	-3.073996	0.393755	-3.317984
H	-2.601717	2.030980	-2.819238
C	-4.085848	-0.906351	-0.484948
H	-5.137760	-0.592990	-0.521125
H	-3.904067	-1.327942	0.512069
H	-3.955549	-1.703902	-1.227648
C	-3.336084	1.928473	0.403942
H	-4.407037	2.170906	0.385016
H	-2.780014	2.844503	0.171664
H	-3.080546	1.617719	1.425587
C	1.345289	-1.252212	1.972003
C	-1.266247	-0.961725	2.025037
O	-2.090662	-1.310869	2.738413
H	0.346747	0.841301	1.830927
O	-0.390704	2.868665	1.341924
H	-0.087198	1.660049	1.545208
C	-1.224993	-2.773583	-0.733462
O	-0.049213	-3.543286	-0.441583
C	1.126789	-2.809368	-0.813217
H	-1.615633	-3.023428	-1.733434
H	-1.988710	-3.017869	0.012321
H	1.936429	-3.082756	-0.129965
H	1.432340	-3.060788	-1.842129
N	2.164559	-1.753562	2.648420
Co	0.023188	-0.418497	0.908136
C	0.564816	3.723848	1.999000
H	1.376726	3.114681	2.411681
H	0.966436	4.445825	1.285270
H	0.047274	4.245332	2.806215

TS5,6-Co-b-H2O Gsolv= -3046.357665

C	0.052274	-1.890498	-0.802668
O	0.097086	-3.136724	-0.909116
H	-0.709332	-3.801736	0.558944
C	-1.146189	-1.044819	-0.576361
C	-0.709011	0.310735	-0.664957
C	-1.278044	1.678973	-0.835410
H	-2.122738	1.932193	-0.190612
H	-1.612900	1.786141	-1.876408
C	-0.044395	2.590775	-0.574176
C	1.198394	1.736541	-0.931725
H	1.433913	1.875368	-1.996296

H	2.095885	1.996154	-0.364041
C	0.703689	0.344669	-0.738129
C	1.210362	-0.987633	-0.676214
C	-1.161679	0.164152	2.241115
C	1.502612	0.122339	1.949431
O	2.428306	0.468367	2.527362
H	0.255030	-1.816823	1.944269
O	-0.884094	-3.685079	1.526417
H	-1.842149	-3.541532	1.609858
H	-0.330513	-2.560951	1.708701
C	-0.081299	3.067395	0.887201
O	-1.103599	3.440903	1.429359
O	1.109748	3.083999	1.465004
C	-0.061909	3.881139	-1.382428
O	0.945338	4.426766	-1.792830
O	-1.288020	4.356858	-1.540545
C	1.138778	3.510058	2.839661
H	2.184334	3.458740	3.142475
H	0.766092	4.534173	2.923819
H	0.528177	2.836093	3.449408
C	-1.407618	5.611139	-2.236037
H	-2.474299	5.832222	-2.258423
H	-0.866946	6.392451	-1.695353
H	-1.016466	5.515323	-3.252233
C	2.617620	-1.409908	-0.712599
C	3.060344	-2.504484	0.043689
C	3.546097	-0.724841	-1.503214
C	4.391271	-2.898437	0.002481
H	2.355385	-3.036517	0.681194
C	4.880158	-1.124346	-1.536804
H	3.222150	0.117570	-2.112649
C	5.326279	-2.214066	-0.785125
H	4.719422	-3.749755	0.598317
H	5.587775	-0.581454	-2.162346
C	-2.538348	-1.518507	-0.550561
C	-2.902630	-2.723859	-1.164994
C	-3.550912	-0.751174	0.047797
C	-4.230462	-3.143587	-1.177917
H	-2.143331	-3.333987	-1.645758
C	-4.871317	-1.178334	0.032696
H	-3.301395	0.184317	0.543652
C	-5.237764	-2.383471	-0.579925
H	-4.489562	-4.081559	-1.667918
H	-5.639049	-0.566849	0.506465
C	6.765124	-2.629692	-0.795275
H	6.865471	-3.720888	-0.823547
H	7.296728	-2.210389	-1.656080
H	7.280195	-2.285153	0.111032
C	-6.667441	-2.827539	-0.591155
H	-7.309112	-2.083768	-1.079576
H	-6.787074	-3.778745	-1.119913
H	-7.051830	-2.955069	0.428498
Co	0.115887	-0.526828	1.013367
N	-1.926404	0.550247	3.045429

TS5,6-Co-b Gsolv= -3085.591731

C	-0.181466	-1.741545	-0.960799
O	-0.353198	-2.968623	-1.122274
H	-1.370439	-3.555288	0.366274
C	-1.220554	-0.710590	-0.722879
C	-0.553898	0.550395	-0.726636
C	-0.874781	2.002831	-0.837421
H	-1.679488	2.367342	-0.194612
H	-1.159151	2.215785	-1.876962
C	0.487381	2.673678	-0.506095
C	1.576203	1.636454	-0.884073
H	1.864130	1.782805	-1.934700
H	2.487011	1.712298	-0.284384
C	0.845589	0.342427	-0.772463
C	1.113782	-1.057907	-0.763894
C	-1.129353	0.308664	2.162703
C	1.507288	-0.106784	1.926918
O	2.456521	0.055500	2.546232
H	0.045955	-1.834020	1.792568
O	-1.348372	-3.504908	1.350331
H	-0.596864	-2.493623	1.520363
C	0.496181	3.076312	0.978196
O	-0.469868	3.564884	1.531862
O	1.671368	2.898228	1.561483
C	0.719415	3.988220	-1.239031
O	1.824659	4.388757	-1.553554
O	-0.405408	4.656258	-1.446200
C	1.749839	3.266690	2.950644
H	2.773226	3.050859	3.256283
H	1.533382	4.331556	3.069388
H	1.040363	2.671208	3.534170
C	-0.276592	5.945082	-2.074147
H	-1.290394	6.336628	-2.151181

H	0.341429	6.601809	-1.456280
H	0.165347	5.834985	-3.067780
C	2.429351	-1.710767	-0.790338
C	2.644058	-2.933151	-0.136499
C	3.501710	-1.117366	-1.464522
C	3.893585	-3.537818	-0.164988
H	1.827684	-3.401414	0.411039
C	4.752709	-1.729519	-1.486747
H	3.356070	-0.175780	-1.991856
C	4.971475	-2.946988	-0.837791
H	4.044554	-4.485515	0.351475
H	5.574023	-1.253773	-2.021326
C	-2.672451	-0.937128	-0.758563
C	-3.215332	-2.052153	-1.410457
C	-3.559772	-0.027834	-0.159802
C	-4.592734	-2.256392	-1.445686
H	-2.556270	-2.765622	-1.896021
C	-4.930416	-0.239617	-0.198274
H	-3.174536	0.841470	0.367905
C	-5.475034	-1.360935	-0.838374
H	-4.990005	-3.130616	-1.960368
H	-5.597207	0.476972	0.280911
C	6.319462	-3.599545	-0.837139
H	6.243881	-4.673030	-1.046777
H	6.983051	-3.148971	-1.582762
H	6.805674	-3.500255	0.142089
C	-6.956491	-1.574582	-0.869682
H	-7.465635	-0.748487	-1.381854
H	-7.217204	-2.504138	-1.386434
H	-7.371365	-1.621827	0.144829
Co	0.070087	-0.492491	0.923868
N	-1.853780	0.762963	2.968919
C	-2.645987	-3.200101	1.899259
H	-2.531702	-3.184171	2.984586
H	-2.999370	-2.225631	1.544296
H	-3.346641	-3.985975	1.608686

TS5,6-Co-c-H2O Gsolv= -2548.280349

C	0.006360	-0.988262	-0.866394
O	0.008895	-2.232918	-0.974914
H	0.068301	-3.046024	0.629737
C	-1.180295	-0.109876	-0.710951
C	-0.712987	1.229462	-0.823627
C	0.697567	1.232754	-0.804509
C	1.177874	-0.106257	-0.688509
C	-1.423969	1.225666	1.911047
C	1.273862	1.119013	1.944389
O	2.133244	1.545547	2.568400
H	-0.205156	-0.783927	1.950791
O	0.154619	-2.954248	1.610053
H	-0.620472	-3.392244	1.998581
H	-0.016392	-1.704513	1.734023
C	1.163371	2.641930	-0.948995
O	-0.012964	3.407249	-0.658962
C	-1.179589	2.636361	-0.976756
H	1.496170	2.817791	-1.985322
H	1.962047	2.950990	-0.266573
H	-1.486641	2.811657	-2.021070
C	2.586660	-0.522898	-0.663706
C	2.993569	-1.672439	0.026556
C	3.551766	0.242894	-1.330899
C	4.331861	-2.051518	0.037107
H	2.260506	-2.261746	0.571036
C	4.891353	-0.136794	-1.315553
H	3.252598	1.133430	-1.881721
C	5.285456	-1.286344	-0.634063
H	4.632915	-2.944872	0.579738
H	5.627715	0.466907	-1.841104
H	6.331453	-1.583738	-0.622358
C	-2.580118	-0.549358	-0.680688
C	-2.956593	-1.722500	-0.012163
C	-3.569067	0.222433	-1.304031
C	-4.290321	-2.115150	0.023026
H	-2.203150	-2.317731	0.499110
C	-4.903862	-0.171817	-1.264856
H	-3.293189	1.130898	-1.837448
C	-5.268641	-1.341991	-0.602440
H	-4.569272	-3.024816	0.550170
H	-5.659658	0.437553	-1.755043
H	-6.311247	-1.649635	-0.570048
H	-1.993883	2.940987	-0.312163
N	-2.319072	1.694657	2.510637
Co	-0.025002	0.421465	0.917211

TS5,6-Co-c Gsolv= -2587.516160

C	0.092923	-0.939734	-0.892436
O	0.022084	-2.185163	-0.910605
H	-0.979333	-2.680828	0.656610

C	-1.029265	0.028803	-0.818564
C	-0.452686	1.330413	-0.922903
C	0.956486	1.221659	-0.912033
C	1.326958	-0.137791	-0.727467
C	-1.198603	1.348915	1.883343
C	1.456849	1.289583	1.829806
O	2.306192	1.735080	2.453947
H	0.272674	-0.683798	1.867490
O	-1.003491	-2.489652	1.622214
H	-0.325750	-1.414333	1.677317
C	1.536844	2.575960	-1.129769
O	0.428881	3.452863	-0.899795
C	-0.805208	2.763186	-1.143821
H	1.890551	2.658900	-2.170478
H	2.356230	2.857648	-0.459826
H	-1.140308	2.911167	-2.183342
C	2.686112	-0.684156	-0.616640
C	2.943082	-1.800607	0.191264
C	3.746051	-0.088818	-1.311286
C	4.231963	-2.312474	0.293061
H	2.129313	-2.255714	0.753030
C	5.036600	-0.602206	-1.204892
H	3.559799	0.771049	-1.953037
C	5.282723	-1.715289	-0.404196
H	4.419667	-3.176316	0.926778
H	5.850112	-0.130748	-1.751481
H	6.290493	-2.115447	-0.319638
C	-2.460045	-0.302362	-0.884858
C	-2.894990	-1.576647	-1.279590
C	-3.427118	0.665311	-0.570476
C	-4.253398	-1.876982	-1.333908
H	-2.164863	-2.336982	-1.539306
C	-4.782234	0.360709	-0.621334
H	-3.122287	1.662384	-0.261271
C	-5.202694	-0.915045	-0.997403
H	-4.569141	-2.871472	-1.641578
H	-5.513344	1.124004	-0.364842
H	-6.263262	-1.153097	-1.034117
H	-1.558754	3.177287	-0.467379
N	-2.027069	1.844887	2.552967
Co	0.160902	0.536969	0.840018
C	-2.342945	-2.205624	2.073431
H	-2.276603	-2.000011	3.143319
H	-2.756309	-1.337139	1.548392
H	-2.967496	-3.084780	1.900059

