

Supporting Material for Using Computational Methods to Explore Improvements on Knölker's Iron Catalyst

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M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

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Figure S1 The geometry of 5a optimized at the theory level of B3LYP/LACVP*

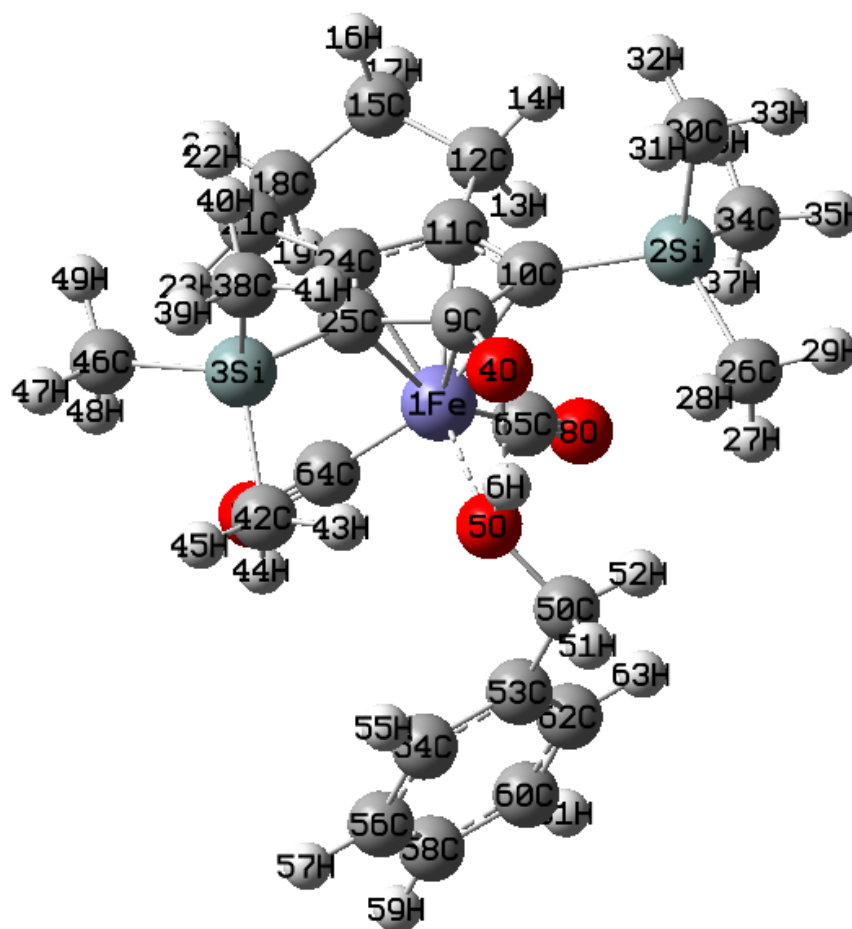


Table S1 Differences of bond lengths between crystal and B3LYP-optimized 5a structure in gas (Å)

Bonds	Bond Lengths (Å)	
	Crystal	B3LYP/LACVP*
Fe-C9	2.2222	2.26624
Fe-C10	2.12563	2.15853
Fe-C11	2.09239	2.13509
Fe-C24	2.0813	2.11598
Fe-C25	2.12628	2.1419
Fe-C64	1.78222	1.78346
Fe-C65	1.7841	1.77794
Fe-O5	2.04422	2.06787
O5-H6	0.83391	1.00411
O5-C50	1.44313	1.43983
C9-C10	1.47669	1.47325

C10-C11	1.44005	1.44238
C11-C24	1.43031	1.43169
C24-C25	1.44252	1.44189
C9-C25	1.46409	1.47368
C9-O4	1.27674	1.26924
O4-H6	1.82198	1.71315
C65-O8	1.14676	1.15499
C64-O7	1.14244	1.15255
C10-Si2	1.88146	1.89346
C25-Si3	1.88633	1.8944
SRE ^a	0.0023	
RMSE ^b	0.0479	
a. Square Root Error; b. Root Mean Square Error.		

Table S2 Differences of bond angles between crystal and B3LYP-optimized 5a structure in gas (degree, °)

Bond Angles	Degrees of Bond Angles (°)	
	Crystal	B3LYP-optimized
C64-Fe-C65	92.29	95.067
C64-Fe-O5	98.721	96.248
C65-Fe-O5	100.456	100.936
Fe-O5-H6	105.208	102.563
O5-H6-O4	147.61	148.21
C9-O4-H6	88.573	90.21
C9-C10-C11	106.045	106.57
C10-C11-C24	109.554	109.191
C11-C24-C25	108.96	109.085
C9-C25-C24	106.701	106.692
C10-C9-C25	108.135	107.555
C10-C9-O4	125.814	125.873
C25-C9-O4	124.623	125.101
SRE ^a	1.9296	
RMSE ^b	1.3891	
a. Square Root Error; b. Root Mean Square Error		

Table S3 B3LYP-calculated energies and thermochemistry in gas at 298 K and 1 atm (Hartree)

Complexes	$E_{\text{SCF}}(\text{B3LYP})$	$H_{\text{corr}}(\text{B3LYP})$	$G_{\text{corr}}(\text{B3LYP})$
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1a	-1592.866688	0.443442	0.352987
PhCHO	-345.5734553	0.117453	0.079703
2aTS	-1938.425513	0.558175	0.452045
3a	-1938.437178	0.565147	0.456569
4a	-1591.654313	0.422861	0.332132
PhCH₂OH	-346.7706079	0.141674	0.102285
5a	-1938.461280	0.567266	0.459965
1b	-776.7296623	0.243579	0.180182
2bTS	-1122.291978	0.358672	0.279291
3b	-1122.304922	0.365663	0.284086
4b	-775.5187385	0.223215	0.160345
5b	-1122.326493	0.367479	0.286786
1c	-1543.656371	0.468216	0.374118
2cTS	-1889.213115	0.582464	0.472500
3c	-1889.225402	0.590044	0.478294
4c	-1542.442591	0.447773	0.354189
5c	-1889.251763	0.592119	0.481070
1d	-1016.328663	0.095967	0.037808
2dTS	-1361.893581	0.210767	0.135836
3d	-1361.909719	0.218287	0.142097
4d	-1015.120419	0.075654	0.018064
5d	-1361.932239	0.220171	0.144284
1e	-1573.002264	0.456790	0.366449
2eTS	-1918.541162	0.571892	0.466423
3e	-1918.544595	0.577816	0.469255
4e	-1571.772879	0.435873	0.346435
5e	-1918.565932	0.579358	0.472203
1f	-1612.300537	0.486444	0.393551
2fTS	-1957.834218	0.601768	0.492748
3f	-1957.839347	0.607687	0.495756
4f	-1611.068832	0.465397	0.373486
5f	-1957.859093	0.609182	0.498255
1g	-1804.044621	0.541718	0.439642
2gTS	-2149.577677	0.657015	0.541182
3g	-2149.580962	0.663058	0.544636
4g	-1802.809435	0.520988	0.420261
5g	-2149.605481	0.664140	0.545837

1h	-1672.161935	0.449022	0.357060
2hTS	-2017.708725	0.563156	0.455018
3h	-2017.720550	0.569955	0.459328
4h	-1670.944454	0.427681	0.336268
5h	-2017.743247	0.571601	0.461431
1i	-2052.458380	0.483206	0.390602
2iTS	-2398.023332	0.600117	0.491140
3i	-2398.036107	0.605477	0.493647
4i	-2051.252031	0.462786	0.370051
5i	-2398.059201	0.607125	0.498254
1j	-2514.556845	0.658908	0.543307
2jTS	-2860.116714	0.776029	0.646446
3j	-2860.129140	0.781120	0.648820
4j	-2513.352396	0.638494	0.522111
5j	-2860.153566	0.782891	0.650361
1k	-2288.365702	0.668693	0.557213
2kTS	-2633.927814	0.786916	0.662863
3k	-2633.944535	0.792128	0.661602
4k	-2287.166100	0.648202	0.536382
5k	-2633.965954	0.793040	0.667148
1l	-2648.131548	0.453998	0.353039
2lTS	-2993.686717	0.568045	0.450886
3l	-2993.697642	0.575623	0.456573
4l	-2646.910902	0.433285	0.330239
5l	-2993.720497	0.577647	0.458761
2i'TS	-2437.335131	0.629983	0.519679
3i'	-2437.350277	0.635382	0.522235
5i'	-2437.376826	0.636557	0.524280
2j'TS	-2899.426527	0.805339	0.673649
3j'	-2899.441801	0.810870	0.674506
5j'	-2899.466817	0.812423	0.676123
PhCOCH₃	-384.895995	0.147220	0.105870
PhCH(OH)CH₃(L/R)	-386.087174	0.170885	0.128001

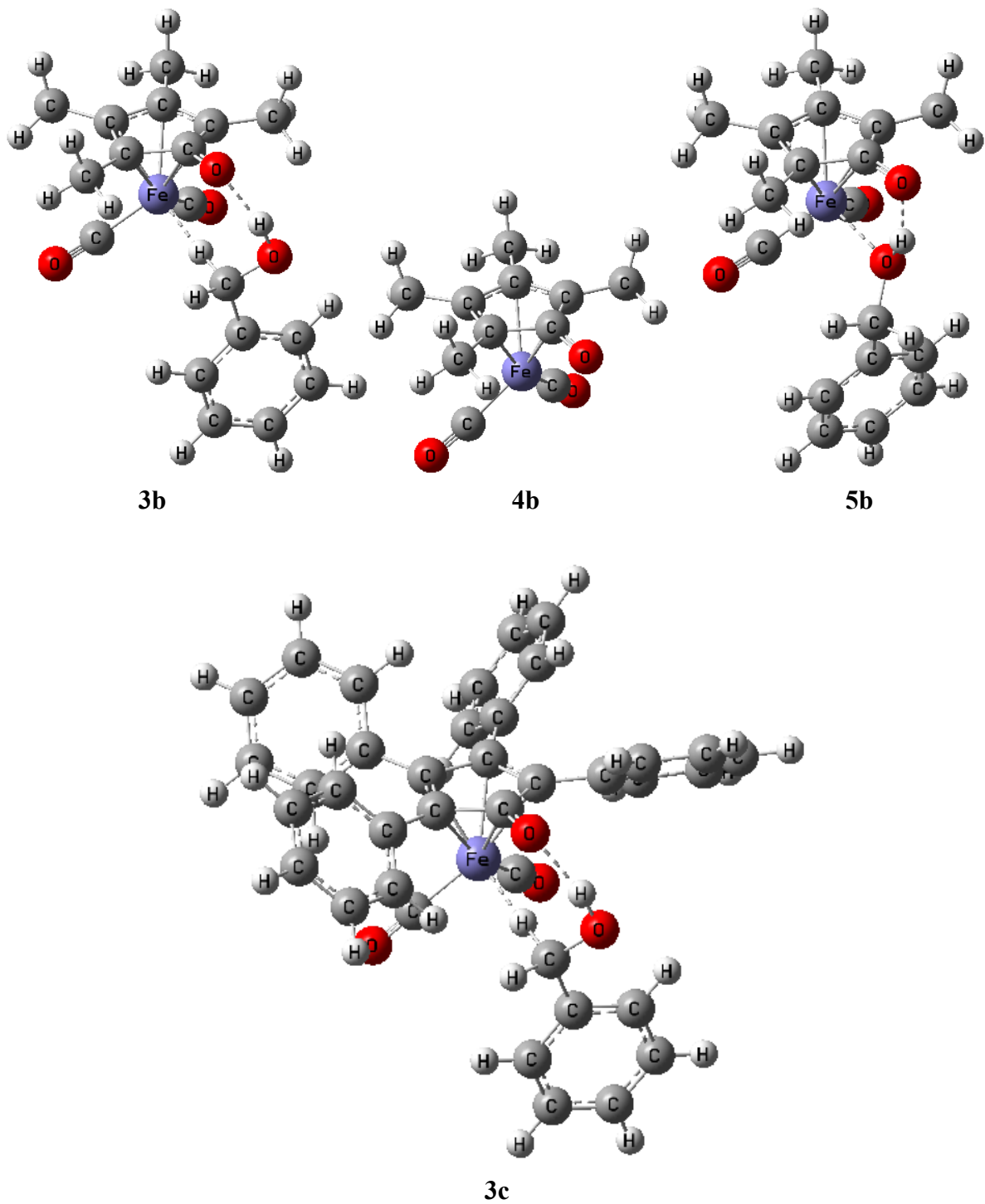
Table S4 Single-point energies^a obtained at the M06/6-311+G* level with SMD solvent model in toluene (Hartree)

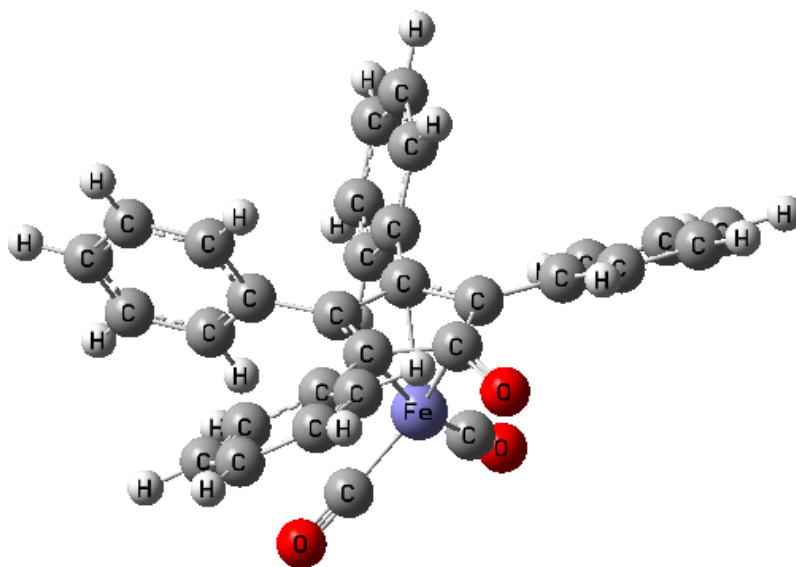
Complexes	<i>E</i>(M06) + ΔG(sol,M06)
1a	-2732.664422
PhCHO	-345.4120839
2aTS	-3078.069761
3a	-3078.085278
4a	-2731.452744
PhCH₂OH	-346.6063348
5a	-3078.107584
1b	-1916.677182
2bTS	-2262.082667
3b	-2262.101053
4b	-1915.467576
5b	-2262.121675
1c	-2683.200240
2cTS	-3028.604693
3c	-3028.620040
4c	-2681.987110
5c	-3028.643174
1d	-2156.406158
2dTS	-2501.811981
3d	-2501.833528
4d	-2155.201560
5d	-2501.856962
1e	-2712.790377
2eTS	-3058.179262
3e	-3058.183002
4e	-2711.559197
5e	-3058.203032
1f	-2752.064826
2fTS	-3097.449388
3f	-3097.454440
4f	-2750.832872
5f	-3097.471591
1g	-2943.710020
2gTS	-3289.092825

3g	-3289.096332
4g	-2942.474602
5g	-3289.118775
1h	-2811.950186
2hTS	-3157.346450
3h	-3157.362270
4h	-2810.732794
5h	-3157.383340
1i	-3192.292241
2iTS	-3537.708700
3i	-3537.723165
4i	-3191.088834
5i	-3537.742207
1j	-3654.142354
2jTS	-3999.557152
3j	-3999.571452
4j	-3652.938660
5j	-3999.586948
1k	-3428.061569
2kTS	-3773.475039
3k	-3773.494999
4k	-3426.866474
5k	-3773.511405
1l	-3787.991055
2lTS	-4133.390036
3l	-4133.407087
4l	-3786.769153
5l	-4133.425603
2i'TS	-3576.998459
3i'	-3577.015652
5i'	-3577.038645
2j'TS	-4038.847565
3j'	-4038.864096
5j'	-4038.881244
PhCOCH₃	-384.710495
PhCH(OH)CH₃(L/R)	-385.899833

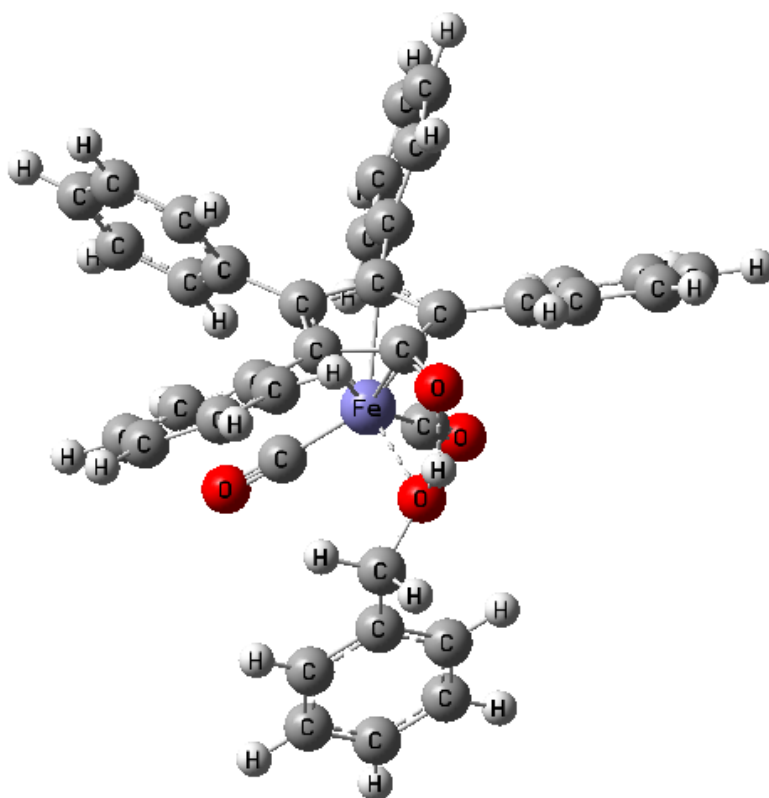
a. single-point calculations were performed at the B3LYP-optimized structures

Figure S2 All other related-structures were optimized at the theory level of B3LYP/LACVP* in gas.

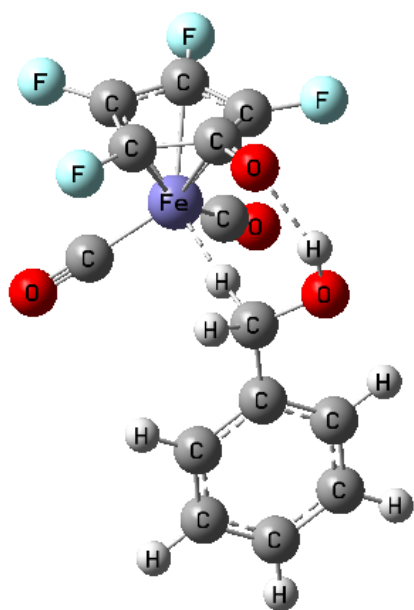




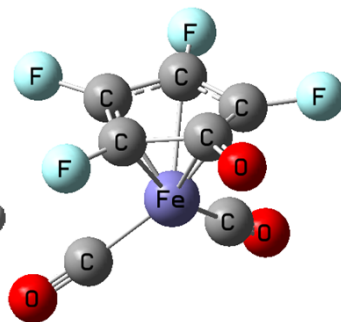
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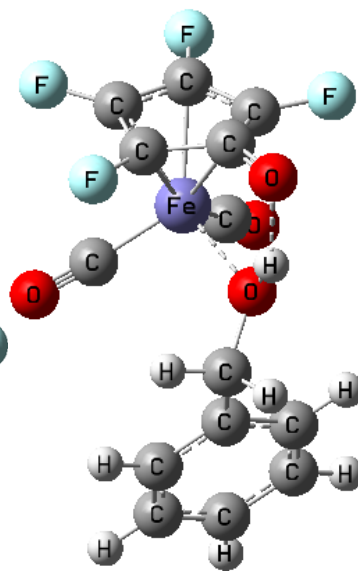
5c



