Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Cleavage Mechanism of Aliphatic C-C bond Catalyzed by 2,4′-Dihydroxyacetophenone Dioxygenase from *Alcaligenes* sp. 4HAP: A QM/MM Study

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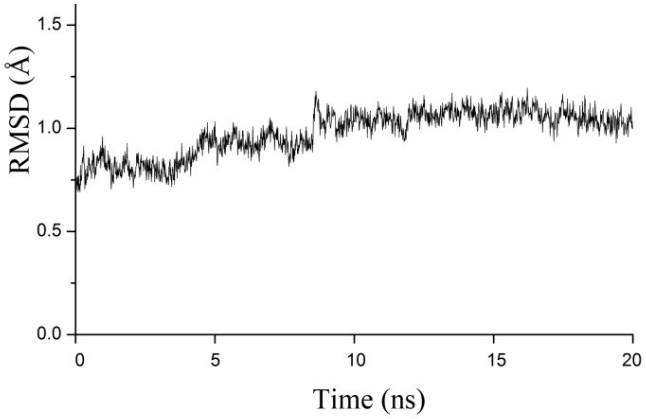

Figure S1. RMSD of DAD in complex with 2,4'-DHAP obtained from 20 ns MD simulation. The reference structure for RMSD is the energy-minimized structure of enzyme-substrate complex which was carried out before MD simulation. Before the molecular dynamics (MD) simulation, the system had been slowly heated from 0 K to 300 K for 200 ps and additional 200ps equilibration, which was not included in the MD simulation, thus, the initial value of RMSD is not zero.

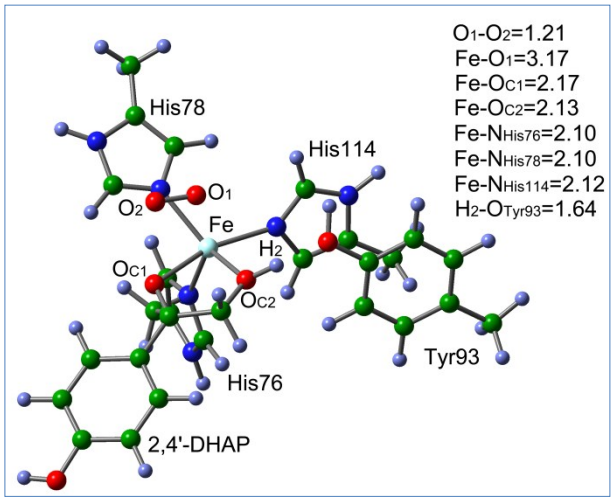

Figure S2. QM/MM optimized structure of ESO2 complex at septet spin state. Distances are given in angstrom.

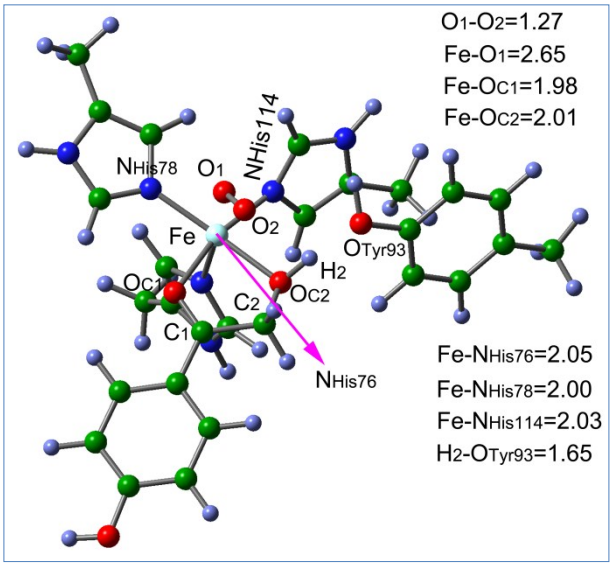

Figure S3. QM/MM optimized structure of ESO2 complex at open-shell singlet spin state. Distances are given in angstrom.

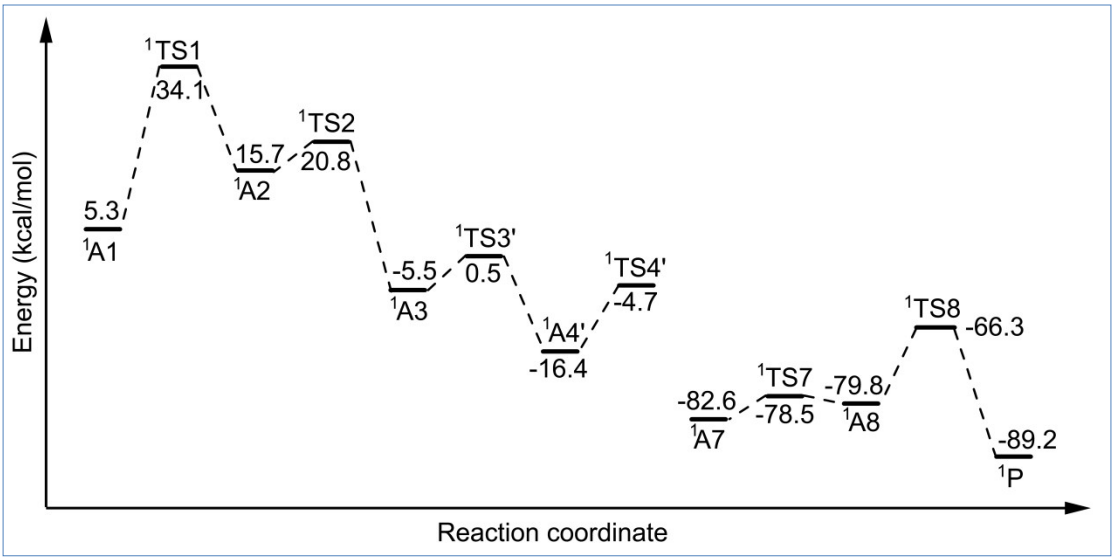

Figure S4. Potential energy profile of the catalytic reaction of DAD enzyme at open-shell singlet state surface. All energies are given in kcal/mol relative to ^{5}A1. In the open-shell singlet state, A5 and A6 were not recognized on the basis of our calculations.

Table S1 The defininations of the reaction coordinates along the catalytic path.

A1-A2	$R(C_2\text{-}H_1)\text{-}R(H_1\text{-}O_2)$
A2-A3	$R(Fe\text{-}O_1)\text{-}R(O_1\text{-}C_2)$
A3-A4	$R(O_2\text{-}H_1)\text{-}R(O_{C1}\text{-}H_1)\text{-}R(O_2\text{-}C_1)$
A4-P	$R(O_1\text{-}O_2)\text{-}R(C_1\text{-}O_2)\text{-}R(C_2\text{-}O_1)$
A3-A4'	$\text{dihedral}(O_{21}\text{-}O_{20}\text{-}C_{13}\text{-}C_{12})$
A4'-A5	$R(O_1\text{-}O_2)\text{-}R(Fe\text{-}O_2)$
A5-A6	$R(C_1\text{-}C_2)\text{-}R(O_1\text{-}C_1)$
A6-A7	$R(Fe\text{-}O_2)\text{-}R(O_2\text{-}C_2)$
A7-A8	$\text{dihedral}(H_1\text{-}O_2\text{-}C_2\text{-}O_1)$
A8-P	$R(O_2\text{-}H_1)\text{-}R(O_{C1}\text{-}H_1)$

Absolute QM/MM single-point energies, zero point energies, and Cartesian coordinates of QM regions of all computed species

Model ^{5}A1

E=-3130.499657 au ZPE=0.5613524043 au

C	8.920	6.423	-3.470
H	8.409	7.291	-3.109
H	8.688	6.276	-4.504
N	8.481	3.932	-3.166
H	8.803	3.645	-4.103
C	8.484	5.227	-2.687
C	8.129	3.107	-2.160
H	8.069	2.034	-2.260
N	7.893	3.801	-1.048
C	8.101	5.126	-1.375
H	7.978	5.913	-0.649
C	7.787	7.981	3.879
H	8.528	7.606	4.554
H	6.963	8.375	4.436
N	6.014	6.767	2.522
H	5.303	7.505	2.661
C	7.307	6.869	2.997
C	5.919	5.662	1.754
H	5.010	5.322	1.281
N	7.095	5.043	1.702
C	7.965	5.787	2.474
H	8.995	5.496	2.586
C	13.811	-2.253	0.017
H	14.565	-2.444	0.751
H	14.146	-1.483	-0.646
C	12.536	-1.807	0.706
C	11.417	-1.409	-0.040
H	11.465	-1.444	-1.120
C	10.257	-0.948	0.566
H	9.419	-0.622	-0.040
C	10.198	-0.855	1.956
O	9.033	-0.342	2.525
H	9.260	0.119	3.372
C	12.435	-1.739	2.100
H	13.275	-2.058	2.711
C	11.279	-1.270	2.731
H	11.233	-1.212	3.814
C	13.118	1.811	-0.011
H	13.012	0.771	-0.241
H	13.935	1.945	0.666
N	11.770	2.465	1.994
H	12.579	2.311	2.624
C	11.856	2.313	0.623
C	10.518	2.820	2.323
H	10.176	2.987	3.332
N	9.768	2.924	1.220
C	10.603	2.609	0.157
H	10.245	2.618	-0.857
C	4.264	1.261	-0.808
C	2.952	-0.212	-2.217
H	2.774	-1.175	-2.678
C	4.019	-0.010	-1.371
H	4.662	-0.850	-1.139
C	2.069	0.847	-2.489
O	1.030	0.570	-3.296
H	0.535	1.382	-3.497
C	3.374	2.318	-1.103
H	3.540	3.289	-0.652
C	2.284	2.117	-1.926
H	1.584	2.925	-2.115
C	5.418	1.510	0.022
O	5.681	2.644	0.477
C	6.394	0.385	0.361
H	6.481	-0.333	-0.459
H	6.003	-0.146	1.239
O	7.663	0.963	0.625
H	8.129	0.487	1.368
O	7.300	2.538	2.930
O	6.151	2.696	3.372
Fe	7.688	3.152	0.972

Model ^{5}TS1

E=-3130.481161 au ZPE=0.5558587378 au

C	8.922	6.410	-3.452
H	8.408	7.276	-3.091
H	8.685	6.259	-4.484
N	8.486	3.917	-3.138
H	8.797	3.628	-4.078
C	8.498	5.214	-2.663
C	8.145	3.097	-2.122
H	8.074	2.024	-2.220
N	7.928	3.795	-1.010
C	8.133	5.118	-1.346

H	8.024	5.910	-0.624
C	7.857	8.055	3.904
H	8.599	7.692	4.584
H	7.025	8.441	4.456
N	6.102	6.809	2.557
H	5.378	7.534	2.701
C	7.396	6.935	3.024
C	6.026	5.714	1.777
H	5.123	5.357	1.306
N	7.219	5.127	1.709
C	8.078	5.878	2.483
H	9.117	5.612	2.577
C	13.798	-2.249	-0.004
H	14.548	-2.437	0.736
H	14.137	-1.482	-0.669
C	12.518	-1.799	0.676
C	11.410	-1.389	-0.080
H	11.470	-1.422	-1.158
C	10.246	-0.922	0.516
H	9.412	-0.598	-0.096
C	10.178	-0.837	1.905
O	9.009	-0.319	2.467
H	9.224	0.134	3.324
C	12.405	-1.738	2.069
H	13.237	-2.064	2.687
C	11.247	-1.263	2.691
H	11.191	-1.210	3.773
C	13.090	1.829	0.010
H	12.977	0.788	-0.211
H	13.911	1.964	0.683
N	11.742	2.462	2.019
H	12.547	2.285	2.648
C	11.834	2.344	0.645
C	10.493	2.825	2.353
H	10.148	2.976	3.363
N	9.751	2.969	1.247
C	10.590	2.673	0.178
H	10.241	2.721	-0.836
C	4.254	1.271	-0.696
C	3.106	-0.295	-2.146
H	2.990	-1.280	-2.581
C	4.087	-0.032	-1.211
H	4.750	-0.832	-0.903
C	2.235	0.731	-2.550
O	1.289	0.406	-3.451
H	0.782	1.196	-3.702
C	3.380	2.295	-1.124
H	3.495	3.292	-0.717
C	2.369	2.028	-2.025
H	1.676	2.811	-2.316
C	5.381	1.608	0.139
O	5.726	2.809	0.327
C	6.227	0.607	0.824
H	6.016	-0.460	0.796
H	5.974	1.042	2.126
O	7.565	0.955	0.721
H	8.127	0.464	1.416
O	7.144	2.554	2.830
O	6.148	1.692	3.089
Fe	7.662	3.186	1.068

Model ^{5}A2

E=-3130.515042 au ZPE=0.5555867853 au

C	8.880	6.365	-3.408
H	8.364	7.231	-3.050
H	8.646	6.212	-4.441
N	8.446	3.873	-3.091
H	8.767	3.583	-4.027
C	8.455	5.170	-2.618
C	8.085	3.056	-2.079
H	8.006	1.984	-2.184
N	7.854	3.754	-0.969
C	8.072	5.076	-1.305
H	7.955	5.869	-0.586
C	7.790	8.059	3.907
H	8.528	7.680	4.582
H	6.965	8.451	4.464
N	6.024	6.862	2.524
H	5.311	7.597	2.664
C	7.311	6.952	3.018
C	5.940	5.772	1.734
H	5.038	5.451	1.236
N	7.115	5.152	1.687
C	7.973	5.877	2.487
H	9.000	5.581	2.612
C	13.807	-2.264	-0.011
H	14.563	-2.449	0.723
H	14.133	-1.488	-0.672

C	12.527	-1.835	0.679
C	11.410	-1.432	-0.067
H	11.467	-1.440	-1.146
C	10.236	-1.010	0.542
H	9.395	-0.690	-0.063
C	10.169	-0.966	1.932
O	8.976	-0.516	2.513
H	9.178	-0.055	3.371
C	12.420	-1.800	2.073
H	13.262	-2.118	2.681
C	11.251	-1.370	2.708
H	11.197	-1.337	3.792
C	13.055	1.797	0.045
H	12.950	0.757	-0.182
H	13.876	1.934	0.717
N	11.711	2.420	2.061
H	12.523	2.252	2.684
C	11.795	2.298	0.686
C	10.463	2.781	2.402
H	10.127	2.949	3.414
N	9.714	2.916	1.300
C	10.545	2.617	0.227
H	10.189	2.660	-0.786
C	4.328	1.165	-0.749
C	3.103	-0.298	-2.247
H	2.956	-1.257	-2.728
C	4.131	-0.096	-1.354
H	4.791	-0.924	-1.124
C	2.221	0.756	-2.546
O	1.234	0.486	-3.419
H	0.730	1.293	-3.618
C	3.436	2.214	-1.064
H	3.569	3.180	-0.592
C	2.390	2.015	-1.944
H	1.691	2.818	-2.154
C	5.462	1.423	0.111
O	5.698	2.607	0.566
C	6.404	0.401	0.444
H	6.229	-0.667	0.371
H	5.370	2.718	2.454
O	7.579	0.827	0.890
H	8.105	0.226	1.548
O	7.185	2.683	2.955
O	5.839	2.678	3.318
Fe	7.632	3.165	1.139

Model ^{5}TS2

E=-3130.495990 au ZPE=0.5615801553 au

C	8.936	6.470	-3.454
H	8.428	7.344	-3.102
H	8.699	6.310	-4.485
N	8.463	3.991	-3.127
H	8.763	3.693	-4.067
C	8.502	5.287	-2.655
C	8.135	3.179	-2.101
H	8.046	2.107	-2.196
N	7.957	3.883	-0.986
C	8.171	5.199	-1.327
H	8.089	5.992	-0.600
C	7.822	8.020	3.924
H	8.571	7.656	4.596
H	7.000	8.414	4.485
N	6.056	6.814	2.557
H	5.353	7.563	2.675
C	7.342	6.898	3.057
C	5.955	5.698	1.810
H	5.057	5.389	1.298
N	7.117	5.048	1.803
C	7.988	5.791	2.572
H	9.012	5.488	2.696
C	13.803	-2.270	-0.001
H	14.544	-2.459	0.748
H	14.148	-1.498	-0.657
C	12.513	-1.829	0.664
C	11.415	-1.426	-0.109
H	11.492	-1.457	-1.186
C	10.238	-0.971	0.466
H	9.412	-0.657	-0.163
C	10.147	-0.889	1.853
O	8.961	-0.373	2.388
H	9.148	0.062	3.262
C	12.376	-1.772	2.055
H	13.200	-2.093	2.686
C	11.203	-1.307	2.658
H	11.130	-1.257	3.739
C	13.037	1.806	0.058
H	12.935	0.765	-0.167
H	13.855	1.946	0.733