TS5,6-Co-H2O Gsolv= -2906.941602

C	-0.012939	-1.158065	-0.727476
O	-0.031329	-2.419049	-0.754219
H	-0.075972	-3.096219	0.852053
C	-1.179827	-0.271499	-0.610754
C	-0.697107	1.066478	-0.813507
C	-1.466437	2.331180	-1.010117
H	-2.362989	2.345844	-0.381124
H	-1.821830	2.341233	-2.053981
C	-0.587547	3.552129	-0.762947
H	-1.135906	4.459637	-1.040860
H	-0.360606	3.630960	0.312732
C	0.705216	3.443059	-1.560729
H	1.290471	4.366875	-1.488422
H	0.449471	3.312985	-2.623268
C	1.561846	2.264172	-1.098621
H	2.304130	2.010937	-1.868243
H	2.141998	2.540341	-0.207514
C	0.733156	1.041471	-0.832471
C	1.177457	-0.308346	-0.613644
Si	-2.952731	-0.928370	-0.595327
C	-3.228833	-1.771045	-2.251187
H	-3.085901	-1.062784	-3.077859
H	-4.253778	-2.159728	-2.316104
H	-2.538109	-2.609951	-2.400919
C	-4.218861	0.442028	-0.399396
H	-4.220983	1.137098	-1.247946
H	-4.073531	1.016139	0.524297
H	-5.213928	-0.021577	-0.348278
C	-3.171984	-2.158002	0.802639
H	-2.943770	-1.708753	1.778231
H	-2.534267	-3.039569	0.664031
H	-4.215256	-2.500504	0.826480
Si	2.936568	-0.995747	-0.554089
C	3.276338	-1.785908	-2.221741
H	4.296180	-2.190088	-2.262117
H	3.176241	-1.044653	-3.025854
H	2.576724	-2.605696	-2.427713
C	4.190249	0.365333	-0.240768
H	5.173964	-0.103165	-0.097731
H	3.969897	0.946201	0.663790
H	4.276704	1.059920	-1.084903

C	3.078661	-2.245800	0.834420
H	4.103224	-2.640252	0.866811
H	2.393497	-3.091743	0.705189
H	2.871663	-1.776562	1.806046
C	-1.371097	1.173812	1.973099
C	1.258564	1.135397	1.972747
O	2.049779	1.629157	2.638466
H	-0.060379	-0.798063	2.089851
O	-0.003064	-3.007780	1.838453
H	-0.838969	-3.328378	2.214722
H	-0.029878	-1.744137	1.914265
N	-2.214580	1.672587	2.622041
Co	0.002445	0.343192	0.964925

TS5,6-Co Gsolv= -2946.176887

C	-0.027265	-0.804009	-1.031400
O	-0.099163	-2.022489	-1.351109
H	-0.008327	-3.076585	0.077769
C	-1.164494	0.085181	-0.738809
C	-0.626094	1.407793	-0.597843
C	-1.341466	2.715615	-0.499852
H	-2.243568	2.621904	0.114217
H	-1.681929	2.978939	-1.514825
C	-0.421734	3.811891	0.026601
H	-0.926315	4.781562	-0.054666
H	-0.220373	3.642217	1.096845
C	0.888554	3.821874	-0.748560
H	1.505329	4.683394	-0.468400
H	0.662292	3.929951	-1.820416
C	1.682615	2.536088	-0.525807
H	2.458339	2.431529	-1.297019
H	2.218478	2.581169	0.432483
C	0.800429	1.323346	-0.580648
C	1.189706	-0.057706	-0.696622
Si	-2.958455	-0.488115	-0.914355
C	-3.192821	-1.009245	-2.703485
H	-2.973658	-0.178970	-3.387277
H	-4.231468	-1.320883	-2.875962
H	-2.537954	-1.848676	-2.967623
C	-4.185860	0.872392	-0.515351
H	-4.100932	1.725955	-1.198987
H	-4.092577	1.238301	0.514835
H	-5.197093	0.457193	-0.629909
C	-3.262772	-1.936200	0.233781
H	-3.124902	-1.641971	1.283012
H	-2.588418	-2.773327	0.013795
H	-4.294092	-2.295596	0.117692
Si	2.943022	-0.754173	-0.837100
C	3.273406	-0.961781	-2.672477
H	4.283463	-1.353427	-2.849256
H	3.188938	0.003649	-3.189259
H	2.555060	-1.654483	-3.129328
C	4.212587	0.411434	-0.090532
H	5.179447	-0.110767	-0.084351
H	3.980269	0.678346	0.948271
H	4.339183	1.335951	-0.665354
C	3.097371	-2.382953	0.072332
H	4.134599	-2.735799	-0.008045
H	2.440720	-3.162707	-0.328706
H	2.871067	-2.253130	1.139457
C	-1.352572	0.936447	2.107606
C	1.271750	0.581637	2.162446
O	2.094049	0.776543	2.936580
H	-0.347608	-1.127542	1.737768
O	0.173978	-3.161364	1.047201
H	-0.013126	-1.955328	1.372258
C	-0.776645	-4.010561	1.715655
H	-0.248217	-4.528885	2.517823
H	-1.586102	-3.403833	2.136192
H	-1.182262	-4.735508	1.007466
N	-2.184784	1.351316	2.826424
Co	-0.016585	0.230044	0.967826

TS5,6-Fe-Casey-H2O Gsolv= -2805.056946

Fe	0.044070	0.620438	0.857675
C	-0.006788	-1.186107	-0.517041
O	-0.029774	-2.434700	-0.246749
H	-0.228960	-2.664117	1.363176
C	-1.176137	-0.310368	-0.608386
C	-0.667286	0.964882	-1.026996
C	0.742874	0.930623	-1.043224
C	1.199699	-0.359277	-0.620960
Si	-2.970280	-0.863785	-0.514872
C	-3.286966	-2.048951	-1.934996
H	-3.100008	-1.569158	-2.904132
H	-4.328822	-2.395281	-1.925795
H	-2.638745	-2.931601	-1.863159
C	-4.061781	0.652259	-0.686319

H	-3.890085	1.174791	-1.636557
H	-3.906523	1.366295	0.132954
H	-5.116728	0.347628	-0.663906
C	-3.335591	-1.726817	1.110409
H	-3.058496	-1.105984	1.973015
H	-2.805461	-2.685538	1.181540
H	-4.411039	-1.938157	1.182376
Si	2.958693	-0.992108	-0.441855
C	3.290070	-2.243422	-1.800797
H	4.316605	-2.626682	-1.731408
H	3.164330	-1.794044	-2.794111
H	2.605480	-3.098055	-1.727472
C	4.129602	0.463263	-0.618660
H	5.168035	0.108676	-0.574113
H	3.997744	1.198887	0.184931
H	3.997476	0.976061	-1.580378
C	3.178696	-1.793309	1.239844
H	4.195358	-2.196211	1.340165
H	2.473434	-2.621577	1.386374
H	3.023230	-1.065326	2.047721
C	-1.265885	1.530018	1.624259
O	-2.134427	2.129585	2.096006
C	1.321864	1.636856	1.536121
O	2.163885	2.311733	1.951168
H	0.185314	-0.228281	2.212997
O	-0.195292	-2.411765	2.335099
H	-1.085525	-2.540574	2.699532
H	-0.039613	-1.173021	2.175805
C	1.242379	2.228203	-1.583669
O	0.083617	3.077562	-1.544774
C	-1.116000	2.284986	-1.557400
H	1.589084	2.096357	-2.621746
H	2.039783	2.715369	-1.011151
H	-1.873488	2.808187	-0.963180
H	-1.492556	2.176119	-2.587949

TS5,6-Fe-Casey Gsolv= -2844.289548

Fe	0.041092	-0.425487	0.946272
C	-0.002634	0.828605	-0.925378
O	0.009712	2.103065	-1.049323
H	-0.351030	2.778815	0.387453
C	1.182492	-0.024945	-0.791664
C	0.686048	-1.366869	-0.761538
C	-0.722460	-1.353544	-0.709472
C	-1.193647	0.002694	-0.723304
Si	2.967512	0.556214	-0.872995
C	3.264468	1.377860	-2.534748
H	3.070934	0.685918	-3.364133
H	4.305460	1.717734	-2.614328
H	2.615135	2.252701	-2.665191
C	4.074250	-0.947291	-0.689722
H	3.906383	-1.674729	-1.494728
H	3.921462	-1.455515	0.271299
H	5.127331	-0.639808	-0.737077
C	3.302771	1.783343	0.503447
H	3.182380	1.320448	1.491898
H	2.618852	2.639597	0.436053
H	4.329032	2.167669	0.431835
Si	-2.985069	0.564256	-0.845553
C	-3.247285	1.254785	-2.570944
H	-4.281991	1.598201	-2.700304
H	-3.045627	0.493394	-3.335219
H	-2.582977	2.107612	-2.761136
C	-4.070563	-0.944566	-0.589169
H	-5.123951	-0.663286	-0.721343
H	-3.965048	-1.359307	0.421755
H	-3.849559	-1.740484	-1.312160
C	-3.421652	1.860396	0.435809
H	-4.504074	2.045504	0.406520
H	-2.913985	2.813300	0.244307
H	-3.164497	1.530828	1.450987
C	1.303434	-1.204772	1.907627
O	2.137016	-1.724731	2.516887
C	-1.276621	-0.980267	1.987971
O	-2.152224	-1.362374	2.639178
H	0.321695	0.822489	1.909230
O	-0.480959	2.812101	1.384959
H	-0.160635	1.620678	1.596836
C	-1.211925	-2.762249	-0.763763
O	-0.029880	-3.537158	-0.500736
C	1.142245	-2.784265	-0.852299
H	-1.606268	-2.993438	-1.767166
H	-1.968720	-3.035165	-0.020056
H	1.951597	-3.078085	-0.175307
H	1.451359	-3.013049	-1.885533
C	0.494507	3.670054	2.002025
H	1.307638	3.062742	2.417498
H	0.894626	4.368050	1.262779