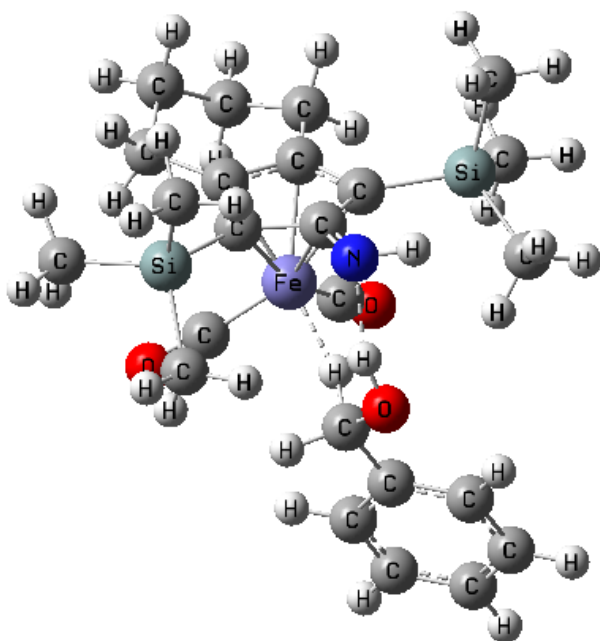
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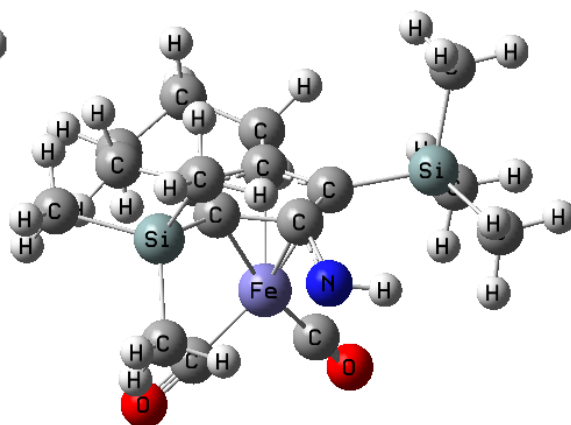
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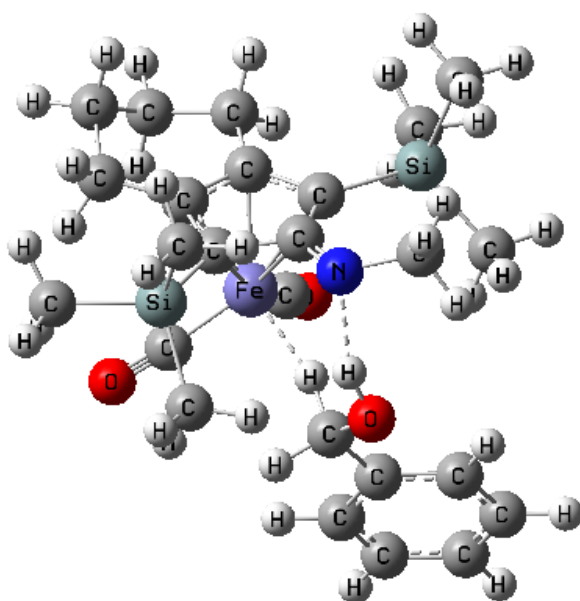
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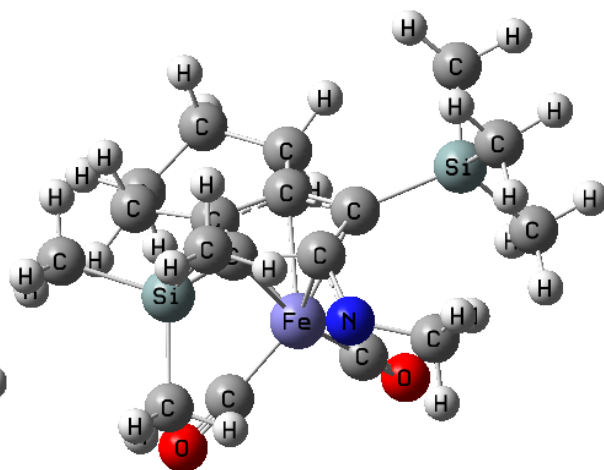
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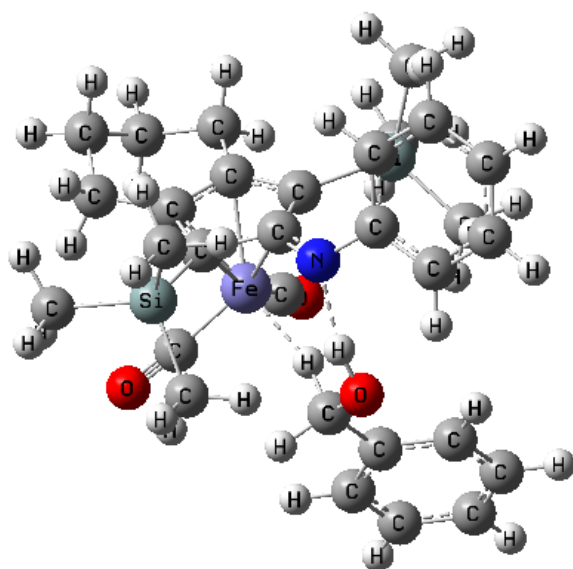
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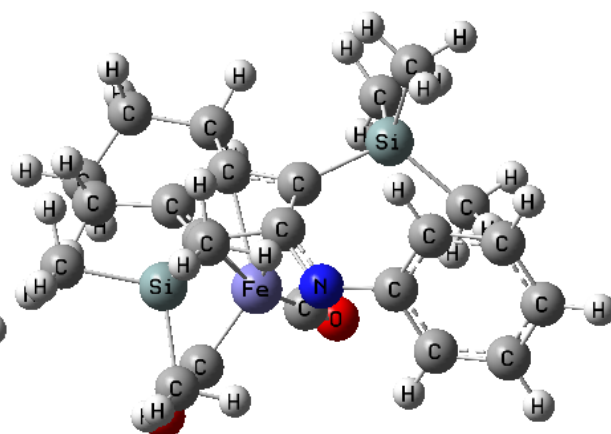
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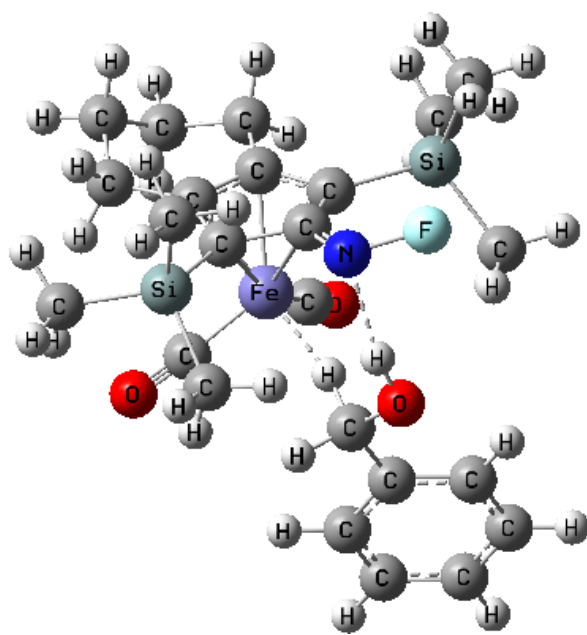
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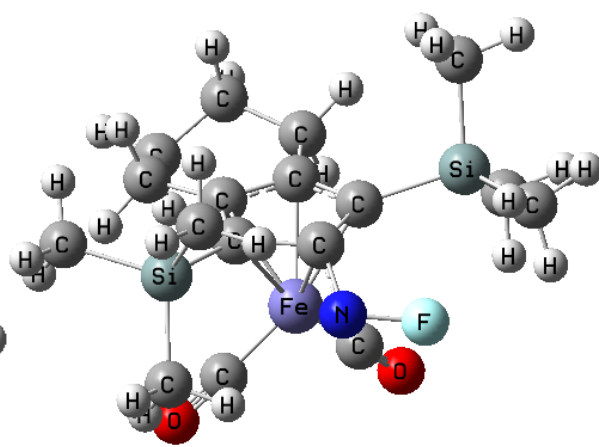
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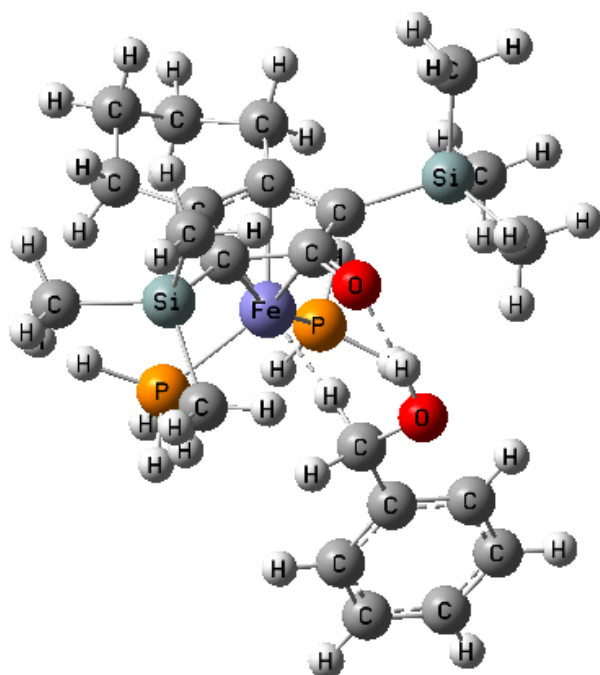
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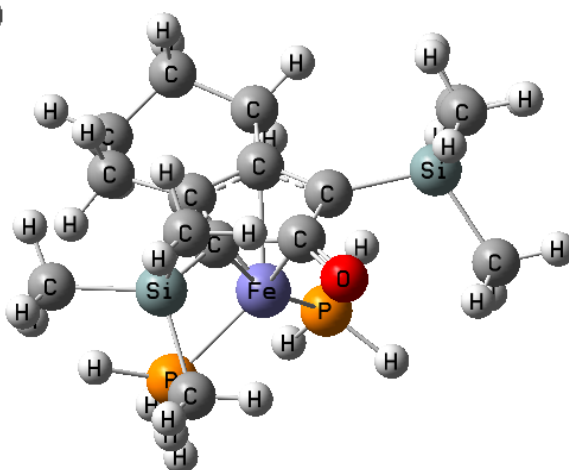
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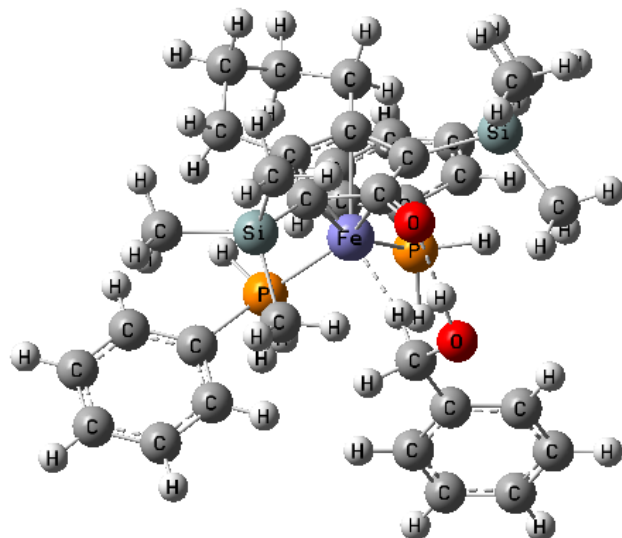
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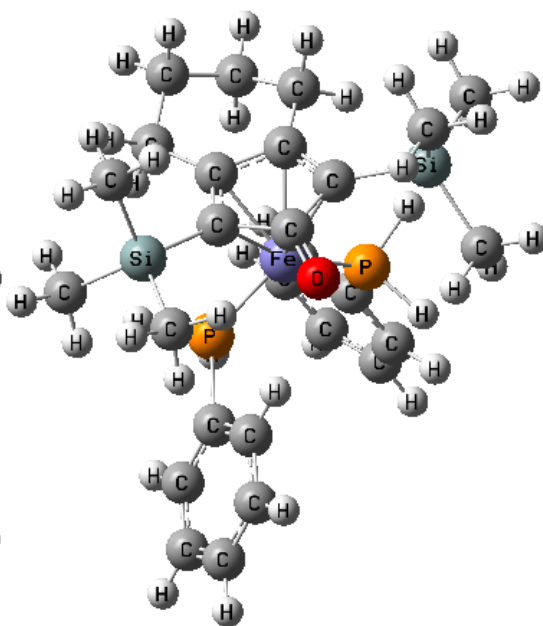
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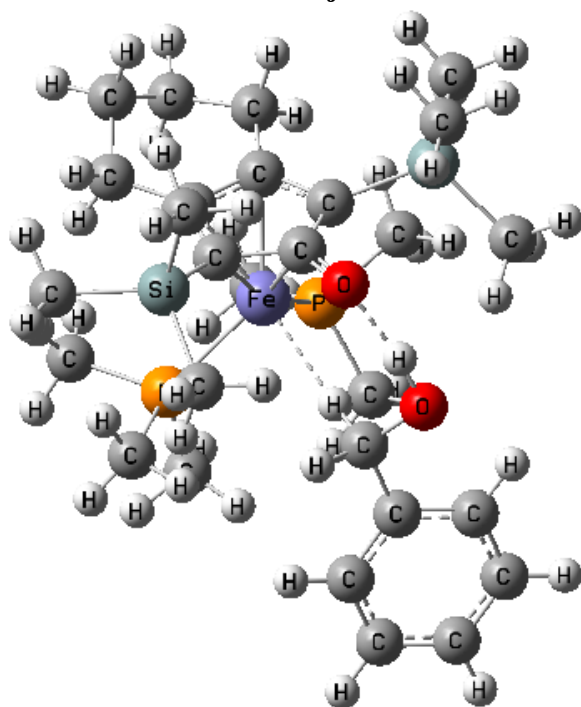
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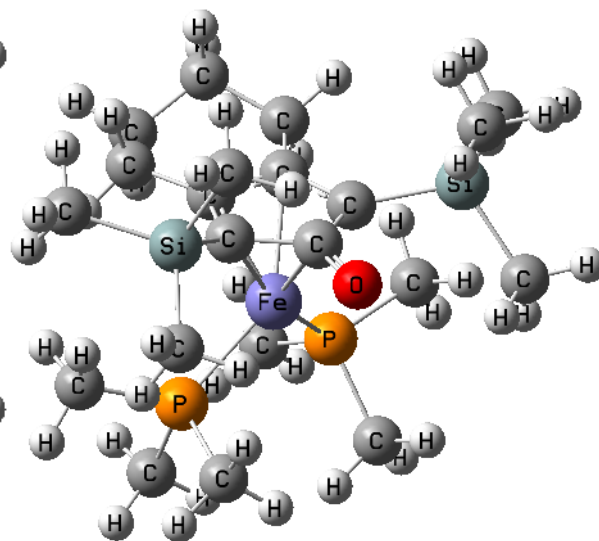
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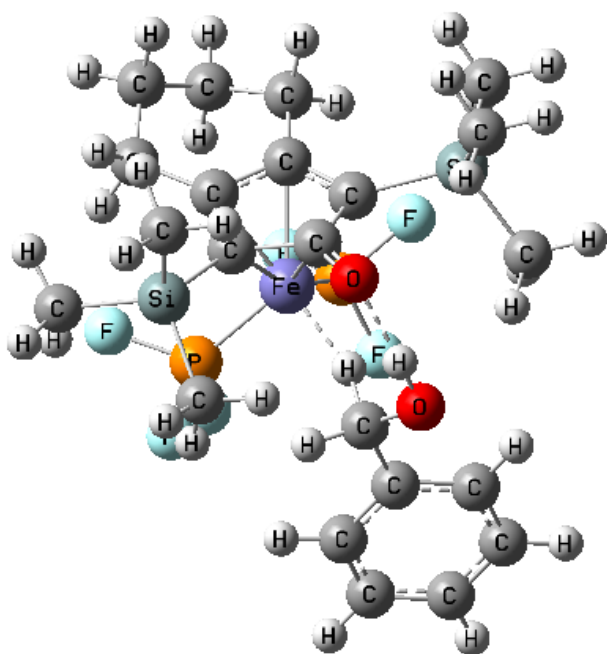
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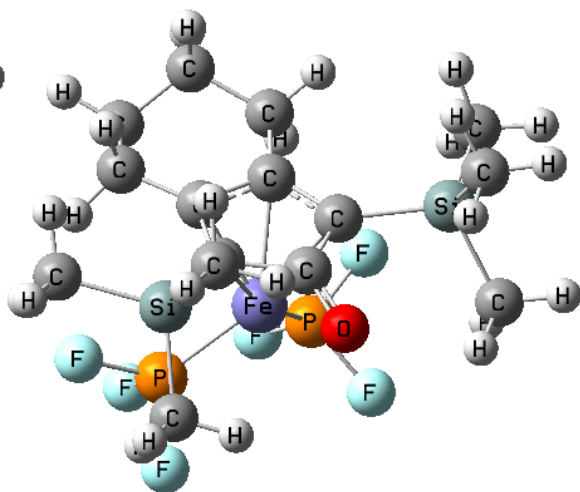
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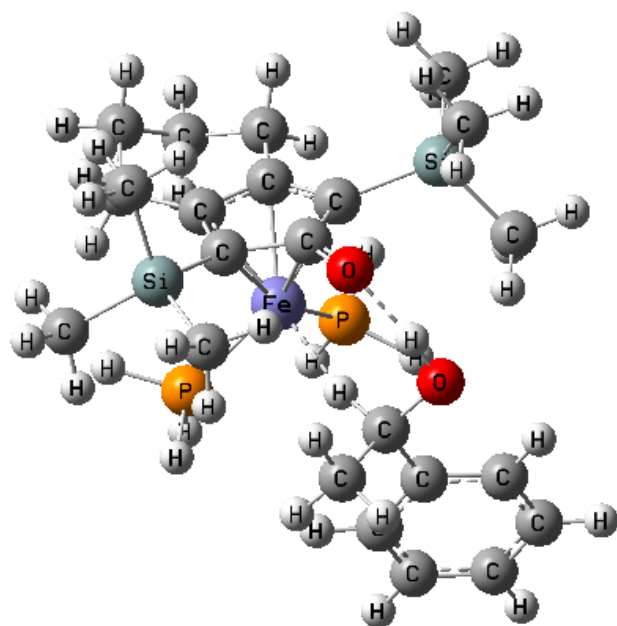
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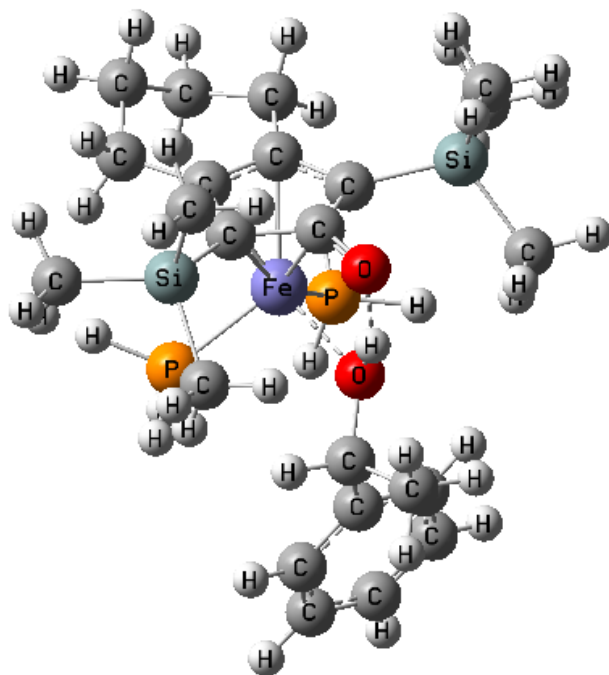
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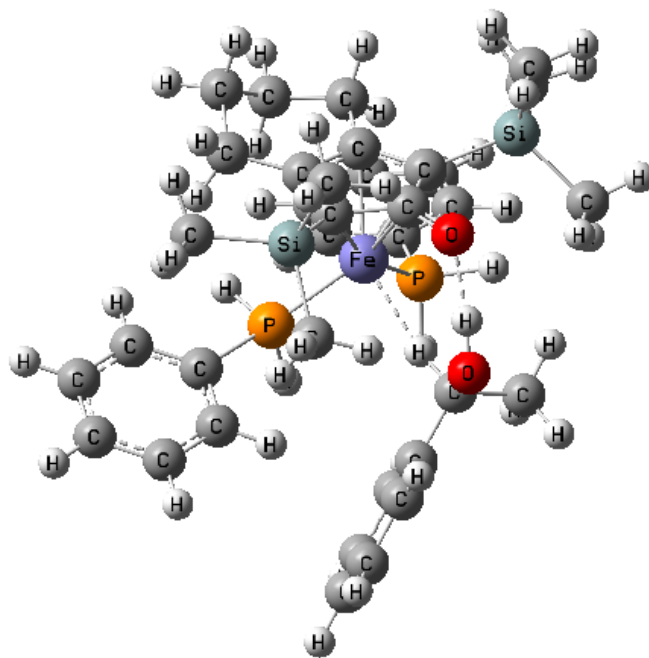
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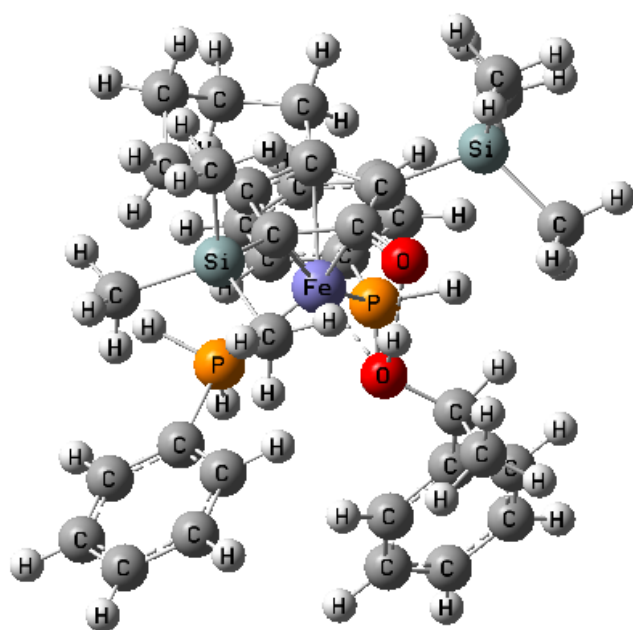
3i'



5i'



3j'



5j'

Cartesian Coordinates of B3LYP-Optimized Structures in Gas

1a

Fe	0.011628	0.480358	1.073896
C	0.013660	-1.254125	-0.206949
O	0.101225	-2.570743	0.129380
H	-0.689435	-2.825631	0.630274
C	-1.187448	-0.495530	-0.400170
C	-0.728075	0.802396	-0.886537
C	-1.562677	1.964374	-1.364838
H	-2.415667	2.135574	-0.701415
H	-1.983334	1.712860	-2.351301
C	-0.720308	3.244351	-1.489827
H	-1.301952	4.016912	-2.006561
H	-0.493103	3.631432	-0.487055
C	0.587395	2.966635	-2.242153
H	1.138840	3.898214	-2.415293
H	0.345184	2.555758	-3.232822
C	1.486843	1.971560	-1.484339
H	2.258764	1.590369	-2.163235
H	2.022341	2.490050	-0.680006
C	0.688585	0.808333	-0.934580
C	1.185001	-0.474490	-0.452760
Si	-2.943297	-1.193229	-0.322658
C	-3.347808	-1.953617	-2.010456
H	-3.328969	-1.197241	-2.804388
H	-4.346033	-2.409056	-2.010296
H	-2.624862	-2.732706	-2.280043
C	-4.238474	0.120326	0.096404
H	-4.342652	0.868394	-0.696692
H	-4.015677	0.645113	1.031268
H	-5.214970	-0.366626	0.214263
C	-3.042181	-2.556690	1.001518
H	-2.586025	-2.248918	1.950482
H	-2.594574	-3.508640	0.684807
H	-4.096385	-2.777688	1.210582
Si	2.947923	-1.169499	-0.319335
C	3.211749	-2.334771	-1.790844
H	4.214214	-2.780012	-1.765771
H	3.105458	-1.808708	-2.747391
H	2.481366	-3.151819	-1.775754
C	4.237218	0.218540	-0.377044

H	5.232864	-0.213749	-0.214101
H	4.073857	0.964300	0.408949
H	4.262634	0.739668	-1.340014
C	3.155830	-2.116678	1.301716
H	4.147746	-2.583909	1.347815
H	2.400111	-2.901766	1.396227
H	3.057243	-1.449500	2.165429
C	-1.243095	1.323974	1.961349
O	-2.083845	1.849446	2.557029
C	1.335835	1.240260	1.935358
O	2.224175	1.713025	2.504681
H	0.001189	-0.486700	2.234863

PhCHO

C	2.215023	-0.251734	0.000000
C	1.734889	1.060059	0.000000
C	0.360138	1.292141	0.000000
C	-0.535303	0.214855	0.000000
C	-0.047356	-1.101214	0.000000
C	1.324093	-1.331962	0.000000
H	3.286280	-0.434955	0.000000
H	2.429759	1.895082	0.000000
H	-0.026020	2.309485	0.000000
H	-0.761706	-1.918932	0.000000
H	1.705413	-2.349330	0.000000
C	-1.993588	0.470743	0.000000
H	-2.273069	1.548678	0.000000
O	-2.849826	-0.392555	0.000000

2aTS

Fe	-0.121288	-0.121565	-0.725476
C	-0.979226	0.248265	1.251073
O	-0.418509	-0.008164	2.417877
H	0.606854	-0.439283	2.343439
C	-0.829112	1.483051	0.513562
C	-1.655022	1.332925	-0.668131
C	-1.975867	2.357210	-1.728052
H	-1.084920	2.927989	-2.005730
H	-2.682424	3.084746	-1.300071
C	-2.614408	1.709719	-2.966525
H	-2.980216	2.492726	-3.640866

H	-1.854285	1.141526	-3.520348
C	-3.761298	0.777409	-2.557693
H	-4.280570	0.389547	-3.441649
H	-4.501617	1.357887	-1.988907
C	-3.267079	-0.402215	-1.697985
H	-4.119970	-0.861368	-1.185484
H	-2.850979	-1.185075	-2.342821
C	-2.251745	0.034692	-0.661856
C	-1.788960	-0.691795	0.500686
Si	0.045646	2.996928	1.267015
C	-0.853447	3.376657	2.887972
H	-1.904071	3.640088	2.714359
H	-0.381852	4.215882	3.414256
H	-0.828583	2.501333	3.545222
C	-0.074329	4.504437	0.122372
H	-1.108543	4.784085	-0.107429
H	0.457992	4.356404	-0.824439
H	0.391496	5.363080	0.622985
C	1.868127	2.628225	1.587487
H	2.425418	2.535625	0.647745
H	1.990832	1.692191	2.140791
H	2.326335	3.438293	2.169031
Si	-2.321839	-2.365389	1.228325
C	-3.459317	-1.982881	2.691823
H	-3.802632	-2.905231	3.176692
H	-4.346698	-1.419068	2.379401
H	-2.926996	-1.384598	3.439589
C	-3.250166	-3.410520	-0.053807
H	-3.436054	-4.406456	0.368309
H	-2.668103	-3.551194	-0.972255
H	-4.222757	-2.990068	-0.331429
C	-0.840737	-3.382714	1.816355
H	-1.195546	-4.248042	2.390894
H	-0.168488	-2.805935	2.458492
H	-0.261998	-3.771799	0.969716
C	0.996834	0.864453	-1.681681
O	1.702006	1.542635	-2.291044
C	-0.112400	-1.515102	-1.812010
O	-0.143951	-2.431822	-2.513330
H	1.162091	-0.722402	0.055069
C	1.987359	-1.354288	0.934199
H	1.558297	-2.354541	0.754308
O	1.824721	-0.845390	2.115110

C	3.314902	-1.170975	0.248124
C	3.624117	-1.932090	-0.887139
C	4.261411	-0.273649	0.755282
C	4.860302	-1.790870	-1.515943
H	2.894027	-2.639366	-1.276806
C	5.498790	-0.133572	0.126670
H	4.018102	0.293932	1.646612
C	5.799919	-0.887599	-1.010584
H	5.092991	-2.386539	-2.394590
H	6.231988	0.561497	0.527349
H	6.765021	-0.777426	-1.497941

3a

Fe	-0.152279	-0.180904	-0.691557
C	-1.066995	0.252545	1.368354
O	-0.597671	-0.032025	2.499914
H	1.078499	-0.286539	2.466348
C	-0.771145	1.455658	0.555148
C	-1.582538	1.348293	-0.625875
C	-1.841619	2.394248	-1.679969
H	-0.926833	2.946866	-1.919543
H	-2.539722	3.130551	-1.254024
C	-2.470208	1.789631	-2.945211
H	-2.784966	2.595685	-3.618040
H	-1.721146	1.196765	-3.487606
C	-3.668159	0.905215	-2.575809
H	-4.177173	0.546138	-3.477641
H	-4.398815	1.516024	-2.026750
C	-3.256730	-0.300988	-1.708412
H	-4.144428	-0.717374	-1.218415
H	-2.866748	-1.103010	-2.345725
C	-2.244236	0.071366	-0.644581
C	-1.851641	-0.670739	0.520869
Si	0.125273	3.009467	1.194222
C	0.839899	2.742002	2.918708
H	0.079263	2.386282	3.619932
H	1.243353	3.691109	3.295109
H	1.649374	2.006083	2.910097
C	-1.163815	4.402761	1.293713
H	-2.009542	4.113505	1.929392
H	-1.563296	4.685145	0.312935
H	-0.713536	5.301234	1.734514

C	1.522348	3.545728	0.031336
H	1.184388	3.742845	-0.992227
H	2.312639	2.788082	-0.018047
H	1.977268	4.470666	0.408787
Si	-2.436607	-2.337269	1.213166
C	-3.632724	-1.965543	2.632570
H	-3.985324	-2.890200	3.106274
H	-4.513568	-1.410636	2.287174
H	-3.131789	-1.361449	3.396991
C	-3.314953	-3.376714	-0.108867
H	-3.573015	-4.353902	0.319201
H	-2.678035	-3.563067	-0.981433
H	-4.247108	-2.922084	-0.461774
C	-0.970478	-3.338886	1.865162
H	-1.324508	-4.244980	2.372959
H	-0.391443	-2.750559	2.583367
H	-0.302226	-3.657748	1.055732
C	0.912339	0.689385	-1.824570
O	1.544516	1.266589	-2.595702
C	-0.213161	-1.648448	-1.691259
O	-0.310785	-2.594939	-2.344624
H	1.276517	-0.717151	0.235345
C	2.027699	-1.151984	1.007701
O	2.019543	-0.397891	2.160774
C	3.371217	-1.142227	0.322857
C	3.690762	-2.151733	-0.594009
C	4.298561	-0.124521	0.573067
C	4.916277	-2.140790	-1.260093
H	2.980113	-2.954475	-0.782250
C	5.526707	-0.116778	-0.090269
H	4.055062	0.642845	1.299771
C	5.837485	-1.120590	-1.010275
H	5.154584	-2.931270	-1.966672
H	6.243794	0.673850	0.114547
H	6.794489	-1.112347	-1.525036
H	1.667640	-2.179367	1.159129

4a

Fe	6.284889	6.683393	2.492152
Si	6.587793	3.113750	2.855298
Si	9.464365	8.217173	3.233097
O	8.281594	5.429459	4.353981