N	11.679	2.433	2.066
H	12.487	2.268	2.694
C	11.774	2.306	0.692
C	10.423	2.779	2.396
H	10.080	2.940	3.407
N	9.679	2.901	1.290
C	10.523	2.607	0.225
H	10.178	2.641	-0.792
C	4.259	1.184	-0.686
C	3.167	-0.417	-2.139
H	3.088	-1.404	-2.576
C	4.131	-0.126	-1.192
H	4.823	-0.902	-0.880
C	2.272	0.583	-2.558
O	1.349	0.238	-3.479
H	0.832	1.019	-3.735
C	3.356	2.179	-1.124
H	3.441	3.183	-0.727
C	2.359	1.882	-2.029
H	1.646	2.644	-2.327
C	5.393	1.593	0.110
O	5.723	2.821	0.156
C	6.289	0.665	0.790
H	5.978	-0.294	1.190
H	5.043	3.061	2.391
O	7.594	0.902	0.635
H	8.153	0.395	1.344
O	6.685	2.127	2.503
O	5.571	2.733	3.143
Fe	7.583	3.150	1.036

Model ^{5}A3

E=-3130.559584 au ZPE=0.5669586703 au

C	8.963	6.509	-3.549
H	8.464	7.383	-3.187
H	8.746	6.379	-4.589
N	8.465	4.026	-3.282
H	8.789	3.740	-4.219
C	8.489	5.315	-2.789
C	8.086	3.196	-2.290
H	7.996	2.127	-2.407
N	7.853	3.884	-1.174
C	8.091	5.208	-1.483
H	7.978	5.992	-0.750
C	7.906	8.002	3.947
H	8.667	7.644	4.608
H	7.096	8.402	4.520
N	6.111	6.779	2.636
H	5.411	7.529	2.762
C	7.409	6.873	3.102
C	6.000	5.664	1.888
H	5.094	5.342	1.399
N	7.167	5.022	1.849
C	8.050	5.772	2.598
H	9.079	5.478	2.696
C	13.672	-2.172	-0.006
H	14.444	-2.332	0.718
H	13.980	-1.412	-0.693
C	12.400	-1.732	0.699
C	11.263	-1.333	-0.021
H	11.284	-1.376	-1.102
C	10.122	-0.854	0.614
H	9.263	-0.533	0.034
C	10.104	-0.747	2.004
O	8.969	-0.209	2.613
H	9.240	0.282	3.431
C	12.334	-1.654	2.095
H	13.189	-1.971	2.686
C	11.200	-1.171	2.752
H	11.183	-1.105	3.835
C	13.148	1.810	-0.089
H	13.043	0.772	-0.328
H	13.958	1.937	0.599
N	11.799	2.519	1.895
H	12.605	2.387	2.534
C	11.881	2.309	0.534
C	10.546	2.891	2.209
H	10.206	3.090	3.212
N	9.792	2.944	1.107
C	10.624	2.581	0.058
H	10.263	2.552	-0.955
C	4.294	1.427	-0.608
C	3.334	-0.267	-2.051
H	3.251	-1.290	-2.397
C	4.170	0.078	-1.005
H	4.751	-0.699	-0.520
C	2.555	0.719	-2.682
O	1.734	0.319	-3.673

H	1.243	1.081	-4.022
C	3.521	2.409	-1.271
H	3.593	3.440	-0.948
C	2.651	2.063	-2.282
H	2.037	2.819	-2.759
C	5.215	1.876	0.406
O	5.518	3.078	0.545
C	5.989	0.960	1.382
H	5.677	-0.088	1.401
H	4.430	2.680	2.739
O	7.341	1.116	1.030
H	7.947	0.597	1.655
O	5.922	1.526	2.693
O	4.532	1.752	3.017
Fe	7.735	3.292	0.829

Model ^{5}TS3'

E=-3130.553974 au ZPE=0.5666156908 au

C	8.983	6.543	-3.575
H	8.489	7.423	-3.218
H	8.771	6.412	-4.616
N	8.462	4.066	-3.303
H	8.787	3.772	-4.238
C	8.495	5.357	-2.816
C	8.077	3.244	-2.308
H	7.979	2.175	-2.420
N	7.849	3.939	-1.196
C	8.094	5.260	-1.510
H	7.986	6.049	-0.781
C	7.905	8.019	3.950
H	8.665	7.666	4.615
H	7.095	8.425	4.519
N	6.105	6.775	2.662
H	5.403	7.525	2.785
C	7.407	6.883	3.114
C	5.993	5.652	1.927
H	5.086	5.318	1.448
N	7.167	5.018	1.883
C	8.052	5.783	2.614
H	9.085	5.499	2.703
C	13.653	-2.158	-0.013
H	14.430	-2.313	0.706
H	13.955	-1.401	-0.707
C	12.385	-1.717	0.698
C	11.247	-1.303	-0.013
H	11.261	-1.337	-1.095
C	10.116	-0.813	0.632
H	9.258	-0.474	0.060
C	10.108	-0.713	2.023
O	8.986	-0.161	2.643
H	9.271	0.315	3.465
C	12.326	-1.649	2.095
H	13.180	-1.980	2.679
C	11.202	-1.157	2.762
H	11.191	-1.098	3.846
C	13.154	1.824	-0.094
H	13.042	0.786	-0.329
H	13.966	1.949	0.592
N	11.809	2.534	1.891
H	12.612	2.390	2.530
C	11.892	2.334	0.529
C	10.559	2.920	2.204
H	10.220	3.113	3.209
N	9.810	2.992	1.101
C	10.639	2.626	0.052
H	10.279	2.608	-0.962
C	4.251	1.443	-0.576
C	3.282	-0.225	-2.045
H	3.195	-1.243	-2.406
C	4.116	0.100	-0.992
H	4.690	-0.691	-0.521
C	2.513	0.774	-2.666
O	1.701	0.390	-3.670
H	1.217	1.158	-4.016
C	3.482	2.437	-1.224
H	3.560	3.463	-0.889
C	2.613	2.110	-2.243
H	2.005	2.878	-2.708
C	5.215	1.876	0.406
O	5.566	3.064	0.519
C	5.999	0.908	1.324
H	5.883	-0.153	1.091
H	5.114	2.831	3.087
O	7.362	1.273	1.145
H	7.973	0.718	1.727
O	5.674	1.061	2.697
O	4.610	2.016	2.916
Fe	7.750	3.336	0.797

Model ^{5}A4'

E=-3130.560055 au ZPE=0.5650352558 au

C	8.986	6.545	-3.554
H	8.489	7.420	-3.189
H	8.764	6.417	-4.593
N	8.479	4.066	-3.292
H	8.793	3.781	-4.233
C	8.515	5.352	-2.794
C	8.115	3.233	-2.299
H	8.018	2.164	-2.421
N	7.901	3.916	-1.177
C	8.137	5.241	-1.483
H	8.035	6.022	-0.744
C	7.924	7.999	3.964
H	8.691	7.657	4.627
H	7.115	8.404	4.534
N	6.115	6.715	2.733
H	5.407	7.457	2.863
C	7.429	6.853	3.141
C	6.002	5.587	2.006
H	5.083	5.220	1.577
N	7.187	4.980	1.922
C	8.079	5.766	2.623
H	9.121	5.502	2.677
C	13.602	-2.129	-0.006
H	14.392	-2.270	0.702
H	13.883	-1.373	-0.709
C	12.339	-1.698	0.723
C	11.187	-1.287	0.034
H	11.182	-1.311	-1.048
C	10.061	-0.811	0.704
H	9.191	-0.473	0.150
C	10.074	-0.725	2.095
O	8.959	-0.196	2.749
H	9.267	0.292	3.556
C	12.303	-1.639	2.122
H	13.170	-1.966	2.689
C	11.186	-1.164	2.812
H	11.193	-1.113	3.896
C	13.170	1.824	-0.089
H	13.067	0.787	-0.331
H	13.981	1.951	0.597
N	11.823	2.526	1.900
H	12.630	2.395	2.538
C	11.903	2.319	0.539
C	10.570	2.900	2.214
H	10.233	3.100	3.218
N	9.815	2.956	1.115
C	10.645	2.592	0.066
H	10.284	2.565	-0.948
C	4.222	1.437	-0.555
C	3.250	-0.226	-2.027
H	3.170	-1.242	-2.394
C	4.089	0.097	-0.974
H	4.668	-0.694	-0.509
C	2.477	0.773	-2.641
O	1.664	0.393	-3.648
H	1.180	1.163	-3.988
C	3.451	2.431	-1.196
H	3.533	3.457	-0.860
C	2.573	2.106	-2.210
H	1.961	2.875	-2.668
C	5.215	1.876	0.406
O	5.609	3.053	0.432
C	5.898	0.934	1.412
H	5.799	-0.129	1.175
H	6.021	2.486	3.625
O	7.260	1.324	1.430
H	7.866	0.699	1.937
O	5.297	1.010	2.681
O	5.200	2.392	3.113
Fe	7.747	3.309	0.814

Model ^{5}TS4'

E=-3130.545158 au ZPE=0.5642942460 au

C	8.939	6.444	-3.471
H	8.435	7.317	-3.112
H	8.703	6.295	-4.504
N	8.470	3.957	-3.155
H	8.779	3.662	-4.093
C	8.497	5.255	-2.683
C	8.121	3.143	-2.137
H	8.030	2.071	-2.231
N	7.915	3.847	-1.026
C	8.135	5.166	-1.365
H	8.032	5.961	-0.643
C	7.903	8.063	3.914
H	8.646	7.687	4.586

H	7.082	8.458	4.475
N	6.120	6.849	2.576
H	5.407	7.581	2.729
C	7.418	6.953	3.035
C	6.026	5.758	1.788
H	5.117	5.413	1.322
N	7.208	5.155	1.710
C	8.080	5.888	2.484
H	9.115	5.607	2.570
C	13.799	-2.246	-0.012
H	14.557	-2.429	0.720
H	14.129	-1.482	-0.684
C	12.527	-1.795	0.680
C	11.396	-1.422	-0.062
H	11.433	-1.486	-1.141
C	10.240	-0.956	0.546
H	9.385	-0.665	-0.055
C	10.201	-0.829	1.934
O	9.042	-0.311	2.501
H	9.269	0.158	3.339
C	12.444	-1.696	2.073
H	13.292	-1.997	2.681
C	11.293	-1.218	2.706
H	11.256	-1.138	3.787
C	13.118	1.777	-0.054
H	13.006	0.741	-0.295
H	13.937	1.899	0.624
N	11.808	2.509	1.946
H	12.632	2.396	2.566
C	11.860	2.280	0.586
C	10.561	2.871	2.285
H	10.248	3.088	3.292
N	9.779	2.901	1.200
C	10.591	2.535	0.135
H	10.210	2.488	-0.869
C	4.275	1.394	-0.587
C	3.258	-0.232	-2.071
H	3.164	-1.238	-2.462
C	4.135	0.065	-1.044
H	4.736	-0.734	-0.625
C	2.460	0.783	-2.626
O	1.614	0.428	-3.612
H	1.124	1.206	-3.925
C	3.474	2.404	-1.167
H	3.563	3.419	-0.802
C	2.565	2.105	-2.159
H	1.932	2.883	-2.573
C	5.290	1.789	0.358
O	5.623	2.985	0.501
C	6.129	0.797	1.194
H	5.748	-0.235	1.153
H	7.636	2.118	3.417
O	7.441	0.909	0.650
H	8.055	0.458	1.295
O	6.114	1.076	2.548
O	7.042	2.538	2.772
Fe	7.690	3.218	1.022

Model ^{5}A5

E=-3130.563673 au ZPE=0.5594894907 au

C	8.884	6.340	-3.361
H	8.361	7.205	-3.010
H	8.627	6.159	-4.384
N	8.553	3.844	-2.966
H	8.862	3.544	-3.903
C	8.500	5.155	-2.533
C	8.259	3.039	-1.928
H	8.270	1.963	-1.986
N	8.000	3.762	-0.835
C	8.135	5.085	-1.213
H	7.987	5.892	-0.515
C	7.783	7.983	3.888
H	8.520	7.630	4.579
H	6.941	8.363	4.428
N	6.061	6.717	2.505
H	5.332	7.439	2.624
C	7.342	6.853	3.006
C	6.004	5.598	1.753
H	5.112	5.228	1.272
N	7.195	5.007	1.737
C	8.032	5.775	2.518
H	9.062	5.501	2.665
C	13.860	-2.279	-0.009
H	14.618	-2.475	0.720
H	14.196	-1.512	-0.676
C	12.593	-1.823	0.689
C	11.467	-1.430	-0.048
H	11.502	-1.479	-1.128

C	10.314	-0.964	0.566
H	9.468	-0.652	-0.034
C	10.271	-0.857	1.956
O	9.118	-0.334	2.536
H	9.362	0.065	3.409
C	12.508	-1.745	2.083
H	13.353	-2.062	2.687
C	11.360	-1.269	2.721
H	11.325	-1.205	3.804
C	13.227	1.802	-0.018
H	13.122	0.760	-0.239
H	14.051	1.944	0.650
N	11.898	2.531	1.986
H	12.716	2.421	2.614
C	11.971	2.305	0.625
C	10.646	2.887	2.312
H	10.303	3.104	3.311
N	9.888	2.925	1.208
C	10.712	2.564	0.156
H	10.345	2.507	-0.851
C	4.283	1.323	-0.827
C	2.972	-0.161	-2.216
H	2.792	-1.127	-2.671
C	4.056	0.049	-1.395
H	4.711	-0.775	-1.149
C	2.063	0.886	-2.457
O	1.012	0.597	-3.238
H	0.493	1.399	-3.418
C	3.371	2.372	-1.089
H	3.526	3.341	-0.632
C	2.267	2.156	-1.889
H	1.546	2.951	-2.051
C	5.448	1.600	-0.038
O	5.723	2.652	0.529
C	6.610	0.445	0.023
H	6.814	0.246	-1.050
H	8.034	1.850	3.021
O	7.776	1.049	0.575
H	8.129	0.488	1.319
O	6.143	-0.589	0.657
O	7.639	2.718	2.843
Fe	7.835	3.149	1.118

Model ^{5}TS5

E=-3130.537155 au ZPE=0.5578039390 au

C	8.881	6.356	-3.362
H	8.365	7.228	-3.017
H	8.629	6.174	-4.386
N	8.498	3.868	-2.972
H	8.801	3.564	-3.909
C	8.479	5.178	-2.532
C	8.183	3.066	-1.935
H	8.154	1.990	-1.998
N	7.947	3.792	-0.840
C	8.117	5.112	-1.212
H	7.993	5.919	-0.508
C	7.783	8.024	3.896
H	8.518	7.668	4.587
H	6.945	8.414	4.436
N	6.044	6.756	2.538
H	5.317	7.479	2.663
C	7.331	6.893	3.020
C	5.979	5.638	1.784
H	5.080	5.265	1.317
N	7.169	5.050	1.748
C	8.016	5.817	2.520
H	9.048	5.545	2.653
C	13.921	-2.328	0.008
H	14.661	-2.543	0.750
H	14.280	-1.557	-0.641
C	12.646	-1.865	0.685
C	11.537	-1.475	-0.078
H	11.595	-1.530	-1.156
C	10.370	-1.009	0.506
H	9.541	-0.699	-0.117
C	10.299	-0.895	1.893
O	9.129	-0.368	2.448
H	9.354	0.049	3.318
C	12.532	-1.780	2.076
H	13.364	-2.093	2.700
C	11.370	-1.300	2.686
H	11.311	-1.229	3.768
C	13.177	1.794	-0.021
H	13.072	0.752	-0.242
H	13.993	1.934	0.657
N	11.840	2.553	1.961
H	12.655	2.451	2.593

C	11.915	2.301	0.605
C	10.584	2.907	2.279
H	10.237	3.139	3.273
N	9.827	2.917	1.175
C	10.653	2.541	0.130
H	10.287	2.459	-0.876
C	4.355	1.304	-0.770
C	3.015	-0.143	-2.171
H	2.780	-1.115	-2.586
C	4.048	0.022	-1.279
H	4.608	-0.844	-0.949
C	2.221	0.961	-2.535
O	1.196	0.709	-3.359
H	0.721	1.529	-3.583
C	3.573	2.410	-1.168
H	3.782	3.386	-0.748
C	2.507	2.244	-2.029
H	1.869	3.086	-2.276
C	5.471	1.526	0.128
O	5.798	2.622	0.644
C	6.677	0.404	0.085
H	6.725	-0.229	-0.809
H	8.010	1.851	2.999
O	7.894	0.911	0.460
H	8.259	0.446	1.276
O	5.753	0.166	1.015
O	7.650	2.736	2.838
Fe	7.779	3.171	1.104