H	0.001983	4.222235	2.804851

TS5,6-Fe-H2O Gsolv= -2808.401236

Fe	0.002835	0.349503	1.005392
C	-0.012131	-1.167839	-0.670277
O	-0.022085	-2.450121	-0.652207
H	-0.036148	-2.993596	0.873186
C	-1.181637	-0.301102	-0.604580
C	-0.702432	1.049737	-0.797770
C	-1.485075	2.308699	-1.011389
H	-2.377005	2.335979	-0.374291
H	-1.853493	2.307348	-2.050699
C	-0.611576	3.538775	-0.788692
H	-1.164923	4.439750	-1.079316
H	-0.379029	3.638341	0.284308
C	0.678735	3.421711	-1.589580
H	1.257122	4.351894	-1.540520
H	0.416143	3.268882	-2.647836
C	1.545719	2.256399	-1.111068
H	2.280424	1.997960	-1.886488
H	2.135461	2.556066	-0.233712
C	0.720363	1.034287	-0.816014
C	1.171934	-0.322412	-0.610780
Si	-2.943453	-0.962633	-0.602521
C	-3.241465	-1.812171	-2.252546
H	-3.107912	-1.105438	-3.082273
H	-4.265821	-2.204157	-2.307205
H	-2.549653	-2.649247	-2.408913
C	-4.216449	0.404632	-0.399867
H	-4.205805	1.122871	-1.228614
H	-4.093461	0.956683	0.540972
H	-5.211433	-0.061787	-0.378158
C	-3.194196	-2.179357	0.804831
H	-2.971865	-1.717045	1.776437
H	-2.566380	-3.071343	0.690555
H	-4.242193	-2.508219	0.822034
Si	2.928508	-0.995754	-0.569109
C	3.263141	-1.835832	-2.216377
H	4.286845	-2.230679	-2.256692
H	3.145311	-1.121740	-3.042569
H	2.569978	-2.668713	-2.390122
C	4.191434	0.374157	-0.318746
H	5.178694	-0.090268	-0.186340
H	3.988691	0.975952	0.576263
H	4.257652	1.049212	-1.180590
C	3.125280	-2.214099	0.844568
H	4.158452	-2.586617	0.868066
H	2.456981	-3.077265	0.743165
H	2.921207	-1.730919	1.810122
C	-1.273802	1.185203	1.897491
O	-2.114677	1.747310	2.460268
C	1.313544	1.109711	1.918144
O	2.175771	1.615167	2.501600
H	-0.038584	-0.741954	2.188396
O	0.016093	-2.943943	1.878725
H	-0.827939	-3.273175	2.226378
H	-0.014941	-1.688718	1.965890

TS5,6-Fe Gsolv= -2847.635456

Fe	-0.053838	0.239169	1.011968
C	-0.005777	-0.852216	-0.947103
O	-0.029990	-2.114545	-1.186416
H	0.287925	-2.901733	0.189951
C	-1.172666	0.000659	-0.746658
C	-0.679145	1.350824	-0.616363
C	-1.446243	2.636820	-0.575270
H	-2.363227	2.535425	0.016884
H	-1.772255	2.865650	-1.603256
C	-0.577970	3.778000	-0.056328
H	-1.113835	4.727906	-0.169498
H	-0.391405	3.640538	1.021557
C	0.745723	3.816126	-0.808065
H	1.325724	4.707033	-0.539785
H	0.531483	3.891545	-1.885528
C	1.583597	2.565256	-0.545643
H	2.365186	2.476793	-1.313063
H	2.113957	2.659880	0.412532
C	0.741963	1.319050	-0.572258
C	1.181026	-0.055414	-0.672833
Si	-2.937662	-0.629298	-0.926265
C	-3.179424	-1.183720	-2.705619
H	-2.998776	-0.355960	-3.403621
H	-4.205849	-1.540558	-2.863195
H	-2.493613	-2.000281	-2.964691
C	-4.205805	0.695591	-0.522310
H	-4.160303	1.550369	-1.208105
H	-4.108190	1.068531	0.505629
H	-5.205546	0.248843	-0.617864

C	-3.231341	-2.065826	0.243648
H	-3.125426	-1.742024	1.288560
H	-2.536191	-2.895069	0.063062
H	-4.253270	-2.447900	0.114286
Si	2.954023	-0.671678	-0.856093
C	3.252154	-0.880160	-2.699197
H	4.266466	-1.252357	-2.894441
H	3.138775	0.080927	-3.218962
H	2.539973	-1.589072	-3.141266
C	4.205351	0.549684	-0.165367
H	5.196839	0.078858	-0.223458
H	4.017113	0.789252	0.888916
H	4.254476	1.487820	-0.729792
C	3.257990	-2.289461	0.040791
H	4.309057	-2.573518	-0.107591
H	2.629835	-3.110693	-0.321740
H	3.092201	-2.176609	1.120596
C	-1.313918	0.945437	2.026896
O	-2.152480	1.409270	2.675913
C	1.266837	0.623839	2.124824
O	2.144057	0.883134	2.833889
H	-0.404055	-1.085577	1.838428
O	0.423371	-3.026061	1.182270
H	0.097318	-1.854016	1.490291
C	-0.530449	-3.947939	1.733600
H	-0.039279	-4.503807	2.534865
H	-1.388714	-3.399104	2.139082
H	-0.866729	-4.639506	0.957367

TS5,6-Fe-Renaud-H2O Gsolv= -2602.916759

Fe	0.084687	0.129867	1.121186
C	0.044617	-1.040904	-0.780658
O	-0.028664	-2.307133	-0.935064
H	-0.897567	-2.898253	0.346130
C	-1.054811	-0.102102	-0.623542
C	-0.470434	1.225094	-0.543628
C	-0.219052	3.521450	-0.120953
H	-0.713778	4.488309	-0.261194
H	-0.014498	3.399664	0.953624
C	1.083974	3.480721	-0.899642
H	1.751361	4.279777	-0.562425
H	0.889352	3.653227	-1.967261
C	0.954312	1.109058	-0.599467
C	1.273449	-0.296451	-0.546355
C	-1.174227	0.818588	2.152543
O	-1.989773	1.305437	2.815916
C	1.388268	0.579510	2.235611
O	2.224672	0.779511	3.012543
H	0.145444	-1.225740	1.982754
O	-1.078417	-2.962269	1.333017
H	-0.471953	-1.928693	1.651611
C	-2.477900	-2.835328	1.640290
H	-2.626396	-3.216003	2.652341
H	-2.789084	-1.784949	1.587224
H	-3.057193	-3.431892	0.931501
C	2.607494	-0.923172	-0.653304
C	3.104415	-1.764781	0.347611
C	3.382292	-0.708274	-1.800259
C	4.355684	-2.363072	0.214800
H	2.504210	-1.940724	1.239901
C	4.635820	-1.300684	-1.930901
H	2.996062	-0.070911	-2.594578
C	5.127892	-2.127428	-0.921512
H	4.729659	-3.011398	1.004360
H	5.228678	-1.118724	-2.824719
H	6.107816	-2.588792	-1.021722
C	-2.481287	-0.437935	-0.792238
C	-3.496988	0.296034	-0.159552
C	-2.856074	-1.505091	-1.621459
C	-4.835180	-0.041383	-0.329777
H	-3.237373	1.142073	0.472121
C	-4.197338	-1.843036	-1.790667
H	-2.088718	-2.075898	-2.136930
C	-5.193457	-1.119388	-1.140276
H	-5.603291	0.540660	0.175234
H	-4.461963	-2.676793	-2.437806
H	-6.240297	-1.385218	-1.269109
N	1.783200	2.197628	-0.729336
N	-1.142704	2.461413	-0.539424
C	2.994744	2.275021	0.073423
H	3.447485	1.288366	0.199844
H	3.725002	2.923025	-0.421854
H	2.777338	2.693982	1.069847
C	-1.803014	2.756670	-1.813272
H	-1.091779	2.875749	-2.647512
H	-2.498200	1.952807	-2.073644
H	-2.377403	3.683426	-1.709414

TS5,6-Fe-Renaud Gsolv= -2602.916759

Fe	0.084687	0.129867	1.121186
C	0.044617	-1.040904	-0.780658
O	-0.028664	-2.307133	-0.935064
H	-0.897567	-2.898253	0.346130
C	-1.054811	-0.102102	-0.623542
C	-0.470434	1.225094	-0.543628
C	-0.219052	3.521450	-0.120953
H	-0.713778	4.488309	-0.261194
H	-0.014498	3.399664	0.953624
C	1.083974	3.480721	-0.899642
H	1.751361	4.279777	-0.562425
H	0.889352	3.653227	-1.967261
C	0.954312	1.109058	-0.599467
C	1.273449	-0.296451	-0.546355
C	-1.174227	0.818588	2.152543
O	-1.989773	1.305437	2.815916
C	1.388268	0.579510	2.235611
O	2.224672	0.779511	3.012543
H	0.145444	-1.225740	1.982754
O	-1.078417	-2.962269	1.333017
H	-0.471953	-1.928693	1.651611
C	-2.477900	-2.835328	1.640290
H	-2.626396	-3.216003	2.652341
H	-2.789084	-1.784949	1.587224
H	-3.057193	-3.431892	0.931501
C	2.607494	-0.923172	-0.653304
C	3.104415	-1.764781	0.347611
C	3.382292	-0.708274	-1.800259
C	4.355684	-2.363072	0.214800
H	2.504210	-1.940724	1.239901
C	4.635820	-1.300684	-1.930901
H	2.996062	-0.070911	-2.594578
C	5.127892	-2.127428	-0.921512
H	4.729659	-3.011398	1.004360
H	5.228678	-1.118724	-2.824719
H	6.107816	-2.588792	-1.021722
C	-2.481287	-0.437935	-0.792238
C	-3.496988	0.296034	-0.159552
C	-2.856074	-1.505091	-1.621459
C	-4.835180	-0.041383	-0.329777
H	-3.237373	1.142073	0.472121
C	-4.197338	-1.843036	-1.790667
H	-2.088718	-2.075898	-2.136930
C	-5.193457	-1.119388	-1.140276
H	-5.603291	0.540660	0.175234
H	-4.461963	-2.676793	-2.437806
H	-6.240297	-1.385218	-1.269109
N	1.783200	2.197628	-0.729336
N	-1.142704	2.461413	-0.539424
C	2.994744	2.275021	0.073423
H	3.447485	1.288366	0.199844
H	3.725002	2.923025	-0.421854
H	2.777338	2.693982	1.069847
C	-1.803014	2.756670	-1.813272
H	-1.091779	2.875749	-2.647512
H	-2.498200	1.952807	-2.073644
H	-2.377403	3.683426	-1.709414