O	5.682448	9.546220	2.314741
O	3.546752	5.764850	1.982902
C	8.088054	5.628234	3.137739
C	7.226066	4.797166	2.255663
C	7.183665	5.457118	0.993514
C	6.580742	4.965618	-0.304785
H	5.486297	4.978153	-0.237682
H	6.857567	3.914932	-0.447432
C	7.038706	5.796693	-1.518175
H	8.059737	5.501831	-1.799414
H	6.399175	5.565745	-2.377812
C	7.022789	7.300452	-1.217629
H	6.011144	7.608665	-0.919975
H	7.277082	7.873078	-2.117019
C	8.018497	7.639816	-0.097552
H	9.043609	7.518725	-0.481290
H	7.929100	8.688244	0.200372
C	7.865202	6.729557	1.093264
C	8.385062	6.890079	2.413430
C	5.692793	3.329494	4.505749
H	4.770765	3.913244	4.395844
H	6.341004	3.844667	5.221002
H	5.417619	2.353478	4.925022
C	8.092872	1.986792	3.073536
H	8.795784	2.424132	3.791184
H	8.626722	1.835484	2.127447
H	7.794893	1.000108	3.449468
C	5.391073	2.337412	1.604509
H	4.989308	1.406163	2.024199
H	5.874023	2.081811	0.654656
H	4.536915	2.988732	1.386019
C	11.165918	7.439560	3.522031
H	11.838694	8.140850	4.031232
H	11.642786	7.145625	2.579018
H	11.072746	6.544554	4.146882
C	8.699672	8.733450	4.882532
H	8.522776	7.851552	5.505982
H	7.744420	9.254112	4.744390
H	9.370685	9.411909	5.424276
C	9.655516	9.748226	2.130462
H	10.302000	10.475401	2.638483
H	8.698748	10.247711	1.937345
H	10.121244	9.517896	1.165563

C	5.893493	8.416327	2.423101
C	4.609752	6.142852	2.228518

PhCH₂OH

C	-0.282174	-2.319161	0.009496
C	0.020988	-1.559865	1.142001
C	0.086481	-0.168970	1.057553
C	-0.146206	0.481529	-0.161070
C	-0.440753	-0.287564	-1.292711
C	-0.514192	-1.679027	-1.209095
H	-0.333053	-3.402763	0.075413
H	0.205137	-2.052163	2.093574
H	0.325278	0.426489	1.934141
H	-0.611598	0.206241	-2.247460
H	-0.742935	-2.262758	-2.097051
C	-0.100716	1.995769	-0.242421
H	0.057410	2.305856	-1.288040
H	-1.060443	2.422757	0.072935
O	0.860378	2.586391	0.624861
H	1.721285	2.194212	0.407875

5a

Fe	0.076976	-0.071253	0.460334
Si	-2.174218	-2.568772	-1.106429
Si	-0.767434	3.126947	-1.104772
O	-1.033871	0.206766	-2.453448
O	1.250258	-0.206298	-1.237097
H	0.573031	-0.146527	-1.976030
O	1.797786	1.779172	1.952731
O	0.842048	-2.486218	1.935497
C	-1.386671	0.270073	-1.235867
C	-1.741975	-0.874744	-0.379350
C	-1.986115	-0.342216	0.938707
C	-2.615601	-1.041534	2.126923
H	-1.917904	-1.763613	2.567210
H	-3.469945	-1.631303	1.774578
C	-3.089042	-0.045540	3.202781
H	-4.036698	0.411577	2.883841
H	-3.299904	-0.586278	4.132773
C	-2.062528	1.068308	3.442604
H	-1.101382	0.627899	3.742316

H	-2.385907	1.716119	4.265856
C	-1.871496	1.911229	2.172112
H	-2.779199	2.509865	1.999437
H	-1.056817	2.629468	2.301735
C	-1.648829	1.049096	0.954074
C	-1.200442	1.440044	-0.359380
C	-0.925317	-3.090757	-2.426728
H	0.045757	-3.351851	-1.989415
H	-0.777229	-2.282116	-3.148057
H	-1.290268	-3.975522	-2.963464
C	-3.886193	-2.407609	-1.904963
H	-3.870313	-1.649709	-2.696667
H	-4.648677	-2.111026	-1.174255
H	-4.206008	-3.356623	-2.353408
C	-2.229373	-3.921340	0.224374
H	-2.379895	-4.894993	-0.259633
H	-3.049262	-3.783894	0.937469
H	-1.295217	-3.981328	0.794606
C	-2.163862	3.578220	-2.301810
H	-1.959997	4.527293	-2.813297
H	-3.126263	3.677689	-1.784964
H	-2.267711	2.795763	-3.061326
C	0.872935	3.059181	-2.043999
H	0.829925	2.311660	-2.841864
H	1.704621	2.800301	-1.379164
H	1.092217	4.034141	-2.497571
C	-0.624473	4.469481	0.229465
H	-0.383962	5.426649	-0.250982
H	0.175990	4.257894	0.948452
H	-1.555509	4.611689	0.789543
C	2.265995	-1.185879	-1.523119
H	2.484264	-1.116645	-2.596345
H	1.888197	-2.194278	-1.318471
C	3.506632	-0.910585	-0.711580
C	4.151204	0.331729	-0.804726
H	3.738175	1.099588	-1.453642
C	5.306430	0.585018	-0.067460
H	5.796355	1.551847	-0.145681
C	5.836851	-0.403150	0.768113
H	6.738740	-0.205310	1.341059
C	5.204599	-1.642990	0.863409
H	5.609507	-2.414867	1.512244
C	4.042474	-1.892433	0.128736

H	3.547278	-2.857249	0.211535
C	1.156754	1.030332	1.355495
C	0.582375	-1.533196	1.336898

1b

Fe	0.008464	0.455100	1.070944
C	0.018217	-1.262762	-0.252960
O	0.106998	-2.581986	0.056849
H	-0.694429	-2.850897	0.533266
C	-1.163400	-0.479256	-0.417548
C	-0.732620	0.829505	-0.874018
C	0.689264	0.847044	-0.902685
C	1.165901	-0.456055	-0.475293
C	-1.240532	1.321932	1.947804
O	-2.090682	1.855848	2.521229
C	1.365280	1.096083	1.984634
O	2.279345	1.476793	2.580342
H	-0.090326	-0.548236	2.198303
C	-2.571827	-0.995779	-0.343335
H	-3.274334	-0.213252	-0.042185
H	-2.904479	-1.387749	-1.313987
H	-2.669704	-1.804687	0.390556
C	2.583043	-0.947613	-0.438756
H	2.674674	-1.797345	0.243001
H	2.906282	-1.281023	-1.434037
H	3.276721	-0.167957	-0.109711
C	1.562376	1.970037	-1.384806
H	1.778069	1.863579	-2.456890
H	1.086248	2.943805	-1.238229
H	2.521987	1.988164	-0.859281
C	-1.648050	1.934908	-1.318629
H	-1.189589	2.917849	-1.178273
H	-1.891421	1.830312	-2.384682
H	-2.592035	1.928012	-0.765386

2bTS

Fe	-0.169035	-0.199534	-0.764923
C	-1.044937	0.072049	1.260910
O	-0.518579	-0.318426	2.393455
H	0.607761	-0.241274	2.371349
C	-0.803112	1.318266	0.569219

C	-1.625065	1.319168	-0.616517
C	-2.264653	0.043697	-0.722442
C	-1.862768	-0.753952	0.413117
H	1.136262	-0.711415	0.047090
C	2.014436	-1.044589	1.041653
H	1.619703	-2.071177	1.153036
O	1.862461	-0.242278	2.049471
C	3.308531	-0.992502	0.281009
C	3.645390	-2.025595	-0.603000
C	4.196462	0.072816	0.469254
C	4.854375	-1.992755	-1.296483
H	2.958477	-2.857833	-0.745374
C	5.405650	0.105410	-0.224976
H	3.931965	0.854088	1.174160
C	5.736263	-0.924453	-1.109945
H	5.110461	-2.799459	-1.978026
H	6.094048	0.932412	-0.072230
H	6.679760	-0.898142	-1.648604
C	-2.349821	-2.119910	0.795504
H	-3.345381	-2.063631	1.255915
H	-2.420427	-2.794476	-0.063743
H	-1.672250	-2.560269	1.532174
C	-3.280455	-0.357962	-1.752929
H	-3.118747	0.153612	-2.706056
H	-3.257491	-1.435277	-1.942664
H	-4.293485	-0.107602	-1.409136
C	-1.841166	2.491487	-1.529953
H	-2.680443	3.101751	-1.169891
H	-0.961444	3.139735	-1.573655
H	-2.075971	2.174331	-2.549937
C	-0.001951	2.453641	1.135571
H	-0.602264	3.033737	1.849257
H	0.874224	2.073463	1.668280
H	0.342934	3.138826	0.355029
C	0.917417	0.761257	-1.786185
C	-0.163892	-1.649579	-1.780775
O	1.604640	1.418456	-2.437735
O	-0.200441	-2.608063	-2.422998

3b

Fe	-0.161185	-0.098850	-0.752871
C	-1.067122	0.238871	1.354773

O	-0.568519	-0.032559	2.472429
H	1.133426	0.013272	2.427516
C	-0.831866	1.444353	0.540774
C	-1.653599	1.361564	-0.628056
C	-2.239771	0.046457	-0.676071
C	-1.796621	-0.683548	0.475475
H	1.272073	-0.591823	0.183813
C	2.014885	-0.944353	1.007779
O	2.049859	-0.036930	2.043679
C	3.347434	-1.083867	0.317296
C	3.598682	-2.199544	-0.491587
C	4.333081	-0.100324	0.454826
C	4.815473	-2.328313	-1.160760
H	2.840532	-2.973773	-0.594317
C	5.552226	-0.232047	-0.212143
H	4.140243	0.753054	1.095711
C	5.795956	-1.342391	-1.023160
H	5.000354	-3.199816	-1.783038
H	6.314327	0.534036	-0.095685
H	6.746049	-1.442682	-1.541048
H	1.610914	-1.923177	1.306295
C	-3.246449	-0.428219	-1.683436
H	-4.261271	-0.163209	-1.356166
H	-3.086791	0.022837	-2.667036
H	-3.215351	-1.515345	-1.800375
C	-1.938814	2.478046	-1.590242
H	-2.813736	3.049707	-1.251926
H	-1.099932	3.175997	-1.660482
H	-2.154393	2.105672	-2.595780
C	-0.061889	2.627887	1.046054
H	0.267042	3.284318	0.234236
H	-0.673476	3.225527	1.735499
H	0.821912	2.293442	1.596814
C	-2.221066	-2.054060	0.911980
H	-1.525447	-2.428986	1.668673
H	-3.218264	-2.028004	1.372369
H	-2.258031	-2.768836	0.083225
C	0.872669	0.889432	-1.818231
C	-0.157871	-1.547646	-1.785833
O	1.491079	1.572158	-2.511069
O	-0.224578	-2.490994	-2.447189

4b

Fe	0.021560	0.358452	1.023473
C			
	0.001746	-1.313828	-0.273620
O	0.015001	-2.386997	0.364763
C	-1.184131	-0.460493	-0.485440
C	-0.737049	0.820239	-0.908875
C	0.709972	0.822849	-0.934451
C	1.176348	-0.456173	-0.527068
C	-1.284352	1.112091	1.969206
O	-2.161210	1.631013	2.511167
C	1.356824	1.117888	1.922417
O	2.250000	1.640834	2.432960
C	-2.585702	-0.969520	-0.346079
H	-3.267172	-0.228454	0.084886
H	-2.991488	-1.265785	-1.322890
H	-2.582000	-1.857530	0.293077
C	2.583765	-0.960143	-0.437056
H	2.605694	-1.848041	0.201889
H	2.956019	-1.255140	-1.427511
H	3.277309	-0.216565	-0.030361
C	1.564519	1.969207	-1.388671
H	1.688437	1.940661	-2.479920
H	1.121573	2.935472	-1.130858
H	2.562907	1.923457	-0.944404
C	-1.611241	1.963436	-1.332649
H	-1.162915	2.931336	-1.090757
H	-1.773625	1.934226	-2.418824
H	-2.593103	1.914213	-0.853304

5b

Fe	0.096622	0.004913	0.477123
O	0.940212	-0.779189	-2.441186
O	1.322426	2.025906	2.213132
O	-1.008560	-1.721985	2.580912
C	0.045497	-0.156944	-1.799020
C	-1.098359	-0.758861	-1.105598
C	-1.801496	0.277521	-0.402747
C	-1.037268	1.486505	-0.505356
C	0.142445	1.208335	-1.279061
C	0.867110	1.191849	1.556994
C	-0.537131	-1.047487	1.773900

C	3.085312	-0.962656	0.432161
H	3.345944	0.096427	0.311377
H	3.738833	-1.549352	-0.226802
O	1.732627	-1.194924	-0.002104
H	1.690043	-1.204775	-1.009031
C	1.196227	2.176883	-1.727152
H	0.834589	2.796414	-2.559474
H	1.519535	2.853461	-0.928729
H	2.065374	1.620378	-2.091577
C	-1.459370	2.839182	-0.007151
H	-0.596574	3.471841	0.221072
H	-2.050354	3.356836	-0.775086
H	-2.074895	2.769521	0.894327
C	-3.158864	0.145241	0.226603
H	-3.940435	0.354649	-0.516546
H	-3.331749	-0.866854	0.604086
H	-3.296007	0.843508	1.057323
C	-1.538805	-2.172798	-1.339505
H	-2.305436	-2.222085	-2.125146
H	-0.684433	-2.765188	-1.680218
H	-1.953846	-2.641170	-0.440841
C	3.262524	-1.394303	1.866683
C	2.852678	-2.671485	2.276123
C	3.862381	-0.542099	2.799862
C	3.037750	-3.083736	3.594638
H	2.380174	-3.335100	1.557092
C	4.056730	-0.956890	4.119772
H	4.176109	0.453578	2.494859
C	3.642995	-2.227666	4.519924
H	2.711955	-4.074018	3.901579
H	4.522938	-0.283663	4.834077
H	3.788347	-2.550646	5.547286

1c

O	2.215635	-0.380528	3.324836
C	-0.016232	-1.795017	-0.359473
C	-1.183050	-0.970618	-0.277385
C	-0.722028	0.408174	-0.273015
C	0.708129	0.399611	-0.276212
C	1.158994	-0.990215	-0.320298
C	-2.569146	-1.477430	-0.422821
C	-2.844325	-2.444639	-1.408622

H	-2.043334	-2.793662	-2.055019
C	-4.137428	-2.940843	-1.587186
H	-4.324650	-3.687073	-2.354758
C	-5.183138	-2.471807	-0.792858
H	-6.190318	-2.855497	-0.930119
C	-4.925843	-1.501089	0.179199
H	-5.733937	-1.126879	0.801832
C	-3.634994	-1.011226	0.365455
H	-3.451445	-0.264625	1.129692
C	-1.592927	1.599542	-0.447471
C	-2.413359	1.669927	-1.586021
H	-2.416502	0.845582	-2.293169
C	-3.217562	2.784867	-1.818784
H	-3.843875	2.819871	-2.706191
C	-3.218156	3.850135	-0.916343
C	-2.408698	3.790924	0.219166
H	-2.405344	4.612303	0.930660
C	-1.604151	2.675228	0.452352
H	-0.986532	2.632338	1.342700
C	1.573005	1.593026	-0.479854
C	2.121306	1.815607	-1.753336
H	1.916939	1.106765	-2.551081
C	2.921397	2.930366	-2.000775
H	3.335825	3.085803	-2.993264
C	3.189739	3.842321	-0.977643
C	2.654370	3.629710	0.293378
H	2.862387	4.330284	1.097763
C	1.853928	2.512936	0.540132
H	1.452039	2.341153	1.534080
C	2.550740	-1.477162	-0.473835
C	2.813406	-2.602150	-1.275752
H	1.991212	-3.126196	-1.749099
C	4.118638	-3.054715	-1.466284
H	4.295914	-3.927429	-2.089404
C	5.189757	-2.393196	-0.864736
H	6.206476	-2.747605	-1.011834
C	4.942712	-1.271707	-0.070534
H	5.766649	-0.747129	0.405795
C	3.639645	-0.817207	0.122178
H	3.469852	0.054834	0.742668
C	1.337253	-0.431717	2.578033
Fe	-0.011489	-0.577349	1.459075
C	-1.185112	0.040818	2.606378

O	-1.966555	0.407427	3.374693
H	-0.228249	-1.879389	2.184816
O	0.004555	-3.147395	-0.444740
H	-0.872635	-3.481832	-0.188134
H	-3.846756	4.718302	-1.095180
H	3.814680	4.710420	-1.169248

2cTS

Fe	0.156577	-0.457395	-0.557653
C	-0.115340	-0.549447	1.645585
O	0.538389	-1.320448	2.467484
H	1.644810	-1.463355	2.138622
C	0.279888	0.773045	1.186191
C	-0.767817	1.256163	0.315124
C	-1.737838	0.208592	0.140292
C	-1.310335	-0.933078	0.931506
H	1.493345	-1.304453	-0.258360
C	2.519766	-2.051823	0.345379
H	1.965051	-3.002756	0.251030
O	2.727036	-1.593865	1.536054
C	3.599616	-1.883319	-0.676229
C	3.607055	-2.682901	-1.826522
C	4.615662	-0.939254	-0.478951
C	4.620889	-2.541780	-2.773445
H	2.819409	-3.418778	-1.976901
C	5.627300	-0.799171	-1.427382
H	4.600060	-0.334470	0.421796
C	5.631822	-1.597649	-2.575255
H	4.624609	-3.167989	-3.661392
H	6.416600	-0.068705	-1.271188
H	6.423122	-1.486788	-3.311865
C	1.101607	0.450136	-1.755477
C	-0.325508	-1.716874	-1.704639
O	1.716637	1.034535	-2.534858
O	-0.608569	-2.568493	-2.429748
C	1.446597	1.518892	1.717345
C	2.234335	2.361863	0.914579
C	1.766050	1.407748	3.082339
C	3.304411	3.069931	1.458615
H	2.012358	2.465441	-0.141636
C	2.837092	2.118082	3.624317
H	1.178074	0.751228	3.714026

C	3.611146	2.951771	2.816340
H	3.900735	3.713941	0.817646
H	3.066684	2.015189	4.681540
H	4.447327	3.502647	3.238697
C	-0.895909	2.638411	-0.216034
C	-0.785834	3.724200	0.668660
C	-1.183988	2.897646	-1.565335
C	-0.955317	5.032251	0.214362
H	-0.566835	3.540765	1.715899
C	-1.347955	4.205679	-2.018678
H	-1.280046	2.069592	-2.260230
C	-1.233832	5.278024	-1.131144
H	-0.866415	5.858659	0.914282
H	-1.564292	4.386191	-3.068096
H	-1.360241	6.297189	-1.486228
C	-3.057956	0.373167	-0.527886
C	-3.529725	-0.509682	-1.511532
C	-3.898513	1.422117	-0.115790
C	-4.795784	-0.342964	-2.072554
H	-2.907699	-1.333055	-1.842771
C	-5.165687	1.586772	-0.674891
H	-3.554652	2.112223	0.648410
C	-5.618840	0.705816	-1.658068
H	-5.137649	-1.036675	-2.835903
H	-5.797081	2.405567	-0.340554
H	-6.604552	0.834565	-2.096891
C	-2.057143	-2.187330	1.195294
C	-1.396826	-3.426346	1.234969
C	-3.432416	-2.154513	1.478644
C	-2.092731	-4.597625	1.527863
H	-0.330158	-3.465886	1.043147
C	-4.128211	-3.327727	1.772055
H	-3.960005	-1.206674	1.476536
C	-3.463178	-4.554165	1.793739
H	-1.562377	-5.545978	1.549897
H	-5.192399	-3.279271	1.987252
H	-4.006058	-5.467874	2.020438

3c

Fe	0.241786	-0.368074	-0.506798
C	-0.076375	-0.386747	1.776850
O	0.631472	-0.957269	2.637297

H	2.293115	-1.006544	2.164485
C	0.139096	0.954267	1.184560
C	-0.937933	1.210380	0.270247
C	-1.729757	0.005212	0.136148
C	-1.146166	-1.010782	0.978475
H	1.798230	-1.129832	-0.078351
C	2.711624	-1.677718	0.404928
O	3.084244	-1.047138	1.566232
C	3.799794	-1.657725	-0.635822
C	3.805603	-2.615266	-1.658004
C	4.795868	-0.674437	-0.608161
C	4.790791	-2.588731	-2.645414
H	3.040291	-3.388893	-1.677380
C	5.783039	-0.651837	-1.594047
H	4.793215	0.055419	0.194246
C	5.782167	-1.605055	-2.615395
H	4.788446	-3.338904	-3.431603
H	6.556465	0.111075	-1.563459
H	6.552852	-1.585096	-3.381319
H	2.325882	-2.697347	0.560993
C	1.113407	0.651282	-1.687708
C	-0.085952	-1.649363	-1.699802
O	1.647179	1.314080	-2.463121
O	-0.282534	-2.493260	-2.460167
C	-1.696304	-2.346262	1.312688
C	-0.840572	-3.447619	1.480373
C	-3.068730	-2.528531	1.553686
C	-1.341257	-4.695410	1.847599
H	0.225728	-3.317695	1.333916
C	-3.569430	-3.777371	1.922078
H	-3.747662	-1.687682	1.461340
C	-2.709777	-4.867461	2.065397
H	-0.659666	-5.533306	1.968405
H	-4.634757	-3.894564	2.102720
H	-3.101016	-5.840039	2.351748
C	-3.045125	-0.065087	-0.558109
C	-3.382220	-1.094801	-1.451162
C	-4.025042	0.895074	-0.249361
C	-4.649144	-1.151110	-2.030754
H	-2.657429	-1.862234	-1.692908
C	-5.294491	0.833822	-0.824015
H	-3.791172	1.692899	0.447919
C	-5.610484	-0.187099	-1.721447

H	-4.884186	-1.954531	-2.723503
H	-6.034862	1.587061	-0.568747
H	-6.597525	-0.233235	-2.173463
C	1.166454	1.902814	1.675699
C	1.533384	1.877691	3.034391
C	1.776576	2.857189	0.841048
C	2.472674	2.778573	3.536564
H	1.086260	1.140976	3.690902
C	2.716106	3.753412	1.345722
H	1.516849	2.903680	-0.210220
C	3.069002	3.719642	2.696962
H	2.739088	2.739881	4.589501
H	3.174821	4.478729	0.678876
H	3.803529	4.418115	3.088935
C	-1.283755	2.521129	-0.339586
C	-1.402754	3.648502	0.490484
C	-1.556674	2.662212	-1.709218
C	-1.782894	4.882521	-0.036913
H	-1.196669	3.555044	1.552154
C	-1.928757	3.898281	-2.235898
H	-1.477159	1.798925	-2.362115
C	-2.043389	5.012925	-1.402307
H	-1.871022	5.742680	0.621121
H	-2.129638	3.989118	-3.299842
H	-2.332934	5.975816	-1.814203

4c

O	-0.000219	-3.031030	-0.221809
O	2.161291	-0.309389	3.228497
C	-0.000078	-1.811820	-0.504563
C	-1.193276	-0.935946	-0.444411
C	-0.726468	0.406791	-0.316433
C	0.726474	0.406692	-0.316145
C	1.193248	-0.936045	-0.444208
C	-2.578559	-1.439356	-0.542060
C	-2.825707	-2.640209	-1.234054
H	-1.993615	-3.193493	-1.652434
C	-4.123062	-3.130863	-1.370393
H	-4.288976	-4.059917	-1.909216
C	-5.201853	-2.437941	-0.818765
H	-6.212759	-2.822431	-0.924457
C	-4.970423	-1.247809	-0.125505

H	-5.800491	-0.701679	0.314627
C	-3.675379	-0.753132	0.012544
H	-3.517691	0.169181	0.559630
C	-1.552554	1.639951	-0.401675
C	-2.190453	1.929754	-1.618798
H	-2.087123	1.240890	-2.452456
C	-2.952534	3.088338	-1.762379
H	-3.437257	3.298218	-2.711917
C	-3.096142	3.971835	-0.690348
C	-2.471398	3.689160	0.525133
H	-2.582458	4.367053	1.367034
C	-1.703222	2.532615	0.668250
H	-1.230792	2.311418	1.619679
C	1.552655	1.639786	-0.401626
C	2.190303	1.929346	-1.618975
H	2.086518	1.240438	-2.452528
C	2.952690	3.087662	-1.762835
H	3.437179	3.297371	-2.712529
C	3.096937	3.971164	-0.690867
C	2.472450	3.688760	0.524786
H	2.583974	4.366644	1.366629
C	1.703925	2.532455	0.668182
H	1.231638	2.311537	1.619757
C	2.578447	-1.439607	-0.541735
C	2.825558	-2.640655	-1.233405
H	1.993466	-3.194090	-1.651546
C	4.122910	-3.131349	-1.369720
H	4.288709	-4.060559	-1.908312
C	5.201771	-2.438290	-0.818431
H	6.212671	-2.822796	-0.924112
C	4.970393	-1.247951	-0.125484
H	5.800508	-0.701680	0.314390
C	3.675384	-0.753224	0.012540
H	3.517774	0.169194	0.559436
C	1.305527	-0.523647	2.487278
C	-1.306033	-0.523671	2.487393
O	-2.161636	-0.309562	3.228821
H	-3.694236	4.872165	-0.800917
H	3.695346	4.871260	-0.801638
Fe	-0.000271	-0.794447	1.303733

5c

Fe	-0.404063	-0.377048	-0.253257
O	-0.490443	-0.608152	2.895085
O	-1.987211	1.184459	-2.171824
O	-0.006716	-2.628019	-2.104151
C	0.205310	-0.134332	1.952979
C	1.168891	-0.880962	1.129592
C	1.639562	0.003036	0.085585
C	0.903085	1.239067	0.168118
C	-0.055661	1.128644	1.239927
C	-1.394341	0.555928	-1.409219
C	-0.168604	-1.747355	-1.382083
C	-3.302161	-0.928877	0.777849
H	-3.374834	0.163764	0.825235
H	-3.773044	-1.338491	1.680881
O	-1.915512	-1.333025	0.814514
H	-1.585055	-1.247711	1.757638
C	-3.979730	-1.466647	-0.457319
C	-3.790802	-2.799242	-0.850868
C	-4.839723	-0.652861	-1.203042
C	-4.447948	-3.303485	-1.972546
H	-3.120184	-3.433931	-0.278522
C	-5.506833	-1.159972	-2.320327
H	-4.986213	0.384409	-0.910610
C	-5.310169	-2.485755	-2.708821
H	-4.289824	-4.336403	-2.271026
H	-6.170843	-0.516045	-2.890633
H	-5.823550	-2.880566	-3.581443
C	-1.004721	2.162719	1.715595
C	-1.351943	2.221662	3.079314
C	-1.573807	3.115306	0.847855
C	-2.228210	3.198967	3.551981
H	-0.941490	1.486055	3.759497
C	-2.449164	4.088999	1.324577
H	-1.329303	3.100690	-0.208016
C	-2.781659	4.137528	2.680391
H	-2.477642	3.223723	4.609738
H	-2.872319	4.811703	0.631636
H	-3.464821	4.897257	3.050945
C	1.274039	2.488059	-0.549192
C	1.727900	3.574321	0.218745
C	1.237217	2.623920	-1.944015
C	2.139344	4.757365	-0.392582
H	1.756925	3.485739	1.300852