Model ^{5}A6

E=-3130.576584 au ZPE=0.5635345707 au

C	8.842	6.265	-3.327
H	8.318	7.133	-2.986
H	8.592	6.077	-4.350
N	8.429	3.774	-2.933
H	8.733	3.468	-3.868
C	8.450	5.086	-2.493
C	8.080	2.982	-1.898
H	8.003	1.907	-1.961
N	7.870	3.715	-0.802
C	8.089	5.029	-1.173
H	7.989	5.840	-0.472
C	7.746	7.986	3.897
H	8.483	7.623	4.583
H	6.910	8.371	4.442
N	6.014	6.759	2.492
H	5.297	7.494	2.609
C	7.291	6.864	3.011
C	5.942	5.646	1.733
H	5.048	5.298	1.239
N	7.120	5.030	1.728
C	7.964	5.773	2.527
H	8.984	5.474	2.691
C	14.020	-2.398	-0.061
H	14.799	-2.624	0.637
H	14.349	-1.626	-0.725
C	12.791	-1.929	0.689
C	11.634	-1.541	-0.003
H	11.606	-1.631	-1.080
C	10.528	-1.028	0.657
H	9.652	-0.722	0.095
C	10.577	-0.866	2.040
O	9.475	-0.272	2.652
H	9.747	0.182	3.494
C	12.783	-1.814	2.082
H	13.648	-2.145	2.650
C	11.688	-1.280	2.765
H	11.709	-1.169	3.844
C	13.120	1.810	0.021
H	13.006	0.768	-0.192
H	13.938	1.948	0.697
N	11.777	2.533	2.010
H	12.589	2.402	2.641
C	11.862	2.333	0.645
C	10.521	2.887	2.331
H	10.164	3.075	3.331
N	9.773	2.948	1.224
C	10.607	2.607	0.169
H	10.250	2.580	-0.844
C	4.226	1.272	-0.836
C	2.985	-0.123	-2.369
H	2.769	-1.081	-2.826
C	3.943	0.008	-1.391
H	4.486	-0.862	-1.047
C	2.263	1.005	-2.790
O	1.338	0.788	-3.740
H	0.889	1.615	-3.982
C	3.501	2.398	-1.266

H	3.690	3.363	-0.810
C	2.519	2.268	-2.232
H	1.937	3.131	-2.539
C	5.268	1.406	0.156
O	5.713	2.466	0.620
C	6.850	0.117	1.347
H	7.051	-0.894	1.688
H	7.245	1.827	3.001
O	7.920	0.859	0.943
H	8.665	0.586	1.571
O	5.762	0.194	0.536
O	7.503	2.759	2.906
Fe	7.683	3.133	1.160

Model ^{5}TS6

E=-3130.552018 au ZPE=0.5622632074 au

C	8.886	6.345	-3.368
H	8.368	7.219	-3.032
H	8.641	6.157	-4.393
N	8.451	3.861	-2.975
H	8.749	3.551	-3.912
C	8.478	5.172	-2.535
C	8.110	3.069	-1.939
H	8.025	1.995	-2.001
N	7.914	3.805	-0.842
C	8.129	5.118	-1.211
H	8.037	5.928	-0.506
C	7.780	7.973	3.906
H	8.522	7.615	4.589
H	6.945	8.354	4.455
N	6.047	6.734	2.517
H	5.328	7.467	2.634
C	7.327	6.847	3.025
C	5.974	5.620	1.759
H	5.080	5.265	1.271
N	7.156	5.012	1.747
C	8.005	5.761	2.535
H	9.030	5.472	2.680
C	13.982	-2.380	-0.059
H	14.749	-2.604	0.653
H	14.324	-1.612	-0.721
C	12.741	-1.905	0.668
C	11.593	-1.524	-0.043
H	11.580	-1.630	-1.118
C	10.481	-0.998	0.594
H	9.610	-0.701	0.019
C	10.511	-0.813	1.976
O	9.410	-0.190	2.556
H	9.671	0.250	3.408
C	12.713	-1.773	2.059
H	13.571	-2.095	2.644
C	11.610	-1.228	2.721
H	11.621	-1.107	3.799
C	13.124	1.817	0.023
H	13.004	0.775	-0.189
H	13.944	1.952	0.697
N	11.780	2.531	2.016
H	12.588	2.386	2.649
C	11.869	2.347	0.650
C	10.526	2.898	2.335
H	10.171	3.074	3.338
N	9.784	2.982	1.226
C	10.620	2.642	0.173
H	10.269	2.633	-0.843
C	4.162	1.309	-0.810
C	3.055	-0.241	-2.294
H	2.905	-1.237	-2.694
C	3.953	-0.004	-1.275
H	4.514	-0.823	-0.842
C	2.311	0.822	-2.830
O	1.436	0.513	-3.807
H	0.972	1.313	-4.104
C	3.428	2.373	-1.365
H	3.569	3.377	-0.982
C	2.496	2.132	-2.357
H	1.903	2.947	-2.758
C	5.165	1.584	0.192
O	5.656	2.695	0.429
C	6.746	0.530	1.588
H	6.910	-0.385	2.152
H	6.755	1.614	2.712
O	7.816	0.966	0.859
H	8.607	0.701	1.433
O	5.587	0.470	0.858
O	7.223	2.486	2.825
Fe	7.677	3.162	1.070

Model ^{5}A7

E=-3130.688276 au ZPE=0.5692427303 au

C	8.939	6.468	-3.504
H	8.440	7.339	-3.133
H	8.718	6.346	-4.544
N	8.435	3.985	-3.263
H	8.765	3.710	-4.201
C	8.470	5.267	-2.751
C	8.033	3.146	-2.288
H	7.925	2.080	-2.426
N	7.796	3.818	-1.164
C	8.057	5.145	-1.450
H	7.945	5.919	-0.706
C	7.837	7.932	3.931
H	8.601	7.576	4.590
H	7.029	8.335	4.506
N	6.024	6.685	2.661
H	5.326	7.436	2.788
C	7.335	6.798	3.090
C	5.901	5.556	1.935
H	4.981	5.205	1.493
N	7.075	4.930	1.864
C	7.972	5.699	2.580
H	9.006	5.411	2.659
C	13.666	-2.170	-0.030
H	14.477	-2.316	0.653
H	13.926	-1.408	-0.734
C	12.426	-1.747	0.739
C	11.246	-1.346	0.092
H	11.200	-1.380	-0.990
C	10.146	-0.871	0.802
H	9.250	-0.545	0.282
C	10.218	-0.774	2.190
O	9.132	-0.237	2.886
H	9.470	0.239	3.691
C	12.443	-1.686	2.138
H	13.330	-2.016	2.672
C	11.355	-1.208	2.868
H	11.401	-1.147	3.950
C	13.103	1.821	-0.058
H	13.008	0.782	-0.297
H	13.906	1.955	0.637
N	11.726	2.489	1.918
H	12.528	2.351	2.560
C	11.826	2.312	0.554
C	10.464	2.842	2.225
H	10.112	3.016	3.229
N	9.723	2.916	1.117
C	10.571	2.585	0.070
H	10.223	2.577	-0.948
C	4.112	1.383	-0.912
C	3.088	-0.206	-2.417
H	2.926	-1.217	-2.772
C	3.889	0.056	-1.324
H	4.365	-0.756	-0.789
C	2.469	0.854	-3.095
O	1.702	0.526	-4.157
H	1.273	1.322	-4.511
C	3.495	2.440	-1.601
H	3.653	3.458	-1.265
C	2.669	2.179	-2.681
H	2.182	2.994	-3.205
C	5.016	1.679	0.190
O	5.469	2.799	0.446
C	6.140	0.741	2.091
H	6.308	-0.288	2.421
H	4.556	1.258	3.050
O	7.376	1.323	1.800
H	8.127	0.757	2.170
O	5.368	0.578	0.895
O	5.489	1.525	3.013
Fe	7.614	3.198	0.844

Model ^{5}TS7

E=-3130.684981 au ZPE=0.5682478973 au

C	8.931	6.458	-3.498
H	8.432	7.329	-3.129
H	8.712	6.335	-4.538
N	8.427	3.975	-3.255
H	8.763	3.699	-4.191
C	8.459	5.257	-2.745
C	8.012	3.138	-2.283
H	7.905	2.072	-2.420
N	7.763	3.812	-1.162
C	8.031	5.138	-1.448
H	7.914	5.913	-0.706
C	7.835	7.932	3.934
H	8.598	7.573	4.593

H	7.028	8.336	4.509
N	6.020	6.695	2.658
H	5.327	7.451	2.782
C	7.330	6.800	3.091
C	5.893	5.567	1.931
H	4.973	5.226	1.482
N	7.062	4.932	1.867
C	7.962	5.696	2.585
H	8.994	5.402	2.668
C	13.673	-2.172	-0.031
H	14.482	-2.319	0.654
H	13.936	-1.411	-0.735
C	12.433	-1.747	0.735
C	11.255	-1.345	0.084
H	11.212	-1.381	-0.998
C	10.154	-0.868	0.790
H	9.260	-0.543	0.268
C	10.223	-0.769	2.179
O	9.136	-0.227	2.867
H	9.470	0.246	3.675
C	12.446	-1.685	2.134
H	13.331	-2.015	2.672
C	11.356	-1.203	2.860
H	11.400	-1.142	3.942
C	13.096	1.823	-0.057
H	12.998	0.784	-0.295
H	13.898	1.955	0.639
N	11.719	2.496	1.916
H	12.518	2.354	2.559
C	11.820	2.319	0.551
C	10.458	2.854	2.221
H	10.105	3.026	3.225
N	9.717	2.931	1.112
C	10.566	2.598	0.067
H	10.219	2.591	-0.952
C	4.118	1.364	-0.882
C	3.109	-0.211	-2.412
H	2.948	-1.218	-2.777
C	3.904	0.041	-1.312
H	4.378	-0.777	-0.783
C	2.489	0.855	-3.081
O	1.725	0.538	-4.147
H	1.294	1.336	-4.494
C	3.501	2.427	-1.562
H	3.647	3.441	-1.210
C	2.684	2.177	-2.651
H	2.195	2.996	-3.168
C	4.983	1.653	0.249
O	5.393	2.778	0.563
C	6.146	0.713	2.113
H	6.376	-0.300	2.444
H	4.700	1.826	2.781
O	7.373	1.316	1.742
H	8.135	0.773	2.117
O	5.336	0.549	0.952
O	5.514	1.416	3.108
Fe	7.604	3.198	0.848

Model ^{5}A8

E=-3130.687680 au ZPE=0.5682400269 au

C	8.915	6.443	-3.503
H	8.417	7.316	-3.136
H	8.699	6.320	-4.544
N	8.414	3.959	-3.257
H	8.756	3.682	-4.190
C	8.438	5.244	-2.751
C	7.992	3.124	-2.287
H	7.888	2.058	-2.421
N	7.731	3.803	-1.170
C	7.999	5.129	-1.459
H	7.872	5.907	-0.722
C	7.829	7.925	3.943
H	8.592	7.567	4.602
H	7.021	8.327	4.518
N	6.025	6.695	2.643
H	5.332	7.454	2.759
C	7.327	6.793	3.099
C	5.902	5.567	1.918
H	4.987	5.231	1.453
N	7.069	4.921	1.876
C	7.961	5.683	2.607
H	8.990	5.385	2.705
C	13.705	-2.188	-0.037
H	14.516	-2.343	0.644
H	13.970	-1.426	-0.740
C	12.471	-1.757	0.735
C	11.292	-1.353	0.088
H	11.242	-1.395	-0.994

C	10.197	-0.869	0.798
H	9.300	-0.543	0.280
C	10.275	-0.764	2.185
O	9.195	-0.212	2.877
H	9.534	0.270	3.678
C	12.493	-1.691	2.133
H	13.377	-2.026	2.667
C	11.409	-1.201	2.863
H	11.459	-1.134	3.945
C	13.113	1.823	-0.075
H	13.010	0.784	-0.309
H	13.916	1.955	0.619
N	11.743	2.514	1.896
H	12.541	2.371	2.541
C	11.840	2.326	0.533
C	10.485	2.884	2.200
H	10.135	3.062	3.204
N	9.745	2.959	1.091
C	10.588	2.611	0.048
H	10.237	2.599	-0.970
C	4.146	1.381	-0.764
C	3.174	-0.164	-2.347
H	3.032	-1.164	-2.742
C	3.963	0.068	-1.239
H	4.455	-0.756	-0.736
C	2.528	0.909	-2.981
O	1.767	0.610	-4.053
H	1.321	1.409	-4.378
C	3.505	2.452	-1.410
H	3.622	3.456	-1.021
C	2.695	2.221	-2.508
H	2.186	3.045	-2.995
C	4.993	1.648	0.383
O	5.379	2.778	0.740
C	6.245	0.745	2.179
H	6.444	-0.252	2.564
H	5.370	2.329	2.780
O	7.462	1.289	1.692
H	8.230	0.779	2.106
O	5.384	0.547	1.049
O	5.673	1.491	3.169
Fe	7.638	3.201	0.838

Model ^{5}TS8

E=-3130.655693 au ZPE=0.5638701460 au

C	8.895	6.405	-3.483
H	8.392	7.276	-3.117
H	8.679	6.279	-4.523
N	8.411	3.915	-3.224
H	8.752	3.638	-4.158
C	8.426	5.204	-2.727
C	7.989	3.083	-2.252
H	7.888	2.016	-2.381
N	7.717	3.767	-1.139
C	7.979	5.095	-1.437
H	7.841	5.877	-0.706
C	7.820	7.940	3.946
H	8.578	7.582	4.611
H	7.007	8.340	4.515
N	6.028	6.709	2.632
H	5.329	7.461	2.754
C	7.327	6.810	3.096
C	5.915	5.590	1.892
H	5.002	5.252	1.425
N	7.087	4.954	1.848
C	7.970	5.711	2.594
H	9.001	5.420	2.696
C	13.717	-2.195	-0.048
H	14.527	-2.350	0.633
H	13.983	-1.434	-0.752
C	12.483	-1.762	0.723
C	11.303	-1.363	0.075
H	11.252	-1.408	-1.006
C	10.204	-0.885	0.786
H	9.303	-0.570	0.267
C	10.284	-0.780	2.172
O	9.203	-0.236	2.871
H	9.549	0.243	3.670
C	12.506	-1.694	2.121
H	13.393	-2.025	2.655
C	11.421	-1.209	2.850
H	11.469	-1.141	3.932
C	13.161	1.814	-0.092
H	13.059	0.775	-0.328
H	13.969	1.945	0.597
N	11.803	2.506	1.889
H	12.607	2.368	2.530

C	11.891	2.313	0.526
C	10.551	2.880	2.202
H	10.206	3.063	3.207
N	9.805	2.952	1.096
C	10.637	2.599	0.046
H	10.277	2.585	-0.968
C	4.174	1.351	-0.745
C	3.245	-0.168	-2.381
H	3.122	-1.160	-2.802
C	4.040	0.054	-1.275
H	4.559	-0.766	-0.791
C	2.559	0.906	-2.973
O	1.797	0.620	-4.050
H	1.330	1.418	-4.347
C	3.486	2.421	-1.343
H	3.553	3.412	-0.910
C	2.686	2.203	-2.453
H	2.142	3.027	-2.904
C	4.963	1.553	0.459
O	5.154	2.783	0.899
C	6.307	1.103	2.614
H	6.373	0.109	3.050
H	5.284	2.635	2.028
O	7.513	1.501	2.056
H	8.232	0.799	2.220
O	5.475	0.569	1.079
O	5.563	1.995	3.100
Fe	7.734	3.240	0.884

Model ^{5}P

E=-3130.686529 au ZPE=0.5670300877 au

C	8.975	6.549	-3.552
H	8.494	7.430	-3.182
H	8.760	6.436	-4.594
N	8.421	4.080	-3.326
H	8.756	3.798	-4.261
C	8.472	5.358	-2.809
C	7.991	3.244	-2.363
H	7.856	2.182	-2.497
N	7.748	3.918	-1.240
C	8.039	5.240	-1.514
H	7.931	6.013	-0.769
C	7.895	7.863	3.916
H	8.666	7.501	4.563
H	7.089	8.249	4.504
N	6.094	6.660	2.597
H	5.402	7.416	2.731
C	7.395	6.741	3.058
C	5.971	5.549	1.844
H	5.054	5.240	1.365
N	7.133	4.898	1.790
C	8.025	5.639	2.541
H	9.053	5.335	2.634
C	13.580	-2.141	-0.027
H	14.407	-2.264	0.641
H	13.811	-1.381	-0.744
C	12.347	-1.735	0.763
C	11.142	-1.360	0.146
H	11.063	-1.411	-0.933
C	10.053	-0.888	0.882
H	9.138	-0.585	0.382
C	10.171	-0.771	2.265
O	9.111	-0.226	3.006
H	9.496	0.256	3.787
C	12.402	-1.660	2.161
H	13.305	-1.975	2.675
C	11.330	-1.186	2.915
H	11.406	-1.112	3.995
C	13.108	1.795	-0.091
H	13.043	0.757	-0.342
H	13.895	1.941	0.619
N	11.695	2.467	1.860
H	12.493	2.365	2.513
C	11.809	2.248	0.502
C	10.418	2.776	2.148
H	10.054	2.976	3.143
N	9.681	2.780	1.033
C	10.547	2.452	0.003
H	10.201	2.389	-1.015
C	4.276	1.381	-1.182
C	3.025	-0.203	-2.510
H	2.915	-1.165	-2.997
C	4.175	0.134	-1.826
H	5.011	-0.549	-1.753
C	1.968	0.720	-2.586
O	0.876	0.344	-3.284
H	0.290	1.109	-3.396
C	3.206	2.292	-1.249

H	3.279	3.251	-0.753
C	2.060	1.968	-1.953
H	1.228	2.664	-1.993
C	5.506	1.710	-0.492
O	5.451	2.772	0.409
C	6.289	1.259	3.043
H	6.497	0.575	3.877
H	4.987	2.502	1.244
O	7.339	1.450	2.241
H	8.103	0.797	2.460
O	6.602	1.188	-0.658
O	5.214	1.798	2.885
Fe	7.626	3.146	0.720