TS5,6-Fe-williams-1-H2O Gsolv= -2758.873247

Fe	0.005548	-0.580343	1.302621
C	-0.124316	-1.636444	-0.760620
O	-0.252438	-2.835781	-1.101074
H	-1.577245	-3.758696	-0.222406
C	-1.194822	-0.685662	-0.418592
C	-0.613169	0.616111	-0.280265
C	0.815433	0.467983	-0.277961
C	1.113471	-0.935810	-0.439366
C	-1.011817	0.326502	2.475181
O	-1.635415	0.926627	3.234461
C	1.439482	-0.508702	2.375669
O	2.358717	-0.519029	3.068536
H	-0.349625	-1.918905	2.252374
O	-2.222221	-4.253985	0.324838
H	-2.975894	-3.654841	0.406613
H	-0.499675	-2.166285	1.485255
C	-2.625127	-1.027391	-0.553958
C	-3.072045	-1.510966	-1.791068
C	-3.544632	-0.890555	0.490439
C	-4.410256	-1.843419	-1.980384
H	-2.363244	-1.615513	-2.611126
C	-4.884540	-1.221977	0.300281
H	-3.212486	-0.534379	1.463709
C	-5.320819	-1.699972	-0.934256
H	-4.742466	-2.214480	-2.947404
H	-5.587750	-1.111040	1.122597
H	-6.366437	-1.961304	-1.080034
C	2.447254	-1.549872	-0.586515

C	2.784991	-2.692567	0.149057
C	3.376886	-1.031779	-1.497012
C	4.027217	-3.298961	-0.013932
H	2.068515	-3.096021	0.864624
C	4.621961	-1.636091	-1.655554
H	3.121678	-0.153486	-2.088831
C	4.951048	-2.769505	-0.914275
H	4.276698	-4.183169	0.568408
H	5.335402	-1.220694	-2.363870
H	5.924312	-3.239169	-1.037717
C	1.777331	1.587782	-0.390048
C	2.868256	1.764150	0.465137
C	1.613506	2.470093	-1.466606
C	3.769787	2.804764	0.255463
H	3.028633	1.088169	1.300226
C	2.516484	3.507516	-1.678316
H	0.775283	2.333878	-2.148794
C	3.597554	3.679641	-0.815268
H	4.610554	2.930583	0.933730
H	2.374456	4.180833	-2.520514
H	4.302370	4.491907	-0.977080
C	-1.343881	1.898977	-0.233646
C	-2.388184	2.118793	-1.139583
C	-0.974583	2.929790	0.639901
C	-3.053737	3.342083	-1.167021
H	-2.671645	1.334366	-1.839039
C	-1.643068	4.148779	0.613569
H	-0.162007	2.774975	1.348703
C	-2.686196	4.358576	-0.288680
H	-3.860808	3.499105	-1.878833
H	-1.349755	4.937273	1.302691
H	-3.209082	5.311954	-0.306152

TS5,6-Fe-williams-1 Gsolv= -2798.091636

Fe	0.012898	-0.569255	1.147003
C	-0.044287	-1.457993	-0.938445
O	-0.097295	-2.678892	-1.291292
H	-1.033844	-3.431814	-0.081733
C	-1.159131	-0.581910	-0.610882
C	-0.630740	0.732059	-0.314988
C	0.796875	0.656697	-0.342285
C	1.157924	-0.717890	-0.590511
C	-1.235871	-0.160148	2.343149
O	-2.021876	0.103572	3.147434
C	1.300219	-0.259094	2.325144
O	2.125415	-0.097665	3.117070
H	0.149343	-2.050234	1.722261
O	-1.264547	-3.547525	0.884383
H	-0.593986	-2.552537	1.321057
C	-2.578085	-0.931526	-0.826615
C	-2.929658	-1.648885	-1.978738
C	-3.600299	-0.530844	0.044170
C	-4.260072	-1.961935	-2.247918
H	-2.153543	-1.953620	-2.676964
C	-4.929623	-0.841647	-0.225801
H	-3.365012	0.038979	0.939978
C	-5.266136	-1.561982	-1.371160
H	-4.509545	-2.517043	-3.149706
H	-5.705725	-0.520108	0.465317
H	-6.305359	-1.806537	-1.578990
C	2.519349	-1.255683	-0.785113
C	3.030424	-2.263112	0.040256
C	3.310054	-0.775129	-1.836014
C	4.308927	-2.773280	-0.173830
H	2.422485	-2.634287	0.865488
C	4.590037	-1.281269	-2.047368
H	2.916366	0.004143	-2.487907
C	5.093444	-2.280689	-1.215614
H	4.695876	-3.552735	0.478993
H	5.194794	-0.894342	-2.864665
H	6.094250	-2.674166	-1.379139
C	1.732586	1.801398	-0.291542
C	2.955767	1.741482	0.389040
C	1.435132	2.955737	-1.029635
C	3.842816	2.813084	0.353295
H	3.230150	0.849197	0.947091
C	2.324358	4.026470	-1.067503
H	0.505895	3.013073	-1.593684
C	3.528724	3.962165	-0.370442
H	4.783954	2.747435	0.894397
H	2.074066	4.911532	-1.648051
H	4.222481	4.799373	-0.396397
C	-1.426329	1.967167	-0.155363
C	-2.317438	2.333743	-1.170498
C	-1.268687	2.810259	0.949809
C	-3.037544	3.522183	-1.081825
H	-2.436056	1.688893	-2.040373
C	-1.987344	3.999127	1.036672

H	-0.574650	2.530301	1.742734
C	-2.874486	4.357945	0.021878
H	-3.725137	3.796911	-1.878566
H	-1.856754	4.645480	1.901659
H	-3.438020	5.285482	0.092721
C	-0.622729	-4.739687	1.372270
H	0.453529	-4.703695	1.166914
H	-0.795679	-4.786591	2.448880
H	-1.067857	-5.609232	0.884279

TS5,6-Fe-williams-2-H2O Gsolv= -2947.819888

Fe	0.092614	-0.509947	1.035355
C	0.039342	-1.905383	-0.751808
O	0.077788	-3.175102	-0.795690
H	-0.675490	-3.698268	0.612513
C	-1.149211	-1.056229	-0.597207
C	-0.696830	0.304395	-0.685217
C	-1.245245	1.678856	-0.904708
H	-2.106679	1.961258	-0.294927
H	-1.534222	1.783534	-1.960102
C	-0.009303	2.569994	-0.604605
C	1.224915	1.706128	-0.966220
H	1.448466	1.836951	-2.034474
H	2.127198	1.971055	-0.407993
C	0.712713	0.322263	-0.742914
C	1.203096	-1.018978	-0.666460
C	-1.139732	0.141203	2.138291
O	-1.945015	0.552144	2.858531
C	1.491192	0.149650	1.899552
O	2.455602	0.539081	2.403278
H	0.310721	-1.767540	1.995374
O	-0.884673	-3.601168	1.587814
H	-1.843703	-3.456866	1.647270
H	-0.334269	-2.482624	1.761198
C	-0.045325	2.986171	0.874766
O	-1.074215	3.195219	1.488927
O	1.164573	3.158484	1.388670
C	-0.009454	3.883237	-1.373123
O	0.992059	4.402779	-1.828462
O	-1.224045	4.411577	-1.448425
C	1.213331	3.531509	2.776968
H	2.271413	3.566788	3.035891
H	0.751979	4.512244	2.920233
H	0.695807	2.779855	3.382256
C	-1.328818	5.689049	-2.101931
H	-2.385931	5.950585	-2.067465
H	-0.733136	6.432998	-1.566152
H	-0.989274	5.611071	-3.137976
C	2.608924	-1.452195	-0.699287
C	3.061201	-2.512916	0.099290
C	3.531751	-0.809183	-1.530831
C	4.389776	-2.915646	0.057300
H	2.363977	-3.011795	0.771283
C	4.865020	-1.214368	-1.563817
H	3.202891	0.008264	-2.171333
C	5.317562	-2.272390	-0.772408
H	4.721858	-3.741035	0.686877
H	5.566397	-0.701672	-2.221359
C	-2.550724	-1.510821	-0.585580
C	-2.921716	-2.757497	-1.106348
C	-3.570226	-0.687505	-0.079201
C	-4.255064	-3.162993	-1.112854
H	-2.160291	-3.416275	-1.514136
C	-4.896593	-1.097314	-0.090514
H	-3.326733	0.287660	0.337852
C	-5.266853	-2.346066	-0.605235
H	-4.513822	-4.137833	-1.525501
H	-5.664863	-0.437240	0.312179
C	6.753922	-2.698136	-0.784981
H	6.846724	-3.790267	-0.811379
H	7.285823	-2.285853	-1.649051
H	7.274955	-2.356084	0.118837
C	-6.702018	-2.774515	-0.611308
H	-7.312072	-2.113615	-1.240233
H	-6.813256	-3.795807	-0.990625
H	-7.132814	-2.736898	0.396925

TS5,6-Fe-williams-2 Gsolv= -2987.053658

Fe	0.072744	-0.470246	0.968815
C	-0.167413	-1.782809	-0.867991
O	-0.339741	-3.037484	-0.945249
H	-1.265180	-3.471033	0.499919
C	-1.207556	-0.759647	-0.718166
C	-0.546927	0.512446	-0.737889
C	-0.875637	1.959412	-0.919760
H	-1.701189	2.347155	-0.318362
H	-1.116972	2.141429	-1.976606
C	0.471649	2.640528	-0.559604

C	1.570224	1.610254	-0.925554
H	1.842428	1.742369	-1.982121
H	2.485748	1.718921	-0.337468
C	0.849156	0.312118	-0.767418
C	1.122551	-1.092043	-0.729914
C	-1.087296	0.276055	2.090096
O	-1.843366	0.746186	2.827867
C	1.521131	-0.021800	1.883469
O	2.513463	0.216641	2.425933
H	0.166341	-1.785324	1.869530
O	-1.316918	-3.397306	1.490903
H	-0.565958	-2.398961	1.640783
C	0.459962	3.006942	0.933276
O	-0.547133	3.294923	1.551160
O	1.678122	3.041805	1.457958
C	0.688160	3.959415	-1.287523
O	1.750130	4.304855	-1.769516
O	-0.411969	4.702435	-1.297858
C	1.751876	3.388241	2.852208
H	2.807399	3.329436	3.116579
H	1.375366	4.402910	3.006908
H	1.167198	2.677798	3.445577
C	-0.304474	5.994949	-1.921080
H	-1.281419	6.462176	-1.800934
H	0.466824	6.588696	-1.423662
H	-0.066293	5.880189	-2.981795
C	2.446124	-1.732074	-0.761549
C	2.697595	-2.930491	-0.076159
C	3.497564	-1.145295	-1.474051
C	3.956380	-3.516229	-0.112146
H	1.902059	-3.393444	0.505180
C	4.759802	-1.735620	-1.501364
H	3.327825	-0.220120	-2.023218
C	5.011482	-2.930864	-0.824773
H	4.133548	-4.443369	0.432977
H	5.564083	-1.258140	-2.060166
C	-2.660409	-0.987461	-0.780874
C	-3.191418	-2.119407	-1.411894
C	-3.562774	-0.065245	-0.225577
C	-4.568129	-2.330351	-1.463255
H	-2.520052	-2.845273	-1.862161
C	-4.932855	-0.281080	-0.281574
H	-3.192148	0.825533	0.278508
C	-5.464297	-1.422108	-0.896996
H	-4.953766	-3.221661	-1.957592
H	-5.609088	0.447128	0.166256
C	6.361590	-3.579228	-0.856177
H	6.340723	-4.513170	-1.432578
H	7.110662	-2.923332	-1.312316
H	6.703296	-3.837701	0.153382
C	-6.945125	-1.639507	-0.953236
H	-7.432570	-0.885174	-1.584220
H	-7.189474	-2.625515	-1.362334
H	-7.398757	-1.559572	0.042163
C	-2.642581	-3.076003	1.948739
H	-3.335858	-3.844772	1.599392
H	-2.610967	-3.073582	3.039911
H	-2.955984	-2.092241	1.580107