C	1.644505	3.810665	-2.555285
H	0.877747	1.803257	-2.554423
C	2.098243	4.880507	-1.783106
H	2.489521	5.584185	0.219367
H	1.603512	3.896999	-3.637753
H	2.414322	5.804193	-2.260200
C	2.874278	-0.179627	-0.725638
C	4.107694	-0.184548	-0.052878
C	2.872394	-0.319907	-2.120082
C	5.303330	-0.317792	-0.756811
H	4.123702	-0.085616	1.028810
C	4.069605	-0.457323	-2.825026
H	1.928891	-0.335745	-2.655901
C	5.288715	-0.455062	-2.146640
H	6.246811	-0.317668	-0.217722
H	4.045845	-0.569089	-3.905725
H	6.220298	-0.563476	-2.695351
C	1.698248	-2.219922	1.482984
C	1.631163	-2.671004	2.815638
C	2.298053	-3.065458	0.529982
C	2.148851	-3.915034	3.175616
H	1.156548	-2.045026	3.560546
C	2.811734	-4.308318	0.894239
H	2.366863	-2.753947	-0.505557
C	2.741422	-4.741150	2.219993
H	2.085558	-4.237993	4.211703
H	3.267151	-4.940139	0.136058
H	3.141478	-5.711331	2.502779

1d

Fe	0.007059	0.480791	1.054014
C	0.051617	-1.321443	-0.176265
O	0.148768	-2.616474	0.171943
H	-0.696727	-2.906131	0.554599
C	-1.124655	-0.531378	-0.352094
C	-0.748547	0.746827	-0.895855
C	0.659147	0.798887	-0.928776
C	1.154220	-0.466617	-0.439634
C	-1.230263	1.412621	1.908891
O	-2.047669	1.981754	2.484921
C	1.368238	1.142054	1.978056
O	2.258381	1.526356	2.596649

H	-0.124478	-0.441424	2.232405
F	-1.588551	1.687381	-1.316212
F	1.407777	1.783592	-1.419559
F	2.436724	-0.824333	-0.420943
F	-2.371688	-1.016846	-0.267637

2dTS

Fe	-0.196962	0.170721	-0.780700
C	-1.037109	-0.005917	1.331807
O	-0.520328	-0.597819	2.348894
H	0.718305	-0.585768	2.316715
C	-0.788997	1.336389	0.845732
C	-1.630026	1.606387	-0.288272
C	-2.270794	0.399203	-0.642593
C	-1.818489	-0.613797	0.272537
C	0.979217	1.295003	-1.505434
O	1.756163	2.019604	-1.945877
C	-0.175367	-0.993069	-2.124677
O	-0.150264	-1.772710	-2.971410
H	1.035520	-0.570800	-0.181427
C	1.926771	-1.324271	0.922521
O	1.842900	-0.630230	1.997608
C	3.195546	-1.369105	0.173214
C	3.374075	-2.341885	-0.822491
C	4.231674	-0.469532	0.467287
C	4.578096	-2.416100	-1.518111
H	2.567290	-3.034971	-1.049961
C	5.433257	-0.546355	-0.231758
H	4.081989	0.271166	1.245815
C	5.607597	-1.516917	-1.224010
H	4.715345	-3.171374	-2.286369
H	6.236654	0.148166	-0.003761
H	6.546937	-1.573500	-1.767093
F	-3.189260	0.249495	-1.593778
F	-2.289493	-1.864290	0.298258
F	-1.831990	2.795161	-0.849845
F	-0.100444	2.269185	1.510649
H	1.261960	-2.191028	0.815979

3d

Fe	-0.766371	0.291868	0.330539
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C	-1.688863	-1.215098	-1.260954
O	-1.139246	-1.905807	-2.127730
H	0.546330	-2.264167	-1.607710
C	-1.832476	-1.486708	0.185226
C	-2.621432	-0.463933	0.798387
C	-2.752763	0.596404	-0.137028
C	-2.037448	0.222791	-1.315931
H	0.704983	-0.219863	-0.404137
C	1.511208	-0.672331	-1.132344
O	1.397850	-2.040819	-1.162693
C	2.835621	-0.210456	-0.589610
C	3.273802	1.093909	-0.852371
C	3.627858	-1.061279	0.189699
C	4.488559	1.546081	-0.338120
H	2.666619	1.755488	-1.467230
C	4.845003	-0.607916	0.700132
H	3.291201	-2.075252	0.376665
C	5.276567	0.694894	0.440829
H	4.822735	2.557645	-0.551399
H	5.458549	-1.275050	1.299448
H	6.225149	1.044549	0.839050
H	1.265019	-0.193879	-2.090207
C	-0.071545	0.016777	1.970381
C	-0.326423	2.034485	0.255402
O	0.338768	-0.178463	3.023902
O	-0.079665	3.154653	0.197038
F	-3.477470	1.694607	0.043459
F	-2.015776	0.952422	-2.436392
F	-3.210911	-0.516570	1.987451
F	-1.585171	-2.673371	0.748150

4d

Fe	0.484357	0.185966	-0.404637
C	-1.735365	-0.470896	-0.700012
O	-2.356466	-0.571998	-1.748703
C	-0.770427	-1.433255	-0.097005
C	-0.284269	-0.932943	1.136576
C	-0.702293	0.429482	1.253020
C	-1.442957	0.758177	0.090289
C	2.027945	-0.734287	-0.585183
O	2.994350	-1.350227	-0.648994
C	1.242988	1.824288	-0.364770

O	1.698495	2.874782	-0.284659
F	0.378975	-1.600159	2.071340
F	-0.480357	1.198064	2.310816
F	-2.035600	1.935032	-0.119405
F	-0.615294	-2.690623	-0.515349

5d

Fe	-0.652974	0.050590	-0.226835
O	-1.732328	-0.092555	2.787479
O	0.620076	-2.042079	-1.868707
O	0.606941	2.349552	-1.590112
C	-2.108719	-0.055981	1.601814
C	-2.171637	1.120267	0.712507
C	-2.587454	0.728697	-0.600255
C	-2.557479	-0.685335	-0.654293
C	-2.119134	-1.159619	0.623293
C	0.164778	-1.214788	-1.213643
C	0.142951	1.446503	-1.055999
C	1.718322	-0.783780	1.663752
H	1.437633	-1.824447	1.462157
H	1.974971	-0.697749	2.726865
O	0.582166	0.084182	1.440115
H	-0.042213	0.018613	2.211964
C	2.877284	-0.358099	0.800095
C	3.316387	0.974159	0.814538
C	3.547482	-1.287701	-0.002544
C	4.403127	1.366599	0.035175
H	2.797280	1.701261	1.433239
C	4.643112	-0.897415	-0.776503
H	3.211020	-2.321571	-0.025034
C	5.070895	0.430382	-0.760536
H	4.732501	2.401911	0.050209
H	5.154647	-1.629205	-1.395538
H	5.919759	0.737003	-1.365524
F	-2.051294	-2.456113	0.951296
F	-2.956117	-1.427155	-1.683481
F	-3.022740	1.528945	-1.569040
F	-2.163694	2.386901	1.141679

1e

Fe	-0.011293	0.487506	1.084533
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C	-0.010615	-1.305103	-0.173714
C	-1.184000	-0.505752	-0.405136
C	-0.691852	0.777484	-0.899872
C	-1.487131	1.947096	-1.424631
H	-2.353614	2.151650	-0.789578
H	-1.886954	1.684174	-2.416766
C	-0.614867	3.206498	-1.552785
H	-1.165356	3.978824	-2.103059
H	-0.408986	3.611120	-0.552304
C	0.707966	2.886335	-2.259665
H	1.283535	3.802367	-2.437745
H	0.486914	2.456253	-3.247095
C	1.562600	1.892513	-1.450652
H	2.347979	1.481894	-2.097702
H	2.081491	2.420044	-0.641456
C	0.722730	0.757746	-0.901770
C	1.181328	-0.526704	-0.385285
Si	-2.963322	-1.154608	-0.351717
C	-3.250625	-2.180532	-1.920120
H	-3.160686	-1.563015	-2.822050
H	-4.250956	-2.631334	-1.923845
H	-2.516147	-2.990586	-2.000525
C	-4.245614	0.236136	-0.273662
H	-4.257968	0.850276	-1.180058
H	-4.092642	0.897390	0.586356
H	-5.242248	-0.211903	-0.170178
C	-3.233734	-2.259681	1.173098
H	-2.775886	-1.830444	2.071698
H	-2.853800	-3.281348	1.045898
H	-4.309957	-2.354843	1.364567
Si	2.964371	-1.160005	-0.293937
C	3.384301	-1.977106	-1.952887
H	4.399947	-2.392237	-1.943571
H	3.327231	-1.259149	-2.780014
H	2.689864	-2.795128	-2.178375
C	4.202040	0.231581	0.048106
H	5.207530	-0.201328	0.128801
H	3.990373	0.749601	0.989217
H	4.233829	0.981356	-0.748800
C	3.169067	-2.443759	1.094099
H	4.237379	-2.562028	1.314560
H	2.798253	-3.440606	0.824274
H	2.678724	-2.126513	2.022104

C	-1.320454	1.293257	1.925128
O	-2.202159	1.790475	2.485813
C	1.255955	1.324892	1.959423
O	2.099930	1.852585	2.549342
H	-0.012232	-0.463148	2.262584
N	-0.028531	-2.658028	0.152681
H	0.796872	-2.961707	0.654743
H	-0.858561	-2.937896	0.661566

2eTS

Fe	-0.187520	-0.013426	-0.754066
C	-0.913599	0.149659	1.355946
H	0.675094	-1.136911	2.169141
C	-0.748322	1.449855	0.705672
C	-1.653636	1.455704	-0.420002
C	-2.013973	2.598434	-1.335969
H	-1.128286	3.176623	-1.612306
H	-2.669154	3.288439	-0.781654
C	-2.752400	2.110469	-2.591660
H	-3.135489	2.973499	-3.148484
H	-2.048614	1.589358	-3.255334
C	-3.899185	1.168833	-2.208448
H	-4.487275	0.892111	-3.091026
H	-4.581856	1.702380	-1.531731
C	-3.390109	-0.109724	-1.515545
H	-4.223473	-0.600428	-1.003041
H	-3.040519	-0.826766	-2.267143
C	-2.296714	0.179142	-0.506807
C	-1.783483	-0.682924	0.525886
Si	0.301855	2.853966	1.440587
C	-0.477376	3.329584	3.104906
H	-1.492544	3.720242	2.962940
H	0.112645	4.111360	3.599295
H	-0.550710	2.483004	3.797639
C	0.335927	4.397273	0.344397
H	-0.656426	4.834895	0.192158
H	0.781223	4.202419	-0.637652
H	0.956871	5.157480	0.835657
C	2.086519	2.272956	1.685436
H	2.604589	2.203690	0.721699
H	2.158064	1.285526	2.152827
H	2.641087	2.985335	2.309130

Si	-2.364235	-2.415386	1.078370
C	-3.219373	-2.191361	2.751564
H	-3.585810	-3.151445	3.135887
H	-4.077952	-1.512562	2.677272
H	-2.519068	-1.772329	3.481130
C	-3.600098	-3.165417	-0.152773
H	-3.810030	-4.196593	0.159718
H	-3.204976	-3.212080	-1.174208
H	-4.558917	-2.636710	-0.182662
C	-0.941827	-3.651232	1.225204
H	-1.312538	-4.567643	1.702652
H	-0.102392	-3.276609	1.818055
H	-0.562338	-3.933802	0.235339
C	0.919382	1.026281	-1.665784
O	1.601673	1.748063	-2.253007
C	-0.314144	-1.248274	-2.019245
O	-0.455157	-2.044729	-2.843362
H	1.154993	-0.844121	-0.043160
C	1.868280	-1.671672	0.510788
H	1.480480	-2.595303	0.047554
O	1.719320	-1.609633	1.834689
C	3.253834	-1.352212	-0.014271
C	3.567997	-1.589778	-1.358960
C	4.238322	-0.842587	0.837593
C	4.842763	-1.308315	-1.849255
H	2.811768	-2.003649	-2.024213
C	5.515638	-0.562603	0.348178
H	3.992079	-0.689017	1.882620
C	5.820722	-0.789958	-0.995423
H	5.075071	-1.498014	-2.894002
H	6.276061	-0.171095	1.019252
H	6.815815	-0.572888	-1.374778
N	-0.266016	-0.316975	2.438584
H	0.225922	0.436977	2.916537

3e

Fe	-0.189774	-0.068028	-0.741615
C	-1.008542	0.180797	1.399144
H	1.026661	-1.086795	2.280595
C	-0.835483	1.440220	0.640015
C	-1.706933	1.350751	-0.499517
C	-2.091087	2.433170	-1.477139

H	-1.218620	3.022857	-1.771795
H	-2.772029	3.128916	-0.961879
C	-2.801943	1.864386	-2.714846
H	-3.211991	2.688250	-3.310466
H	-2.075360	1.341519	-3.351738
C	-3.915798	0.897269	-2.298643
H	-4.488212	0.563994	-3.171940
H	-4.621560	1.430692	-1.645870
C	-3.361137	-0.332222	-1.554596
H	-4.179085	-0.845147	-1.037948
H	-2.964605	-1.055696	-2.276143
C	-2.301053	0.042403	-0.538857
C	-1.780692	-0.741291	0.541458
Si	0.051724	2.973678	1.323720
C	1.598850	2.471570	2.305729
H	1.381225	2.309143	3.368726
H	2.341951	3.277159	2.255650
H	2.069833	1.559474	1.924830
C	-1.158774	3.863573	2.483381
H	-1.499041	3.204083	3.290647
H	-2.048345	4.214622	1.946217
H	-0.684234	4.738263	2.945858
C	0.583647	4.187399	-0.030686
H	-0.265375	4.668492	-0.528081
H	1.208171	3.719613	-0.798874
H	1.178842	4.983961	0.434194
Si	-2.272558	-2.480650	1.137785
C	-3.329919	-2.261234	2.691754
H	-3.644923	-3.231469	3.095721
H	-4.235245	-1.677530	2.484014
H	-2.757676	-1.735619	3.463066
C	-3.275144	-3.412414	-0.179346
H	-3.423579	-4.444681	0.163277
H	-2.754658	-3.463944	-1.142815
H	-4.268390	-2.984883	-0.352759
C	-0.764977	-3.558593	1.515849
H	-1.096520	-4.498684	1.975252
H	-0.064342	-3.078874	2.204348
H	-0.224909	-3.819547	0.597498
C	0.848305	0.936366	-1.772306
O	1.469735	1.618038	-2.466694
C	-0.228916	-1.413680	-1.897851
O	-0.324019	-2.279494	-2.657365

H	1.338732	-0.740423	0.091147
C	2.055133	-1.449689	0.653323
O	1.982178	-1.228989	2.014877
C	3.435245	-1.183822	0.098072
C	3.751700	-1.608120	-1.199587
C	4.403989	-0.514268	0.852718
C	5.011880	-1.356329	-1.740586
H	3.008785	-2.144278	-1.787677
C	5.667865	-0.266881	0.312194
H	4.162809	-0.206889	1.864288
C	5.974743	-0.681998	-0.984723
H	5.244182	-1.691321	-2.748037
H	6.415663	0.249254	0.908899
H	6.958941	-0.488059	-1.402786
H	1.714701	-2.455521	0.367441
N	-0.457698	-0.196415	2.532246
H	0.028967	0.589678	2.966058

4e

Fe	-0.002263	0.316640	1.153064
Si	-2.951095	-1.157324	-0.404271
Si	2.989645	-1.168115	-0.236346
O	2.067424	1.591953	2.776115
O	-2.150155	1.304052	2.867713
C	0.048582	-1.240785	-0.016087
C	-1.170847	-0.500097	-0.399964
C	-0.705864	0.749815	-0.921697
C	-1.535863	1.888108	-1.475721
H	-2.049378	2.404173	-0.655549
H	-2.325171	1.483202	-2.121146
C	-0.683373	2.895814	-2.267975
H	-0.441928	2.475686	-3.254896
H	-1.267846	3.805388	-2.448226
C	0.622944	3.224835	-1.534864
H	0.395631	3.617358	-0.534206
H	1.174636	4.008166	-2.067396
C	1.504721	1.972464	-1.410341
H	1.909961	1.719036	-2.401685
H	2.369778	2.170002	-0.770521
C	0.728387	0.784574	-0.900523
C	1.231955	-0.446925	-0.382717
C	-3.163523	-2.617634	0.785334

H	-2.994621	-2.337007	1.831958
H	-2.509560	-3.463271	0.543412
H	-4.196984	-2.980240	0.713803
C	-3.305143	-1.764582	-2.166067
H	-2.603389	-2.553612	-2.461619
H	-3.223236	-0.956662	-2.903132
H	-4.319691	-2.176131	-2.238770
C	-4.213726	0.171750	0.068652
H	-5.218771	-0.269328	0.064800
H	-4.224980	1.013626	-0.631418
H	-4.032820	0.571367	1.072076
C	2.962825	-2.775549	-1.238289
H	3.949682	-3.255031	-1.238535
H	2.677380	-2.599202	-2.282540
H	2.245025	-3.482493	-0.807670
C	3.492314	-1.535936	1.545100
H	2.728121	-2.151107	2.028699
H	3.618836	-0.621750	2.134707
H	4.446176	-2.078964	1.561285
C	4.264151	0.008386	-1.006505
H	5.244325	-0.485581	-1.012478
H	4.375373	0.937379	-0.435617
H	4.026559	0.273368	-2.043140
C	1.244013	1.068101	2.156396
C	-1.293362	0.907771	2.197640
N	0.160600	-1.993090	1.091308
H	-0.759561	-2.324543	1.384071

5e

Fe	0.026753	-0.098223	0.495800
Si	-2.372893	-2.421206	-1.118448
Si	-0.397181	3.144823	-1.114543
O	1.201251	-0.513753	-1.169672
H	0.533384	-0.497573	-1.929935
O	1.913377	1.609162	1.950834
O	0.468540	-2.487112	2.133951
C	-1.352333	0.341557	-1.310554
C	-1.819778	-0.741371	-0.428410
C	-2.077959	-0.153189	0.857934
C	-2.822456	-0.755947	2.032436
H	-2.220339	-1.533634	2.515867
H	-3.717968	-1.263581	1.657302

C	-3.232467	0.308017	3.068484
H	-4.114930	0.852659	2.703003
H	-3.534460	-0.187716	3.998528
C	-2.106490	1.314497	3.330243
H	-1.209697	0.784267	3.679499
H	-2.393898	2.012339	4.125553
C	-1.775132	2.102473	2.053397
H	-2.605582	2.790854	1.831676
H	-0.893844	2.730000	2.210430
C	-1.591430	1.191453	0.863859
C	-1.053632	1.500365	-0.443423
C	-1.062639	-3.216673	-2.226957
H	-0.173803	-3.518537	-1.660405
H	-0.760084	-2.526264	-3.018899
H	-1.473945	-4.121319	-2.693215
C	-3.944318	-2.116001	-2.132876
H	-3.735095	-1.405619	-2.940107
H	-4.750319	-1.699186	-1.516426
H	-4.315399	-3.045364	-2.583063
C	-2.749179	-3.659702	0.272836
H	-2.936529	-4.645444	-0.172278
H	-3.635818	-3.395846	0.859034
H	-1.907697	-3.771083	0.966781
C	-1.691730	3.835058	-2.318993
H	-1.340731	4.762342	-2.788902
H	-2.629869	4.060914	-1.797287
H	-1.928167	3.123702	-3.118885
C	1.252461	2.903521	-2.019206
H	1.189881	2.196404	-2.853238
H	2.016702	2.526708	-1.330261
H	1.602341	3.862428	-2.422239
C	-0.099928	4.434810	0.242275
H	0.288234	5.349382	-0.224594
H	0.642595	4.106065	0.978086
H	-1.015989	4.705330	0.778107
C	2.164120	-1.573173	-1.311420
H	2.350246	-1.699763	-2.385451
H	1.749378	-2.512689	-0.927747
C	3.443417	-1.228083	-0.590759
C	4.159970	-0.072483	-0.935381
H	3.775920	0.580897	-1.714496
C	5.349946	0.243106	-0.282456
H	5.895630	1.141874	-0.557363

C	5.843896	-0.596496	0.721051
H	6.773223	-0.351047	1.227969
C	5.139515	-1.749358	1.068431
H	5.515756	-2.405438	1.848707
C	3.943280	-2.060164	0.416538
H	3.393070	-2.956112	0.694845
C	1.203973	0.910543	1.366836
C	0.336179	-1.546835	1.474160
N	-1.009405	0.118193	-2.569928
H	-0.689976	0.983944	-3.009234

1f

Fe	-0.034632	-0.619989	1.062501
C	-0.009900	1.158198	-0.088744
C	1.192075	0.399912	-0.354422
C	0.732210	-0.859792	-0.920303
C	1.563896	-2.003258	-1.449566
H	2.400113	-2.222686	-0.779976
H	2.008873	-1.697343	-2.409606
C	0.715324	-3.266054	-1.667881
H	1.301605	-4.011457	-2.218181
H	0.465583	-3.709765	-0.694041
C	-0.575064	-2.930676	-2.424587
H	-1.130242	-3.843919	-2.668980
H	-0.312493	-2.456166	-3.381183
C	-1.478198	-1.982652	-1.614562
H	-2.245475	-1.559751	-2.273209
H	-2.019142	-2.550765	-0.848370
C	-0.684874	-0.855747	-0.986400
C	-1.179083	0.394013	-0.433071
Si	2.986754	1.002762	-0.203374
C	3.515005	1.721975	-1.879525
H	3.459381	0.962654	-2.669371
H	4.552784	2.076228	-1.836785
H	2.888286	2.565450	-2.189944
C	4.208279	-0.383163	0.220806
H	4.334089	-1.098314	-0.598838
H	3.927615	-0.940995	1.119488
H	5.191170	0.068592	0.407922
C	3.161580	2.327699	1.144206
H	2.757038	1.983573	2.103719
H	2.681075	3.277669	0.886092

H	4.226947	2.540516	1.298863
Si	-2.972265	1.006643	-0.222016
C	-3.375231	2.245393	-1.604000
H	-4.447394	2.479784	-1.596839
H	-3.132689	1.843320	-2.595326
H	-2.833973	3.189941	-1.482874
C	-4.204913	-0.428791	-0.377550
H	-5.207677	-0.047715	-0.144222
H	-3.995543	-1.240261	0.327731
H	-4.246540	-0.855619	-1.385192
C	-3.235844	1.814144	1.464447
H	-4.248601	2.232657	1.529552
H	-2.511188	2.615907	1.628255
H	-3.121748	1.085135	2.274405
C	1.193796	-1.522209	1.928800
O	2.006949	-2.094463	2.519331
C	-1.366014	-1.417983	1.876982
O	-2.250070	-1.924091	2.423759
H	-0.025667	0.278863	2.271055
N	-0.103381	2.493058	0.402957
H	0.528302	2.627411	1.185491
C	0.108433	3.530670	-0.611351
H	1.113333	3.526756	-1.063983
H	-0.620102	3.404113	-1.416493
H	-0.060353	4.511181	-0.153835

2fTS

Fe	-0.215836	0.002791	-0.830061
C	-0.890349	0.087595	1.312522
H	0.635685	-1.338512	1.967557
C	-0.717383	1.421597	0.704989
C	-1.653067	1.470609	-0.404609
C	-2.031719	2.645185	-1.274674
H	-1.149995	3.210102	-1.578971
H	-2.644555	3.334017	-0.672547
C	-2.832656	2.216111	-2.513102
H	-3.220267	3.107437	-3.020145
H	-2.167178	1.708957	-3.225589
C	-3.977947	1.279828	-2.119363
H	-4.606528	1.044063	-2.985850
H	-4.623821	1.794734	-1.393796
C	-3.451947	-0.027839	-1.501204

H	-4.267802	-0.539246	-0.982020
H	-3.131388	-0.710440	-2.296570
C	-2.322204	0.211256	-0.519822
C	-1.790145	-0.694001	0.455363
Si	0.399798	2.866512	1.276811
C	-0.274261	3.611972	2.888571
H	-0.300784	2.918099	3.731977
H	-1.294571	3.985054	2.733509
H	0.343757	4.470519	3.181837
C	0.423852	4.328467	0.063025
H	-0.544604	4.826261	-0.048039
H	0.798790	4.064852	-0.931413
H	1.121174	5.067944	0.479907
C	2.210574	2.308365	1.414299
H	2.729435	2.523003	0.472323
H	2.332887	1.239495	1.607995
H	2.732664	2.858468	2.207226
Si	-2.389419	-2.443473	0.942390
C	-3.212122	-2.304253	2.642087
H	-3.615670	-3.274801	2.957027
H	-4.042793	-1.587775	2.628425
H	-2.489744	-1.971391	3.393184
C	-3.681074	-3.106434	-0.284441
H	-3.890284	-4.151039	-0.019078
H	-3.328003	-3.103063	-1.322068
H	-4.634951	-2.569357	-0.247312
C	-1.007323	-3.732476	0.970880
H	-1.400356	-4.663535	1.399959
H	-0.137346	-3.426925	1.558200
H	-0.668119	-3.965772	-0.046243
C	0.897747	1.031549	-1.745283
O	1.585716	1.731206	-2.352704
C	-0.407546	-1.178006	-2.137414
O	-0.593623	-1.938951	-2.985924
H	1.127957	-0.912566	-0.196095
C	1.825659	-1.781471	0.297181
H	1.433920	-2.667386	-0.232116
O	1.666506	-1.814795	1.623695
C	3.221480	-1.443871	-0.186988
C	3.552319	-1.590350	-1.540507
C	4.198777	-1.006074	0.711954
C	4.837187	-1.290204	-1.992038
H	2.801508	-1.948143	-2.243409