Mode ^{3}A1

E=-3130.511071 au ZPE=0.5613524034 au

C	8.904	6.391	-3.424
H	8.393	7.258	-3.060
H	8.656	6.237	-4.453
N	8.492	3.897	-3.092
H	8.803	3.605	-4.031
C	8.489	5.196	-2.627
C	8.164	3.078	-2.070
H	8.124	2.003	-2.155
N	7.939	3.784	-0.964
C	8.125	5.107	-1.308
H	8.013	5.904	-0.591
C	7.894	7.898	3.875
H	8.649	7.548	4.548
H	7.051	8.246	4.435
N	6.182	6.642	2.482
H	5.452	7.360	2.619
C	7.468	6.776	2.974
C	6.121	5.538	1.713
H	5.229	5.166	1.235
N	7.319	4.953	1.678
C	8.163	5.715	2.460
H	9.198	5.449	2.577
C	13.816	-2.256	0.008
H	14.556	-2.457	0.754
H	14.172	-1.492	-0.651
C	12.537	-1.791	0.677
C	11.444	-1.361	-0.090
H	11.513	-1.398	-1.167
C	10.287	-0.867	0.493
H	9.470	-0.520	-0.130
C	10.206	-0.771	1.882
O	9.051	-0.208	2.421
H	9.259	0.215	3.295
C	12.409	-1.728	2.068
H	13.226	-2.073	2.695
C	11.256	-1.224	2.678
H	11.193	-1.166	3.760
C	13.050	1.892	0.052
H	12.919	0.848	-0.145
H	13.869	2.027	0.727
N	11.680	2.558	2.039
H	12.468	2.356	2.681
C	11.799	2.446	0.667
C	10.430	2.936	2.352
H	10.056	3.065	3.355
N	9.717	3.099	1.231
C	10.572	2.802	0.177
H	10.249	2.859	-0.844
C	4.362	1.440	-0.731
C	3.048	-0.079	-2.094
H	2.867	-1.058	-2.521
C	4.113	0.149	-1.251
H	4.752	-0.688	-0.995
C	2.174	0.975	-2.414
O	1.150	0.678	-3.229
H	0.646	1.480	-3.447
C	3.473	2.486	-1.064
H	3.632	3.470	-0.642
C	2.390	2.261	-1.888
H	1.694	3.065	-2.107
C	5.528	1.713	0.069
O	5.819	2.871	0.464
C	6.495	0.605	0.443
H	6.565	-0.173	-0.319
H	6.156	0.162	1.387
O	7.792	1.197	0.610
H	8.293	0.709	1.344
O	7.620	2.662	2.841
O	6.548	1.975	3.086
Fe	7.731	3.148	0.995

Model ^{3}TS1

E=-3130.469935 au ZPE=0.5558587378 au

C	8.929	6.417	-3.406
H	8.424	7.289	-3.047
H	8.673	6.254	-4.432
N	8.442	3.936	-3.068
H	8.730	3.635	-4.011
C	8.515	5.231	-2.595
C	8.103	3.127	-2.043
H	7.999	2.057	-2.130
N	7.957	3.837	-0.924
C	8.200	5.151	-1.265
H	8.151	5.945	-0.539
C	7.945	7.918	3.868
H	8.703	7.565	4.536
H	7.104	8.263	4.433
N	6.219	6.660	2.500
H	5.490	7.377	2.650
C	7.515	6.801	2.963
C	6.145	5.557	1.733
H	5.248	5.182	1.268
N	7.348	4.980	1.667
C	8.207	5.746	2.428
H	9.245	5.483	2.522
C	13.799	-2.249	-0.002
H	14.530	-2.447	0.754
H	14.163	-1.487	-0.659
C	12.512	-1.782	0.649
C	11.439	-1.336	-0.135
H	11.531	-1.360	-1.211
C	10.274	-0.838	0.429
H	9.469	-0.482	-0.206
C	10.169	-0.759	1.815
O	9.005	-0.189	2.337
H	9.197	0.225	3.220
C	12.358	-1.733	2.038
H	13.161	-2.090	2.677
C	11.197	-1.227	2.630
H	11.112	-1.179	3.711
C	13.010	1.899	0.079
H	12.877	0.855	-0.115
H	13.828	2.035	0.755
N	11.633	2.556	2.062
H	12.418	2.347	2.703
C	11.759	2.457	0.690
C	10.378	2.936	2.369
H	10.003	3.064	3.372
N	9.673	3.112	1.248
C	10.534	2.818	0.197
H	10.220	2.884	-0.826
C	4.311	1.414	-0.670
C	3.120	-0.164	-2.074
H	2.999	-1.150	-2.507
C	4.142	0.113	-1.190
H	4.833	-0.679	-0.924
C	2.215	0.850	-2.433
O	1.236	0.516	-3.293
H	0.715	1.301	-3.528
C	3.398	2.423	-1.045
H	3.504	3.417	-0.629
C	2.353	2.145	-1.903
H	1.631	2.917	-2.152
C	5.462	1.752	0.131
O	5.782	2.962	0.365
C	6.357	0.764	0.732
H	6.238	-0.310	0.622
H	6.092	1.208	2.068
O	7.686	1.209	0.631
H	8.270	0.702	1.312
O	7.430	2.570	2.739
O	6.244	1.930	2.961
Fe	7.667	3.176	0.983

Model ^{3}A2

E=-3130.481900 au ZPE=0.5555867853 au

C	8.879	6.365	-3.406
H	8.363	7.231	-3.048
H	8.643	6.210	-4.438
N	8.444	3.871	-3.083
H	8.763	3.582	-4.022
C	8.455	5.168	-2.612
C	8.087	3.053	-2.068
H	8.009	1.982	-2.179
N	7.861	3.749	-0.951
C	8.074	5.073	-1.297
H	7.958	5.870	-0.582
C	7.790	8.057	3.906
H	8.528	7.680	4.582

H	6.964	8.449	4.462
N	6.027	6.855	2.521
H	5.313	7.593	2.660
C	7.312	6.946	3.016
C	5.942	5.762	1.733
H	5.038	5.447	1.236
N	7.117	5.136	1.688
C	7.975	5.869	2.486
H	9.002	5.577	2.613
C	13.807	-2.264	-0.011
H	14.563	-2.449	0.723
H	14.133	-1.488	-0.672
C	12.527	-1.835	0.679
C	11.410	-1.432	-0.067
H	11.467	-1.440	-1.146
C	10.236	-1.010	0.542
H	9.395	-0.691	-0.063
C	10.169	-0.966	1.932
O	8.976	-0.517	2.513
H	9.178	-0.054	3.371
C	12.419	-1.800	2.073
H	13.262	-2.119	2.681
C	11.251	-1.371	2.708
H	11.197	-1.338	3.792
C	13.052	1.798	0.045
H	12.948	0.758	-0.182
H	13.873	1.936	0.717
N	11.706	2.421	2.060
H	12.520	2.252	2.682
C	11.789	2.300	0.687
C	10.456	2.784	2.402
H	10.125	2.950	3.415
N	9.698	2.923	1.306
C	10.535	2.621	0.231
H	10.186	2.662	-0.785
C	4.331	1.168	-0.747
C	3.103	-0.297	-2.246
H	2.956	-1.257	-2.728
C	4.132	-0.095	-1.352
H	4.792	-0.923	-1.124
C	2.221	0.756	-2.546
O	1.234	0.486	-3.418
H	0.730	1.293	-3.618
C	3.437	2.215	-1.064
H	3.569	3.180	-0.592
C	2.390	2.015	-1.943
H	1.691	2.818	-2.154
C	5.469	1.429	0.112
O	5.704	2.619	0.565
C	6.407	0.408	0.445
H	6.231	-0.661	0.372
H	5.368	2.721	2.448
O	7.582	0.839	0.892
H	8.107	0.233	1.549
O	7.220	2.690	2.889
O	5.867	2.689	3.303
Fe	7.579	3.149	1.150

Model ^{3}TS2

E=-3130.459014 au ZPE=0.5615801553 au

C	8.930	6.455	-3.445
H	8.423	7.330	-3.095
H	8.683	6.287	-4.472
N	8.481	3.973	-3.090
H	8.769	3.671	-4.034
C	8.507	5.276	-2.632
C	8.180	3.162	-2.060
H	8.099	2.089	-2.133
N	8.006	3.884	-0.953
C	8.187	5.204	-1.302
H	8.105	6.001	-0.582
C	7.894	7.862	3.876
H	8.655	7.499	4.534
H	7.061	8.209	4.451
N	6.160	6.654	2.475
H	5.447	7.389	2.614
C	7.448	6.754	2.967
C	6.070	5.559	1.698
H	5.177	5.224	1.196
N	7.250	4.941	1.658
C	8.118	5.680	2.440
H	9.149	5.394	2.549
C	13.816	-2.280	0.008
H	14.537	-2.483	0.772
H	14.189	-1.514	-0.639
C	12.520	-1.817	0.645
C	11.447	-1.403	-0.156
H	11.546	-1.455	-1.230

C	10.271	-0.908	0.385
H	9.464	-0.586	-0.264
C	10.155	-0.792	1.769
O	8.988	-0.210	2.258
H	9.160	0.194	3.147
C	12.354	-1.740	2.031
H	13.155	-2.075	2.684
C	11.182	-1.232	2.601
H	11.090	-1.163	3.680
C	12.976	1.854	0.105
H	12.864	0.809	-0.094
H	13.786	2.002	0.789
N	11.573	2.527	2.074
H	12.357	2.347	2.726
C	11.710	2.387	0.707
C	10.308	2.892	2.362
H	9.933	3.050	3.362
N	9.605	3.013	1.230
C	10.480	2.698	0.197
H	10.174	2.717	-0.830
C	4.304	1.438	-0.642
C	3.155	-0.215	-2.004
H	3.071	-1.216	-2.409
C	4.164	0.114	-1.117
H	4.880	-0.649	-0.825
C	2.233	0.763	-2.413
O	1.268	0.384	-3.282
H	0.746	1.159	-3.545
C	3.370	2.408	-1.070
H	3.450	3.421	-0.695
C	2.338	2.075	-1.926
H	1.605	2.823	-2.208
C	5.435	1.851	0.143
O	5.776	3.129	0.209
C	6.363	1.000	0.840
H	6.111	0.003	1.187
H	5.004	2.651	2.356
O	7.684	1.167	0.411
H	8.277	0.698	1.093
O	6.797	2.025	2.243
O	5.723	2.564	3.014
Fe	7.608	3.187	0.851

Model ^{3}A3

E=-3130.530913 au ZPE=0.5669586703 au

C	8.964	6.506	-3.547
H	8.461	7.370	-3.165
H	8.738	6.393	-4.587
N	8.473	4.020	-3.327
H	8.786	3.754	-4.273
C	8.508	5.295	-2.804
C	8.127	3.164	-2.343
H	8.044	2.097	-2.483
N	7.926	3.822	-1.207
C	8.145	5.154	-1.490
H	8.051	5.919	-0.734
C	7.972	7.948	3.958
H	8.746	7.609	4.615
H	7.156	8.329	4.535
N	6.199	6.687	2.657
H	5.491	7.431	2.776
C	7.497	6.806	3.116
C	6.106	5.566	1.915
H	5.206	5.233	1.423
N	7.286	4.944	1.873
C	8.157	5.717	2.612
H	9.194	5.448	2.698
C	13.677	-2.166	-0.013
H	14.452	-2.329	0.706
H	13.984	-1.408	-0.703
C	12.412	-1.720	0.699
C	11.280	-1.296	-0.014
H	11.296	-1.329	-1.095
C	10.150	-0.801	0.629
H	9.296	-0.458	0.055
C	10.141	-0.707	2.020
O	9.020	-0.150	2.642
H	9.309	0.340	3.456
C	12.351	-1.657	2.096
H	13.200	-1.998	2.681
C	11.229	-1.159	2.762
H	11.217	-1.100	3.846
C	13.059	1.884	-0.040
H	12.931	0.843	-0.253
H	13.862	2.009	0.656
N	11.667	2.581	1.916
H	12.443	2.390	2.574

C	11.796	2.432	0.551
C	10.413	2.983	2.200
H	10.037	3.141	3.197
N	9.712	3.120	1.071
C	10.573	2.781	0.038
H	10.252	2.814	-0.986
C	4.337	1.492	-0.606
C	3.271	-0.199	-1.977
H	3.146	-1.225	-2.300
C	4.144	0.137	-0.961
H	4.710	-0.651	-0.475
C	2.512	0.800	-2.612
O	1.658	0.406	-3.574
H	1.181	1.173	-3.932
C	3.583	2.486	-1.274
H	3.707	3.522	-0.988
C	2.666	2.149	-2.245
H	2.066	2.917	-2.720
C	5.352	1.914	0.319
O	5.770	3.097	0.341
C	6.086	1.004	1.324
H	5.797	-0.051	1.311
H	4.379	2.644	2.735
O	7.451	1.190	1.061
H	8.043	0.667	1.703
O	5.915	1.549	2.635
O	4.494	1.688	2.871
Fe	7.744	3.276	0.791

Model ^{3}TS3' ZPE=0.5666156908 au

C	8.971	6.519	-3.553
H	8.470	7.385	-3.173
H	8.744	6.403	-4.592
N	8.472	4.036	-3.326
H	8.780	3.765	-4.273
C	8.513	5.312	-2.806
C	8.131	3.183	-2.337
H	8.046	2.115	-2.473
N	7.940	3.845	-1.202
C	8.159	5.175	-1.489
H	8.072	5.942	-0.734
C	7.958	7.939	3.948
H	8.731	7.599	4.605
H	7.144	8.325	4.525
N	6.175	6.668	2.664
H	5.468	7.414	2.779
C	7.477	6.795	3.110
C	6.075	5.535	1.941
H	5.173	5.195	1.457
N	7.257	4.913	1.899
C	8.133	5.697	2.619
H	9.171	5.432	2.700
C	13.684	-2.168	-0.014
H	14.462	-2.331	0.702
H	13.989	-1.411	-0.706
C	12.422	-1.721	0.702
C	11.290	-1.290	-0.008
H	11.304	-1.319	-1.090
C	10.164	-0.792	0.639
H	9.311	-0.441	0.067
C	10.157	-0.702	2.030
O	9.040	-0.139	2.651
H	9.328	0.343	3.469
C	12.363	-1.663	2.099
H	13.212	-2.011	2.681
C	11.244	-1.163	2.769
H	11.233	-1.108	3.853
C	13.066	1.887	-0.043
H	12.932	0.847	-0.258
H	13.870	2.007	0.652
N	11.676	2.582	1.915
H	12.453	2.387	2.573
C	11.806	2.441	0.550
C	10.424	2.989	2.200
H	10.049	3.141	3.199
N	9.724	3.137	1.072
C	10.585	2.799	0.038
H	10.265	2.840	-0.986
C	4.331	1.465	-0.592
C	3.251	-0.199	-1.985
H	3.122	-1.219	-2.323
C	4.129	0.117	-0.967
H	4.687	-0.683	-0.493
C	2.502	0.814	-2.608
O	1.651	0.439	-3.580
H	1.180	1.213	-3.929
C	3.578	2.473	-1.240
H	3.705	3.504	-0.935

C	2.659	2.156	-2.216
H	2.061	2.935	-2.676
C	5.368	1.873	0.316
O	5.807	3.047	0.324
C	6.121	0.919	1.261
H	5.966	-0.147	1.073
H	5.082	2.869	3.022
O	7.488	1.240	1.080
H	8.084	0.710	1.707
O	5.798	1.166	2.627
O	4.649	2.040	2.753
Fe	7.754	3.269	0.783

Model ^{3}A4'

E=-3130.535882 au ZPE=0.5650352558 au

C	9.003	6.547	-3.570
H	8.502	7.407	-3.177
H	8.767	6.440	-4.608
N	8.501	4.064	-3.369
H	8.796	3.805	-4.324
C	8.557	5.331	-2.831
C	8.181	3.196	-2.388
H	8.086	2.131	-2.541
N	8.016	3.841	-1.240
C	8.232	5.175	-1.508
H	8.159	5.929	-0.739
C	7.960	7.895	3.926
H	8.735	7.559	4.582
H	7.148	8.284	4.504
N	6.162	6.594	2.696
H	5.451	7.331	2.825
C	7.477	6.747	3.095
C	6.058	5.459	1.976
H	5.140	5.087	1.548
N	7.249	4.863	1.886
C	8.136	5.664	2.577
H	9.181	5.415	2.623
C	13.623	-2.128	-0.007
H	14.408	-2.276	0.705
H	13.914	-1.373	-0.707
C	12.361	-1.690	0.715
C	11.224	-1.251	0.018
H	11.233	-1.263	-1.065
C	10.099	-0.766	0.679
H	9.242	-0.408	0.117
C	10.097	-0.698	2.071
O	8.980	-0.158	2.716
H	9.284	0.338	3.520
C	12.308	-1.650	2.114
H	13.162	-2.000	2.688
C	11.191	-1.164	2.797
H	11.186	-1.123	3.881
C	13.096	1.893	-0.059
H	12.981	0.852	-0.279
H	13.893	2.024	0.643
N	11.677	2.559	1.890
H	12.449	2.373	2.555
C	11.823	2.423	0.526
C	10.417	2.951	2.161
H	10.030	3.101	3.155
N	9.726	3.092	1.027
C	10.602	2.766	0.002
H	10.294	2.804	-1.025
C	4.310	1.488	-0.727
C	3.174	-0.176	-2.075
H	3.027	-1.198	-2.401
C	4.086	0.141	-1.087
H	4.652	-0.661	-0.626
C	2.412	0.838	-2.677
O	1.526	0.460	-3.619
H	1.052	1.237	-3.958
C	3.546	2.497	-1.355
H	3.690	3.528	-1.059
C	2.593	2.179	-2.300
H	1.985	2.959	-2.744
C	5.375	1.880	0.162
O	5.848	3.037	0.142
C	6.007	0.918	1.180
H	5.934	-0.140	0.910
H	5.943	2.438	3.410
O	7.356	1.318	1.297
H	7.940	0.707	1.852
O	5.313	0.958	2.402
O	5.162	2.334	2.841
Fe	7.761	3.255	0.704