TS5,6-Fe-wills-1-H2O Gsolv= -2449.741947

Fe	-0.043824	0.446446	0.962034
C	-0.000442	-1.024068	-0.766732
O	0.011144	-2.293540	-0.796545
H	0.107019	-2.903860	0.749815
C	-1.188940	-0.158986	-0.691906
C	-0.725458	1.186117	-0.829399
C	0.680371	1.200162	-0.796597
C	1.164583	-0.142410	-0.662149
C	-1.285298	1.358522	1.837210
O	-2.117122	1.962913	2.364247
C	1.332347	1.057274	1.895531
O	2.274176	1.457449	2.432360
H	-0.318827	-0.689473	2.057018
O	0.189576	-2.829838	1.744915
H	-0.576302	-3.287349	2.127585
H	-0.029348	-1.597389	1.845887
C	1.142936	2.605181	-0.996148
O	-0.042395	3.376510	-0.746225
C	-1.200126	2.584922	-1.049420
H	1.483360	2.755296	-2.034269
H	1.930231	2.947035	-0.315315
H	-1.492443	2.720022	-2.104140
C	2.578439	-0.546908	-0.663588
C	3.027704	-1.674728	0.037555
C	3.514318	0.214382	-1.377340
C	4.371216	-2.035940	0.011337
H	2.324006	-2.262742	0.620851
C	4.859585	-0.145219	-1.398036

H	3.185363	1.088257	-1.937943
C	5.293206	-1.274314	-0.706540
H	4.701462	-2.913677	0.562773
H	5.568654	0.457802	-1.960977
H	6.343073	-1.557775	-0.722981
C	-2.589562	-0.602553	-0.673759
C	-2.970142	-1.794501	-0.039129
C	-3.581408	0.178817	-1.282226
C	-4.303561	-2.190136	-0.018033
H	-2.215786	-2.405341	0.451755
C	-4.916671	-0.216400	-1.254582
H	-3.306853	1.098979	-1.796134
C	-5.283565	-1.402919	-0.623270
H	-4.580950	-3.115301	0.482838
H	-5.671208	0.405002	-1.731947
H	-6.325864	-1.712709	-0.601086
H	-2.026363	2.919911	-0.413284

TS5,6-Fe-wills-1 Gsolv= -2488.980347

Fe	-0.158232	-0.537289	0.886973
C	-0.088664	0.958526	-0.818090
O	-0.002269	2.222166	-0.771315
H	0.911556	2.580503	0.717435
C	1.021519	-0.001966	-0.810566
C	0.440205	-1.311058	-0.909375
C	-0.962016	-1.197499	-0.887508
C	-1.326163	0.169745	-0.700178
C	1.150994	-1.273594	1.832952
O	2.016362	-1.763695	2.422195
C	-1.467241	-1.315667	1.784888
O	-2.361158	-1.817054	2.318652
H	-0.373864	0.652608	1.925838
O	0.993530	2.391676	1.690199
H	0.324577	1.342561	1.745578
C	-1.553907	-2.541363	-1.144262
O	-0.445826	-3.433417	-0.961624
C	0.792017	-2.737465	-1.179129
H	-1.925263	-2.595797	-2.180914
H	-2.361693	-2.846008	-0.469333
H	1.131178	-2.861254	-2.220696
C	-2.690582	0.709013	-0.607467
C	-2.971423	1.850230	0.157922
C	-3.743073	0.075553	-1.281140
C	-4.268951	2.345143	0.238258
H	-2.168419	2.340837	0.704296
C	-5.042883	0.569448	-1.194782
H	-3.542642	-0.803667	-1.892012
C	-5.310225	1.707107	-0.436648
H	-4.470683	3.229286	0.839207
H	-5.846990	0.064112	-1.725248
H	-6.324449	2.093999	-0.368197
C	2.453503	0.323038	-0.903011
C	2.888321	1.595643	-1.303263
C	3.424865	-0.646691	-0.606687
C	4.246991	1.893286	-1.375458
H	2.154397	2.356987	-1.550239
C	4.780603	-0.346180	-0.677478
H	3.123267	-1.646025	-0.297938
C	5.200205	0.929460	-1.055124
H	4.560286	2.888060	-1.685626
H	5.513003	-1.112887	-0.434296
H	6.260714	1.165387	-1.105997
H	1.540868	-3.178165	-0.512647
C	2.351704	2.128089	2.087643
H	2.760708	1.270376	1.541771
H	2.955014	3.018172	1.895502
H	2.332581	1.916242	3.158388

TS5,6-Fe-wills-2-H2O Gsolv= -2489.007622

Fe	0.128117	0.349445	0.987955
C	0.117184	-1.114964	-0.736085
O	0.138237	-2.385703	-0.755265
H	0.090767	-2.984189	0.811358
C	-1.071201	-0.269984	-0.634682
C	-0.634086	1.091138	-0.759662
C	0.772102	1.111771	-0.825288
C	1.281089	-0.211132	-0.684576
C	-1.276241	0.665806	2.025108
O	-2.213419	0.823132	2.682739
C	1.225496	1.448789	1.836684
O	1.949336	2.186008	2.354702
H	0.639448	-0.739140	2.038307
O	0.217408	-2.906177	1.800319
H	-0.617159	-3.157296	2.226337
H	0.337264	-1.653079	1.864302
C	1.210112	2.513704	-1.089467
O	0.038451	3.286195	-0.812705
C	-1.148711	2.479630	-0.993721

H	1.500794	2.615062	-2.148669
H	2.031822	2.887915	-0.468415
H	-1.468556	2.553925	-2.049418
C	-2.231392	3.003422	-0.087838
H	-1.867338	3.057756	0.945096
H	-2.543199	4.005210	-0.401297
H	-3.108660	2.345951	-0.120099
C	-2.462843	-0.749223	-0.676231
C	-2.912468	-1.787637	0.149102
C	-3.363612	-0.176101	-1.584080
C	-4.224488	-2.244244	0.065422
H	-2.232017	-2.226366	0.875392
C	-4.677762	-0.630197	-1.665128
H	-3.027701	0.624866	-2.241600
C	-5.112354	-1.667494	-0.842075
H	-4.556740	-3.049276	0.717257
H	-5.361937	-0.173698	-2.377054
H	-6.138231	-2.023233	-0.905228
C	2.697157	-0.604853	-0.679670
C	3.122907	-1.806432	-0.093573
C	3.659853	0.232298	-1.261138
C	4.469801	-2.154003	-0.089106
H	2.394409	-2.465250	0.371590
C	5.008261	-0.115400	-1.251426
H	3.354332	1.159837	-1.742329
C	5.419591	-1.310214	-0.664714
H	4.780733	-3.087491	0.375192
H	5.738012	0.549965	-1.707572
H	6.472440	-1.582751	-0.655414

TS5,6-Fe-wills-2 Gsolv= -2528.242763

Fe	0.146036	0.284280	0.977504
C	0.172896	-0.849576	-0.969917
O	0.182673	-2.103053	-1.192602
H	0.092277	-2.922907	0.292453
C	-1.004889	-0.005690	-0.784651
C	-0.540403	1.345420	-0.626448
C	0.870158	1.342064	-0.660235
C	1.350015	0.009952	-0.739205
C	-1.324651	0.301542	1.963714
O	-2.312266	0.299809	2.564853
C	1.064751	1.331730	2.068063
O	1.646233	2.050106	2.762159
H	0.780447	-0.908161	1.831138
O	0.267994	-2.998049	1.273157
H	0.470283	-1.782327	1.509797
C	1.349591	2.753141	-0.658221
O	0.191382	3.498999	-0.274852
C	-1.016936	2.768849	-0.594946
H	1.672136	3.032152	-1.675144
H	2.164707	2.983347	0.037080
H	-1.343047	3.054352	-1.611808
C	-2.071055	3.142988	0.414891
H	-1.696269	2.962698	1.430216
H	-2.331610	4.202322	0.319774
H	-2.981188	2.550762	0.264297
C	-2.401153	-0.433680	-0.965190
C	-2.854714	-1.689385	-0.538482
C	-3.308808	0.418960	-1.609074
C	-4.175369	-2.076104	-0.742741
H	-2.169319	-2.364604	-0.034432
C	-4.631206	0.032482	-1.812073
H	-2.974545	1.390272	-1.970520
C	-5.070774	-1.216362	-1.378184
H	-4.507583	-3.053148	-0.398429
H	-5.318136	0.710090	-2.314311
H	-6.103624	-1.519105	-1.534443
C	2.757557	-0.411165	-0.793410
C	3.170242	-1.659249	-0.305377
C	3.719289	0.441172	-1.353145
C	4.506191	-2.040192	-0.377081
H	2.442403	-2.327066	0.148388
C	5.057214	0.060237	-1.419362
H	3.417814	1.406463	-1.757529
C	5.455848	-1.182724	-0.932479
H	4.809009	-3.010310	0.011135
H	5.788014	0.736429	-1.857509
H	6.500131	-1.482308	-0.983527
C	-0.880431	-3.443697	2.013527
H	-1.379061	-4.244332	1.462962
H	-0.523853	-3.821895	2.973243
H	-1.574215	-2.610766	2.180497

TS5,6-Fe-wills-3-H2O Gsolv= -2666.663558

Fe	0.298580	0.371856	0.963334
C	0.141688	-1.192545	-0.660406
O	0.074586	-2.463701	-0.583503
H	0.037656	-2.930602	1.016435