C	5.486026	-0.707337	0.261281
H	3.937955	-0.923894	1.761653
C	5.808091	-0.844176	-1.090548
H	5.082794	-1.408714	-3.044207
H	6.240634	-0.372192	0.968466
H	6.810844	-0.612768	-1.440103
N	-0.274701	-0.522763	2.340655
C	0.273014	0.209871	3.474148
H	-0.535475	0.689363	4.040191
H	0.754309	-0.517980	4.134106
H	1.020580	0.972189	3.231831

3f

Fe	-0.246054	-0.029357	-0.840244
C	-0.953306	0.117715	1.380943
H	0.894736	-1.500164	1.991505
C	-0.726798	1.421113	0.677095
C	-1.663555	1.437906	-0.424854
C	-2.049833	2.589098	-1.322288
H	-1.169618	3.141327	-1.652184
H	-2.651129	3.295669	-0.728645
C	-2.869063	2.133874	-2.539277
H	-3.261027	3.014715	-3.061124
H	-2.214826	1.608434	-3.248730
C	-4.011020	1.209745	-2.109030
H	-4.652722	0.957020	-2.961040
H	-4.645263	1.740988	-1.384911
C	-3.476681	-0.085275	-1.472488
H	-4.286221	-0.590580	-0.936531
H	-3.160458	-0.780180	-2.258666
C	-2.339008	0.172861	-0.505161
C	-1.796530	-0.705845	0.476970
Si	0.349904	2.916689	1.190473
C	2.118249	2.406197	1.640096
H	2.196759	1.722698	2.487416
H	2.696990	3.306859	1.883168
H	2.607048	1.927134	0.783400
C	-0.501784	3.884602	2.590528
H	-0.692439	3.308160	3.500621
H	-1.467519	4.271833	2.241279
H	0.113606	4.749817	2.869038
C	0.575620	4.206940	-0.189065

H	-0.339800	4.758263	-0.425465
H	0.986929	3.798121	-1.117077
H	1.302580	4.939858	0.185914
Si	-2.370244	-2.458494	0.966861
C	-3.336108	-2.323563	2.589595
H	-3.725732	-3.302925	2.894519
H	-4.190113	-1.641729	2.493139
H	-2.689497	-1.944814	3.386721
C	-3.513503	-3.211371	-0.353057
H	-3.689380	-4.262666	-0.090096
H	-3.068751	-3.200749	-1.354876
H	-4.494006	-2.727383	-0.412292
C	-0.949242	-3.697207	1.142835
H	-1.355019	-4.641177	1.529701
H	-0.157568	-3.373162	1.822253
H	-0.495908	-3.919623	0.168869
C	0.833735	0.954913	-1.844663
O	1.490419	1.616368	-2.527266
C	-0.437220	-1.267735	-2.095363
O	-0.637397	-2.057176	-2.915913
H	1.260054	-0.892715	-0.099537
C	1.934455	-1.707746	0.345534
O	1.830012	-1.715326	1.729139
C	3.338890	-1.407784	-0.124131
C	3.724411	-1.753557	-1.425900
C	4.258670	-0.766733	0.712806
C	5.005134	-1.452433	-1.889454
H	3.020387	-2.267615	-2.077889
C	5.542944	-0.472134	0.251281
H	3.960895	-0.516748	1.724992
C	5.918718	-0.809101	-1.050731
H	5.292122	-1.727246	-2.901021
H	6.252094	0.020533	0.911573
H	6.918613	-0.578236	-1.408481
H	1.572267	-2.641921	-0.108027
N	-0.468627	-0.435455	2.464279
C	0.172353	0.313275	3.527324
H	1.233505	0.044052	3.605943
H	0.095914	1.399726	3.437838
H	-0.296399	0.023702	4.477458

4f

Fe	0.128432	0.216530	1.128823
Si	-3.011155	-0.788171	-0.696659
Si	2.927099	-1.066399	-0.771350
O	2.327773	1.145229	2.809311
O	-1.859599	0.908981	3.151005
C	0.012070	-1.075402	-0.341712
C	-1.197054	-0.221287	-0.482657
C	-0.684948	1.103925	-0.713237
C	-1.468581	2.391242	-0.875477
H	-1.908316	2.672725	0.089554
H	-2.308093	2.229293	-1.555103
C	-0.604451	3.549905	-1.408037
H	-0.466896	3.432926	-2.492725
H	-1.139596	4.495412	-1.261675
C	0.773301	3.595199	-0.738638
H	0.655241	3.692122	0.349266
H	1.337159	4.471353	-1.079627
C	1.564071	2.318461	-1.058814
H	1.852644	2.331273	-2.120669
H	2.497711	2.288058	-0.489303
C	0.748860	1.076174	-0.801757
C	1.209195	-0.256587	-0.625368
C	-4.036930	-0.780324	0.896771
H	-4.064809	0.219880	1.343881
H	-3.670152	-1.470149	1.663375
H	-5.069999	-1.066064	0.660213
C	-3.013955	-2.498283	-1.516568
H	-2.611382	-3.297367	-0.889444
H	-2.431772	-2.478887	-2.446094
H	-4.043286	-2.772025	-1.781231
C	-3.929625	0.331748	-1.929647
H	-4.840364	-0.194346	-2.244221
H	-3.345813	0.534944	-2.835017
H	-4.244866	1.288869	-1.501691
C	2.705015	-2.577613	-1.890678
H	3.665174	-3.078501	-2.066906
H	2.291334	-2.298742	-2.867568
H	2.024239	-3.299875	-1.428514
C	3.666645	-1.591326	0.885037
H	2.964818	-2.235372	1.423013
H	3.901248	-0.732996	1.523493
H	4.597600	-2.149245	0.720865
C	4.132718	0.127870	-1.624575

H	5.064296	-0.406541	-1.851146
H	4.397709	0.984056	-0.993910
H	3.740690	0.515076	-2.572452
C	1.456674	0.748939	2.159302
C	-1.064816	0.616610	2.361860
N	0.238919	-2.042604	0.557657
C	-0.806552	-2.875061	1.117941
H	-0.495256	-3.184875	2.120437
H	-1.793722	-2.406124	1.200039
H	-0.905615	-3.791263	0.517273

5f

Fe	0.106001	0.004132	0.558855
Si	-1.821912	-2.806162	-0.794016
Si	-1.001764	3.138217	-1.005390
O	1.323562	0.164073	-1.142866
H	0.655536	0.317760	-1.871809
O	1.610241	1.932716	2.175816
O	1.167423	-2.337710	1.963163
C	-1.412780	0.230677	-1.224071
C	-1.624249	-0.962106	-0.348738
C	-1.925221	-0.436460	0.973837
C	-2.531567	-1.163476	2.160916
H	-1.790897	-1.811731	2.641218
H	-3.326000	-1.827087	1.803059
C	-3.123242	-0.196008	3.202473
H	-4.090213	0.183091	2.841325
H	-3.328294	-0.744527	4.129412
C	-2.196320	0.994459	3.465390
H	-1.214675	0.633329	3.801800
H	-2.596450	1.625363	4.267880
C	-2.032061	1.831871	2.189038
H	-2.974577	2.364043	1.987643
H	-1.273070	2.605225	2.330082
C	-1.719739	0.976858	0.984581
C	-1.269439	1.388993	-0.310615
C	-0.402059	-3.500266	-1.849203
H	0.518539	-3.541820	-1.254144
H	-0.188981	-2.951730	-2.768284
H	-0.647543	-4.533087	-2.129236
C	-3.503313	-3.100039	-1.633954
H	-3.632873	-2.559896	-2.577181

H	-4.317631	-2.789958	-0.966777
H	-3.639283	-4.169324	-1.841192
C	-1.812349	-3.955094	0.723582
H	-1.749079	-4.983673	0.343987
H	-2.719060	-3.893596	1.332119
H	-0.949455	-3.801860	1.379124
C	-2.527541	3.589254	-2.035261
H	-2.425949	4.590771	-2.472325
H	-3.439757	3.583905	-1.425783
H	-2.660032	2.870464	-2.850141
C	0.559934	3.283228	-2.065721
H	0.476269	2.672150	-2.968265
H	1.450876	2.962209	-1.514476
H	0.707567	4.328685	-2.365850
C	-0.824985	4.424184	0.384491
H	-0.632542	5.404093	-0.071883
H	0.017673	4.208769	1.052367
H	-1.727454	4.525355	0.997029
C	2.360677	-0.735750	-1.578675
H	2.582001	-0.489252	-2.625702
H	2.003047	-1.770865	-1.540849
C	3.595715	-0.569361	-0.729736
C	4.202040	0.688778	-0.600726
H	3.761974	1.547250	-1.101416
C	5.354560	0.842402	0.167462
H	5.813846	1.822685	0.262588
C	5.921440	-0.262180	0.811251
H	6.821384	-0.141915	1.408315
C	5.327188	-1.517901	0.685054
H	5.759507	-2.380176	1.185365
C	4.167197	-1.667905	-0.079162
H	3.701330	-2.646610	-0.167523
C	1.050317	1.156905	1.530454
C	0.780582	-1.412214	1.387040
N	-1.098486	0.399533	-2.489111
C	-1.292635	-0.623348	-3.496569
H	-1.724738	-0.155058	-4.391026
H	-0.339181	-1.070194	-3.819293
H	-1.959676	-1.441362	-3.202648

1g

Fe	1.480234	-0.099107	-1.003756
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C	-0.443624	0.061504	-0.168771
C	0.146532	-1.182321	0.263933
C	1.325430	-0.797995	1.022543
C	2.289290	-1.688849	1.768106
H	2.544966	-2.572650	1.177003
H	1.788361	-2.060051	2.675762
C	3.564816	-0.931292	2.170829
H	4.153889	-1.546568	2.861039
H	4.186811	-0.764552	1.280500
C	3.219290	0.416865	2.814708
H	4.123294	0.910298	3.190330
H	2.572785	0.238758	3.686089
C	2.498299	1.351151	1.825554
H	2.035889	2.178308	2.377413
H	3.228323	1.811370	1.149110
C	1.430898	0.617718	1.041005
C	0.337669	1.186785	0.273989
Si	-0.606008	-2.916915	0.033193
C	-1.777088	-3.243354	1.486442
H	-1.247062	-3.199772	2.446019
H	-2.225076	-4.241590	1.402316
H	-2.590310	-2.510516	1.518771
C	0.714018	-4.278026	0.022672
H	1.200667	-4.406585	0.995354
H	1.491963	-4.111726	-0.729613
H	0.223827	-5.229958	-0.219623
C	-1.558607	-3.031473	-1.599719
H	-0.949958	-2.696099	-2.447998
H	-2.485097	-2.448472	-1.582344
H	-1.833495	-4.077355	-1.786421
Si	-0.095350	3.023348	-0.007430
C	-1.292516	3.566450	1.358362
H	-1.546074	4.627773	1.241502
H	-0.850250	3.442135	2.354821
H	-2.225935	2.994087	1.332071
C	1.449723	4.118702	0.099651
H	1.157513	5.150906	-0.133603
H	2.222599	3.829981	-0.620150
H	1.901716	4.128150	1.096959
C	-0.880156	3.287765	-1.705918
H	-1.007077	4.361968	-1.891960
H	-1.861390	2.810374	-1.777412
H	-0.247567	2.881999	-2.503701

C	2.380744	-1.449989	-1.668274
O	2.952839	-2.343781	-2.125954
C	2.540481	1.109198	-1.707001
O	3.224607	1.905599	-2.189733
H	0.807653	-0.075644	-2.352295
N	-1.646128	0.192405	-0.912678
H	-1.602727	-0.104350	-1.876374
C	-2.913606	0.193441	-0.329888
C	-4.050232	0.121178	-1.159625
C	-3.102420	0.294194	1.061135
C	-5.329897	0.152096	-0.612621
H	-3.919556	0.047977	-2.237454
C	-4.392277	0.327555	1.593994
H	-2.240686	0.343903	1.718708
C	-5.515608	0.257177	0.768669
H	-6.189633	0.094012	-1.275415
H	-4.513765	0.406422	2.671514
H	-6.515308	0.281948	1.191629

2gTS

Fe	0.128209	-1.377182	0.155389
C	0.951578	0.667326	-0.120092
H	-0.665471	1.145018	-1.622030
C	0.704183	0.358946	1.296293
C	1.551613	-0.779444	1.593902
C	1.819038	-1.428608	2.929930
H	0.893610	-1.560429	3.492977
H	2.442727	-0.741199	3.522484
C	2.550045	-2.772167	2.786013
H	2.875266	-3.116082	3.774640
H	1.855038	-3.530378	2.398707
C	3.747950	-2.640619	1.840221
H	4.325343	-3.571730	1.809472
H	4.423403	-1.864556	2.227718
C	3.304855	-2.268064	0.414136
H	4.168646	-1.915637	-0.157948
H	2.946406	-3.162482	-0.108849
C	2.243293	-1.187324	0.409792
C	1.813128	-0.364660	-0.687916
Si	-0.369402	1.301976	2.580410
C	0.644438	2.690830	3.379430
H	1.603931	2.320491	3.762154

H	0.086556	3.095262	4.233929
H	0.847279	3.513479	2.689948
C	-0.901446	0.194847	4.034554
H	-0.076388	-0.044867	4.713324
H	-1.395059	-0.737354	3.745288
H	-1.630993	0.774597	4.615751
C	-1.961844	1.962033	1.814307
H	-2.559895	1.154493	1.376739
H	-1.788812	2.713972	1.040844
H	-2.565309	2.426517	2.605191
Si	2.447075	-0.262987	-2.488530
C	3.353829	1.386888	-2.679063
H	3.757005	1.488042	-3.694626
H	4.196639	1.462580	-1.980780
H	2.684602	2.232476	-2.492809
C	3.675604	-1.661881	-2.867647
H	3.921878	-1.616663	-3.936564
H	3.262466	-2.658749	-2.675170
H	4.618971	-1.572240	-2.317732
C	1.051515	-0.426670	-3.752204
H	1.445208	-0.215588	-4.754911
H	0.219159	0.256491	-3.562160
H	0.658324	-1.450961	-3.768257
C	-1.037551	-2.098812	1.281233
O	-1.763623	-2.604074	2.020110
C	0.277041	-2.855514	-0.815174
O	0.434599	-3.814914	-1.436466
H	-1.189885	-0.858529	-0.836103
C	-1.900470	-0.511481	-1.761925
H	-1.567373	-1.220067	-2.539336
O	-1.671319	0.774747	-2.052304
C	-3.300586	-0.844404	-1.294302
C	-3.735368	-2.175909	-1.273652
C	-4.175329	0.168725	-0.888013
C	-5.022702	-2.493438	-0.840725
H	-3.065336	-2.967036	-1.606879
C	-5.464563	-0.148359	-0.457129
H	-3.835117	1.197698	-0.930934
C	-5.890439	-1.478424	-0.428269
H	-5.350803	-3.529525	-0.831395
H	-6.139963	0.645252	-0.147967
H	-6.895049	-1.723218	-0.093733
N	0.365446	1.588248	-0.930252

C	0.287581	2.948083	-0.631981
C	-0.745241	3.731490	-1.194452
C	1.299304	3.609260	0.097004
C	-0.767846	5.111000	-1.010271
H	-1.522146	3.241017	-1.772195
C	1.265536	4.992722	0.270673
H	2.126845	3.031524	0.498772
C	0.231714	5.756145	-0.274678
H	-1.576611	5.689734	-1.449964
H	2.064394	5.476812	0.827878
H	0.211122	6.833814	-0.140843

3g

Fe	0.304071	-1.345240	0.263231
C	0.947134	0.802911	-0.230983
H	-1.010014	0.869269	-1.847302
C	0.767899	0.541967	1.221379
C	1.723314	-0.491277	1.549079
C	2.126997	-1.002234	2.911027
H	1.252612	-1.171311	3.541140
H	2.712802	-0.212003	3.406509
C	2.978250	-2.278237	2.827208
H	3.387556	-2.506362	3.818151
H	2.343119	-3.128501	2.542159
C	4.105146	-2.111061	1.803718
H	4.771433	-2.981333	1.809871
H	4.718431	-1.243853	2.087777
C	3.550414	-1.904574	0.382967
H	4.342939	-1.523525	-0.268555
H	3.254784	-2.871046	-0.041631
C	2.388481	-0.932925	0.356685
C	1.820531	-0.255334	-0.769244
Si	-0.338790	1.445019	2.506171
C	0.567130	2.949664	3.224044
H	1.570011	2.677412	3.577110
H	0.007329	3.324190	4.090848
H	0.666568	3.768825	2.509056
C	-0.729096	0.370368	4.028627
H	0.125690	0.247640	4.701805
H	-1.137223	-0.618183	3.802250
H	-1.500138	0.910703	4.594246
C	-2.018973	1.914928	1.783408

H	-1.957965	2.639888	0.968977
H	-2.631514	2.355204	2.581090
H	-2.551789	1.030659	1.413632
Si	2.353359	-0.272026	-2.603109
C	3.183910	1.385175	-2.985051
H	3.540671	1.407174	-4.022501
H	4.049961	1.558478	-2.334206
H	2.485098	2.215513	-2.845776
C	3.604820	-1.660011	-2.948322
H	3.771784	-1.705123	-4.032432
H	3.242449	-2.646575	-2.637341
H	4.581149	-1.493437	-2.480500
C	0.903975	-0.586845	-3.776801
H	1.247567	-0.460171	-4.811673
H	0.061149	0.090035	-3.618037
H	0.539049	-1.617192	-3.682930
C	-0.714045	-2.108472	1.501177
O	-1.326753	-2.652928	2.313355
C	0.531742	-2.874168	-0.609265
O	0.757308	-3.862032	-1.163469
H	-1.252911	-0.972352	-0.706026
C	-1.963026	-0.831300	-1.602930
H	-1.591458	-1.543732	-2.354074
O	-1.911641	0.478376	-2.045424
C	-3.337103	-1.237845	-1.124594
C	-3.676444	-2.595310	-1.056235
C	-4.272833	-0.277893	-0.723454
C	-4.927607	-2.990004	-0.582035
H	-2.960706	-3.347276	-1.384225
C	-5.527049	-0.672928	-0.254733
H	-4.010735	0.771944	-0.796164
C	-5.856760	-2.027867	-0.178336
H	-5.179635	-4.046162	-0.535863
H	-6.249448	0.080189	0.049285
H	-6.833777	-2.332952	0.186872
N	0.341041	1.635839	-1.070193
C	0.025434	2.963109	-0.787133
C	-1.121129	3.557873	-1.360754
C	0.926201	3.800703	-0.093154
C	-1.366924	4.919400	-1.208685
H	-1.817293	2.936785	-1.914988
C	0.676287	5.166022	0.040510
H	1.843888	3.373920	0.301594

C	-0.474497	5.736325	-0.506914
H	-2.262613	5.348690	-1.650928
H	1.395108	5.789189	0.567550
H	-0.665439	6.800571	-0.403232

4g

Fe	0.620673	0.204191	1.090210
Si	-1.810525	2.141152	-0.824737
Si	1.871706	-2.606982	-0.830710
O	2.410191	-1.007330	3.062456
O	-0.485313	2.095362	3.022185
C	-0.099633	-0.433395	-0.621809
C	-0.237533	1.048920	-0.638241
C	1.122190	1.533724	-0.609832
C	1.612734	2.967810	-0.640621
H	1.369435	3.465268	0.305091
H	1.071983	3.516273	-1.416725
C	3.124831	3.078912	-0.910924
H	3.316564	2.928528	-1.983120
H	3.456773	4.096538	-0.674706
C	3.927796	2.044369	-0.117465
H	3.732053	2.164298	0.956936
H	5.003492	2.194745	-0.265167
C	3.541008	0.627162	-0.561263
H	3.935446	0.446509	-1.572293
H	4.005805	-0.124024	0.084607
C	2.045835	0.435005	-0.595775
C	1.327156	-0.788743	-0.642055
C	-3.191953	1.809795	0.421372
H	-2.825681	1.852862	1.452584
H	-3.703518	0.857417	0.281444
H	-3.934678	2.610868	0.307127
C	-2.430538	1.925692	-2.603275
H	-2.781393	0.907390	-2.795305
H	-1.642963	2.155199	-3.331454
H	-3.268714	2.607329	-2.795556
C	-1.426557	3.989041	-0.588341
H	-2.391066	4.513326	-0.587934
H	-0.822712	4.432053	-1.385846
H	-0.944050	4.208279	0.370431
C	0.829651	-3.330807	-2.236003
H	1.135308	-4.362311	-2.451585

H	0.938899	-2.751776	-3.161160
H	-0.231821	-3.343457	-1.967535
C	1.638249	-3.635704	0.735724
H	0.607353	-3.551644	1.092425
H	2.307770	-3.322953	1.544147
H	1.845546	-4.692157	0.521736
C	3.696233	-2.686555	-1.349921
H	3.947217	-3.724265	-1.604662
H	4.380549	-2.376580	-0.552256
H	3.908545	-2.074296	-2.234292
C	1.675071	-0.552408	2.295956
C	-0.059066	1.325565	2.271978
N	-0.849967	-1.308742	0.069211
C	-2.238969	-1.386318	0.107884
C	-2.900227	-1.618112	1.329304
C	-2.995391	-1.422994	-1.081849
C	-4.275105	-1.832324	1.359596
H	-2.316666	-1.613840	2.245482
C	-4.371563	-1.647405	-1.040720
H	-2.485009	-1.306618	-2.033689
C	-5.024236	-1.844801	0.177737
H	-4.767284	-1.992773	2.315615
H	-4.934104	-1.672332	-1.970946
H	-6.096258	-2.016840	0.207033

5g

Fe	-0.872312	0.587028	-0.367919
Si	2.005184	-0.508412	-2.400084
Si	0.304065	1.614263	2.943324
O	-0.963431	-1.224761	0.611303
H	-0.011979	-1.311879	0.978775
O	-3.306230	1.684321	0.849649
O	-2.195166	0.016641	-2.919427
C	1.244525	0.371563	0.459499
C	1.218626	0.546491	-1.009014
C	0.620860	1.849659	-1.238929
C	0.566917	2.639001	-2.534004
H	-0.184887	2.221032	-3.212449
H	1.527615	2.537421	-3.051619
C	0.274020	4.131843	-2.293929
H	1.185385	4.630677	-1.934238
H	0.012312	4.606928	-3.246580

C	-0.839697	4.333602	-1.260662
H	-1.751951	3.819787	-1.594453
H	-1.089111	5.396922	-1.166434
C	-0.408671	3.785018	0.107612
H	0.369802	4.440857	0.526409
H	-1.240317	3.814396	0.816295
C	0.168771	2.395338	-0.000294
C	0.462455	1.458709	1.052950
C	1.907093	-2.373229	-2.105626
H	0.867807	-2.724232	-2.114001
H	2.372890	-2.704018	-1.175633
H	2.420398	-2.875129	-2.936448
C	3.804932	0.034512	-2.659625
H	4.444379	-0.237472	-1.816133
H	3.879797	1.118902	-2.810025
H	4.209594	-0.450044	-3.557418
C	1.141926	-0.240051	-4.075178
H	1.573291	-0.968187	-4.775149
H	1.311511	0.752322	-4.503497
H	0.062989	-0.419105	-4.051123
C	2.051841	1.780794	3.652036
H	2.022462	1.866043	4.745687
H	2.560107	2.672373	3.264390
H	2.657985	0.906049	3.395461
C	-0.581704	0.130778	3.712883
H	-0.011306	-0.788201	3.554581
H	-1.579254	-0.007825	3.280682
H	-0.700727	0.284937	4.793079
C	-0.687538	3.162314	3.425247
H	-0.740050	3.215094	4.520562
H	-1.719195	3.132747	3.054958
H	-0.227611	4.094049	3.077894
C	-1.454480	-2.465308	0.078788
H	-1.067382	-3.266939	0.721564
H	-1.062981	-2.627046	-0.932671
C	-2.963251	-2.480071	0.070630
C	-3.680312	-2.199809	1.243169
H	-3.139090	-1.949799	2.151829
C	-5.073596	-2.233722	1.244682
H	-5.618270	-2.012159	2.158625
C	-5.769731	-2.555901	0.075277
H	-6.856036	-2.583751	0.077941
C	-5.064344	-2.840764	-1.094038

H	-5.597744	-3.088957	-2.007641
C	-3.667663	-2.798681	-1.095252
H	-3.121742	-3.013652	-2.011111
C	-2.370028	1.219819	0.365005
C	-1.671255	0.195902	-1.906534
N	1.543078	-0.697755	1.214857
C	2.678574	-1.478662	1.097419
C	2.628727	-2.844103	1.462075
C	3.945441	-0.940958	0.769043
C	3.774541	-3.634509	1.457478
H	1.671032	-3.269005	1.754053
C	5.087566	-1.740427	0.768674
H	4.022999	0.120141	0.548565
C	5.015558	-3.094727	1.103881
H	3.698414	-4.682795	1.737315
H	6.047299	-1.294179	0.516926
H	5.908665	-3.712805	1.105810

1h

Fe	0.079355	0.476767	1.099968
C	-0.051103	-1.144546	-0.266675
C	-1.184618	-0.297752	-0.482558
C	-0.613052	0.990629	-0.857601
C	-1.336944	2.260273	-1.234952
H	-2.189506	2.436431	-0.572393
H	-1.753603	2.143091	-2.245826
C	-0.392043	3.471966	-1.221433
H	-0.902135	4.337863	-1.659576
H	-0.146464	3.735651	-0.183526
C	0.895876	3.163421	-1.994267
H	1.526212	4.056959	-2.071794
H	0.632034	2.874422	-3.021633
C	1.699028	2.027306	-1.332528
H	2.438412	1.642566	-2.046430
H	2.272101	2.424275	-0.486666
C	0.800428	0.893801	-0.882961
C	1.194068	-0.441784	-0.461842
Si	-3.013706	-0.862065	-0.511166
C	-3.112035	-2.469420	-1.506667
H	-2.702672	-2.338939	-2.515745
H	-4.159866	-2.778473	-1.612014
H	-2.564999	-3.281862	-1.021739