Model ^{3}TS4'

E=-3130.527067 au ZPE=0.5642942460 au

C	8.942	6.447	-3.481
H	8.434	7.306	-3.094
H	8.701	6.326	-4.516
N	8.465	3.955	-3.245
H	8.765	3.690	-4.196
C	8.513	5.232	-2.725
C	8.137	3.101	-2.252
H	8.048	2.034	-2.386
N	7.962	3.764	-1.113
C	8.179	5.095	-1.403
H	8.101	5.858	-0.645
C	7.969	7.997	3.948
H	8.731	7.634	4.606
H	7.157	8.388	4.525
N	6.169	6.762	2.659
H	5.460	7.499	2.807
C	7.476	6.876	3.089
C	6.069	5.664	1.880
H	5.153	5.320	1.426
N	7.250	5.061	1.783
C	8.131	5.810	2.530
H	9.171	5.540	2.592
C	13.804	-2.241	-0.007
H	14.563	-2.431	0.723
H	14.135	-1.473	-0.675
C	12.534	-1.792	0.690
C	11.407	-1.400	-0.048
H	11.445	-1.444	-1.128
C	10.251	-0.938	0.567
H	9.401	-0.633	-0.034
C	10.210	-0.841	1.957
O	9.046	-0.347	2.546
H	9.291	0.156	3.358
C	12.450	-1.714	2.084
H	13.296	-2.030	2.688
C	11.300	-1.245	2.723
H	11.260	-1.182	3.806
C	13.052	1.814	-0.037
H	12.930	0.776	-0.265
H	13.853	1.934	0.662
N	11.692	2.600	1.910
H	12.490	2.474	2.557
C	11.785	2.347	0.559
C	10.435	2.991	2.197
H	10.094	3.236	3.186
N	9.692	3.014	1.087
C	10.535	2.615	0.061
H	10.191	2.550	-0.955
C	4.284	1.453	-0.601
C	3.226	-0.194	-2.030
H	3.120	-1.207	-2.400
C	4.117	0.115	-1.021
H	4.722	-0.680	-0.595
C	2.430	0.817	-2.594
O	1.564	0.448	-3.557
H	1.074	1.223	-3.880
C	3.490	2.461	-1.193
H	3.596	3.484	-0.854
C	2.557	2.148	-2.158
H	1.922	2.922	-2.575
C	5.334	1.834	0.306
O	5.755	3.011	0.367
C	6.084	0.813	1.186
H	5.528	-0.124	1.320
H	7.828	1.939	3.188
O	7.350	0.665	0.635
H	7.937	0.218	1.299
O	6.152	1.262	2.545
O	7.147	2.372	2.644
Fe	7.698	3.219	0.835

Model ^{3}A5

E=-3130.564798 au ZPE=0.5594894907 au

C	8.884	6.340	-3.361
H	8.362	7.205	-3.010
H	8.626	6.158	-4.384
N	8.553	3.844	-2.966
H	8.862	3.544	-3.903
C	8.500	5.155	-2.532
C	8.258	3.039	-1.928
H	8.269	1.963	-1.986
N	7.998	3.762	-0.835
C	8.134	5.085	-1.213
H	7.987	5.892	-0.515
C	7.783	7.983	3.887
H	8.520	7.631	4.578

H	6.941	8.363	4.427
N	6.061	6.716	2.504
H	5.333	7.438	2.623
C	7.342	6.851	3.005
C	6.004	5.596	1.753
H	5.112	5.226	1.273
N	7.194	5.004	1.738
C	8.032	5.773	2.518
H	9.062	5.500	2.665
C	13.860	-2.279	-0.009
H	14.618	-2.475	0.720
H	14.196	-1.512	-0.676
C	12.593	-1.823	0.689
C	11.467	-1.430	-0.048
H	11.502	-1.479	-1.127
C	10.314	-0.964	0.566
H	9.468	-0.653	-0.034
C	10.270	-0.856	1.955
O	9.118	-0.333	2.536
H	9.362	0.065	3.409
C	12.508	-1.745	2.083
H	13.353	-2.063	2.687
C	11.360	-1.269	2.721
H	11.325	-1.205	3.804
C	13.227	1.803	-0.018
H	13.123	0.761	-0.239
H	14.051	1.945	0.650
N	11.898	2.531	1.986
H	12.716	2.422	2.614
C	11.971	2.305	0.625
C	10.645	2.887	2.311
H	10.303	3.104	3.310
N	9.888	2.925	1.208
C	10.712	2.564	0.156
H	10.345	2.507	-0.851
C	4.283	1.324	-0.827
C	2.973	-0.161	-2.215
H	2.793	-1.126	-2.671
C	4.057	0.050	-1.394
H	4.713	-0.774	-1.148
C	2.064	0.885	-2.457
O	1.013	0.596	-3.237
H	0.494	1.398	-3.418
C	3.370	2.372	-1.089
H	3.525	3.342	-0.633
C	2.267	2.157	-1.889
H	1.546	2.951	-2.051
C	5.448	1.602	-0.039
O	5.728	2.652	0.527
C	6.612	0.441	0.021
H	6.816	0.249	-1.054
H	8.032	1.851	3.023
O	7.772	1.055	0.579
H	8.127	0.492	1.321
O	6.145	-0.586	0.660
O	7.638	2.718	2.844
Fe	7.830	3.147	1.118

Model ^{3}TS5

E=-3130.528221 au ZPE=0.5578039390 au

C	8.853	6.295	-3.367
H	8.337	7.158	-3.000
H	8.592	6.133	-4.392
N	8.473	3.798	-3.023
H	8.786	3.510	-3.962
C	8.462	5.099	-2.558
C	8.147	2.980	-2.000
H	8.112	1.906	-2.087
N	7.914	3.683	-0.892
C	8.093	5.008	-1.241
H	7.975	5.803	-0.525
C	7.861	7.850	3.847
H	8.613	7.507	4.526
H	7.012	8.195	4.399
N	6.159	6.559	2.473
H	5.423	7.270	2.601
C	7.448	6.722	2.947
C	6.107	5.434	1.730
H	5.214	5.035	1.277
N	7.311	4.868	1.690
C	8.152	5.658	2.443
H	9.189	5.407	2.562
C	13.920	-2.331	-0.010
H	14.657	-2.544	0.736
H	14.282	-1.562	-0.660
C	12.643	-1.866	0.660
C	11.555	-1.441	-0.115
H	11.632	-1.473	-1.191

C	10.388	-0.963	0.458
H	9.577	-0.622	-0.173
C	10.299	-0.874	1.845
O	9.133	-0.323	2.386
H	9.353	0.072	3.269
C	12.506	-1.810	2.050
H	13.321	-2.154	2.681
C	11.344	-1.317	2.651
H	11.270	-1.261	3.732
C	13.087	1.842	0.009
H	12.964	0.799	-0.195
H	13.902	1.979	0.689
N	11.747	2.620	1.978
H	12.556	2.499	2.614
C	11.829	2.383	0.621
C	10.489	2.982	2.291
H	10.137	3.196	3.287
N	9.740	3.012	1.185
C	10.572	2.638	0.140
H	10.216	2.572	-0.870
C	4.362	1.320	-0.729
C	3.041	-0.148	-2.125
H	2.804	-1.128	-2.523
C	4.036	0.026	-1.194
H	4.564	-0.837	-0.806
C	2.287	0.964	-2.553
O	1.298	0.711	-3.418
H	0.834	1.528	-3.669
C	3.621	2.430	-1.188
H	3.843	3.412	-0.789
C	2.576	2.257	-2.071
H	1.964	3.103	-2.367
C	5.467	1.538	0.200
O	5.806	2.693	0.640
C	6.698	0.477	0.116
H	6.767	-0.239	-0.707
H	8.035	1.799	3.051
O	7.908	1.034	0.485
H	8.331	0.524	1.260
O	5.745	0.315	1.059
O	7.581	2.623	2.824
Fe	7.729	3.039	1.079

Model ^{3}A6

E=-3130.567102 au ZPE=0.5635345707 au

C	8.836	6.250	-3.319
H	8.313	7.111	-2.958
H	8.578	6.079	-4.343
N	8.420	3.753	-2.967
H	8.723	3.460	-3.907
C	8.454	5.055	-2.502
C	8.078	2.944	-1.941
H	8.005	1.870	-2.024
N	7.888	3.654	-0.828
C	8.111	4.972	-1.178
H	8.032	5.771	-0.461
C	7.858	7.869	3.877
H	8.613	7.525	4.553
H	7.011	8.214	4.433
N	6.158	6.596	2.480
H	5.428	7.314	2.599
C	7.440	6.741	2.977
C	6.106	5.473	1.734
H	5.216	5.089	1.261
N	7.304	4.891	1.714
C	8.140	5.670	2.485
H	9.171	5.404	2.625
C	14.033	-2.400	-0.053
H	14.796	-2.641	0.657
H	14.387	-1.634	-0.711
C	12.801	-1.909	0.677
C	11.669	-1.491	-0.037
H	11.659	-1.580	-1.114
C	10.566	-0.945	0.600
H	9.714	-0.611	0.017
C	10.593	-0.781	1.983
O	9.500	-0.144	2.566
H	9.751	0.273	3.434
C	12.766	-1.798	2.070
H	13.610	-2.152	2.655
C	11.674	-1.232	2.732
H	11.680	-1.122	3.811
C	13.030	1.906	0.095
H	12.885	0.861	-0.086
H	13.857	2.041	0.761
N	11.688	2.622	2.084
H	12.486	2.437	2.718

C	11.790	2.483	0.713
C	10.435	2.995	2.405
H	10.062	3.128	3.408
N	9.710	3.134	1.292
C	10.554	2.823	0.232
H	10.221	2.860	-0.787
C	4.222	1.441	-0.813
C	2.885	0.039	-2.260
H	2.661	-0.914	-2.723
C	3.933	0.181	-1.383
H	4.537	-0.677	-1.126
C	2.070	1.143	-2.555
O	1.035	0.903	-3.373
H	0.565	1.725	-3.590
C	3.421	2.550	-1.140
H	3.618	3.510	-0.679
C	2.346	2.405	-2.000
H	1.700	3.249	-2.212
C	5.327	1.566	0.105
O	5.753	2.613	0.627
C	6.971	0.236	1.171
H	7.195	-0.792	1.436
H	6.987	1.804	2.957
O	8.040	1.028	0.839
H	8.759	0.746	1.510
O	5.908	0.354	0.337
O	7.511	2.619	2.886
Fe	7.699	3.036	1.147

Model ^{3}TS6

E=-3130.541247 au ZPE=0.5622632074 au

C	8.872	6.320	-3.352
H	8.356	7.187	-2.995
H	8.614	6.148	-4.376
N	8.423	3.832	-2.999
H	8.716	3.535	-3.941
C	8.478	5.132	-2.532
C	8.087	3.024	-1.972
H	7.998	1.952	-2.054
N	7.924	3.737	-0.857
C	8.154	5.053	-1.203
H	8.091	5.849	-0.480
C	7.873	7.858	3.883
H	8.632	7.514	4.554
H	7.031	8.204	4.445
N	6.162	6.590	2.500
H	5.435	7.313	2.621
C	7.448	6.730	2.988
C	6.098	5.469	1.754
H	5.205	5.095	1.280
N	7.293	4.879	1.727
C	8.140	5.656	2.490
H	9.173	5.390	2.616
C	14.029	-2.406	-0.056
H	14.786	-2.645	0.662
H	14.388	-1.641	-0.712
C	12.790	-1.915	0.662
C	11.657	-1.515	-0.061
H	11.652	-1.623	-1.136
C	10.548	-0.969	0.562
H	9.688	-0.660	-0.024
C	10.567	-0.780	1.944
O	9.475	-0.131	2.500
H	9.715	0.286	3.368
C	12.748	-1.784	2.053
H	13.592	-2.124	2.647
C	11.650	-1.214	2.702
H	11.652	-1.091	3.779
C	13.021	1.892	0.098
H	12.881	0.848	-0.089
H	13.843	2.027	0.770
N	11.663	2.604	2.079
H	12.456	2.423	2.719
C	11.776	2.462	0.710
C	10.405	2.974	2.389
H	10.029	3.107	3.391
N	9.688	3.109	1.271
C	10.542	2.796	0.218
H	10.218	2.829	-0.804
C	4.183	1.454	-0.750
C	2.941	-0.038	-2.187
H	2.758	-1.015	-2.617
C	3.938	0.162	-1.258
H	4.546	-0.671	-0.927
C	2.126	1.037	-2.577
O	1.137	0.750	-3.440
H	0.661	1.559	-3.694
C	3.392	2.535	-1.179

H	3.560	3.521	-0.765
C	2.357	2.328	-2.073
H	1.710	3.151	-2.356
C	5.252	1.662	0.194
O	5.741	2.771	0.503
C	6.881	0.601	1.492
H	7.069	-0.324	2.026
H	6.664	1.764	2.746
O	7.945	1.054	0.724
H	8.734	0.809	1.300
O	5.739	0.514	0.717
O	7.428	2.372	2.713
Fe	7.676	3.057	1.054

Model ^{3}A7

E=-3130.658825 au ZPE=0.5692427303 au

C	8.923	6.442	-3.481
H	8.416	7.302	-3.096
H	8.690	6.326	-4.519
N	8.433	3.957	-3.270
H	8.746	3.700	-4.218
C	8.481	5.227	-2.733
C	8.073	3.095	-2.296
H	7.973	2.031	-2.449
N	7.878	3.744	-1.152
C	8.117	5.077	-1.420
H	8.028	5.832	-0.654
C	7.863	7.878	3.930
H	8.632	7.531	4.588
H	7.050	8.267	4.506
N	6.071	6.614	2.648
H	5.368	7.360	2.765
C	7.377	6.739	3.085
C	5.966	5.481	1.922
H	5.052	5.126	1.471
N	7.143	4.862	1.861
C	8.026	5.642	2.581
H	9.063	5.370	2.665
C	13.651	-2.160	-0.033
H	14.463	-2.304	0.649
H	13.909	-1.399	-0.739
C	12.412	-1.737	0.737
C	11.236	-1.321	0.092
H	11.189	-1.350	-0.990
C	10.140	-0.838	0.805
H	9.247	-0.504	0.286
C	10.216	-0.747	2.193
O	9.139	-0.199	2.897
H	9.491	0.277	3.696
C	12.430	-1.684	2.136
H	13.311	-2.027	2.670
C	11.347	-1.196	2.868
H	11.396	-1.139	3.951
C	13.029	1.867	-0.020
H	12.927	0.825	-0.241
H	13.818	2.006	0.689
N	11.598	2.539	1.916
H	12.374	2.375	2.581
C	11.744	2.384	0.554
C	10.328	2.898	2.187
H	9.939	3.053	3.180
N	9.631	3.002	1.051
C	10.513	2.686	0.029
H	10.203	2.699	-0.999
C	4.203	1.468	-0.935
C	3.081	-0.139	-2.350
H	2.877	-1.155	-2.664
C	3.919	0.134	-1.288
H	4.379	-0.675	-0.735
C	2.476	0.916	-3.048
O	1.668	0.576	-4.073
H	1.247	1.369	-4.442
C	3.606	2.520	-1.650
H	3.814	3.544	-1.364
C	2.733	2.249	-2.689
H	2.257	3.060	-3.228
C	5.164	1.760	0.115
O	5.669	2.879	0.304
C	6.171	0.852	2.102
H	6.319	-0.175	2.447
H	4.506	1.304	2.950
O	7.414	1.456	1.931
H	8.156	0.839	2.232
O	5.515	0.671	0.833
O	5.421	1.632	2.942
Fe	7.648	3.131	0.792