C	-0.986246	-0.262175	-0.596626
C	-0.452557	1.052754	-0.817033
C	0.951057	0.953765	-0.906822
C	1.371954	-0.389742	-0.687553
Si	3.126686	-1.063034	-0.679041
C	3.405933	-1.973734	-2.296654
H	2.706482	-2.813312	-2.400465
H	4.426439	-2.374429	-2.351559
H	3.258845	-1.304425	-3.153989
C	4.296772	0.395985	-0.535405
H	5.335847	0.041254	-0.528712
H	4.130486	0.954174	0.395898
H	4.190561	1.092748	-1.377044
C	3.386129	-2.225311	0.768149
H	4.413791	-2.612441	0.754197
H	2.704117	-3.083573	0.726515
H	3.234101	-1.708839	1.725024
C	-1.075409	0.821807	1.982870
O	-2.004251	1.069437	2.625358
C	1.438483	1.484913	1.734428
O	2.171271	2.236252	2.219434
H	0.773958	-0.659166	2.083944
O	0.185162	-2.799668	1.998917
H	-0.663598	-2.948290	2.444907
H	0.400375	-1.560459	1.977097
C	1.495311	2.290174	-1.284987
O	0.389202	3.176400	-1.078252
C	-0.865110	2.456380	-1.141006
H	1.791896	2.277489	-2.346921
H	2.344367	2.653128	-0.695614
H	-1.233280	2.478415	-2.182990
C	-2.409947	-0.635693	-0.581700
C	-2.910800	-1.618823	0.281797
C	-3.294642	-0.015163	-1.474374
C	-4.257046	-1.970486	0.252756
H	-2.244044	-2.095437	0.996649
C	-4.642380	-0.364861	-1.501280
H	-2.919748	0.740066	-2.164136
C	-5.128689	-1.345026	-0.638150
H	-4.628823	-2.731786	0.935147
H	-5.312450	0.128636	-2.201870
H	-6.181276	-1.618215	-0.657174
C	-1.852219	3.138509	-0.230042
H	-1.436367	3.219480	0.781745
H	-2.078409	4.145314	-0.596656
H	-2.789068	2.570354	-0.183925

TS5,6-Fe-wills-3 Gsolv= -2705.897728

Fe	0.329615	0.278722	0.949697
C	0.158642	-0.926504	-0.949796
O	0.051000	-2.187596	-1.114828
H	-0.013844	-2.929066	0.387166
C	-0.939635	0.017571	-0.741385
C	-0.352582	1.328744	-0.667173
C	1.049941	1.191656	-0.760267
C	1.417935	-0.180877	-0.802816
Si	3.147601	-0.911636	-0.908552
C	3.430543	-1.457944	-2.681958
H	2.690102	-2.211289	-2.980285
H	4.428971	-1.897989	-2.802589
H	3.348474	-0.610561	-3.374632
C	4.371267	0.425495	-0.426708
H	5.392925	0.025155	-0.468614
H	4.196121	0.781114	0.597387
H	4.327567	1.288030	-1.104289
C	3.336146	-2.375740	0.245019
H	4.346143	-2.794844	0.140929
H	2.617771	-3.172967	0.017915
H	3.203405	-2.080474	1.293894
C	-1.081374	0.507577	1.995784
O	-2.037589	0.639317	2.632249
C	1.414193	1.263231	1.943839
O	2.100982	1.944138	2.577157
H	0.845329	-0.937147	1.852531
O	0.182702	-3.002153	1.366456
H	0.490822	-1.796645	1.560737
C	1.655285	2.550576	-0.858988
O	0.583232	3.426301	-0.495098
C	-0.700865	2.788396	-0.694227
H	1.974796	2.732767	-1.898429
H	2.505331	2.752580	-0.198315
H	-1.068122	3.044087	-1.704794
C	-2.373757	-0.294590	-0.842695
C	-2.902676	-1.515585	-0.400192
C	-3.245949	0.632592	-1.430900
C	-4.259517	-1.793546	-0.533105
H	-2.246294	-2.251554	0.054903
C	-4.603971	0.355114	-1.562076

H	-2.856844	1.576414	-1.808682
C	-5.117821	-0.859221	-1.111923
H	-4.648574	-2.745934	-0.179341
H	-5.260367	1.090342	-2.022500
H	-6.178509	-1.077521	-1.213066
C	-1.649930	3.316709	0.351554
H	-1.223867	3.170456	1.351799
H	-1.825765	4.386911	0.199253
H	-2.615178	2.799683	0.299842
C	-0.987630	-3.309309	2.140577
H	-1.561662	-4.091103	1.638028
H	-0.650857	-3.667660	3.115066
H	-1.606376	-2.412771	2.270828

TS5,6-Fe-wills-4-H2O Gsolv= -2627.398744

Fe	0.191384	0.504839	0.914523
C	0.036531	-1.106051	-0.681340
O	-0.053484	-2.373203	-0.589137
H	-0.017306	-2.840483	0.984109
C	-1.077034	-0.149054	-0.641995
C	-0.508040	1.141195	-0.903795
C	0.894796	1.024543	-0.934766
C	1.280746	-0.333713	-0.692350
Si	3.014804	-1.058687	-0.639810
C	3.246756	-2.185561	-2.122221
H	2.540209	-3.024656	-2.097144
H	4.263502	-2.599575	-2.136483
H	3.093037	-1.641218	-3.062643
C	4.232832	0.366400	-0.715187
H	5.259673	-0.021239	-0.681865
H	4.111859	1.053910	0.132092
H	4.126657	0.942805	-1.643537
C	3.269745	-2.022681	0.947999
H	4.295631	-2.412623	0.989944
H	2.584370	-2.876214	1.021721
H	3.116061	-1.382678	1.827400
C	-1.101109	1.368454	1.758950
O	-1.989587	1.922127	2.248678
C	1.522054	1.331455	1.747263
O	2.394685	1.876297	2.273893
H	0.206647	-0.509770	2.158450
O	0.076979	-2.720827	1.976255
H	-0.774060	-2.967115	2.372530
H	0.135128	-1.463336	1.986140
C	1.466404	2.356521	-1.292519
O	0.364973	3.256951	-1.092132
C	-0.875783	2.548869	-1.236407
H	1.779046	2.360636	-2.349675
H	2.305482	2.703568	-0.680639
H	-1.618076	3.016898	-0.579927
H	-1.235355	2.616070	-2.276757
C	-2.510636	-0.463565	-0.570202
C	-2.986707	-1.564036	0.157654
C	-3.439854	0.353415	-1.229724
C	-4.348860	-1.842145	0.212501
H	-2.283308	-2.198842	0.691096
C	-4.803320	0.076953	-1.169042
H	-3.094369	1.205063	-1.813900
C	-5.264053	-1.023795	-0.449789
H	-4.698618	-2.700530	0.782148
H	-5.506208	0.723080	-1.690442
H	-6.328574	-1.241907	-0.403497

TS5,6-Fe-wills-4 Gsolv= -2666.632306

Fe	-0.216298	-0.459233	0.916034
C	-0.075840	0.838743	-0.960271
O	0.058212	2.095696	-1.110630
H	0.192130	2.816475	0.370300
C	1.000642	-0.152540	-0.791177
C	0.357850	-1.437565	-0.788825
C	-1.038548	-1.251291	-0.777552
C	-1.348515	0.146490	-0.768437
Si	-3.039826	0.966266	-0.795787
C	-3.321976	1.695183	-2.502042
H	-2.559179	2.445134	-2.746220
H	-4.304364	2.181781	-2.559723
H	-3.288046	0.914404	-3.272578
C	-4.332200	-0.350215	-0.452636
H	-5.334288	0.093150	-0.525970
H	-4.231935	-0.779294	0.552518
H	-4.281765	-1.167798	-1.184025
C	-3.132219	2.303085	0.514821
H	-4.142252	2.733488	0.541101
H	-2.424632	3.118443	0.319625
H	-2.917192	1.891344	1.510381
C	1.005565	-1.332374	1.852152
O	1.828972	-1.919243	2.411558
C	-1.579651	-0.959812	1.932317

O	-2.478289	-1.299800	2.574468
H	0.028271	0.741354	1.955804
O	0.134476	2.870970	1.368931
H	-0.007189	1.634895	1.589168
C	-1.697812	-2.584212	-0.891244
O	-0.634278	-3.506978	-0.610906
C	0.632139	-2.901538	-0.908698
H	-2.076143	-2.731811	-1.916402
H	-2.514589	-2.778820	-0.187862
H	1.372150	-3.315319	-0.214883
H	0.944090	-3.141777	-1.938857
C	2.448813	0.103058	-0.803305
C	2.967207	1.403231	-0.691482
C	3.357840	-0.961200	-0.916068
C	4.341092	1.625122	-0.680993
H	2.284348	2.243507	-0.609981
C	4.731142	-0.736806	-0.905551
H	2.995124	-1.981964	-1.018208
C	5.232062	0.558350	-0.785465
H	4.716596	2.642358	-0.588526
H	5.411937	-1.580776	-0.993545
H	6.305331	0.734147	-0.776013
C	1.392454	3.270141	1.938835
H	1.208614	3.541094	2.980026
H	2.113458	2.444584	1.892487
H	1.777802	4.133477	1.391850

TS5,6-Fe-wills-5-H2O Gsolv= -2705.917162

Fe	0.084585	0.412586	0.942297
C	0.071418	-1.038234	-0.793766
O	0.170009	-2.308874	-0.817877
H	0.259412	-2.924934	0.719753
C	-1.163903	-0.270036	-0.619085
C	-0.813410	1.113945	-0.764322
C	0.586316	1.209553	-0.891104
C	1.185973	-0.082375	-0.790616
Si	3.015727	-0.510943	-0.849533
C	3.372280	-1.492992	-2.410978
H	4.454621	-1.588780	-2.569359
H	2.947954	-1.002501	-3.295992
H	2.950171	-2.504384	-2.347094
C	3.977224	1.102255	-0.861006
H	5.054250	0.895373	-0.918314
H	3.798638	1.681943	0.054844
H	3.719813	1.731318	-1.723009
C	3.501945	-1.514916	0.668643
H	2.820518	-2.373101	0.764040
H	3.330856	-0.886319	1.557265
C	-1.278842	0.715616	2.031798
O	-2.190101	0.855773	2.728864
C	1.206894	1.507537	1.766873
O	1.941839	2.233275	2.285942
H	0.596072	-0.672751	2.003242
O	0.408825	-2.866366	1.708740
H	-0.388913	-3.201188	2.147312
H	0.414663	-1.604268	1.800515
C	0.936716	2.630740	-1.182321
O	-0.269708	3.343053	-0.883562
C	-1.415893	2.467068	-0.990910
H	1.194605	2.734873	-2.249363
H	1.748303	3.062439	-0.586708
H	-1.790239	2.500258	-2.030900
C	4.951136	-1.995512	0.625368
H	5.232362	-2.537849	1.537067
H	5.124622	-2.674649	-0.219778
H	5.654960	-1.158908	0.518852
C	-2.526901	-0.825057	-0.572467
C	-2.865436	-1.885439	0.278026
C	-3.517459	-0.295990	-1.411072
C	-4.157072	-2.403982	0.286957
H	-2.115394	-2.291018	0.953829
C	-4.811315	-0.811216	-1.398562
H	-3.268409	0.521645	-2.086610
C	-5.135261	-1.868571	-0.550476
H	-4.402606	-3.224069	0.958211
H	-5.566832	-0.386285	-2.055881
H	-6.145709	-2.270867	-0.538323
C	-2.482639	2.954972	-0.046429
H	-2.080120	3.040263	0.969892
H	-2.848083	3.938667	-0.359802
H	-3.332455	2.261976	-0.034109