C	-4.081537	0.412888	-1.426724
H	-3.703461	0.641874	-2.429526
H	-4.194043	1.356203	-0.882102
H	-5.086627	-0.011721	-1.547849
C	-3.739286	-1.087521	1.218386
H	-3.786476	-0.137812	1.762161
H	-3.141542	-1.785720	1.810183
H	-4.760835	-1.482571	1.147820
Si	2.946159	-1.177249	-0.448339
C	3.289799	-1.885653	-2.171824
H	4.285111	-2.345089	-2.216736
H	3.249865	-1.105528	-2.941562
H	2.555020	-2.653225	-2.442489
C	4.257507	0.120161	-0.029192
H	5.238715	-0.370628	0.002717
H	4.088614	0.582678	0.948661
H	4.316551	0.918420	-0.775387
C	3.093213	-2.572070	0.836452
H	4.157406	-2.752524	1.033839
H	2.680325	-3.530601	0.497095
H	2.629936	-2.309609	1.795326
C	-1.171586	1.281177	2.032230
O	-2.005594	1.794072	2.645292
C	1.391811	1.171427	2.026920
O	2.265879	1.607106	2.646319
H	0.035324	-0.554436	2.198997
N	-0.088560	-2.535226	-0.040121
H	0.745629	-2.819263	0.469425
F	-1.108457	-2.840738	0.924452

2hTS

Fe	-0.198716	-0.104428	-0.826173
C	-0.888884	0.197391	1.253229
H	0.561714	-1.146574	2.096141
C	-0.635936	1.463047	0.586925
C	-1.555035	1.477046	-0.541290
C	-1.844184	2.598816	-1.508602
H	-0.924472	3.095989	-1.822113
H	-2.440050	3.360731	-0.983210
C	-2.628145	2.108943	-2.735588
H	-2.950467	2.972472	-3.328749
H	-1.969869	1.508397	-3.378773

C	-3.836621	1.271800	-2.306277
H	-4.449185	0.996716	-3.172489
H	-4.474867	1.881978	-1.651576
C	-3.411208	-0.005698	-1.558770
H	-4.270798	-0.409550	-1.015145
H	-3.123167	-0.780718	-2.278159
C	-2.288514	0.252458	-0.574552
C	-1.830555	-0.607399	0.488820
Si	0.466147	2.905788	1.216187
C	-0.302628	3.584360	2.808193
H	-1.324762	3.940430	2.627880
H	0.280147	4.436658	3.179976
H	-0.340424	2.825598	3.593712
C	0.492950	4.347124	-0.022812
H	-0.488207	4.797988	-0.202794
H	0.933403	4.075742	-0.988847
H	1.132815	5.128339	0.409120
C	2.272518	2.390331	1.422124
H	2.740981	2.204755	0.448538
H	2.378972	1.489616	2.029038
H	2.834157	3.200075	1.905892
Si	-2.535787	-2.279813	1.100052
C	-3.336430	-1.946746	2.781183
H	-3.756085	-2.869682	3.200292
H	-4.151706	-1.217360	2.700023
H	-2.600857	-1.552277	3.489349
C	-3.850215	-2.963678	-0.084380
H	-4.123611	-3.968312	0.263655
H	-3.487166	-3.067139	-1.113170
H	-4.769797	-2.369287	-0.104473
C	-1.196802	-3.604571	1.244303
H	-1.609568	-4.476461	1.768147
H	-0.308541	-3.271181	1.789170
H	-0.876805	-3.944990	0.251457
C	0.985360	0.819157	-1.768115
O	1.724077	1.457786	-2.379922
C	-0.428706	-1.355619	-2.057216
O	-0.626442	-2.165373	-2.855392
H	1.051701	-1.000708	-0.158404
C	1.773728	-1.864903	0.439621
H	1.361318	-2.765055	-0.051528
O	1.585525	-1.792783	1.739291
C	3.159139	-1.542942	-0.076006

C	3.512044	-1.858698	-1.394290
C	4.107397	-0.955846	0.767712
C	4.793687	-1.580251	-1.868476
H	2.782184	-2.332148	-2.049321
C	5.390537	-0.678945	0.294357
H	3.827505	-0.741334	1.793511
C	5.735877	-0.986006	-1.024137
H	5.059571	-1.831837	-2.891838
H	6.124127	-0.227165	0.957118
H	6.736168	-0.771107	-1.390749
N	-0.299482	-0.348689	2.354811
F	0.474673	0.651957	3.024472

3h

Fe	-0.186881	-0.132470	-0.791399
C	-1.075610	0.266358	1.306102
H	1.069859	-0.931832	2.338970
C	-0.875949	1.467034	0.477589
C	-1.722605	1.273169	-0.678169
C	-2.105929	2.268440	-1.745941
H	-1.241969	2.852163	-2.069286
H	-2.809816	2.987609	-1.299286
C	-2.778820	1.593132	-2.950852
H	-3.184621	2.363369	-3.616811
H	-2.030076	1.034716	-3.529301
C	-3.889060	0.643852	-2.489500
H	-4.432442	0.232398	-3.347793
H	-4.620384	1.213717	-1.898909
C	-3.332589	-0.512960	-1.638983
H	-4.153416	-0.993823	-1.096240
H	-2.912821	-1.285984	-2.292277
C	-2.298737	-0.040859	-0.637677
C	-1.788527	-0.744301	0.501925
Si	0.060559	3.052596	1.004910
C	1.869905	2.667813	1.400011
H	1.974732	1.768658	2.010709
H	2.324879	3.506370	1.942775
H	2.443626	2.526514	0.475904
C	-0.866898	3.869806	2.439995
H	-0.919378	3.214886	3.312731
H	-1.891282	4.129846	2.144489
H	-0.365709	4.800116	2.736338

C	0.102917	4.340006	-0.393855
H	-0.884614	4.725807	-0.667915
H	0.600301	3.980306	-1.301448
H	0.690222	5.192700	-0.027310
Si	-2.288915	-2.452058	1.186807
C	-3.493561	-2.148553	2.614082
H	-3.811242	-3.096328	3.066206
H	-4.394389	-1.620336	2.278663
H	-3.017697	-1.542365	3.392270
C	-3.123399	-3.519067	-0.141816
H	-3.259686	-4.529662	0.264434
H	-2.512670	-3.615442	-1.047023
H	-4.112557	-3.154630	-0.437432
C	-0.795419	-3.437519	1.801539
H	-1.149509	-4.332355	2.329419
H	-0.166205	-2.872295	2.494359
H	-0.170449	-3.781505	0.968608
C	0.879260	0.846524	-1.825864
O	1.518612	1.518388	-2.511152
C	-0.180963	-1.524994	-1.892340
O	-0.246163	-2.420701	-2.618962
H	1.332877	-0.744403	0.110094
C	2.045540	-1.411023	0.720636
O	2.007474	-1.052336	2.059644
C	3.420056	-1.230190	0.124443
C	3.764841	-1.925182	-1.042025
C	4.352267	-0.363722	0.706038
C	5.019421	-1.750288	-1.626254
H	3.050831	-2.613374	-1.491054
C	5.609885	-0.194365	0.124492
H	4.087347	0.161492	1.616746
C	5.946047	-0.882411	-1.043345
H	5.275991	-2.297402	-2.529520
H	6.329671	0.476063	0.586850
H	6.926071	-0.748756	-1.493575
H	1.683405	-2.433705	0.544590
N	-0.609769	-0.087317	2.485309
F	0.027063	1.045373	3.103178

4h

Fe	0.093500	0.144806	1.202767
Si	-2.993225	-1.016728	-0.607268

Si	2.994499	-1.035411	-0.616789
O	2.235114	1.208929	2.878720
O	-1.941923	0.696751	3.225986
C	0.053109	-1.174769	-0.240518
C	-1.188002	-0.410886	-0.408899
C	-0.743387	0.925836	-0.703648
C	-1.601490	2.149514	-0.950037
H	-2.021714	2.497380	0.001436
H	-2.457524	1.883442	-1.578727
C	-0.806651	3.290525	-1.609297
H	-0.651032	3.062471	-2.673524
H	-1.395935	4.213862	-1.569097
C	0.556500	3.488024	-0.935555
H	0.412276	3.694520	0.133842
H	1.073269	4.356028	-1.360966
C	1.434638	2.238302	-1.106234
H	1.762980	2.170671	-2.154294
H	2.345763	2.321841	-0.506809
C	0.687738	0.973553	-0.765277
C	1.224921	-0.326291	-0.511368
C	-3.285345	-2.852160	-0.282027
H	-3.283370	-3.092325	0.784179
H	-2.536938	-3.487195	-0.765996
H	-4.269036	-3.117665	-0.691179
C	-3.404198	-0.739823	-2.444160
H	-2.750434	-1.348324	-3.081175
H	-3.308758	0.300514	-2.772670
H	-4.437217	-1.052913	-2.642227
C	-4.166192	-0.005264	0.479866
H	-5.200562	-0.322260	0.295820
H	-4.112828	1.070860	0.282253
H	-3.958342	-0.159673	1.544089
C	2.896140	-2.467959	-1.850401
H	3.883107	-2.924441	-1.995855
H	2.534448	-2.135342	-2.830858
H	2.216457	-3.247117	-1.487952
C	3.633864	-1.662974	1.044644
H	2.930144	-2.374446	1.486777
H	3.788439	-0.848335	1.760263
H	4.597091	-2.169866	0.902990
C	4.197126	0.268402	-1.286528
H	5.172451	-0.206481	-1.453636
H	4.357546	1.094143	-0.584267

H	3.873443	0.693204	-2.243425
C	1.383573	0.765760	2.235221
C	-1.135787	0.473723	2.429647
N	0.300750	-2.058686	0.757661
F	-0.916897	-2.691677	1.146229

5h

Fe	0.055259	-0.204067	0.540891
Si	-2.459070	-2.357168	-1.117181
Si	-0.314165	3.207187	-0.778434
O	1.168735	-0.562255	-1.183093
H	0.506490	-0.520546	-1.923086
O	2.045833	1.354899	2.029049
O	0.492895	-2.690746	2.027485
C	-1.393852	0.416627	-1.169086
C	-1.836236	-0.729280	-0.357020
C	-2.030156	-0.219578	0.973903
C	-2.751957	-0.887153	2.127338
H	-2.157375	-1.713729	2.531773
H	-3.674396	-1.340516	1.747784
C	-3.095003	0.109969	3.249843
H	-3.972612	0.703318	2.955860
H	-3.379094	-0.443210	4.152608
C	-1.930274	1.062662	3.537740
H	-1.038668	0.484635	3.817866
H	-2.168209	1.711830	4.388544
C	-1.618933	1.930398	2.308685
H	-2.435171	2.655115	2.165493
H	-0.717343	2.521234	2.481215
C	-1.502230	1.105302	1.049430
C	-1.004006	1.502541	-0.257530
C	-1.210453	-3.091580	-2.334917
H	-0.296124	-3.423778	-1.829118
H	-0.941164	-2.372984	-3.114107
H	-1.649519	-3.971976	-2.821399
C	-4.074740	-1.975160	-2.028202
H	-3.904134	-1.219296	-2.802621
H	-4.842187	-1.590094	-1.345711
H	-4.478731	-2.873162	-2.512168
C	-2.769851	-3.675144	0.213560
H	-2.991315	-4.628359	-0.283622
H	-3.619716	-3.445107	0.864546

H	-1.892441	-3.837601	0.850246
C	-1.592047	4.083238	-1.868975
H	-1.230978	5.076320	-2.165575
H	-2.535680	4.225084	-1.327061
H	-1.800525	3.506965	-2.773697
C	1.381213	3.070744	-1.611447
H	1.359158	2.390311	-2.464803
H	2.132424	2.710655	-0.898384
H	1.705159	4.058976	-1.962790
C	-0.030747	4.341068	0.723621
H	0.369142	5.289698	0.340946
H	0.708343	3.946054	1.429866
H	-0.945469	4.578163	1.276891
C	2.139297	-1.606494	-1.400859
H	2.313934	-1.662996	-2.482407
H	1.733339	-2.569746	-1.069850
C	3.420187	-1.292710	-0.671223
C	4.104795	-0.095819	-0.928765
H	3.690983	0.614175	-1.639818
C	5.298599	0.189388	-0.268860
H	5.819695	1.120752	-0.473458
C	5.827208	-0.721153	0.651707
H	6.759503	-0.498381	1.163552
C	5.153868	-1.915017	0.911362
H	5.557295	-2.625766	1.627444
C	3.953209	-2.196170	0.254380
H	3.426652	-3.124619	0.463725
C	1.296644	0.718036	1.426936
C	0.359753	-1.712632	1.425974
N	-1.178308	0.211917	-2.457358
F	-0.666666	1.433663	-3.047204

1i

Fe	-0.017149	-0.587151	-0.980829
C	-0.005366	1.265766	0.037780
O	-0.060935	2.529421	-0.503567
H	0.526799	2.553845	-1.274394
C	-1.184688	0.555292	0.411308
C	-0.697571	-0.655164	1.064196
C	-1.501048	-1.730486	1.751730
H	-2.378527	-2.013684	1.159647
H	-1.895565	-1.328178	2.698216

C	-0.645223	-2.971180	2.055307
H	-1.198635	-3.646812	2.718999
H	-0.454406	-3.523814	1.124521
C	0.690577	-2.570533	2.693904
H	1.256030	-3.459581	2.998865
H	0.485933	-1.997799	3.609843
C	1.545984	-1.715777	1.739876
H	2.353653	-1.240515	2.310763
H	2.041506	-2.367411	1.007044
C	0.716936	-0.653865	1.051181
C	1.189047	0.550113	0.376765
Si	-2.906882	1.321201	0.288767
C	-3.018717	2.688607	1.598786
H	-2.878067	2.290394	2.611107
H	-3.993534	3.191830	1.569920
H	-2.243959	3.444646	1.426886
C	-4.272384	0.047185	0.637075
H	-4.203140	-0.376517	1.645012
H	-4.269748	-0.784075	-0.078089
H	-5.249987	0.539773	0.555805
C	-3.215211	2.081154	-1.416372
H	-3.169816	1.332487	-2.215015
H	-2.461743	2.843674	-1.634299
H	-4.205384	2.553440	-1.452006
Si	2.921763	1.278897	0.260588
C	3.202182	2.404628	1.760658
H	4.188250	2.884752	1.723022
H	3.141477	1.842818	2.700709
H	2.444103	3.195628	1.799560
C	4.278962	-0.047956	0.245396
H	5.257607	0.441141	0.156060
H	4.185224	-0.741811	-0.597222
H	4.294744	-0.641258	1.165654
C	3.110696	2.318419	-1.320191
H	4.168051	2.562567	-1.482578
H	2.574256	3.272738	-1.253525
H	2.757069	1.783027	-2.209991
H	-0.036708	0.189464	-2.318089
P	-1.632780	-1.713787	-1.916595
H	-2.323855	-2.784057	-1.275239
H	-2.799538	-1.039561	-2.357537
H	-1.386011	-2.400026	-3.134938
P	1.553384	-1.699132	-2.006102

H	2.663831	-1.000682	-2.545739
H	2.323894	-2.740069	-1.404004
H	1.237101	-2.410616	-3.193803

2iTS

Fe	-0.086050	-0.172668	-0.677316
C	-1.040257	0.259524	1.201540
O	-0.548549	0.081120	2.443079
H	0.449767	-0.165935	2.443122
C	-0.923808	1.470419	0.435491
C	-1.710272	1.234779	-0.764900
C	-2.062790	2.212701	-1.857616
H	-1.194800	2.810628	-2.154670
H	-2.795083	2.931957	-1.459275
C	-2.674506	1.506325	-3.076879
H	-3.069399	2.252919	-3.776545
H	-1.892446	0.948775	-3.612284
C	-3.784485	0.542509	-2.639148
H	-4.290468	0.110386	-3.510921
H	-4.544790	1.112042	-2.085869
C	-3.242312	-0.588497	-1.744161
H	-4.078137	-1.070274	-1.223721
H	-2.799418	-1.372466	-2.372393
C	-2.251908	-0.077157	-0.720416
C	-1.800921	-0.735508	0.493175
Si	-0.242480	3.063378	1.205375
C	-1.288009	3.417295	2.743923
H	-2.343962	3.565731	2.486418
H	-0.939821	4.318787	3.263662
H	-1.227671	2.573792	3.439512
C	-0.402110	4.537913	0.016935
H	-1.439519	4.732746	-0.277016
H	0.189720	4.414604	-0.898252
H	-0.031328	5.439825	0.521106
C	1.578180	2.903555	1.693787
H	2.236047	2.959585	0.817644
H	1.777707	1.953181	2.198660
H	1.860860	3.721705	2.368688
Si	-2.322358	-2.354466	1.320395
C	-3.548639	-1.923141	2.698142
H	-3.885383	-2.821427	3.230846
H	-4.437196	-1.415723	2.302843

H	-3.076155	-1.253577	3.425420
C	-3.168333	-3.534077	0.092180
H	-3.383995	-4.482579	0.600782
H	-2.535012	-3.768369	-0.772201
H	-4.119806	-3.145748	-0.286913
C	-0.844312	-3.276192	2.061839
H	-1.194095	-4.120624	2.669596
H	-0.246923	-2.621643	2.703432
H	-0.186632	-3.685013	1.285017
H	1.215358	-0.668632	0.147128
C	2.115247	-1.157833	1.183854
H	1.713402	-2.185466	1.101442
O	1.912854	-0.510164	2.261432
C	3.427009	-0.993096	0.455853
C	3.833274	-1.936862	-0.496087
C	4.271604	0.081741	0.758229
C	5.057373	-1.801586	-1.151980
H	3.193223	-2.791194	-0.711069
C	5.495679	0.219049	0.102688
H	3.958188	0.789279	1.518668
C	5.890059	-0.718620	-0.856094
H	5.366737	-2.543507	-1.883750
H	6.147976	1.054195	0.345077
H	6.846078	-0.612876	-1.362157
P	0.125652	-2.008450	-1.876722
H	-0.947820	-2.495086	-2.667858
H	1.124270	-2.114615	-2.881612
H	0.424122	-3.245775	-1.246387
P	1.362280	1.000084	-1.865191
H	2.454634	1.621239	-1.213705
H	2.121205	0.399894	-2.904695
H	0.937606	2.132252	-2.607856

3i

Fe	-0.116128	-0.173439	-0.697933
C	-1.077102	0.209671	1.315093
O	-0.573178	-0.001677	2.458261
H	1.074707	-0.204383	2.462134
C	-0.918463	1.418943	0.485533
C	-1.716793	1.200098	-0.699112
C	-2.132298	2.210570	-1.738659
H	-1.296433	2.853725	-2.033772

H	-2.872066	2.883221	-1.276689
C	-2.768606	1.546397	-2.968815
H	-3.203604	2.314469	-3.619669
H	-1.994137	1.032105	-3.556466
C	-3.841335	0.538757	-2.537184
H	-4.366697	0.132301	-3.409831
H	-4.595117	1.066077	-1.935309
C	-3.244268	-0.615781	-1.710340
H	-4.050402	-1.148941	-1.194074
H	-2.795077	-1.353448	-2.387815
C	-2.242088	-0.127841	-0.684511
C	-1.774349	-0.801894	0.501903
Si	-0.312144	3.061422	1.201169
C	0.836751	2.818779	2.678207
H	0.306585	2.339338	3.506203
H	1.217085	3.790071	3.020774
H	1.689614	2.177821	2.433810
C	-1.851274	4.019728	1.773991
H	-2.413314	3.441641	2.517187
H	-2.532485	4.244629	0.943921
H	-1.569055	4.973263	2.238416
C	0.601123	4.149783	-0.066113
H	0.000611	4.394167	-0.949797
H	1.538401	3.693984	-0.406477
H	0.865942	5.100000	0.415834
Si	-2.259106	-2.438038	1.310288
C	-3.428325	-2.048363	2.748595
H	-3.708579	-2.957641	3.295262
H	-4.351649	-1.569290	2.400141
H	-2.936753	-1.364890	3.449104
C	-3.157109	-3.610306	0.108546
H	-3.365610	-4.555945	0.625709
H	-2.561005	-3.853935	-0.779197
H	-4.118370	-3.211946	-0.234897
C	-0.743727	-3.358269	1.978707
H	-1.054494	-4.234605	2.561839
H	-0.162019	-2.702229	2.633361
H	-0.086047	-3.717095	1.176852
H	1.396795	-0.573750	0.279408
C	2.127232	-1.017459	1.044803
O	2.042137	-0.327956	2.237645
C	3.501153	-0.909590	0.423312
C	3.955123	-1.897308	-0.460256

C	4.325400	0.188929	0.695824
C	5.202692	-1.783211	-1.076350
H	3.336730	-2.772337	-0.652802
C	5.575539	0.301212	0.084460
H	3.983872	0.936973	1.403293
C	6.015991	-0.680058	-0.806956
H	5.544598	-2.561247	-1.754039
H	6.210010	1.154668	0.309559
H	6.990728	-0.592219	-1.279412
H	1.825824	-2.072571	1.130156
P	0.098125	-2.045163	-1.890612
H	0.731282	-3.188378	-1.334436
H	-1.062389	-2.715269	-2.344873
H	0.801089	-2.083048	-3.125852
P	1.254604	1.018263	-2.002460
H	1.780154	0.477344	-3.207023
H	0.812330	2.242934	-2.553365
H	2.491547	1.490307	-1.496520

4i

Fe	-0.002551	-0.532283	0.958749
Si	2.900237	1.295946	-0.278859
Si	-2.887916	1.316719	-0.307374
O	0.011178	2.399381	0.513365
C	0.005497	1.322333	-0.134865
C	1.197799	0.498733	-0.439932
C	0.718015	-0.714796	-1.035374
C	1.518960	-1.825994	-1.681092
H	1.992849	-2.456397	-0.916698
H	2.342828	-1.390518	-2.257256
C	0.650800	-2.704739	-2.599576
H	0.439373	-2.159829	-3.530823
H	1.208864	-3.605334	-2.883061
C	-0.679359	-3.076639	-1.932853
H	-0.480821	-3.602101	-0.987601
H	-1.246135	-3.769336	-2.566742
C	-1.521322	-1.818762	-1.664600
H	-1.905806	-1.439177	-2.624344
H	-2.407638	-2.064711	-1.069488
C	-0.717038	-0.717848	-1.019629
C	-1.190263	0.506488	-0.435010
C	3.201933	1.889541	1.494370

H	3.355307	1.062014	2.197998
H	2.338690	2.472354	1.830904
H	4.092707	2.528787	1.542022
C	2.940527	2.789447	-1.442902
H	2.127358	3.477844	-1.188917
H	2.813253	2.487645	-2.489772
H	3.889258	3.335237	-1.364339
C	4.309752	0.116024	-0.773145
H	5.272936	0.613545	-0.599983
H	4.272996	-0.154359	-1.834868
H	4.317573	-0.814831	-0.193309
C	-2.892689	2.800848	-1.484389
H	-3.836704	3.357196	-1.425688
H	-2.751847	2.488835	-2.526518
H	-2.076346	3.482787	-1.223153
C	-3.223225	1.928662	1.453544
H	-2.368032	2.518571	1.798584
H	-3.384474	1.108379	2.163895
H	-4.117006	2.564878	1.479863
C	-4.291261	0.142010	-0.828890
H	-5.248699	0.676546	-0.776735
H	-4.379314	-0.739114	-0.181509
H	-4.172658	-0.212128	-1.859513
P	-1.649477	-1.549526	2.048568
H	-1.476439	-2.817254	2.670009
H	-2.247969	-0.922167	3.174633
H	-2.856656	-1.860547	1.378605
P	1.625397	-1.592666	2.043933
H	2.246111	-0.988225	3.170267
H	1.422468	-2.858858	2.659326
H	2.820804	-1.931713	1.365622

5i

Fe	0.014912	-0.054741	0.510918
Si	-2.014253	-2.676960	-1.171420
Si	-1.007743	3.030055	-1.219277
O	-0.853172	0.059052	-2.439283
O	1.345512	-0.107154	-1.114874
H	0.653916	-0.074079	-1.861264
C	-1.328415	0.143835	-1.250355
C	-1.699561	-0.988463	-0.397665
C	-2.088149	-0.427681	0.882647

C	-2.806290	-1.117004	2.024416
H	-2.131111	-1.779495	2.582008
H	-3.582308	-1.773477	1.613978
C	-3.455031	-0.113139	2.996521
H	-4.383571	0.274414	2.553466
H	-3.741419	-0.628768	3.921308
C	-2.527661	1.070385	3.298055
H	-1.583796	0.699350	3.723365
H	-2.978653	1.728785	4.050568
C	-2.242137	1.867319	2.016245
H	-3.157243	2.405124	1.721948
H	-1.493918	2.644834	2.203099
C	-1.836972	0.970850	0.872954
C	-1.300295	1.350075	-0.417719
C	-0.533976	-3.280621	-2.187142
H	0.325853	-3.531311	-1.553959
H	-0.229980	-2.505195	-2.896437
H	-0.799367	-4.183149	-2.752429
C	-3.507738	-2.509642	-2.327445
H	-3.302397	-1.747676	-3.087783
H	-4.408683	-2.203717	-1.781436
H	-3.731118	-3.453185	-2.841369
C	-2.395406	-4.016174	0.126501
H	-2.483432	-4.988515	-0.375444
H	-3.337969	-3.838833	0.655968
H	-1.603744	-4.111472	0.879670
C	-2.456402	3.369545	-2.394696
H	-2.329414	4.321241	-2.926292
H	-3.412425	3.410881	-1.858323
H	-2.524199	2.569660	-3.140465
C	0.602893	3.075315	-2.214741
H	0.563777	2.335396	-3.019746
H	1.474819	2.846615	-1.591735
H	0.753048	4.067514	-2.659317
C	-0.940424	4.437494	0.061370
H	-0.779658	5.389682	-0.460917
H	-0.119360	4.323621	0.779903
H	-1.872348	4.532600	0.629789
C	2.395899	-1.022563	-1.445135
H	2.581392	-0.933091	-2.523995
H	2.088836	-2.057630	-1.251687
C	3.656606	-0.698164	-0.678066
C	4.187427	0.600422	-0.701131