Model ^{3}TS7

E=-3130.653057 au ZPE=0.5682478973 au

C	8.918	6.437	-3.477
H	8.415	7.299	-3.091
H	8.685	6.323	-4.515
N	8.422	3.952	-3.265
H	8.743	3.693	-4.210
C	8.470	5.223	-2.730
C	8.044	3.094	-2.294
H	7.941	2.030	-2.447
N	7.835	3.746	-1.154
C	8.087	5.077	-1.421
H	7.995	5.835	-0.659
C	7.868	7.882	3.933
H	8.637	7.532	4.589
H	7.056	8.272	4.511
N	6.074	6.632	2.644
H	5.375	7.383	2.761
C	7.378	6.745	3.087
C	5.964	5.501	1.915
H	5.050	5.160	1.454
N	7.136	4.872	1.860
C	8.021	5.644	2.585
H	9.056	5.365	2.672
C	13.661	-2.163	-0.033
H	14.472	-2.308	0.649
H	13.921	-1.403	-0.740
C	12.423	-1.738	0.736
C	11.249	-1.321	0.089
H	11.203	-1.350	-0.993
C	10.152	-0.838	0.800
H	9.260	-0.503	0.279
C	10.225	-0.748	2.188
O	9.146	-0.198	2.886
H	9.493	0.279	3.687
C	12.437	-1.687	2.135
H	13.318	-2.031	2.670
C	11.354	-1.198	2.866
H	11.400	-1.141	3.948
C	13.019	1.873	-0.024
H	12.915	0.831	-0.244
H	13.807	2.011	0.687
N	11.586	2.545	1.909
H	12.360	2.379	2.575
C	11.734	2.394	0.547
C	10.316	2.903	2.179
H	9.926	3.055	3.172
N	9.619	3.011	1.042
C	10.503	2.698	0.020
H	10.193	2.714	-1.009
C	4.207	1.438	-0.911
C	3.091	-0.150	-2.350
H	2.884	-1.163	-2.675
C	3.920	0.108	-1.278
H	4.370	-0.708	-0.727
C	2.495	0.915	-3.044
O	1.693	0.587	-4.075
H	1.275	1.385	-4.439
C	3.618	2.500	-1.620
H	3.823	3.520	-1.320
C	2.755	2.243	-2.671
H	2.285	3.062	-3.206
C	5.132	1.725	0.168
O	5.613	2.851	0.399
C	6.179	0.811	2.127
H	6.385	-0.203	2.471
H	4.705	1.963	2.672
O	7.420	1.427	1.861
H	8.173	0.835	2.182
O	5.459	0.639	0.901
O	5.456	1.497	3.067
Fe	7.634	3.130	0.801

Model ^{3}A8

E=-3130.656676 au ZPE=0.5682400269 au

C	8.918	6.440	-3.490
H	8.414	7.301	-3.104
H	8.687	6.327	-4.529
N	8.427	3.953	-3.277
H	8.745	3.694	-4.224
C	8.469	5.225	-2.745
C	8.054	3.094	-2.305
H	7.955	2.030	-2.456
N	7.843	3.747	-1.166
C	8.087	5.080	-1.436
H	7.991	5.839	-0.675
C	7.878	7.878	3.940
H	8.649	7.534	4.598

H	7.064	8.266	4.516
N	6.096	6.623	2.639
H	5.395	7.373	2.747
C	7.394	6.737	3.098
C	5.991	5.487	1.918
H	5.084	5.148	1.442
N	7.164	4.852	1.885
C	8.042	5.630	2.613
H	9.076	5.353	2.711
C	13.694	-2.175	-0.036
H	14.508	-2.328	0.642
H	13.955	-1.413	-0.741
C	12.463	-1.745	0.740
C	11.289	-1.320	0.097
H	11.239	-1.347	-0.985
C	10.198	-0.832	0.814
H	9.305	-0.490	0.299
C	10.279	-0.746	2.202
O	9.205	-0.191	2.906
H	9.557	0.299	3.697
C	12.484	-1.699	2.139
H	13.363	-2.052	2.669
C	11.407	-1.205	2.875
H	11.455	-1.151	3.958
C	13.056	1.877	-0.048
H	12.946	0.835	-0.266
H	13.846	2.012	0.661
N	11.635	2.568	1.886
H	12.410	2.401	2.552
C	11.776	2.406	0.524
C	10.369	2.941	2.158
H	9.984	3.099	3.152
N	9.671	3.047	1.023
C	10.546	2.717	-0.001
H	10.230	2.729	-1.027
C	4.264	1.459	-0.880
C	3.145	-0.117	-2.330
H	2.937	-1.126	-2.664
C	3.984	0.133	-1.265
H	4.444	-0.689	-0.728
C	2.533	0.954	-3.001
O	1.719	0.636	-4.026
H	1.289	1.435	-4.373
C	3.659	2.527	-1.566
H	3.853	3.542	-1.246
C	2.789	2.279	-2.613
H	2.306	3.102	-3.129
C	5.174	1.732	0.212
O	5.642	2.862	0.479
C	6.280	0.846	2.130
H	6.413	-0.154	2.535
H	5.486	2.498	2.691
O	7.534	1.369	1.763
H	8.278	0.810	2.170
O	5.518	0.647	0.924
O	5.621	1.607	3.052
Fe	7.691	3.138	0.791

Model ^{3}TS8

E=-3130.624240 au ZPE=0.5638701460 au

C	8.883	6.384	-3.460
H	8.377	7.242	-3.069
H	8.650	6.275	-4.499
N	8.406	3.891	-3.253
H	8.732	3.636	-4.198
C	8.439	5.163	-2.719
C	8.016	3.029	-2.290
H	7.912	1.966	-2.445
N	7.785	3.681	-1.153
C	8.035	5.016	-1.418
H	7.924	5.774	-0.658
C	7.873	7.895	3.944
H	8.641	7.546	4.602
H	7.060	8.286	4.520
N	6.087	6.649	2.638
H	5.387	7.401	2.750
C	7.385	6.758	3.099
C	5.980	5.518	1.912
H	5.070	5.179	1.441
N	7.151	4.882	1.876
C	8.031	5.653	2.609
H	9.064	5.373	2.707
C	13.693	-2.181	-0.053
H	14.509	-2.332	0.623
H	13.951	-1.420	-0.759
C	12.463	-1.753	0.726
C	11.285	-1.328	0.089
H	11.230	-1.357	-0.993

C	10.195	-0.841	0.810
H	9.296	-0.510	0.300
C	10.288	-0.758	2.196
O	9.223	-0.201	2.924
H	9.600	0.266	3.719
C	12.491	-1.709	2.125
H	13.372	-2.064	2.651
C	11.418	-1.216	2.866
H	11.472	-1.161	3.948
C	13.050	1.872	-0.061
H	12.942	0.830	-0.278
H	13.837	2.009	0.651
N	11.628	2.573	1.867
H	12.405	2.412	2.533
C	11.767	2.400	0.506
C	10.364	2.946	2.138
H	9.980	3.113	3.132
N	9.661	3.038	1.003
C	10.535	2.703	-0.019
H	10.216	2.707	-1.045
C	4.400	1.412	-0.896
C	3.232	-0.098	-2.380
H	3.012	-1.092	-2.752
C	4.127	0.108	-1.351
H	4.624	-0.727	-0.871
C	2.576	0.999	-2.961
O	1.726	0.725	-3.971
H	1.278	1.535	-4.264
C	3.729	2.504	-1.470
H	3.902	3.500	-1.085
C	2.821	2.302	-2.499
H	2.294	3.143	-2.936
C	5.327	1.573	0.212
O	5.605	2.794	0.673
C	6.417	1.154	2.669
H	6.385	0.143	3.061
H	5.433	2.595	2.013
O	7.612	1.613	2.326
H	8.329	0.864	2.411
O	5.851	0.562	0.755
O	5.473	1.967	2.914
Fe	7.673	3.149	0.812

Model ^{3}P

E=-3130.656142 au ZPE=0.5670300877 au

C	8.957	6.485	-3.511
H	8.457	7.346	-3.120
H	8.720	6.375	-4.549
N	8.468	4.002	-3.306
H	8.775	3.747	-4.258
C	8.511	5.270	-2.767
C	8.109	3.133	-2.342
H	7.995	2.071	-2.491
N	7.906	3.781	-1.196
C	8.144	5.116	-1.455
H	8.050	5.869	-0.687
C	7.889	7.817	3.923
H	8.665	7.465	4.571
H	7.081	8.201	4.510
N	6.101	6.598	2.598
H	5.409	7.356	2.710
C	7.396	6.685	3.074
C	5.989	5.471	1.863
H	5.076	5.161	1.378
N	7.147	4.812	1.839
C	8.027	5.569	2.588
H	9.055	5.275	2.698
C	13.571	-2.125	-0.038
H	14.398	-2.243	0.630
H	13.802	-1.372	-0.762
C	12.339	-1.711	0.749
C	11.145	-1.309	0.128
H	11.072	-1.350	-0.952
C	10.060	-0.823	0.860
H	9.153	-0.502	0.357
C	10.174	-0.717	2.244
O	9.122	-0.152	2.985
H	9.515	0.321	3.768
C	12.386	-1.650	2.148
H	13.281	-1.986	2.665
C	11.319	-1.160	2.900
H	11.390	-1.094	3.980
C	13.095	1.841	-0.068
H	13.015	0.799	-0.297
H	13.877	1.990	0.646
N	11.657	2.545	1.856
H	12.438	2.424	2.526

C	11.799	2.328	0.502
C	10.380	2.884	2.117
H	9.994	3.081	3.104
N	9.674	2.911	0.981
C	10.557	2.567	-0.029
H	10.234	2.512	-1.053
C	4.333	1.427	-1.214
C	2.942	-0.114	-2.455
H	2.766	-1.074	-2.925
C	4.135	0.176	-1.828
H	4.937	-0.550	-1.780
C	1.925	0.857	-2.487
O	0.777	0.515	-3.104
H	0.210	1.299	-3.187
C	3.311	2.393	-1.254
H	3.450	3.357	-0.781
C	2.116	2.113	-1.893
H	1.318	2.849	-1.908
C	5.609	1.668	-0.577
O	5.677	2.792	0.273
C	6.332	1.389	2.964
H	6.491	0.708	3.811
H	5.208	2.591	1.130
O	7.420	1.559	2.208
H	8.165	0.879	2.443
O	6.634	1.020	-0.719
O	5.273	1.940	2.748
Fe	7.698	3.080	0.691

Model ^{7}A2

E=-3130.515704 au ZPE=0.5555867853 au

C	8.879	6.365	-3.406
H	8.363	7.231	-3.048
H	8.643	6.210	-4.438
N	8.444	3.871	-3.083
H	8.763	3.582	-4.022
C	8.455	5.168	-2.612
C	8.087	3.053	-2.068
H	8.009	1.982	-2.179
N	7.861	3.749	-0.951
C	8.074	5.073	-1.297
H	7.958	5.870	-0.582
C	7.790	8.057	3.906
H	8.528	7.680	4.582
H	6.964	8.449	4.462
N	6.027	6.855	2.521
H	5.313	7.593	2.660
C	7.312	6.946	3.016
C	5.942	5.762	1.733
H	5.038	5.447	1.236
N	7.117	5.136	1.688
C	7.975	5.869	2.486
H	9.002	5.577	2.613
C	13.807	-2.264	-0.011
H	14.563	-2.449	0.723
H	14.133	-1.488	-0.672
C	12.527	-1.835	0.679
C	11.410	-1.432	-0.067
H	11.467	-1.440	-1.146
C	10.236	-1.010	0.542
H	9.395	-0.691	-0.063
C	10.169	-0.966	1.932
O	8.976	-0.517	2.513
H	9.178	-0.054	3.371
C	12.419	-1.800	2.073
H	13.262	-2.119	2.681
C	11.251	-1.371	2.708
H	11.197	-1.338	3.792
C	13.052	1.798	0.045
H	12.948	0.758	-0.182
H	13.873	1.936	0.717
N	11.706	2.421	2.060
H	12.520	2.252	2.682
C	11.789	2.300	0.687
C	10.456	2.784	2.402
H	10.125	2.950	3.415
N	9.698	2.923	1.306
C	10.535	2.621	0.231
H	10.186	2.662	-0.785
C	4.331	1.168	-0.747
C	3.103	-0.297	-2.246
H	2.956	-1.257	-2.728
C	4.132	-0.095	-1.352
H	4.792	-0.923	-1.124
C	2.221	0.756	-2.546
O	1.234	0.486	-3.418
H	0.730	1.293	-3.618

C	3.437	2.215	-1.064
H	3.569	3.180	-0.592
C	2.390	2.015	-1.943
H	1.691	2.818	-2.154
C	5.469	1.429	0.112
O	5.704	2.619	0.565
C	6.407	0.408	0.445
H	6.231	-0.661	0.372
H	5.368	2.721	2.448
O	7.582	0.839	0.892
H	8.107	0.233	1.549
O	7.220	2.690	2.889
O	5.867	2.689	3.303
Fe	7.579	3.149	1.150

Model ^{7}TS2

E=-3130.473841 au ZPE=0.5615801553 au

C	8.998	6.539	-3.500
H	8.487	7.436	-3.145
H	8.773	6.422	-4.562
N	8.466	4.069	-3.211
H	8.747	3.779	-4.161
C	8.551	5.354	-2.713
C	8.131	3.241	-2.206
H	7.991	2.177	-2.322
N	7.998	3.928	-1.074
C	8.242	5.249	-1.382
H	8.195	6.030	-0.639
C	7.863	7.970	3.895
H	8.633	7.591	4.571
H	7.040	8.384	4.486
N	6.061	6.716	2.618
H	5.354	7.458	2.763
C	7.376	6.843	3.034
C	5.937	5.597	1.887
H	5.018	5.237	1.451
N	7.122	4.987	1.802
C	8.026	5.759	2.509
H	9.063	5.482	2.572
C	13.786	-2.261	-0.006
H	14.561	-2.460	0.740
H	14.151	-1.483	-0.689
C	12.501	-1.820	0.667
C	11.393	-1.421	-0.095
H	11.457	-1.460	-1.172
C	10.224	-0.958	0.492
H	9.389	-0.647	-0.126
C	10.148	-0.863	1.881
O	8.980	-0.336	2.427
H	9.185	0.085	3.300
C	12.379	-1.756	2.059
H	13.209	-2.078	2.682
C	11.216	-1.283	2.672
H	11.155	-1.228	3.754
C	12.987	1.819	0.060
H	12.913	0.750	-0.162
H	13.799	1.937	0.782
N	11.584	2.446	2.038
H	12.375	2.266	2.683
C	11.713	2.326	0.666
C	10.325	2.802	2.340
H	9.959	2.953	3.344
N	9.608	2.938	1.213
C	10.478	2.639	0.168
H	10.158	2.673	-0.856
C	4.253	1.249	-0.744
C	3.128	-0.438	-2.082
H	3.043	-1.455	-2.445
C	4.088	-0.095	-1.147
H	4.758	-0.861	-0.769
C	2.268	0.543	-2.600
O	1.341	0.146	-3.507
H	0.851	0.922	-3.819
C	3.385	2.226	-1.285
H	3.490	3.258	-0.972
C	2.394	1.877	-2.183
H	1.718	2.634	-2.567
C	5.368	1.673	0.058
O	5.794	2.931	-0.033
C	6.214	0.857	0.885
H	5.882	-0.101	1.274
H	4.634	2.317	2.226
O	7.564	0.950	0.576
H	8.110	0.499	1.296
O	6.502	1.930	2.292
O	5.332	2.502	2.890
Fe	7.527	3.219	0.862

Model ^{7}A3

E=-3130.486325 au ZPE=0.5669586703 au

C	8.993	6.536	-3.563
H	8.496	7.411	-3.198
H	8.774	6.409	-4.603
N	8.442	4.061	-3.314
H	8.744	3.778	-4.261
C	8.518	5.342	-2.805
C	8.073	3.225	-2.328
H	7.935	2.162	-2.455
N	7.901	3.909	-1.197
C	8.162	5.232	-1.489
H	8.094	6.008	-0.742
C	7.957	7.975	3.925
H	8.725	7.623	4.582
H	7.142	8.359	4.502
N	6.162	6.721	2.650
H	5.453	7.462	2.800
C	7.475	6.845	3.071
C	6.042	5.612	1.906
H	5.130	5.257	1.451
N	7.231	5.003	1.817
C	8.129	5.768	2.537
H	9.167	5.495	2.599
C	13.679	-2.178	-0.014
H	14.458	-2.341	0.701
H	13.981	-1.417	-0.703
C	12.416	-1.738	0.705
C	11.270	-1.335	0.002
H	11.272	-1.383	-1.079
C	10.142	-0.846	0.653
H	9.275	-0.522	0.086
C	10.149	-0.732	2.043
O	9.034	-0.174	2.667
H	9.321	0.282	3.500
C	12.370	-1.661	2.102
H	13.229	-1.989	2.682
C	11.251	-1.168	2.776
H	11.251	-1.101	3.859
C	13.030	1.852	-0.030
H	12.921	0.812	-0.256
H	13.828	1.983	0.671
N	11.621	2.504	1.931
H	12.403	2.317	2.586
C	11.755	2.371	0.562
C	10.365	2.878	2.222
H	9.993	3.029	3.224
N	9.657	3.017	1.092
C	10.526	2.700	0.054
H	10.207	2.734	-0.972
C	4.374	1.403	-0.614
C	3.291	-0.250	-2.043
H	3.149	-1.272	-2.374
C	4.153	0.052	-1.009
H	4.690	-0.754	-0.517
C	2.579	0.768	-2.703
O	1.734	0.394	-3.698
H	1.276	1.177	-4.044
C	3.656	2.418	-1.314
H	3.780	3.449	-1.007
C	2.771	2.107	-2.326
H	2.212	2.897	-2.818
C	5.292	1.781	0.393
O	5.718	3.078	0.465
C	6.049	0.959	1.366
H	5.818	-0.108	1.387
H	4.346	2.487	2.551
O	7.443	1.190	1.078
H	8.050	0.702	1.724
O	5.976	1.527	2.699
O	4.594	1.698	3.068
Fe	7.583	3.290	0.744