TS5,6-Fe-wills-5 Gsolv= -2823.667124

Fe	-0.367321	0.616325	1.100935
C	0.025130	-0.970814	-0.443963
O	0.067437	-2.240573	-0.317536
H	-0.248267	-2.627008	1.265019
C	-1.172895	-0.174867	-0.707924

C	-0.750667	1.192604	-0.826350
C	0.641213	1.247883	-0.590684
C	1.142156	-0.032632	-0.229071
Si	2.924904	-0.454530	0.213984
C	3.717310	1.061007	0.992276
H	4.727445	0.806401	1.340680
H	3.145092	1.396623	1.867369
H	3.806819	1.905637	0.297436
C	3.002369	-1.856660	1.458940
H	4.052352	-2.100323	1.671043
H	2.504089	-2.769735	1.112803
H	2.539773	-1.550627	2.406548
C	3.834695	-0.918217	-1.397685
C	-1.999754	0.794115	1.760971
O	-3.085968	0.884492	2.147317
C	0.300042	1.970975	2.025450
O	0.707658	2.883606	2.606052
H	0.104125	-0.272792	2.340745
O	-0.286664	-2.461626	2.253229
H	-0.146401	-1.208498	2.207851
C	1.112743	2.633812	-0.877139
O	-0.097063	3.395796	-0.946090
C	-1.222661	2.545344	-1.270563
H	1.639094	2.647850	-1.846446
H	1.765903	3.090179	-0.125263
H	-1.347802	2.531081	-2.368800
C	5.314824	-1.156771	-1.095085
H	5.848115	-1.443018	-2.016245
H	5.805725	-0.256020	-0.700870
H	5.464949	-1.967243	-0.367718
C	-2.506201	-0.708693	-1.027948
C	-3.025279	-1.843762	-0.390015
C	-3.276178	-0.095947	-2.026985
C	-4.277583	-2.343224	-0.733323
H	-2.446044	-2.333205	0.387409
C	-4.529532	-0.596112	-2.370867
H	-2.884913	0.771726	-2.555974
C	-5.036523	-1.721443	-1.724241
H	-4.662899	-3.222109	-0.220886
H	-5.108587	-0.106163	-3.150580
H	-6.015584	-2.112913	-1.990872
C	-2.452608	3.121299	-0.617267
H	-2.291527	3.226606	0.462736
H	-2.679208	4.107360	-1.036498
H	-3.319798	2.471349	-0.783193
C	-1.566257	-2.793602	2.814559
H	-1.423593	-2.962712	3.883535
H	-2.275793	-1.970832	2.663419
H	-1.943420	-3.705267	2.345216
C	3.231127	-2.188029	-1.997890
H	3.760693	-2.457411	-2.926415
H	3.310895	-3.045923	-1.315322
H	2.169605	-2.058618	-2.251912
C	3.706420	0.220880	-2.409500
H	2.658524	0.407721	-2.685751
H	4.129648	1.162611	-2.031615
H	4.248127	-0.032177	-3.335467

TS5,6-Mn-a-H2O Gsolv= -2708.944261

C	-0.014063	-1.207566	-0.482452
O	-0.041462	-2.452716	-0.194880
H	-0.394296	-2.652994	1.403067
C	-1.175801	-0.330800	-0.599600
C	-0.658447	0.936122	-1.026114
C	0.750075	0.902801	-1.038789
C	1.197866	-0.383812	-0.596721
Si	-2.987194	-0.834479	-0.523153
C	-3.311188	-2.014668	-1.944505
H	-3.098613	-1.539995	-2.910867
H	-4.360497	-2.337415	-1.949994
H	-2.683765	-2.911301	-1.862394
C	-4.020326	0.719064	-0.710968
H	-3.816089	1.242561	-1.653884
H	-3.849150	1.420067	0.116932
H	-5.086076	0.454325	-0.704947
C	-3.419924	-1.668395	1.099209
H	-3.135593	-1.050179	1.961912
H	-2.943503	-2.653342	1.187739
H	-4.505862	-1.825894	1.147458
Si	2.959150	-1.027916	-0.448167
C	3.185110	-2.427971	-1.677561
H	4.223148	-2.785416	-1.665323
H	2.953778	-2.101403	-2.699444
H	2.532358	-3.276753	-1.438397
C	4.123191	0.384085	-0.862581
H	5.162510	0.031257	-0.831227
H	4.033779	1.213646	-0.149360
H	3.937067	0.776080	-1.871073

C	3.278352	-1.651487	1.291694
H	4.281594	-2.092425	1.361758
H	2.551810	-2.424286	1.574706
H	3.215501	-0.837902	2.026449
C	1.448989	1.619853	1.517185
O	2.325604	2.283869	1.869648
H	0.444384	-0.345197	2.151504
O	-0.393788	-2.380972	2.370345
H	-1.317392	-2.371079	2.668917
H	-0.043814	-1.194646	2.190857
C	1.249814	2.189682	-1.604949
O	0.095754	3.045474	-1.556816
C	-1.107802	2.259336	-1.547930
H	1.575550	2.043029	-2.647700
H	2.059612	2.679595	-1.053205
H	-1.852172	2.783711	-0.937793
H	-1.505810	2.153659	-2.570636
Mn	0.049997	0.635114	0.909268
N	-1.138035	1.511719	1.611539
O	-2.039185	2.161656	1.992383

TS5,6-Mn-a Gsolv= -2748.175683

C	0.008286	0.845639	-0.915060
O	0.009296	2.117260	-1.037695
H	-0.391009	2.838245	0.378959
C	1.197907	0.001186	-0.793481
C	0.713349	-1.344050	-0.784160
C	-0.695271	-1.348376	-0.720617
C	-1.175363	0.004827	-0.708001
Si	2.980124	0.596636	-0.830735
C	3.308579	1.437710	-2.476473
H	3.140243	0.752332	-3.316663
H	4.347808	1.787983	-2.528516
H	2.653579	2.307505	-2.612762
C	4.090221	-0.901490	-0.630213
H	3.944322	-1.628507	-1.439785
H	3.918487	-1.412293	0.326582
H	5.142601	-0.588923	-0.653512
C	3.269780	1.808869	0.569037
H	3.124476	1.330647	1.546886
H	2.583544	2.662475	0.494353
H	4.295836	2.198349	0.531200
Si	-2.972015	0.555786	-0.854309
C	-3.182679	1.353781	-2.540361
H	-4.237639	1.602388	-2.716352
H	-2.857447	0.679835	-3.343081
H	-2.600611	2.280643	-2.617792
C	-4.045721	-0.979328	-0.741369
H	-5.100024	-0.696775	-0.861999
H	-3.947504	-1.487126	0.226602
H	-3.803949	-1.699230	-1.534262
C	-3.466807	1.774445	0.479227
H	-4.547733	1.959726	0.415771
H	-2.955526	2.736734	0.357587
H	-3.251412	1.395538	1.486607
C	-1.376584	-0.990437	1.960495
O	-2.295163	-1.376635	2.543832
H	0.216496	0.899092	1.896938
O	-0.542419	2.898566	1.370025
H	-0.228453	1.694832	1.611605
C	-1.171601	-2.758891	-0.818495
O	0.018548	-3.528544	-0.575132
C	1.186326	-2.754084	-0.893017
H	-1.559861	-2.964880	-1.829634
H	-1.927626	-3.061364	-0.085477
H	1.987239	-3.048548	-0.205589
H	1.518386	-2.960115	-1.923685
C	0.436154	3.753179	1.985907
H	0.838426	4.449742	1.246451
H	-0.054949	4.307458	2.788192
H	1.247998	3.144808	2.402839
Mn	0.074075	-0.469589	0.993950
N	1.191774	-1.269307	1.874931
O	2.011866	-1.911585	2.415891

TS5,6-Mn-b-H2O Gsolv= -2851.707568

C	0.035545	-1.921432	-0.725919
O	0.069299	-3.190652	-0.766585
H	-0.709492	-3.695080	0.665546
C	-1.150134	-1.075425	-0.580903
C	-0.703871	0.283317	-0.669491
C	-1.271974	1.649244	-0.881833
H	-2.123621	1.918819	-0.251665
H	-1.589521	1.744830	-1.929648
C	-0.038779	2.556713	-0.615408
C	1.200007	1.699594	-0.980630
H	1.408444	1.817451	-2.053485
H	2.105894	1.983694	-0.438081

C	0.704862	0.313328	-0.729732
C	1.198969	-1.027522	-0.643892
C	1.607156	0.156495	1.867227
O	2.602425	0.561520	2.288618
H	0.480689	-1.831546	1.919541
O	-0.883743	-3.566316	1.642775
H	-1.830502	-3.363628	1.728952
H	-0.260268	-2.494075	1.773459
C	-0.058766	3.004235	0.855528
O	-1.082033	3.255744	1.463254
O	1.155312	3.155723	1.366115
C	-0.061246	3.855242	-1.407798
O	0.933023	4.383581	-1.869236
O	-1.283982	4.361665	-1.495766
C	1.212286	3.555103	2.746494
H	2.271118	3.580749	3.003299
H	0.765536	4.544997	2.871969
H	0.684376	2.823775	3.367617
C	-1.408521	5.625817	-2.171271
H	-2.470536	5.868046	-2.146718
H	-0.829889	6.389757	-1.644993
H	-1.061892	5.536743	-3.204066
C	2.606632	-1.455592	-0.694367
C	3.068260	-2.539247	0.067103
C	3.522920	-0.781577	-1.508908
C	4.398918	-2.932810	0.006586
H	2.377825	-3.066311	0.723573
C	4.858227	-1.177205	-1.559625
H	3.187773	0.052756	-2.123614
C	5.320275	-2.257222	-0.804118
H	4.737497	-3.777248	0.606693
H	5.553555	-0.639461	-2.203427
C	-2.548228	-1.534534	-0.566397
C	-2.928926	-2.709427	-1.226920
C	-3.549327	-0.788599	0.077427
C	-4.260304	-3.120022	-1.242979
H	-2.177854	-3.302359	-1.742335
C	-4.874156	-1.204155	0.055992
H	-3.291502	0.126453	0.608672
C	-5.256436	-2.379055	-0.603799
H	-4.531256	-4.035217	-1.768723
H	-5.632081	-0.608293	0.564496
C	6.759518	-2.671882	-0.833924
H	6.860421	-3.763069	-0.865433
H	7.279430	-2.251684	-1.701527
H	7.287286	-2.328810	0.065650
C	-6.690179	-2.812080	-0.620361
H	-7.328561	-2.053582	-1.090559
H	-6.817978	-3.749944	-1.170927
H	-7.073513	-2.960812	0.396867
O	-1.823928	0.635208	2.838637
N	-1.010912	0.148552	2.143661
Mn	0.086307	-0.485856	1.105690