H	3.668818	1.375533	-1.258779
C	5.368241	0.895934	-0.021163
H	5.769998	1.905513	-0.049876
C	6.040623	-0.104162	0.688729
H	6.962415	0.126712	1.215858
C	5.524595	-1.399956	0.712544
H	6.041782	-2.184184	1.259043
C	4.337568	-1.691817	0.034382
H	3.941672	-2.705091	0.051795
P	1.305425	1.410043	1.609507
H	2.005279	2.412303	0.894138
H	0.733978	2.269049	2.581877
H	2.406437	0.987108	2.400043
P	0.765261	-1.828778	1.636518
H	-0.147144	-2.564096	2.432765
H	1.322546	-2.956647	0.975371
H	1.787531	-1.731297	2.619437

1j

Fe	0.010163	-0.115433	-0.305120
C	0.474426	1.958027	-0.447547
O	1.023555	2.631303	-1.509264
H	1.874763	2.221076	-1.724617
C	-0.938869	1.815067	-0.310909
C	-1.126004	1.194199	0.994382
C	-2.422334	0.952504	1.727650
H	-3.160677	0.460888	1.085955
H	-2.855147	1.929073	1.996868
C	-2.214341	0.130341	3.010836
H	-3.119979	0.181153	3.627882
H	-2.070730	-0.925865	2.749288
C	-0.998223	0.627123	3.801974
H	-0.915549	0.094020	4.757399
H	-1.138755	1.690254	4.045028
C	0.304755	0.458636	2.998953
H	1.108010	1.017071	3.495912
H	0.616569	-0.594955	3.020646
C	0.139093	0.956331	1.579612
C	1.185657	1.413342	0.669759
Si	-2.153965	2.648048	-1.490087
C	-2.048732	4.520539	-1.197269
H	-2.308085	4.781250	-0.163784

H	-2.731446	5.067044	-1.860476
H	-1.032252	4.884207	-1.386990
C	-3.944814	2.104604	-1.163199
H	-4.293161	2.410269	-0.170313
H	-4.086054	1.020690	-1.244708
H	-4.605874	2.577408	-1.901309
C	-1.726153	2.293925	-3.298902
H	-1.801171	1.227485	-3.537566
H	-0.700237	2.608406	-3.511653
H	-2.403097	2.839138	-3.969095
Si	3.001846	1.736796	1.052421
C	3.102051	3.379878	1.998675
H	4.140768	3.643552	2.235581
H	2.548061	3.332925	2.944186
H	2.674148	4.198601	1.407995
C	3.805898	0.385946	2.110896
H	4.827253	0.693974	2.370186
H	3.270748	0.207453	3.049343
C	4.035449	1.906571	-0.534453
H	5.096905	1.974464	-0.264123
H	3.798959	2.815521	-1.101278
H	3.930491	1.035677	-1.192760
H	0.562600	-0.265874	-1.732817
P	-1.562602	-1.297443	-1.258911
H	-2.253786	-0.703349	-2.342865
H	-1.072005	-2.416840	-1.981431
P	1.203723	-1.883436	0.185119
H	1.544893	-2.147109	1.541970
H	0.623372	-3.163987	-0.051767
C	2.863410	-2.237629	-0.560410
C	3.806989	-3.025233	0.117733
C	3.177127	-1.754718	-1.838182
C	5.038651	-3.321147	-0.468070
C	4.407342	-2.058352	-2.427679
H	2.451847	-1.138419	-2.362209
C	5.340738	-2.838890	-1.743842
H	5.761491	-3.927351	0.071751
H	4.636601	-1.680123	-3.420627
H	6.299428	-3.069915	-2.200616
C	-3.031195	-2.104452	-0.463548
C	-4.308363	-2.043799	-1.040298
C	-2.866975	-2.813912	0.735463
C	-5.395145	-2.677370	-0.433494

H	-4.457299	-1.502292	-1.971452
C	-3.948927	-3.458788	1.336437
H	-1.885569	-2.858919	1.201352
C	-5.216724	-3.388647	0.754191
H	-6.379218	-2.616682	-0.890894
H	-3.804121	-4.009720	2.262089
H	-6.061405	-3.884103	1.225296
H	3.581083	-3.409372	1.109974
H	3.879036	-0.565098	1.573512

2jTS

Fe	0.001482	-0.141566	0.030092
C	-0.267711	-1.537835	-1.607130
O	-0.456535	-1.275086	-2.916814
H	-0.453629	-0.267480	-3.114959
C	1.015571	-1.749434	-1.007381
C	0.737115	-2.132986	0.366318
C	1.705348	-2.650626	1.401421
H	2.587748	-2.008203	1.479030
H	2.073432	-3.633780	1.068849
C	1.045352	-2.815036	2.780474
H	1.708389	-3.392821	3.436115
H	0.919520	-1.830824	3.252297
C	-0.320291	-3.502385	2.659828
H	-0.743524	-3.701243	3.652291
H	-0.184935	-4.479530	2.174369
C	-1.310460	-2.659672	1.834663
H	-2.181044	-3.270436	1.573448
H	-1.703391	-1.844801	2.457762
C	-0.672554	-2.136303	0.564686
C	-1.332340	-1.717592	-0.655048
Si	2.554076	-1.934490	-2.096900
C	2.220873	-3.395130	-3.256650
H	2.052819	-4.323008	-2.696139
H	3.066280	-3.563055	-3.935984
H	1.328454	-3.200227	-3.860574
C	4.101402	-2.338292	-1.070941
H	4.011767	-3.297582	-0.548422
H	4.332986	-1.573074	-0.321442
H	4.966852	-2.412706	-1.742469
C	2.903370	-0.383098	-3.130008
H	3.507697	0.349753	-2.581201

H	1. 976299	0. 108732	-3. 441628
H	3. 465855	-0. 655556	-4. 032171
Si	-3. 122055	-1. 872001	-1. 251607
C	-3. 189328	-3. 419967	-2. 345485
H	-4. 199745	-3. 582283	-2. 742088
H	-2. 900184	-4. 320448	-1. 789590
H	-2. 503537	-3. 313239	-3. 193009
C	-4. 354233	-2. 100130	0. 175445
H	-5. 374785	-2. 058587	-0. 227297
H	-4. 271306	-1. 317738	0. 937063
H	-4. 244609	-3. 071029	0. 672409
C	-3. 679250	-0. 382542	-2. 279554
H	-4. 596333	-0. 636204	-2. 827270
H	-2. 920771	-0. 090115	-3. 011898
H	-3. 905921	0. 482243	-1. 647245
H	-0. 273708	1. 090049	-1. 005593
C	-0. 653650	1. 863348	-2. 187470
H	-1. 718069	1. 869928	-1. 887544
O	-0. 326994	1. 233031	-3. 244907
C	0. 047922	3. 162013	-1. 865514
C	-0. 494017	4. 061058	-0. 938252
C	1. 232265	3. 498594	-2. 531927
C	0. 145998	5. 270339	-0. 664125
H	-1. 425995	3. 816722	-0. 432158
C	1. 874351	4. 706753	-2. 258233
H	1. 623981	2. 807147	-3. 270943
C	1. 336367	5. 593645	-1. 321407
H	-0. 286125	5. 962566	0. 054031
H	2. 791843	4. 962239	-2. 782432
H	1. 835448	6. 536150	-1. 111952
P	-1. 100187	0. 898734	1. 649059
H	-0. 899536	0. 375697	2. 954659
H	-0. 642789	2. 212627	1. 941162
P	1. 824302	1. 072572	0. 421563
H	2. 700203	1. 246897	-0. 671929
H	1. 561471	2. 446386	0. 649759
C	3. 097504	0. 790046	1. 730815
C	4. 464659	0. 757939	1. 417406
C	2. 709187	0. 620329	3. 068695
C	5. 419828	0. 556690	2. 416454
H	4. 788716	0. 894085	0. 388875
C	3. 663487	0. 430898	4. 068629
H	1. 655515	0. 635949	3. 334688

C	5.021585	0.394461	3.743939
H	6.474299	0.530459	2.155259
H	3.345972	0.306704	5.100522
H	5.764347	0.239920	4.521725
C	-2.916164	1.198640	1.823175
C	-3.605036	0.786748	2.973541
C	-3.626137	1.865407	0.813509
C	-4.972873	1.034338	3.110532
H	-3.073848	0.272956	3.770833
C	-4.989943	2.124133	0.955931
H	-3.115276	2.180618	-0.091614
C	-5.667214	1.706146	2.103675
H	-5.492434	0.704637	4.006225
H	-5.524040	2.645564	0.166305
H	-6.730590	1.901391	2.210929

3j

Fe	0.050957	-0.205838	-0.006436
C	-0.272105	-1.340017	-1.943098
O	-0.530630	-0.860576	-3.092278
H	-0.579320	0.754324	-3.170271
C	1.062984	-1.512326	-1.363502
C	0.869014	-2.140750	-0.074544
C	1.901754	-2.797131	0.809022
H	2.775274	-2.153839	0.956435
H	2.273718	-3.691661	0.285133
C	1.321685	-3.230151	2.165186
H	2.041818	-3.877763	2.680184
H	1.177749	-2.349958	2.806252
C	-0.016857	-3.954582	1.980950
H	-0.381302	-4.348264	2.937977
H	0.134842	-4.821333	1.321902
C	-1.079756	-3.027277	1.364362
H	-1.940987	-3.618836	1.037234
H	-1.466649	-2.353757	2.141308
C	-0.534669	-2.256156	0.179681
C	-1.267355	-1.669976	-0.911169
Si	2.563851	-1.409117	-2.505128
C	2.286748	-2.670484	-3.891938
H	2.222336	-3.692624	-3.498496
H	3.099664	-2.645678	-4.628721
H	1.346452	-2.447920	-4.407151

C	4.177437	-1.864103	-1.604847
H	4.165847	-2.894134	-1.230971
H	4.395046	-1.206266	-0.755074
H	5.018126	-1.780103	-2.305835
C	2.783132	0.310306	-3.271474
H	3.232222	1.028071	-2.573826
H	1.820900	0.715658	-3.597705
H	3.444411	0.248882	-4.145447
Si	-3.080835	-1.774877	-1.434704
C	-3.172517	-3.083195	-2.804828
H	-4.193058	-3.182106	-3.196225
H	-2.856589	-4.069498	-2.442646
H	-2.512976	-2.799678	-3.631776
C	-4.238175	-2.315005	-0.026597
H	-5.273604	-2.284065	-0.390691
H	-4.181464	-1.658257	0.848153
H	-4.046068	-3.341828	0.305565
C	-3.719918	-0.129270	-2.118682
H	-4.691128	-0.276811	-2.608677
H	-3.026221	0.280762	-2.858745
H	-3.862989	0.609873	-1.323032
H	-0.193898	1.339337	-1.058032
C	-0.677097	2.108785	-1.758744
H	-1.737795	2.119832	-1.465078
O	-0.493375	1.750350	-3.079099
C	-0.031153	3.442446	-1.442321
C	-0.460334	4.197259	-0.342679
C	1.016037	3.930639	-2.232580
C	0.153322	5.410442	-0.026908
H	-1.288472	3.841208	0.267415
C	1.627466	5.146525	-1.920335
H	1.329767	3.355734	-3.096741
C	1.202587	5.888121	-0.815870
H	-0.194957	5.986824	0.826375
H	2.435395	5.517938	-2.545678
H	1.678092	6.835599	-0.576412
P	-1.110732	0.531044	1.776252
H	-0.926556	-0.283998	2.921634
H	-0.631640	1.728611	2.377919
P	1.893912	0.932682	0.654717
H	2.890118	1.155990	-0.321584
H	1.663000	2.299881	0.960979
C	3.010762	0.491089	2.057798

C	4.403375	0.478122	1.886318
C	2.483871	0.183632	3.321448
C	5.248290	0.163715	2.952710
H	4.833921	0.718114	0.917832
C	3.328964	-0.118220	4.389805
H	1.409105	0.180383	3.478529
C	4.713376	-0.132485	4.207023
H	6.324184	0.154330	2.801121
H	2.904856	-0.347432	5.363682
H	5.370739	-0.374126	5.037602
C	-2.919499	0.837165	2.015412
C	-3.628648	0.183502	3.033979
C	-3.600523	1.751401	1.197858
C	-4.987811	0.438146	3.230132
H	-3.120732	-0.526556	3.681714
C	-4.955764	2.014237	1.401427
H	-3.076371	2.261909	0.395039
C	-5.653220	1.355937	2.416500
H	-5.523268	-0.079572	4.021345
H	-5.466846	2.728347	0.761663
H	-6.709896	1.556008	2.570298

4j

Fe	-0.036640	-0.217629	-0.056774
C	-2.011116	-0.235935	-0.711354
O	-2.152815	0.388091	-1.802684
C	-1.504281	-1.620332	-0.607096
C	-1.167408	-1.829290	0.771685
C	-0.726695	-3.104921	1.445348
H	0.024316	-3.633225	0.847808
H	-1.595472	-3.780142	1.490811
C	-0.214416	-2.866188	2.875235
H	-0.099572	-3.828300	3.389263
H	0.783161	-2.405628	2.842019
C	-1.167877	-1.951209	3.654072
H	-0.849422	-1.860332	4.699830
H	-2.167061	-2.409685	3.668328
C	-1.257975	-0.554182	3.014194
H	-2.098856	-0.002575	3.452090
H	-0.358246	0.023936	3.266217
C	-1.429891	-0.631687	1.511964
C	-1.948432	0.380322	0.632829

Si	-1.689301	-2.767339	-2.091669
C	-3.541423	-2.863432	-2.483762
H	-4.110246	-3.278148	-1.642438
H	-3.736162	-3.491640	-3.362246
H	-3.929222	-1.859658	-2.689710
C	-1.066240	-4.526493	-1.721919
H	-1.587440	-4.982556	-0.872225
H	0.009720	-4.560462	-1.510905
H	-1.244648	-5.166203	-2.595980
C	-0.782918	-2.110772	-3.619975
H	0.307801	-2.182123	-3.531208
H	-1.048203	-1.059841	-3.771624
H	-1.076335	-2.676922	-4.513371
Si	-2.901209	1.946506	1.087726
C	-4.542469	1.352859	1.845941
H	-5.175834	2.204374	2.126155
H	-4.390802	0.743254	2.745249
H	-5.102802	0.743796	1.126323
C	-2.035534	3.046615	2.376657
H	-2.733632	3.827412	2.706019
H	-1.713995	2.498972	3.270109
C	-3.298759	3.008174	-0.423204
H	-4.074097	3.743613	-0.171796
H	-3.647554	2.386034	-1.251643
H	-2.418741	3.556917	-0.775488
P	1.720986	-1.355204	-0.796996
H	1.565029	-2.763461	-0.849666
H	2.065014	-1.182999	-2.163569
P	1.102752	1.523644	0.747156
H	0.671363	2.081420	1.975286
H	2.474055	1.424284	1.097137
C	1.183906	3.006154	-0.346552
C	2.087438	4.053686	-0.108037
C	0.337333	3.068402	-1.464105
C	2.140078	5.149007	-0.969395
C	0.394162	4.168716	-2.325100
H	-0.373542	2.267711	-1.660672
C	1.292842	5.207140	-2.079938
H	2.842639	5.955384	-0.776067
H	-0.266777	4.208236	-3.186491
H	1.336688	6.060131	-2.751970
C	3.426749	-1.245879	-0.098755
C	4.548214	-1.073136	-0.922859

C	3.613064	-1.326997	1.289838
C	5.828511	-0.990569	-0.371004
H	4.425077	-1.005490	-2.000828
C	4.893291	-1.256785	1.840271
H	2.751375	-1.441591	1.942985
C	6.003938	-1.086263	1.010334
H	6.687736	-0.854167	-1.022190
H	5.022825	-1.328732	2.916915
H	7.000502	-1.024663	1.438967
H	2.753531	4.014033	0.750777
H	-1.160480	3.555690	1.956337

5j

Fe	-0.429224	-0.145375	0.002558
Si	-1.827890	3.151401	1.090754
Si	1.709489	-1.041579	2.957512
O	1.091965	1.915562	1.715695
O	1.358521	0.810046	-0.594190
H	1.494993	1.348944	0.260706
C	0.103786	1.094727	1.776722
C	-1.251708	1.370504	1.303615
C	-2.005853	0.142276	1.467909
C	-3.506741	-0.052179	1.391749
H	-3.849346	-0.106521	0.352147
H	-4.003385	0.824049	1.822738
C	-3.963539	-1.313660	2.148810
H	-3.946538	-1.115953	3.230396
H	-5.004197	-1.542467	1.887848
C	-3.056301	-2.514849	1.856398
H	-3.058490	-2.717119	0.776321
H	-3.442559	-3.416646	2.347744
C	-1.621881	-2.241668	2.333811
H	-1.601752	-2.279670	3.434462
H	-0.946807	-3.038627	2.003471
C	-1.126305	-0.881338	1.910574
C	0.210722	-0.343199	2.048546
C	-0.752474	4.149404	-0.110388
H	-0.862113	3.817597	-1.150184
H	0.301528	4.069622	0.171145
H	-1.036580	5.209179	-0.075999
C	-1.731952	3.984945	2.791370
H	-0.703960	3.937340	3.167923

H	-2.378961	3.483545	3.521669
H	-2.031504	5.039832	2.746565
C	-3.621313	3.271975	0.460369
H	-3.840411	4.315793	0.199910
H	-4.352993	2.968091	1.217120
H	-3.804558	2.665679	-0.435003
C	1.556842	-0.477339	4.766241
H	2.402731	-0.831406	5.369505
H	0.636043	-0.850130	5.232057
H	1.538356	0.617304	4.822994
C	3.350413	-0.398311	2.275218
H	3.338416	0.694524	2.240361
H	3.550023	-0.770401	1.265149
H	4.178225	-0.721577	2.920033
C	1.758645	-2.943028	2.943870
H	2.668329	-3.280031	3.457979
H	1.793124	-3.352984	1.927767
H	0.905814	-3.392337	3.465078
C	1.598862	1.650671	-1.733882
H	0.878269	2.478365	-1.732439
H	1.411803	1.036597	-2.619594
C	3.016250	2.180306	-1.762226
C	3.498227	2.972429	-0.708513
H	2.858171	3.184383	0.144819
C	4.799911	3.470996	-0.740986
H	5.163090	4.079899	0.082583
C	5.634818	3.192371	-1.827063
H	6.647973	3.584972	-1.850846
C	5.163183	2.406421	-2.878877
H	5.806853	2.182575	-3.725643
C	3.861327	1.900624	-2.842066
H	3.498288	1.284783	-3.662452
P	0.139354	-2.174609	-0.810042
H	-0.436810	-3.284817	-0.143303
H	-0.376596	-2.517713	-2.093757
P	-1.596098	0.395087	-1.849012
H	-1.838672	1.765458	-2.117189
H	-0.918176	0.133992	-3.073971
C	-3.266919	-0.245208	-2.306982
C	-4.232665	0.592581	-2.884735
C	-3.584029	-1.595023	-2.092772
C	-5.484835	0.090230	-3.244311
H	-4.008823	1.642284	-3.056325

C	-4.831502	-2.099458	-2.462101
H	-2.856117	-2.253036	-1.627331
C	-5.785313	-1.257092	-3.037401
H	-6.223793	0.753026	-3.686313
H	-5.060523	-3.148160	-2.292965
H	-6.759418	-1.647932	-3.318251
C	1.844444	-2.849573	-1.040591
C	2.066165	-4.233964	-1.122627
C	2.929726	-1.973678	-1.181042
C	3.349466	-4.731725	-1.346829
H	1.235774	-4.927266	-1.010161
C	4.213590	-2.476054	-1.413217
H	2.767610	-0.905784	-1.083847
C	4.425447	-3.852159	-1.496738
H	3.509806	-5.805214	-1.402931
H	5.046596	-1.786213	-1.518280
H	5.425027	-4.241323	-1.671300

1k

Fe	0.112872	0.679154	-0.334348
C	-0.156353	-1.356943	-0.768407
O	-0.260590	-1.873177	-2.053540
H	-0.090723	-1.130318	-2.654750
C	1.085262	-1.260270	-0.062721
C	0.714468	-0.779449	1.256331
C	1.589552	-0.669722	2.482428
H	2.538665	-0.171751	2.266044
H	1.859721	-1.689054	2.799934
C	0.873808	0.028954	3.648698
H	1.466162	-0.083989	4.565291
H	0.798104	1.107272	3.447812
C	-0.533936	-0.546260	3.841493
H	-1.007593	-0.121777	4.735576
H	-0.455348	-1.630079	4.009737
C	-1.415588	-0.279181	2.608948
H	-2.331810	-0.877793	2.684121
H	-1.737611	0.768676	2.624779
C	-0.689226	-0.609682	1.320609
C	-1.274820	-0.985482	0.040148
Si	2.598489	-2.175585	-0.717705
C	2.114868	-4.001141	-0.907677
H	1.842427	-4.443233	0.058722

H	2.943545	-4.590508	-1.321098
H	1.255592	-4.102286	-1.578626
C	4.074866	-2.143276	0.479740
H	3.804541	-2.551266	1.460696
H	4.503911	-1.149588	0.636531
H	4.869852	-2.781918	0.072805
C	3.150355	-1.538833	-2.418433
H	3.327195	-0.458014	-2.428584
H	2.379727	-1.750975	-3.167850
H	4.073882	-2.037612	-2.739453
Si	-3.015654	-1.658845	-0.264087
C	-3.061974	-3.350550	0.602843
H	-4.036654	-3.836929	0.468282
H	-2.880109	-3.263411	1.681000
H	-2.294998	-4.017915	0.192343
C	-4.425742	-0.622554	0.486031
H	-5.364594	-1.179914	0.368814
H	-4.564282	0.346415	-0.004958
H	-4.292910	-0.438202	1.557922
C	-3.406581	-1.949821	-2.094570
H	-4.406702	-2.393222	-2.187544
H	-2.679163	-2.638098	-2.533399
H	-3.393954	-1.033676	-2.694455
H	0.280354	0.905789	-1.856593
P	1.836630	2.112335	-0.142742
P	-1.466333	2.248153	-0.599989
C	1.803114	3.403822	1.205618
H	1.819577	2.898673	2.177169
H	2.663175	4.081829	1.148130
H	0.884239	3.994246	1.156193
C	3.561570	1.484880	0.156339
H	4.267592	2.323432	0.166106
H	3.633051	0.963277	1.111939
H	3.850994	0.792104	-0.636265
C	2.244623	3.143347	-1.634764
H	2.477871	2.465473	-2.461269
H	1.404222	3.765228	-1.941011
H	3.109901	3.788055	-1.440783
C	-2.703238	1.858175	-1.929227
H	-3.211963	0.917584	-1.722753
H	-3.449694	2.655603	-2.026846
H	-2.165261	1.748435	-2.875763
C	-1.078147	3.973955	-1.194777

H	-0.373284	4.492313	-0.540165
H	-0.652284	3.927714	-2.200591
H	-2.001386	4.562022	-1.241397
C	-2.594954	2.709856	0.808406
H	-3.354909	3.433250	0.489997
H	-3.098023	1.823620	1.200419
H	-2.006692	3.153707	1.618881

2kTS

Fe	0.064674	-0.191593	0.462606
C	1.249760	0.407282	-1.291855
O	0.859860	0.436025	-2.582879
H	-0.141376	0.631643	-2.670108
C	1.210043	1.519067	-0.381420
C	1.882659	1.034640	0.813339
C	2.365806	1.857000	1.987889
H	1.558287	2.433881	2.450535
H	3.069804	2.606058	1.599363
C	3.094944	1.021899	3.053745
H	3.643584	1.692656	3.726537
H	2.369693	0.477252	3.674617
C	4.038780	0.007039	2.402310
H	4.629223	-0.517404	3.164064
H	4.751596	0.534957	1.752949
C	3.234412	-1.008873	1.575503
H	3.919330	-1.651135	1.011770
H	2.701665	-1.666809	2.268917
C	2.287054	-0.310644	0.619118
C	1.871040	-0.743809	-0.704020
Si	1.035040	3.283140	-1.069444
C	2.234832	3.395511	-2.535531
H	3.268129	3.213961	-2.213976
H	2.198113	4.391414	-2.995419
H	1.987532	2.651028	-3.297815
C	1.604673	4.626743	0.155689
H	2.663608	4.525413	0.419223
H	1.029986	4.674397	1.086455
H	1.489616	5.598868	-0.342173
C	-0.703929	3.740362	-1.669308
H	-1.318005	4.157975	-0.862929
H	-1.227644	2.875415	-2.088138
H	-0.630042	4.508970	-2.449605

Si	2.580527	-2.096281	-1.822728
C	4.124666	-1.348939	-2.637254
H	4.607353	-2.066340	-3.313238
H	4.867890	-1.041722	-1.891087
H	3.855043	-0.462795	-3.223110
C	3.156507	-3.657338	-0.892590
H	3.497496	-4.394459	-1.631582
H	2.374238	-4.139827	-0.296543
H	4.003357	-3.459495	-0.226187
C	1.400980	-2.630168	-3.204817
H	1.874038	-3.408669	-3.817886
H	1.173713	-1.772997	-3.843796
H	0.450359	-3.029655	-2.836851
H	-1.284420	-0.267324	-0.516574
C	-2.037184	-0.276947	-1.852591
H	-1.641907	-1.281832	-2.083872
O	-1.662708	0.702590	-2.569670
C	-3.466017	-0.298839	-1.372382
C	-4.084053	-1.493965	-0.984972
C	-4.223410	0.879668	-1.401252
C	-5.426307	-1.509897	-0.600960
H	-3.517747	-2.422122	-1.001882
C	-5.563927	0.867156	-1.016120
H	-3.745773	1.790965	-1.746407
C	-6.168075	-0.326230	-0.608249
H	-5.895880	-2.445805	-0.308760
H	-6.143167	1.786685	-1.043604
H	-7.214105	-0.336509	-0.313474
P	-0.483697	-2.301866	1.165128
P	-1.215265	0.915760	1.998619
C	-0.748204	0.699461	3.789130
H	0.283715	1.022695	3.947008
H	-1.405607	1.278099	4.448883
H	-0.812962	-0.356756	4.069951
C	-3.051358	0.660983	2.122072
H	-3.514955	0.835080	1.148848
H	-3.305958	-0.347627	2.445030
H	-3.467699	1.370736	2.846168
C	-1.262841	2.765187	1.889019
H	-1.836836	3.184647	2.723462
H	-0.260495	3.191814	1.897460
H	-1.742890	3.047824	0.949309
C	-2.085993	-2.620121	2.057422