Model ^{7}TS3'

E=-3130.480662 au ZPE=0.5666156908 au

C	8.962	6.503	-3.541
H	8.451	7.396	-3.179
H	8.754	6.405	-4.609
N	8.422	4.024	-3.283
H	8.736	3.739	-4.226
C	8.485	5.310	-2.782
C	8.029	3.194	-2.302
H	7.898	2.129	-2.423
N	7.829	3.885	-1.178
C	8.098	5.209	-1.473
H	8.012	5.990	-0.735
C	7.945	7.991	3.936

H	8.726	7.622	4.605
H	7.128	8.407	4.533
N	6.144	6.732	2.672
H	5.436	7.474	2.821
C	7.458	6.860	3.087
C	6.020	5.617	1.937
H	5.104	5.259	1.494
N	7.211	5.009	1.848
C	8.112	5.781	2.558
H	9.151	5.512	2.615
C	13.690	-2.176	-0.032
H	14.501	-2.339	0.685
H	14.013	-1.412	-0.748
C	12.436	-1.732	0.699
C	11.292	-1.303	0.007
H	11.288	-1.336	-1.075
C	10.176	-0.807	0.673
H	9.311	-0.460	0.118
C	10.192	-0.717	2.065
O	9.087	-0.156	2.703
H	9.381	0.286	3.541
C	12.399	-1.676	2.097
H	13.257	-2.026	2.665
C	11.292	-1.177	2.785
H	11.298	-1.126	3.869
C	13.026	1.879	-0.032
H	12.938	0.811	-0.247
H	13.836	1.993	0.693
N	11.624	2.519	1.933
H	12.402	2.304	2.585
C	11.760	2.418	0.561
C	10.378	2.917	2.230
H	10.007	3.047	3.234
N	9.678	3.104	1.102
C	10.542	2.794	0.057
H	10.226	2.864	-0.967
C	4.435	1.380	-0.628
C	3.317	-0.202	-2.112
H	3.153	-1.209	-2.478
C	4.206	0.050	-1.088
H	4.736	-0.782	-0.634
C	2.589	0.848	-2.701
O	1.728	0.522	-3.699
H	1.260	1.318	-3.999
C	3.689	2.426	-1.244
H	3.803	3.437	-0.875
C	2.780	2.164	-2.251
H	2.202	2.976	-2.680
C	5.376	1.692	0.375
O	5.704	2.996	0.659
C	6.137	0.774	1.259
H	6.182	-0.271	0.943
H	5.088	2.566	2.424
O	7.511	1.303	1.215
H	8.132	0.778	1.819
O	5.733	0.737	2.606
O	4.838	1.821	3.010
Fe	7.589	3.302	0.779

Model ^{7}A4'

E=-3130.494539 au ZPE=0.5650352558 au

C	9.010	6.555	-3.560
H	8.501	7.448	-3.195
H	8.796	6.456	-4.626
N	8.456	4.082	-3.315
H	8.751	3.802	-4.265
C	8.538	5.361	-2.801
C	8.093	3.242	-2.330
H	7.952	2.181	-2.461
N	7.934	3.920	-1.194
C	8.195	5.245	-1.481
H	8.135	6.016	-0.728
C	7.921	7.948	3.912
H	8.700	7.584	4.586
H	7.101	8.365	4.507
N	6.116	6.655	2.681
H	5.402	7.389	2.830
C	7.437	6.809	3.070
C	5.998	5.531	1.958
H	5.081	5.146	1.539
N	7.196	4.945	1.849
C	8.098	5.737	2.536
H	9.142	5.482	2.579
C	13.694	-2.180	-0.024
H	14.501	-2.346	0.697
H	14.024	-1.415	-0.737
C	12.437	-1.734	0.699
C	11.297	-1.310	-0.002

H	11.300	-1.345	-1.084
C	10.175	-0.815	0.653
H	9.314	-0.472	0.087
C	10.179	-0.720	2.044
O	9.066	-0.165	2.672
H	9.349	0.278	3.512
C	12.389	-1.673	2.096
H	13.243	-2.018	2.672
C	11.275	-1.175	2.774
H	11.273	-1.121	3.858
C	13.049	1.872	-0.026
H	12.969	0.804	-0.247
H	13.859	1.986	0.700
N	11.639	2.508	1.938
H	12.418	2.311	2.592
C	11.777	2.397	0.568
C	10.385	2.890	2.229
H	10.010	3.025	3.232
N	9.684	3.057	1.099
C	10.555	2.749	0.060
H	10.241	2.806	-0.966
C	4.435	1.345	-0.801
C	3.233	-0.255	-2.200
H	3.045	-1.268	-2.536
C	4.158	0.006	-1.211
H	4.681	-0.827	-0.752
C	2.508	0.790	-2.799
O	1.610	0.450	-3.757
H	1.152	1.247	-4.068
C	3.687	2.389	-1.426
H	3.845	3.409	-1.102
C	2.738	2.115	-2.393
H	2.165	2.925	-2.833
C	5.418	1.668	0.164
O	5.768	2.960	0.376
C	6.181	0.694	1.003
H	6.274	-0.303	0.559
H	4.321	1.607	2.853
O	7.507	1.268	1.137
H	8.094	0.733	1.765
O	5.652	0.405	2.266
O	5.291	1.638	2.948
Fe	7.594	3.280	0.740

Model ^{7}TS4'

E=-3130.488138 au ZPE=0.5642942460 au

C	8.990	6.533	-3.521
H	8.481	7.427	-3.157
H	8.773	6.432	-4.587
N	8.436	4.061	-3.269
H	8.735	3.779	-4.217
C	8.522	5.340	-2.757
C	8.064	3.224	-2.285
H	7.922	2.162	-2.414
N	7.904	3.905	-1.150
C	8.173	5.227	-1.438
H	8.115	6.000	-0.687
C	7.877	7.918	3.907
H	8.653	7.538	4.576
H	7.061	8.334	4.506
N	6.075	6.689	2.608
H	5.375	7.439	2.750
C	7.384	6.797	3.045
C	5.947	5.575	1.870
H	5.033	5.233	1.407
N	7.127	4.947	1.802
C	8.027	5.705	2.528
H	9.060	5.415	2.608
C	13.763	-2.230	-0.017
H	14.552	-2.419	0.717
H	14.114	-1.458	-0.713
C	12.493	-1.780	0.679
C	11.368	-1.376	-0.056
H	11.399	-1.431	-1.135
C	10.225	-0.884	0.561
H	9.377	-0.561	-0.033
C	10.195	-0.764	1.950
O	9.061	-0.200	2.526
H	9.305	0.234	3.383
C	12.411	-1.699	2.073
H	13.252	-2.029	2.676
C	11.275	-1.198	2.715
H	11.247	-1.129	3.797
C	12.996	1.849	0.008
H	12.916	0.781	-0.213
H	13.804	1.964	0.736
N	11.591	2.503	1.971
H	12.379	2.326	2.621

C	11.721	2.368	0.601
C	10.332	2.862	2.266
H	9.962	3.006	3.269
N	9.617	2.991	1.139
C	10.487	2.681	0.098
H	10.167	2.706	-0.927
C	4.376	1.255	-0.821
C	3.215	-0.359	-2.233
H	3.055	-1.373	-2.581
C	4.133	-0.084	-1.241
H	4.689	-0.904	-0.798
C	2.468	0.676	-2.823
O	1.574	0.326	-3.781
H	1.114	1.120	-4.096
C	3.613	2.290	-1.443
H	3.760	3.311	-1.116
C	2.674	2.003	-2.414
H	2.089	2.806	-2.853
C	5.355	1.600	0.139
O	5.703	2.902	0.315
C	6.181	0.693	0.979
H	6.046	-0.375	0.788
H	5.392	2.546	2.804
O	7.551	1.094	0.773
H	8.138	0.647	1.464
O	5.937	0.776	2.387
O	6.265	2.116	2.848
Fe	7.526	3.212	0.765

Model ^{7}A5

E=-3130.579169 au ZPE=0.5594894907 au

C	8.859	6.289	-3.348
H	8.337	7.147	-2.980
H	8.598	6.125	-4.373
N	8.549	3.785	-2.988
H	8.874	3.499	-3.924
C	8.479	5.089	-2.538
C	8.231	2.966	-1.963
H	8.254	1.890	-2.041
N	7.943	3.667	-0.866
C	8.085	4.994	-1.228
H	7.916	5.793	-0.524
C	7.814	8.021	3.891
H	8.549	7.671	4.586
H	6.975	8.414	4.427
N	6.059	6.700	2.610
H	5.326	7.416	2.745
C	7.365	6.884	3.023
C	5.988	5.568	1.881
H	5.078	5.164	1.464
N	7.194	5.011	1.793
C	8.058	5.827	2.495
H	9.109	5.600	2.551
C	13.871	-2.278	-0.023
H	14.629	-2.472	0.707
H	14.206	-1.511	-0.689
C	12.603	-1.824	0.673
C	11.496	-1.386	-0.067
H	11.550	-1.388	-1.147
C	10.336	-0.936	0.546
H	9.504	-0.589	-0.054
C	10.264	-0.893	1.939
O	9.098	-0.402	2.513
H	9.301	0.018	3.387
C	12.494	-1.802	2.067
H	13.327	-2.152	2.670
C	11.338	-1.345	2.705
H	11.284	-1.331	3.789
C	13.204	1.840	-0.006
H	13.081	0.798	-0.218
H	14.046	1.975	0.641
N	11.894	2.410	2.044
H	12.710	2.207	2.654
C	11.970	2.362	0.664
C	10.661	2.781	2.411
H	10.325	2.869	3.433
N	9.913	3.006	1.321
C	10.732	2.752	0.230
H	10.373	2.865	-0.775
C	4.321	1.286	-0.739
C	3.020	-0.160	-2.178
H	2.837	-1.116	-2.653
C	4.090	0.025	-1.335
H	4.735	-0.809	-1.091
C	2.128	0.901	-2.421
O	1.092	0.638	-3.229
H	0.580	1.445	-3.404

C	3.424	2.348	-1.000
H	3.582	3.308	-0.524
C	2.336	2.160	-1.827
H	1.628	2.967	-1.991
C	5.474	1.533	0.076
O	5.734	2.572	0.683
C	6.641	0.395	0.117
H	6.867	0.233	-0.958
H	7.890	3.083	3.770
O	7.783	0.991	0.713
H	8.160	0.429	1.469
O	6.178	-0.679	0.693
O	7.650	2.483	3.049
Fe	7.809	3.036	1.301

Model ^{7}TS5

E=-3130.552424 au ZPE=0.5578039390 au

C	8.861	6.304	-3.353
H	8.342	7.166	-2.990
H	8.604	6.139	-4.378
N	8.526	3.803	-2.991
H	8.852	3.513	-3.925
C	8.471	5.108	-2.542
C	8.194	2.989	-1.966
H	8.196	1.913	-2.043
N	7.915	3.694	-0.871
C	8.075	5.018	-1.232
H	7.915	5.820	-0.528
C	7.817	8.039	3.900
H	8.553	7.689	4.594
H	6.981	8.437	4.437
N	6.052	6.715	2.636
H	5.320	7.432	2.772
C	7.361	6.900	3.038
C	5.974	5.580	1.912
H	5.062	5.171	1.504
N	7.180	5.026	1.817
C	8.051	5.842	2.510
H	9.101	5.613	2.558
C	13.897	-2.295	-0.004
H	14.643	-2.501	0.735
H	14.248	-1.527	-0.661
C	12.625	-1.833	0.678
C	11.535	-1.388	-0.083
H	11.608	-1.392	-1.161
C	10.368	-0.929	0.507
H	9.555	-0.571	-0.111
C	10.273	-0.882	1.897
O	9.096	-0.376	2.450
H	9.285	0.052	3.325
C	12.492	-1.808	2.069
H	13.312	-2.162	2.688
C	11.327	-1.341	2.686
H	11.255	-1.323	3.768
C	13.182	1.852	-0.011
H	13.061	0.809	-0.219
H	14.020	1.991	0.640
N	11.860	2.412	2.029
H	12.668	2.196	2.642
C	11.944	2.377	0.649
C	10.624	2.787	2.390
H	10.287	2.867	3.412
N	9.882	3.024	1.300
C	10.709	2.777	0.212
H	10.357	2.903	-0.795
C	4.358	1.282	-0.696
C	3.047	-0.147	-2.145
H	2.837	-1.107	-2.602
C	4.080	0.011	-1.252
H	4.665	-0.850	-0.955
C	2.216	0.948	-2.455
O	1.190	0.702	-3.279
H	0.699	1.519	-3.477
C	3.545	2.381	-1.047
H	3.734	3.344	-0.590
C	2.471	2.217	-1.899
H	1.806	3.050	-2.106
C	5.465	1.481	0.222
O	5.761	2.577	0.779
C	6.712	0.415	0.154
H	6.813	-0.195	-0.749
H	7.944	3.032	3.760
O	7.892	0.944	0.602
H	8.273	0.447	1.424
O	5.748	0.127	1.041
O	7.669	2.454	3.034
Fe	7.743	3.064	1.296

Model ^{7}A6

E=-3130.591978 au ZPE=0.5635345707 au

C	8.837	6.239	-3.310
H	8.312	7.096	-2.942
H	8.577	6.074	-4.335
N	8.473	3.736	-2.967
H	8.786	3.453	-3.906
C	8.461	5.037	-2.500
C	8.135	2.917	-1.946
H	8.084	1.842	-2.038
N	7.896	3.617	-0.837
C	8.089	4.941	-1.184
H	7.962	5.737	-0.469
C	7.776	7.991	3.894
H	8.510	7.636	4.587
H	6.939	8.384	4.432
N	6.018	6.691	2.595
H	5.291	7.414	2.723
C	7.322	6.858	3.022
C	5.939	5.556	1.869
H	5.028	5.164	1.443
N	7.138	4.982	1.798
C	8.005	5.788	2.508
H	9.052	5.547	2.579
C	14.058	-2.397	-0.059
H	14.842	-2.627	0.632
H	14.384	-1.625	-0.724
C	12.838	-1.926	0.702
C	11.686	-1.508	0.019
H	11.662	-1.561	-1.062
C	10.576	-1.022	0.692
H	9.704	-0.696	0.138
C	10.614	-0.918	2.082
O	9.497	-0.379	2.710
H	9.729	0.001	3.598
C	12.827	-1.854	2.098
H	13.692	-2.202	2.657
C	11.728	-1.348	2.795
H	11.744	-1.277	3.877
C	13.173	1.826	0.008
H	13.054	0.784	-0.205
H	14.008	1.963	0.664
N	11.871	2.479	2.040
H	12.694	2.320	2.650
C	11.931	2.347	0.665
C	10.628	2.834	2.399
H	10.301	2.973	3.418
N	9.860	2.965	1.308
C	10.673	2.668	0.225
H	10.299	2.703	-0.781
C	4.271	1.293	-0.823
C	2.940	-0.030	-2.345
H	2.687	-0.968	-2.825
C	3.943	0.052	-1.409
H	4.480	-0.838	-1.115
C	2.219	1.122	-2.695
O	1.247	0.944	-3.603
H	0.808	1.784	-3.817
C	3.547	2.444	-1.182
H	3.773	3.390	-0.705
C	2.521	2.362	-2.108
H	1.938	3.243	-2.359
C	5.352	1.365	0.133
O	5.781	2.395	0.684
C	6.925	-0.015	1.246
H	7.140	-1.064	1.429
H	7.848	3.196	3.781
O	8.001	0.801	1.036
H	8.682	0.505	1.736
O	5.902	0.149	0.360
O	7.654	2.535	3.100
Fe	7.718	2.986	1.314

Model ^{7}TS6

E=-3130.552424 au ZPE=0.5622632074 au

C	8.882	6.311	-3.382
H	8.356	7.169	-3.019
H	8.633	6.148	-4.410
N	8.500	3.810	-3.043
H	8.802	3.522	-3.986
C	8.493	5.112	-2.579
C	8.181	2.990	-2.020
H	8.128	1.915	-2.102
N	7.964	3.696	-0.912
C	8.142	5.020	-1.258
H	8.025	5.816	-0.540
C	7.806	8.014	3.911
H	8.542	7.669	4.607