TS5,6-Mn-b Gsolv= -2890.940674

C	-0.182055	-1.784870	-0.870328
O	-0.357732	-3.037731	-0.958398
H	-1.289566	-3.480151	0.492647
C	-1.217141	-0.758124	-0.737457
C	-0.549695	0.510164	-0.745586
C	-0.872946	1.961131	-0.911478
H	-1.689305	2.346828	-0.295687
H	-1.129919	2.152534	-1.962849
C	0.481786	2.636290	-0.563262
C	1.571915	1.600366	-0.934995
H	1.832346	1.724229	-1.995636
H	2.493869	1.709292	-0.357512
C	0.845990	0.307406	-0.760314
C	1.110237	-1.097890	-0.714415
C	1.598136	-0.057473	1.871731
O	2.616306	0.175638	2.363332
H	0.241916	-1.866766	1.785354
O	-1.331183	-3.406051	1.483492
H	-0.545699	-2.433583	1.620797
C	0.488325	3.009992	0.928830
O	-0.505355	3.344085	1.544980
O	1.708714	3.002222	1.449789
C	0.700173	3.952509	-1.295850
O	1.764871	4.295306	-1.773938
O	-0.398977	4.696313	-1.313495
C	1.801316	3.350980	2.841917
H	2.858891	3.280087	3.095044
H	1.438485	4.370080	2.999665
H	1.215987	2.647111	3.442363
C	-0.287241	5.987383	-1.938988
H	-1.263546	6.456790	-1.822303
H	0.483951	6.580573	-1.440751
H	-0.046572	5.869975	-2.998849

C	2.430900	-1.745279	-0.749611
C	2.677330	-2.950174	-0.074304
C	3.480972	-1.163893	-1.468750
C	3.930178	-3.547688	-0.126170
H	1.881525	-3.412471	0.506960
C	4.736899	-1.765927	-1.511861
H	3.313505	-0.237082	-2.015687
C	4.984543	-2.966544	-0.842998
H	4.102146	-4.482659	0.407043
H	5.538491	-1.296070	-2.080843
C	-2.669136	-0.981911	-0.791806
C	-3.206809	-2.113625	-1.418083
C	-3.564602	-0.059214	-0.225206
C	-4.584125	-2.322173	-1.457176
H	-2.540344	-2.838763	-1.876587
C	-4.935116	-0.273850	-0.268341
H	-3.187794	0.829929	0.276676
C	-5.473383	-1.413855	-0.880013
H	-4.975833	-3.211379	-1.950400
H	-5.606459	0.454544	0.186417
C	6.336407	-3.611515	-0.869303
H	6.263938	-4.684056	-1.085688
H	6.983727	-3.152415	-1.624102
H	6.839702	-3.516770	0.101683
C	-6.954291	-1.635092	-0.909729
H	-7.367201	-1.692853	0.105261
H	-7.470386	-0.809077	-1.414913
H	-7.210842	-2.563196	-1.431387
O	-1.793240	0.841305	2.720190
N	-1.009436	0.285555	2.044156
Mn	0.039653	-0.447135	1.020674
C	-2.646860	-3.055048	1.949246
H	-3.362497	-3.794711	1.582817
H	-2.615597	-3.077621	3.040043
H	-2.929651	-2.054004	1.602645

TS5,6-Mn-c-H2O Gsolv= -2353.632084

C	-0.001112	-1.150172	-0.585235
O	-0.015954	-2.400891	-0.379344
H	-0.802271	-2.616246	1.123356
C	-1.157698	-0.250314	-0.653084
C	-0.647161	1.046923	-0.985384
C	0.759198	1.014408	-0.996095
C	1.195631	-0.297779	-0.630414
C	1.556622	1.374884	1.622805
O	2.534420	1.849820	2.009865
H	0.306160	-0.510466	2.059230
O	-0.999263	-2.309050	2.053917
H	-1.949942	-2.109437	2.081568
H	-0.388711	-1.220650	2.001119
C	1.264405	2.323483	-1.501302
O	0.112515	3.175162	-1.421809
C	-1.089944	2.392053	-1.459557
H	1.596515	2.224269	-2.547954
H	2.073605	2.780253	-0.920777
H	-1.479024	2.320071	-2.488509
C	2.587223	-0.761520	-0.523772
C	2.942431	-1.800846	0.348658
C	3.592300	-0.146925	-1.281803
C	4.265493	-2.218337	0.447944
H	2.177072	-2.271473	0.961956
C	4.917695	-0.563104	-1.176807
H	3.335184	0.654868	-1.972529
C	5.258941	-1.601816	-0.313494
H	4.524455	-3.023876	1.131711
H	5.684050	-0.074770	-1.774729
H	6.293147	-1.928142	-0.230643
C	-2.576589	-0.634613	-0.589383
C	-2.985884	-1.959996	-0.802094
C	-3.564724	0.332767	-0.343097
C	-4.335251	-2.302534	-0.765155
H	-2.240781	-2.724012	-1.003024
C	-4.911073	-0.012843	-0.304813
H	-3.283390	1.369459	-0.168734
C	-5.304565	-1.334371	-0.512885
H	-4.628389	-3.336072	-0.937049
H	-5.656009	0.755297	-0.109156
H	-6.357458	-1.605052	-0.482037
H	-1.836430	2.900988	-0.840754
O	-1.865116	2.294900	2.131332
N	-1.048552	1.575637	1.689578
Mn	0.049746	0.632396	0.926721

TS5,6-Mn-c Gsolv= -2392.868031

C	0.074126	-0.965276	-0.831146
O	-0.012502	-2.228456	-0.796931
H	-0.960665	-2.596485	0.695335
C	-1.034595	-0.005379	-0.828788

C	-0.452935	1.300197	-0.921580
C	0.948991	1.196118	-0.888994
C	1.310683	-0.173439	-0.704024
C	1.602092	1.218069	1.768303
O	2.556542	1.658449	2.245387
H	0.451295	-0.752239	1.839805
O	-1.017916	-2.408352	1.669075
H	-0.304936	-1.390839	1.711043
C	1.533484	2.540202	-1.163568
O	0.422142	3.427785	-0.977526
C	-0.814204	2.726059	-1.179808
H	1.894384	2.589089	-2.204216
H	2.345178	2.856380	-0.499129
H	-1.170218	2.849589	-2.215723
C	2.677118	-0.710898	-0.615922
C	2.964358	-1.852371	0.146413
C	3.725324	-0.069968	-1.288925
C	4.264277	-2.341778	0.222562
H	2.164866	-2.347549	0.693903
C	5.027560	-0.558037	-1.206304
H	3.519571	0.810575	-1.896043
C	5.301343	-1.696824	-0.452224
H	4.471259	-3.226528	0.820776
H	5.828428	-0.047195	-1.736361
H	6.317485	-2.079102	-0.386647
C	-2.466554	-0.327164	-0.899860
C	-2.908158	-1.592333	-1.316450
C	-3.431388	0.635013	-0.558663
C	-4.267614	-1.889693	-1.366256
H	-2.178834	-2.346180	-1.597470
C	-4.787957	0.333676	-0.606908
H	-3.124621	1.626936	-0.232362
C	-5.214039	-0.933702	-1.004456
H	-4.587325	-2.877534	-1.691505
H	-5.515949	1.092886	-0.329554
H	-6.275193	-1.169731	-1.038007
H	-1.556703	3.160249	-0.501496
O	-1.911114	1.866118	2.328391
N	-1.025660	1.299685	1.803560
Mn	0.137695	0.551956	0.928247
C	-2.356934	-2.087725	2.091030
H	-3.007618	-2.938779	1.878387
H	-2.315544	-1.910590	3.167261
H	-2.724691	-1.192488	1.577151

TS5,6-Mn Gsolv= -2751.522091

C	-0.005861	-0.870135	-0.929160
O	0.006439	-2.125815	-1.182114
H	0.332935	-2.966862	0.180917
C	-1.190541	-0.048936	-0.717226
C	-0.732473	1.314270	-0.616101
C	-1.541333	2.573724	-0.602151
H	-2.431504	2.468123	0.029103
H	-1.915268	2.737039	-1.626851
C	-0.700915	3.771877	-0.171015
H	-1.266105	4.695274	-0.344373
H	-0.503682	3.719115	0.911793
C	0.618698	3.799561	-0.929725
H	1.170352	4.724504	-0.724292
H	0.402984	3.792769	-2.009569
C	1.494416	2.596653	-0.582253
H	2.300362	2.499876	-1.322058
H	1.989296	2.758149	0.386450
C	0.690448	1.325158	-0.569109
C	1.161272	-0.040261	-0.656034
Si	-2.949878	-0.698592	-0.871867
C	-3.268154	-1.003396	-2.698189
H	-3.168470	-0.068070	-3.265398
H	-4.280728	-1.393385	-2.865142
H	-2.553349	-1.725994	-3.112825
C	-4.206604	0.533537	-0.215746
H	-4.286834	1.433458	-0.837347
H	-3.982056	0.842395	0.814366
H	-5.192084	0.047498	-0.207183
C	-3.161070	-2.282583	0.110410
H	-2.983789	-2.102582	1.179380
H	-2.488078	-3.079918	-0.226232
H	-4.193252	-2.642826	0.000907
Si	2.940734	-0.637809	-0.872951
C	3.174989	-0.959659	-2.708493
H	4.194226	-1.314482	-2.911204
H	3.019928	-0.036735	-3.283552
H	2.472247	-1.713785	-3.084482
C	4.207171	0.643716	-0.336797
H	5.198823	0.177532	-0.425913
H	4.087753	0.959115	0.706742
H	4.209614	1.538525	-0.969986
C	3.297572	-2.193010	0.112077

H	4.359244	-2.446285	-0.014896	C	-0.494461	-4.062686	1.676474
H	2.703980	-3.052428	-0.218990	H	-0.029215	-4.602211	2.503808
H	3.116696	-2.039739	1.184298	H	-1.384447	-3.532677	2.035323
C	1.409595	0.595631	2.080343	H	-0.776465	-4.766423	0.889731
O	2.353194	0.849127	2.697872	O	-1.891892	1.700239	2.676653
H	-0.309848	-1.168771	1.832225	N	-1.132673	1.056884	2.049730
O	0.465972	-3.124639	1.165150	Mn	-0.075212	0.278774	1.080701
H	0.137545	-1.950173	1.512752				

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