H	-2.093765	-2.122783	3.031333
H	-2.929584	-2.252086	1.468900
H	-2.213691	-3.695964	2.222314
C	0.629500	-3.261970	2.306890
H	0.181079	-4.233745	2.543362
H	1.602536	-3.432519	1.841916
H	0.784455	-2.711789	3.240442
C	-0.683349	-3.568431	-0.178783
H	0.267834	-3.735840	-0.683654
H	-1.038717	-4.520713	0.231927
H	-1.398377	-3.214597	-0.925352

3k

Fe	0.265904	-0.084953	0.545068
C	1.234901	0.262866	-1.470859
O	0.654673	0.292528	-2.603624
H	-0.969590	0.536864	-2.675934
C	1.404068	1.400324	-0.559776
C	2.162475	0.900395	0.564128
C	2.884439	1.695816	1.626631
H	2.239685	2.451258	2.084281
H	3.685363	2.262464	1.127718
C	3.521898	0.811586	2.709481
H	4.196357	1.417899	3.326808
H	2.745738	0.417509	3.381680
C	4.275440	-0.359311	2.070959
H	4.816486	-0.936328	2.831313
H	5.031424	0.037224	1.378036
C	3.308017	-1.282024	1.310378
H	3.876619	-1.999792	0.710187
H	2.752241	-1.876297	2.041831
C	2.372861	-0.503654	0.406983
C	1.741759	-0.946928	-0.811607
Si	1.258131	3.125407	-1.327781
C	2.266402	3.085018	-2.934042
H	3.322178	2.863774	-2.732177
H	2.221445	4.051603	-3.452213
H	1.881640	2.309445	-3.602331
C	2.050330	4.492115	-0.262496
H	3.108411	4.288313	-0.060816
H	1.552919	4.667847	0.696362
H	2.006843	5.433748	-0.825750

C	-0.521714	3.641084	-1.743382
H	-1.034982	4.122374	-0.901905
H	-1.122998	2.783474	-2.062209
H	-0.509281	4.368168	-2.565699
Si	2.101917	-2.430173	-1.923457
C	3.445196	-1.865021	-3.139513
H	3.724891	-2.668597	-3.832755
H	4.353990	-1.542259	-2.616551
H	3.078171	-1.018203	-3.729566
C	2.808569	-3.937068	-0.986471
H	2.826124	-4.802431	-1.661911
H	2.235807	-4.231133	-0.099239
H	3.841754	-3.763435	-0.663283
C	0.610232	-2.986216	-2.950107
H	0.941237	-3.666943	-3.745409
H	0.156411	-2.107379	-3.417182
H	-0.158530	-3.508132	-2.371417
H	-1.659879	-0.187886	-0.619729
C	-2.273685	-0.357288	-1.557720
H	-2.033533	-1.386125	-1.872201
O	-1.958087	0.579709	-2.536381
C	-3.738462	-0.270811	-1.183258
C	-4.419852	-1.394971	-0.699551
C	-4.435930	0.937462	-1.308170
C	-5.761355	-1.311446	-0.319075
H	-3.904316	-2.352050	-0.642145
C	-5.778078	1.022089	-0.933425
H	-3.919824	1.797305	-1.722162
C	-6.444035	-0.098658	-0.430922
H	-6.275818	-2.196224	0.047478
H	-6.308545	1.964884	-1.041786
H	-7.489941	-0.031393	-0.143287
P	-0.527122	-2.069147	1.534365
P	-0.811402	1.297027	2.048124
C	-0.471893	0.959291	3.847772
H	0.587845	1.143837	4.049636
H	-1.071430	1.609573	4.495505
H	-0.684500	-0.081901	4.101952
C	-2.670018	1.357534	2.018061
H	-3.000635	1.740111	1.048241
H	-3.119454	0.373884	2.152811
H	-3.041324	2.025230	2.804203
C	-0.526620	3.128619	2.048420

H	-1.122964	3.595336	2.840669
H	0.523816	3.369776	2.213447
H	-0.826205	3.546570	1.086300
C	-2.186055	-2.099365	2.383413
H	-2.213270	-1.424181	3.241783
H	-2.972792	-1.802945	1.683604
H	-2.402069	-3.113486	2.738107
C	0.487654	-2.893627	2.858255
H	-0.091224	-3.690062	3.339030
H	1.385491	-3.336585	2.420731
H	0.797252	-2.168241	3.616237
C	-0.811767	-3.517646	0.411697
H	0.125795	-3.838017	-0.042361
H	-1.245120	-4.357147	0.967778
H	-1.495345	-3.232916	-0.392255

4k

Fe	0.101456	0.636674	-0.180784
Si	2.536570	-2.176497	-0.727387
Si	-3.022012	-1.651012	-0.240507
O	-0.327115	-1.746810	-1.940989
C	-0.216338	-1.435730	-0.722467
C	1.057038	-1.270828	0.009658
C	0.717733	-0.762830	1.308001
C	1.618352	-0.561061	2.510712
H	2.201209	0.364115	2.415374
H	2.353549	-1.372546	2.555682
C	0.821549	-0.499355	3.826104
H	0.474725	-1.507755	4.094164
H	1.478024	-0.166720	4.639995
C	-0.395307	0.425223	3.693765
H	-0.061403	1.426946	3.386459
H	-0.899380	0.540591	4.661399
C	-1.382939	-0.133510	2.658048
H	-1.875338	-1.018990	3.089510
H	-2.185620	0.585709	2.461972
C	-0.698658	-0.547307	1.379402
C	-1.309424	-0.958075	0.141609
C	3.032966	-1.482410	-2.423160
H	3.463654	-0.474580	-2.389386
H	2.137028	-1.450048	-3.052050
H	3.769806	-2.137707	-2.905491

C	2.001590	-3.978071	-0.984829
H	1.116554	-4.011460	-1.627770
H	1.749668	-4.460448	-0.032109
H	2.797668	-4.567613	-1.457502
C	4.053363	-2.236434	0.424065
H	4.859998	-2.785464	-0.079669
H	3.825712	-2.782492	1.347851
H	4.451849	-1.257078	0.705732
C	-2.800132	-3.528983	-0.382936
H	-3.746311	-4.029337	-0.625389
H	-2.423091	-3.959123	0.553086
H	-2.076875	-3.754801	-1.173205
C	-3.780500	-1.053929	-1.874341
H	-3.048142	-1.181153	-2.678707
H	-4.106816	-0.008038	-1.862032
H	-4.658483	-1.666570	-2.117151
C	-4.275232	-1.356754	1.165329
H	-5.230617	-1.823985	0.892571
H	-4.479992	-0.303045	1.383967
H	-3.941699	-1.827117	2.097838
P	-1.465176	2.247857	-0.627750
P	1.904243	2.022037	-0.202525
C	-3.136292	2.180196	0.167548
H	-3.805721	2.924945	-0.278186
H	-3.575407	1.191105	0.051844
H	-3.038682	2.389802	1.237732
C	-1.855293	2.074561	-2.437175
H	-2.035402	1.024198	-2.675659
H	-2.730862	2.671071	-2.719580
H	-0.996888	2.412866	-3.027459
C	-1.242015	4.098902	-0.536181
H	-1.191656	4.419951	0.509422
H	-0.328321	4.423181	-1.040469
H	-2.092907	4.603091	-1.008805
C	1.902859	3.437703	1.002636
H	1.009497	4.052055	0.885397
H	1.899730	3.031206	2.019294
H	2.790312	4.069357	0.877878
C	2.191518	2.888896	-1.826412
H	3.033710	3.588216	-1.768930
H	2.410646	2.137110	-2.592118
H	1.300410	3.437410	-2.143495
C	3.633705	1.419832	0.093733

H	3.724553	0.980250	1.089576
H	3.898260	0.657172	-0.639499
H	4.341055	2.253161	0.012199

5k

Fe	0.219084	-0.163356	0.456179
C	1.190509	0.471331	-1.457166
O	0.486282	0.511275	-2.541306
H	-0.803991	0.195454	-1.745332
C	1.257635	1.540110	-0.468559
C	2.059256	1.026346	0.621108
C	2.693151	1.820087	1.737294
H	1.974847	2.490841	2.218348
H	3.449705	2.482059	1.286482
C	3.392825	0.927364	2.771212
H	3.996303	1.545389	3.447749
H	2.643598	0.414477	3.391945
C	4.268470	-0.114991	2.064132
H	4.854541	-0.690044	2.792228
H	4.989963	0.405043	1.417954
C	3.412053	-1.071918	1.216138
H	4.058957	-1.685286	0.579714
H	2.913501	-1.772558	1.896996
C	2.413037	-0.323588	0.352664
C	1.840951	-0.719586	-0.921229
Si	1.021114	3.303558	-1.093843
C	-0.630064	3.600316	-1.975703
H	-0.783835	2.802279	-2.708380
H	-0.599568	4.559172	-2.509599
H	-1.491225	3.623775	-1.301043
C	2.393138	3.593697	-2.375083
H	2.298461	2.871300	-3.193350
H	3.390714	3.472652	-1.934924
H	2.336382	4.602859	-2.803162
C	1.261303	4.629277	0.256336
H	2.284260	4.618393	0.649708
H	0.580476	4.542266	1.110886
H	1.095997	5.620093	-0.186957
Si	2.239413	-2.062205	-2.185077
C	3.066972	-1.212182	-3.664993
H	3.277582	-1.926995	-4.471083
H	4.017929	-0.747539	-3.375286

H	2.411327	-0.428195	-4.055850
C	3.487701	-3.369420	-1.581486
H	3.674080	-4.073115	-2.403710
H	3.157663	-3.957313	-0.719942
H	4.453553	-2.914775	-1.329146
C	0.685134	-2.945054	-2.825154
H	0.945512	-3.696135	-3.582033
H	0.030299	-2.202404	-3.292646
H	0.113867	-3.449925	-2.037121
H	-2.137608	-2.043621	-1.013932
C	-2.338340	-1.063590	-1.455884
O	-1.399870	-0.103253	-0.963977
C	-3.769829	-0.651644	-1.181339
C	-4.704239	-1.579193	-0.705968
C	-4.194139	0.659696	-1.441865
C	-6.035322	-1.209504	-0.492175
H	-4.390144	-2.601276	-0.504525
C	-5.520285	1.032622	-1.225249
H	-3.476051	1.384224	-1.816125
C	-6.445776	0.098841	-0.748960
H	-6.747217	-1.942805	-0.121981
H	-5.835061	2.052082	-1.433238
H	-7.479251	0.390377	-0.581668
H	-2.183061	-1.164425	-2.538327
P	-0.090975	-2.193909	1.522072
P	-1.128463	0.993993	1.948886
C	0.257968	-2.175217	3.351940
H	0.203359	-3.183100	3.779402
H	1.258832	-1.769387	3.527273
H	-0.459513	-1.537143	3.874542
C	-1.736273	-3.077600	1.511841
H	-2.574586	-2.404223	1.693509
H	-1.881314	-3.546325	0.533775
H	-1.744937	-3.869368	2.270007
C	0.936020	-3.666095	1.046528
H	1.999977	-3.457095	1.159103
H	0.676325	-4.526134	1.674711
H	0.750172	-3.922360	0.001448
C	-0.458827	1.603051	3.573544
H	0.336971	2.332407	3.405516
H	-1.250144	2.081720	4.161931
H	-0.039413	0.775239	4.152468
C	-2.684517	0.173540	2.561075

H	-3.293499	-0.139390	1.708007
H	-2.461321	-0.702554	3.175705
H	-3.268117	0.876354	3.166492
C	-1.904018	2.545770	1.306832
H	-2.596556	2.968716	2.043999
H	-1.138864	3.285584	1.071458
H	-2.450148	2.308811	0.391152

11

Fe	0.072649	-0.533404	-0.372068
C	-0.116539	1.577459	-0.505765
O	-0.185150	2.352677	-1.623938
H	-1.012964	2.165623	-2.093732
C	-1.221709	1.049860	0.239173
C	-0.614639	0.400061	1.397730
C	-1.302402	-0.257162	2.567488
H	-2.134067	-0.881646	2.229641
H	-1.736614	0.522036	3.214120
C	-0.304911	-1.091071	3.387777
H	-0.785233	-1.438472	4.309918
H	-0.017855	-1.982697	2.814970
C	0.946741	-0.266376	3.715378
H	1.612053	-0.821862	4.386259
H	0.640100	0.639967	4.256885
C	1.723929	0.137654	2.446474
H	2.393382	0.973309	2.680013
H	2.375841	-0.683424	2.131774
C	0.793800	0.562169	1.328406
C	1.139568	1.260766	0.099450
Si	-3.021737	1.625695	0.035038
C	-3.156906	3.229889	1.033887
H	-2.953208	3.057898	2.097595
H	-4.164099	3.657746	0.954215
H	-2.444077	3.982470	0.677105
C	-4.290213	0.384963	0.685638
H	-4.192289	0.222321	1.764264
H	-4.224725	-0.587294	0.189882
H	-5.296758	0.783553	0.505214
C	-3.414766	2.006387	-1.784252
H	-3.154737	1.178017	-2.452681
H	-2.935827	2.925934	-2.144677
H	-4.495557	2.166827	-1.885326

Si	2.775258	1.964088	-0.568929
C	2.620438	3.852083	-0.491247
H	3.526705	4.333545	-0.879716
H	2.475562	4.200922	0.538687
H	1.770323	4.199896	-1.087491
C	4.256616	1.449526	0.493773
H	5.173702	1.833251	0.028371
H	4.360021	0.363642	0.575594
H	4.208658	1.868648	1.505343
C	3.036290	1.412198	-2.355034
H	3.918595	1.900986	-2.787075
H	2.166035	1.671487	-2.966314
H	3.182238	0.329120	-2.416214
H	0.280004	-0.540511	-1.876081
P	-1.458731	-1.803077	-0.895076
P	1.567356	-1.961660	-0.339878
F	-1.166980	-3.140479	-1.702853
F	-2.597281	-1.243125	-1.872159
F	-2.471164	-2.434525	0.175284
F	1.595673	-3.129221	-1.414407
F	1.801874	-2.874979	0.956205
F	3.094176	-1.514398	-0.493157

21TS

Fe	-0.231384	-0.127676	-0.402339
C	-1.139895	0.642853	1.429009
O	-0.680588	0.542614	2.651530
H	0.342074	-0.002274	2.739106
C	-0.828596	1.714961	0.503560
C	-1.633318	1.457104	-0.674277
C	-1.867580	2.362203	-1.858140
H	-0.937362	2.814469	-2.208001
H	-2.500171	3.195786	-1.515445
C	-2.583484	1.632239	-3.003474
H	-2.881603	2.358358	-3.768705
H	-1.888366	0.931244	-3.485282
C	-3.808575	0.877580	-2.474529
H	-4.376687	0.431764	-3.299191
H	-4.480762	1.596093	-1.983967
C	-3.415983	-0.224973	-1.473053
H	-4.299088	-0.535367	-0.904005
H	-3.086930	-1.117455	-2.011448

C	-2.353237	0.239474	-0.497008
C	-2.005560	-0.331175	0.789122
Si	0.016656	3.316265	1.094564
C	-1.215346	4.114151	2.293369
H	-2.169772	4.343135	1.803630
H	-0.814864	5.052542	2.696986
H	-1.420561	3.443809	3.135307
C	0.338762	4.516005	-0.339375
H	-0.581828	4.864725	-0.819862
H	0.986387	4.084215	-1.110285
H	0.854356	5.400689	0.056315
C	1.646304	2.976983	1.979656
H	2.424894	2.675710	1.271941
H	1.534642	2.181434	2.720865
H	1.988384	3.885050	2.492467
Si	-2.759031	-1.747964	1.818688
C	-3.626225	-0.942731	3.295026
H	-4.055092	-1.704441	3.958193
H	-4.444163	-0.287996	2.969774
H	-2.918702	-0.339721	3.872251
C	-4.041946	-2.752524	0.850490
H	-4.386973	-3.579742	1.484452
H	-3.639494	-3.187676	-0.068727
H	-4.925911	-2.159173	0.589395
C	-1.402888	-2.919298	2.423131
H	-1.829699	-3.675914	3.093446
H	-0.632224	-2.376070	2.979926
H	-0.920655	-3.450022	1.593959
H	0.992252	-0.617543	0.547934
C	1.730074	-1.158763	1.621956
H	1.260241	-2.148179	1.531716
O	1.473362	-0.470332	2.690611
C	3.132325	-1.114310	1.090599
C	3.592154	-2.116208	0.224788
C	4.007857	-0.098676	1.498009
C	4.909004	-2.098983	-0.233915
H	2.919974	-2.911121	-0.085468
C	5.322639	-0.082015	1.036212
H	3.647696	0.657257	2.186809
C	5.775647	-1.079868	0.168139
H	5.258889	-2.881610	-0.901532
H	5.998046	0.706123	1.358172
H	6.802004	-1.066276	-0.188898

P	-0.275571	-2.016749	-1.308055
P	1.269704	0.652056	-1.641475
F	0.911384	1.397439	-3.006353
F	2.368106	-0.335233	-2.229825
F	2.271000	1.761921	-1.091030
F	-1.646193	-2.820371	-1.458820
F	0.559095	-3.227678	-0.674881
F	0.219198	-2.221689	-2.810923

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Fe	-0.192903	-0.036629	-0.374251
C	-1.317726	0.349883	1.573576
O	-0.895204	0.287151	2.756835
H	0.761883	0.146370	2.919594
C	-1.224618	1.516200	0.668502
C	-1.934874	1.151119	-0.529490
C	-2.402528	2.042418	-1.654147
H	-1.626815	2.752779	-1.948274
H	-3.232482	2.651714	-1.265434
C	-2.902395	1.233437	-2.860176
H	-3.370052	1.910537	-3.584262
H	-2.050789	0.762132	-3.367712
C	-3.898985	0.162108	-2.404784
H	-4.335837	-0.355384	-3.266514
H	-4.730188	0.653851	-1.879539
C	-3.239766	-0.871058	-1.471579
H	-4.017433	-1.423205	-0.931088
H	-2.703347	-1.616112	-2.063519
C	-2.317134	-0.229545	-0.455569
C	-1.831728	-0.787007	0.781179
Si	-0.711906	3.221405	1.351564
C	1.145076	3.305162	1.688257
H	1.483987	2.449548	2.280462
H	1.384634	4.222010	2.241794
H	1.719794	3.324110	0.754692
C	-1.685207	3.468050	2.956103
H	-1.492685	2.648976	3.654722
H	-2.765010	3.501746	2.764454
H	-1.404067	4.413241	3.437204
C	-1.177765	4.632754	0.172661
H	-2.249928	4.655585	-0.053558
H	-0.627522	4.598119	-0.772511

H	-0.930448	5.584792	0.660194
Si	-2.258272	-2.429175	1.639247
C	-3.729901	-2.061642	2.773644
H	-4.040459	-2.962443	3.317521
H	-4.597660	-1.698138	2.209637
H	-3.462357	-1.296395	3.510664
C	-2.753906	-3.777944	0.399245
H	-2.871617	-4.725562	0.940549
H	-2.000783	-3.941703	-0.378480
H	-3.707601	-3.568947	-0.097436
C	-0.811036	-3.077569	2.666753
H	-1.144742	-3.919050	3.287176
H	-0.418904	-2.301183	3.329975
H	0.003424	-3.442459	2.031740
H	1.234774	-0.146580	0.696663
C	1.883005	-0.638808	1.549290
O	1.733466	0.084158	2.710298
C	3.305946	-0.625250	1.050524
C	3.810005	-1.724936	0.345477
C	4.133821	0.480664	1.280137
C	5.121148	-1.717356	-0.132967
H	3.180824	-2.595538	0.180018
C	5.444615	0.485547	0.804420
H	3.749018	1.324303	1.842897
C	5.940973	-0.610728	0.094025
H	5.502476	-2.578744	-0.674546
H	6.081800	1.345818	0.991656
H	6.963247	-0.604552	-0.274531
H	1.497853	-1.661579	1.623546
P	0.308977	-1.854259	-1.337532
P	0.897708	1.136681	-1.746184
F	2.477301	1.031796	-1.856575
F	0.566626	0.933468	-3.296632
F	0.798094	2.729500	-1.748339
F	1.561433	-1.913474	-2.321127
F	-0.713215	-2.630504	-2.282789
F	0.717148	-3.115976	-0.440139

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Fe	0.000641	-0.481144	-0.331916
Si	-2.915206	1.747816	-0.428104
Si	2.901410	1.782504	-0.385328

O	-0.005255	1.772518	-1.820619
C	-0.005055	1.549179	-0.583086
C	-1.209876	1.166477	0.189141
C	-0.731061	0.601291	1.410029
C	-1.534544	0.140201	2.606436
H	-2.043545	-0.801214	2.373468
H	-2.332793	0.865914	2.796043
C	-0.666962	-0.028352	3.867136
H	-0.446925	0.960221	4.295017
H	-1.234488	-0.578037	4.626722
C	0.655751	-0.738815	3.556152
H	0.452001	-1.724966	3.116195
H	1.221897	-0.915834	4.477857
C	1.505610	0.099254	2.588655
H	1.880075	0.987652	3.120142
H	2.389890	-0.452922	2.261438
C	0.711257	0.579978	1.401579
C	1.196216	1.162914	0.188304
C	-3.321660	1.018018	-2.122726
H	-3.523296	-0.057404	-2.091997
H	-2.491707	1.192439	-2.814798
H	-4.215679	1.508115	-2.529024
C	-2.773962	3.629826	-0.583977
H	-1.985198	3.895346	-1.296151
H	-2.536247	4.102031	0.377012
H	-3.715439	4.063171	-0.943963
C	-4.299480	1.336235	0.798200
H	-5.257798	1.660545	0.372472
H	-4.179785	1.857742	1.755068
H	-4.376548	0.263354	0.999624
C	2.725116	3.664989	-0.500479
H	3.662619	4.124565	-0.837629
H	2.465612	4.110415	0.467636
H	1.940868	3.932513	-1.217004
C	3.361710	1.102657	-2.086729
H	2.550252	1.289253	-2.797609
H	3.569885	0.028038	-2.078816
H	4.262958	1.609389	-2.454738
C	4.260880	1.372760	0.868866
H	5.203304	1.824400	0.533363
H	4.429950	0.295713	0.965101
H	4.045571	1.775660	1.865349
P	1.560732	-1.868470	-0.565425

P	-1.537143	-1.901960	-0.534071
F	-2.131384	-2.242638	-1.972132
F	-1.334797	-3.403408	-0.046740
F	-2.927329	-1.662607	0.212693
F	2.154146	-2.155567	-2.015284
F	1.386808	-3.386393	-0.120472
F	2.950958	-1.626521	0.180762

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Fe	-0.121774	-0.051052	0.251124
Si	-2.635140	-2.335508	-1.319420
Si	-0.997968	3.244794	-1.232357
O	-1.374080	0.339838	-2.586208
O	0.954043	-0.103054	-1.537641
H	0.217348	0.026588	-2.210913
C	-1.648578	0.399953	-1.348009
C	-2.017564	-0.739206	-0.493310
C	-2.205505	-0.202891	0.839265
C	-2.909067	-0.845158	2.018787
H	-2.257549	-1.566249	2.516300
H	-3.760503	-1.423177	1.642602
C	-3.399874	0.197292	3.040566
H	-4.303359	0.693473	2.657963
H	-3.691252	-0.312375	3.966447
C	-2.331022	1.260640	3.317782
H	-1.410480	0.780798	3.676740
H	-2.662054	1.944134	4.108481
C	-2.030724	2.060381	2.042864
H	-2.899894	2.693781	1.805745
H	-1.194432	2.743882	2.198849
C	-1.802669	1.165280	0.850069
C	-1.357285	1.543932	-0.468630
C	-1.356687	-3.035760	-2.522627
H	-0.486457	-3.447271	-2.001615
H	-1.021749	-2.256456	-3.213724
H	-1.804829	-3.845368	-3.112636
C	-4.197496	-1.861519	-2.280934
H	-3.965399	-1.089298	-3.022406
H	-4.978738	-1.470121	-1.617914
H	-4.612859	-2.728451	-2.809941
C	-3.079419	-3.684532	-0.059932
H	-3.314067	-4.609808	-0.602002

H	-3.963277	-3.426436	0.534473
H	-2.264153	-3.909452	0.635039
C	-2.567854	3.746704	-2.168206
H	-2.433777	4.714022	-2.668719
H	-3.431374	3.836092	-1.497731
H	-2.809389	3.000040	-2.932637
C	0.451313	3.164328	-2.442178
H	0.228961	2.461177	-3.250233
H	1.368894	2.839601	-1.942398
H	0.633506	4.152318	-2.883606
C	-0.633452	4.561850	0.084733
H	-0.410842	5.511560	-0.418868
H	0.235176	4.313375	0.703599
H	-1.487252	4.739312	0.748053
C	1.952925	-1.009173	-2.057260
H	2.050877	-0.781700	-3.125673
H	1.611003	-2.042447	-1.957974
C	3.271405	-0.805643	-1.356147
C	3.912911	0.441057	-1.412532
H	3.442508	1.259441	-1.951187
C	5.141638	0.632584	-0.784148
H	5.628690	1.602741	-0.833093
C	5.749220	-0.422511	-0.096146
H	6.708365	-0.273122	0.392274
C	5.121779	-1.666763	-0.040249
H	5.588005	-2.490394	0.493511
C	3.886915	-1.855901	-0.665812
H	3.398314	-2.825249	-0.616882
P	1.344990	1.132790	1.255627
P	0.490376	-1.915013	1.055726
F	-0.486600	-2.769543	1.984752
F	1.782589	-2.066731	1.972444
F	0.841977	-3.112931	0.049286
F	2.711579	0.492934	1.747596
F	1.975442	2.403406	0.525193
F	0.975684	1.869733	2.622790