H	6.968	8.411	4.445
N	6.051	6.695	2.627
H	5.321	7.417	2.753
C	7.356	6.871	3.053
C	5.972	5.558	1.911
H	5.068	5.159	1.476
N	7.177	4.989	1.844
C	8.045	5.803	2.546
H	9.092	5.565	2.613
C	14.042	-2.397	-0.076
H	14.817	-2.623	0.626
H	14.377	-1.629	-0.742
C	12.812	-1.920	0.666
C	11.661	-1.524	-0.032
H	11.645	-1.601	-1.111
C	10.545	-1.031	0.623
H	9.664	-0.736	0.061
C	10.573	-0.891	2.010
O	9.462	-0.319	2.603
H	9.693	0.056	3.490
C	12.790	-1.823	2.060
H	13.652	-2.157	2.632
C	11.684	-1.307	2.739
H	11.696	-1.217	3.820
C	13.136	1.839	0.026
H	12.997	0.799	-0.184
H	13.972	1.961	0.683
N	11.814	2.460	2.058
H	12.621	2.251	2.675
C	11.902	2.387	0.679
C	10.579	2.852	2.407
H	10.238	2.959	3.426
N	9.843	3.066	1.306
C	10.672	2.782	0.227
H	10.327	2.882	-0.784
C	4.208	1.371	-0.724
C	3.071	-0.164	-2.204
H	2.914	-1.156	-2.609
C	3.985	0.063	-1.195
H	4.555	-0.759	-0.779
C	2.325	0.905	-2.723
O	1.432	0.606	-3.690
H	0.973	1.411	-3.980
C	3.477	2.441	-1.268
H	3.631	3.443	-0.888
C	2.527	2.210	-2.247
H	1.933	3.032	-2.634
C	5.233	1.621	0.266
O	5.763	2.746	0.450
C	6.791	0.718	1.737
H	6.915	-0.147	2.375
H	7.387	2.670	3.590
O	7.878	0.925	0.858
H	8.656	0.627	1.401
O	5.643	0.542	0.942
O	7.348	2.138	2.762
Fe	7.716	3.104	1.151

Model ^{7}A7

E=-3130.552424 au ZPE=0.5692427303 au

C	8.923	6.442	-3.481
H	8.416	7.302	-3.096
H	8.690	6.326	-4.519
N	8.433	3.957	-3.270
H	8.746	3.700	-4.218
C	8.481	5.227	-2.733
C	8.073	3.095	-2.296
H	7.973	2.031	-2.449
N	7.878	3.744	-1.152
C	8.117	5.077	-1.420
H	8.028	5.832	-0.654
C	7.863	7.878	3.930
H	8.632	7.531	4.588
H	7.050	8.267	4.506
N	6.071	6.614	2.648
H	5.368	7.360	2.765
C	7.377	6.739	3.085
C	5.966	5.481	1.922
H	5.052	5.126	1.471
N	7.143	4.862	1.861
C	8.026	5.642	2.581
H	9.063	5.370	2.665
C	13.651	-2.160	-0.033
H	14.463	-2.304	0.649
H	13.909	-1.399	-0.739
C	12.412	-1.737	0.737
C	11.236	-1.321	0.092
H	11.189	-1.350	-0.990

C	10.140	-0.838	0.805
H	9.247	-0.504	0.286
C	10.216	-0.747	2.193
O	9.139	-0.199	2.897
H	9.491	0.277	3.696
C	12.430	-1.684	2.136
H	13.311	-2.027	2.670
C	11.347	-1.196	2.868
H	11.396	-1.139	3.951
C	13.029	1.867	-0.020
H	12.927	0.825	-0.241
H	13.818	2.006	0.689
N	11.598	2.539	1.916
H	12.374	2.375	2.581
C	11.744	2.384	0.554
C	10.328	2.898	2.187
H	9.939	3.053	3.180
N	9.631	3.002	1.051
C	10.513	2.686	0.029
H	10.203	2.699	-0.999
C	4.203	1.468	-0.935
C	3.081	-0.139	-2.350
H	2.877	-1.155	-2.664
C	3.919	0.134	-1.288
H	4.379	-0.675	-0.735
C	2.476	0.916	-3.048
O	1.668	0.576	-4.073
H	1.247	1.369	-4.442
C	3.606	2.520	-1.650
H	3.814	3.544	-1.364
C	2.733	2.249	-2.689
H	2.257	3.060	-3.228
C	5.164	1.760	0.115
O	5.669	2.879	0.304
C	6.171	0.852	2.102
H	6.319	-0.175	2.447
H	4.506	1.304	2.950
O	7.414	1.456	1.931
H	8.156	0.839	2.232
O	5.515	0.671	0.833
O	5.421	1.632	2.942
Fe	7.648	3.131	0.792

Model ^{7}TS7

E=-3130.573979 au ZPE=0.5682478973 au

C	8.971	6.498	-3.518
H	8.457	7.389	-3.154
H	8.753	6.397	-4.583
N	8.417	4.025	-3.270
H	8.716	3.747	-4.219
C	8.508	5.302	-2.754
C	8.039	3.189	-2.285
H	7.885	2.129	-2.421
N	7.881	3.864	-1.148
C	8.158	5.184	-1.435
H	8.101	5.957	-0.684
C	7.856	7.921	3.915
H	8.631	7.546	4.588
H	7.041	8.344	4.510
N	6.055	6.676	2.626
H	5.355	7.428	2.755
C	7.363	6.790	3.066
C	5.929	5.548	1.905
H	5.015	5.197	1.449
N	7.109	4.920	1.851
C	8.006	5.690	2.568
H	9.039	5.402	2.656
C	13.662	-2.168	-0.045
H	14.503	-2.304	0.641
H	13.942	-1.403	-0.778
C	12.431	-1.749	0.738
C	11.241	-1.348	0.108
H	11.176	-1.388	-0.973
C	10.151	-0.872	0.835
H	9.241	-0.560	0.331
C	10.249	-0.770	2.222
O	9.181	-0.225	2.935
H	9.537	0.213	3.752
C	12.469	-1.690	2.136
H	13.360	-2.026	2.658
C	11.395	-1.206	2.882
H	11.457	-1.146	3.963
C	13.049	1.841	-0.037
H	12.992	0.775	-0.272
H	13.851	1.964	0.695
N	11.632	2.476	1.919
H	12.419	2.315	2.574

C	11.763	2.336	0.551
C	10.366	2.819	2.209
H	9.994	2.968	3.211
N	9.651	2.929	1.082
C	10.523	2.630	0.045
H	10.199	2.650	-0.980
C	4.310	1.322	-0.870
C	3.124	-0.235	-2.321
H	2.900	-1.238	-2.668
C	3.992	-0.017	-1.284
H	4.466	-0.847	-0.774
C	2.497	0.851	-2.976
O	1.658	0.544	-3.996
H	1.233	1.353	-4.324
C	3.660	2.413	-1.548
H	3.852	3.425	-1.216
C	2.768	2.174	-2.568
H	2.268	3.004	-3.057
C	5.254	1.560	0.125
O	5.758	2.764	0.387
C	6.247	0.690	2.074
H	6.526	-0.294	2.457
H	5.600	2.084	3.229
O	7.429	1.520	2.110
H	8.211	0.927	2.323
O	5.861	0.478	0.747
O	5.252	1.286	2.814
Fe	7.552	3.201	0.820

Model ^{7}A8

E=-3130.583522 au ZPE=0.5682400269 au

C	8.978	6.488	-3.506
H	8.462	7.377	-3.139
H	8.755	6.386	-4.570
N	8.433	4.012	-3.258
H	8.724	3.736	-4.209
C	8.526	5.289	-2.740
C	8.064	3.173	-2.272
H	7.908	2.113	-2.409
N	7.913	3.847	-1.132
C	8.188	5.169	-1.419
H	8.136	5.940	-0.666
C	7.868	7.923	3.913
H	8.641	7.551	4.589
H	7.048	8.343	4.504
N	6.075	6.669	2.621
H	5.370	7.416	2.751
C	7.383	6.790	3.062
C	5.956	5.544	1.898
H	5.045	5.188	1.442
N	7.141	4.924	1.842
C	8.034	5.695	2.563
H	9.068	5.414	2.651
C	13.678	-2.175	-0.047
H	14.518	-2.317	0.640
H	13.962	-1.410	-0.779
C	12.449	-1.750	0.735
C	11.258	-1.354	0.104
H	11.191	-1.401	-0.976
C	10.168	-0.875	0.830
H	9.257	-0.567	0.325
C	10.267	-0.767	2.216
O	9.199	-0.218	2.924
H	9.550	0.224	3.741
C	12.489	-1.683	2.133
H	13.381	-2.016	2.656
C	11.414	-1.197	2.877
H	11.478	-1.132	3.958
C	13.070	1.845	-0.039
H	13.007	0.778	-0.273
H	13.874	1.964	0.691
N	11.655	2.484	1.920
H	12.441	2.317	2.575
C	11.787	2.347	0.552
C	10.393	2.838	2.211
H	10.020	2.983	3.213
N	9.681	2.960	1.081
C	10.552	2.655	0.044
H	10.228	2.680	-0.980
C	4.372	1.309	-0.938
C	3.147	-0.257	-2.342
H	2.918	-1.263	-2.674
C	4.055	-0.029	-1.337
H	4.547	-0.856	-0.841
C	2.489	0.818	-2.973
O	1.604	0.501	-3.953
H	1.170	1.309	-4.271
C	3.703	2.389	-1.599

H	3.905	3.405	-1.282
C	2.773	2.142	-2.587
H	2.255	2.968	-3.063
C	5.314	1.551	0.062
O	5.783	2.769	0.386
C	6.273	0.711	2.031
H	6.559	-0.248	2.461
H	4.810	1.940	2.280
O	7.482	1.535	2.041
H	8.255	0.942	2.283
O	5.929	0.475	0.695
O	5.303	1.284	2.799
Fe	7.578	3.203	0.836

Model ^{7}TS8

E=-3130.549051 au ZPE=0.5638701460 au

C	8.940	6.440	-3.488
H	8.418	7.328	-3.127
H	8.721	6.333	-4.553
N	8.424	3.958	-3.226
H	8.730	3.679	-4.173
C	8.491	5.241	-2.719
C	8.050	3.121	-2.241
H	7.912	2.057	-2.364
N	7.866	3.804	-1.110
C	8.127	5.130	-1.404
H	8.047	5.908	-0.661
C	7.866	7.931	3.922
H	8.637	7.566	4.604
H	7.038	8.346	4.506
N	6.094	6.668	2.612
H	5.385	7.411	2.740
C	7.396	6.792	3.067
C	5.985	5.545	1.885
H	5.078	5.189	1.420
N	7.173	4.926	1.839
C	8.056	5.700	2.571
H	9.091	5.423	2.669
C	13.651	-2.168	-0.063
H	14.497	-2.295	0.620
H	13.923	-1.404	-0.801
C	12.422	-1.751	0.726
C	11.225	-1.361	0.103
H	11.153	-1.407	-0.977
C	10.135	-0.888	0.834
H	9.217	-0.587	0.337
C	10.244	-0.779	2.219
O	9.179	-0.231	2.938
H	9.539	0.169	3.772
C	12.469	-1.687	2.124
H	13.365	-2.016	2.642
C	11.396	-1.207	2.874
H	11.468	-1.143	3.955
C	13.068	1.818	-0.037
H	13.017	0.752	-0.278
H	13.873	1.942	0.692
N	11.656	2.466	1.924
H	12.451	2.325	2.575
C	11.780	2.300	0.557
C	10.389	2.794	2.220
H	10.026	2.962	3.224
N	9.661	2.870	1.093
C	10.532	2.563	0.055
H	10.199	2.551	-0.967
C	4.452	1.310	-0.929
C	3.269	-0.258	-2.369
H	3.109	-1.254	-2.768
C	4.242	-0.009	-1.424
H	4.877	-0.808	-1.058
C	2.435	0.783	-2.826
O	1.486	0.455	-3.739
H	0.981	1.247	-3.984
C	3.596	2.348	-1.402
H	3.715	3.352	-1.016
C	2.606	2.086	-2.330
H	1.954	2.886	-2.667
C	5.555	1.595	-0.087
O	5.690	2.844	0.504
C	6.338	0.877	2.248
H	6.434	-0.162	2.538
H	5.202	2.268	1.773
O	7.459	1.647	2.429
H	8.241	1.008	2.459
O	6.476	0.758	0.314
O	5.194	1.478	2.441
Fe	7.572	3.164	0.850

Model ^{7}P

E=-3130.608265 au ZPE=0.5670300877 au

C	8.982	6.558	-3.546
H	8.490	7.463	-3.188
H	8.770	6.461	-4.613
N	8.355	4.105	-3.312
H	8.666	3.818	-4.254
C	8.474	5.380	-2.787
C	7.916	3.281	-2.348
H	7.718	2.228	-2.472
N	7.745	3.963	-1.210
C	8.081	5.274	-1.481
H	8.028	6.043	-0.726
C	7.903	7.768	3.883
H	8.692	7.383	4.531
H	7.092	8.164	4.502
N	6.109	6.614	2.514
H	5.427	7.380	2.654
C	7.403	6.660	3.003
C	5.966	5.514	1.756
H	5.055	5.231	1.252
N	7.114	4.830	1.722
C	8.015	5.544	2.495
H	9.033	5.217	2.609
C	13.540	-2.126	-0.036
H	14.390	-2.228	0.645
H	13.796	-1.363	-0.781
C	12.305	-1.727	0.756
C	11.097	-1.350	0.145
H	11.015	-1.398	-0.935
C	10.009	-0.881	0.884
H	9.090	-0.581	0.390
C	10.130	-0.767	2.268
O	9.076	-0.221	3.016
H	9.471	0.223	3.812
C	12.362	-1.658	2.154
H	13.266	-1.975	2.667
C	11.292	-1.184	2.912
H	11.373	-1.116	3.992
C	13.018	1.811	-0.073
H	12.993	0.746	-0.317
H	13.798	1.949	0.679
N	11.550	2.448	1.846
H	12.331	2.322	2.517
C	11.704	2.268	0.485
C	10.270	2.750	2.113
H	9.878	2.919	3.104
N	9.566	2.790	0.971
C	10.460	2.490	-0.047
H	10.140	2.451	-1.074
C	4.474	1.387	-1.107
C	3.616	-0.284	-2.659
H	3.704	-1.229	-3.184
C	4.618	0.162	-1.821
H	5.518	-0.424	-1.672
C	2.461	0.494	-2.862
O	1.538	0.037	-3.754
H	0.875	0.729	-3.894
C	3.277	2.139	-1.295
H	3.148	3.071	-0.760
C	2.296	1.701	-2.159
H	1.393	2.290	-2.292
C	5.465	1.820	-0.213
O	5.283	2.995	0.553
C	6.265	1.324	3.148
H	6.396	0.428	3.768
H	4.918	2.740	1.433
O	7.393	1.682	2.514
H	8.091	0.943	2.585
O	6.778	1.503	-0.239
O	5.230	1.942	3.070
Fe	7.517	3.057	0.637

Model ^{1}A1

E=-3130.491238 au ZPE=0.5613524034 au

C	8.896	6.372	-3.389
H	8.387	7.241	-3.028
H	8.639	6.208	-4.415
N	8.469	3.881	-3.037
H	8.775	3.581	-3.974
C	8.490	5.184	-2.577
C	8.138	3.073	-2.007
H	8.090	1.999	-2.083
N	7.941	3.788	-0.898
C	8.146	5.105	-1.253
H	8.057	5.906	-0.539
C	7.917	7.936	3.870

H	8.667	7.577	4.543
H	7.074	8.285	4.429
N	6.201	6.691	2.479
H	5.472	7.408	2.622
C	7.488	6.823	2.961
C	6.138	5.588	1.706
H	5.241	5.221	1.232
N	7.334	5.003	1.656
C	8.182	5.765	2.430
H	9.218	5.500	2.539
C	13.862	-2.286	0.000
H	14.598	-2.496	0.747
H	14.226	-1.522	-0.655
C	12.585	-1.814	0.667
C	11.499	-1.378	-0.105
H	11.573	-1.414	-1.182
C	10.341	-0.880	0.473
H	9.530	-0.524	-0.152
C	10.254	-0.786	1.861
O	9.098	-0.223	2.391
H	9.296	0.185	3.273
C	12.453	-1.750	2.057
H	13.267	-2.099	2.687
C	11.299	-1.242	2.662
H	11.231	-1.183	3.744
C	13.031	1.890	0.065
H	12.890	0.847	-0.128
H	13.853	2.020	0.738
N	11.673	2.572	2.051
H	12.462	2.371	2.690
C	11.787	2.457	0.680
C	10.422	2.960	2.362
H	10.059	3.102	3.368
N	9.707	3.127	1.244
C	10.559	2.819	0.192
H	10.236	2.871	-0.829
C	4.365	1.412	-0.729
C	3.036	-0.096	-2.089
H	2.852	-1.070	-2.525
C	4.115	0.127	-1.264
H	4.765	-0.707	-1.028
C	2.150	0.958	-2.379
O	1.118	0.669	-3.185
H	0.611	1.472	-3.391
C	3.461	2.457	-1.026
H	3.620	3.436	-0.592
C	2.365	2.237	-1.836
H	1.661	3.039	-2.031
C	5.548	1.677	0.045
O	5.811	2.824	0.496
C	6.567	0.581	0.309
H	6.660	-0.104	-0.537
H	6.249	0.016	1.192
O	7.838	1.199	0.539
H	8.312	0.705	1.277
O	7.416	2.725	2.721
O	6.896	1.619	3.059
Fe	7.686	3.140	1.032

Model ^{1}TS1

E=-3130.439944 au ZPE=0.5558587378 au

C	8.923	6.407	-3.397
H	8.417	7.281	-3.045
H	8.666	6.234	-4.421
N	8.450	3.925	-3.037
H	8.735	3.620	-3.979
C	8.512	5.228	-2.575
C	8.127	3.124	-2.004
H	8.031	2.052	-2.079
N	7.981	3.843	-0.887
C	8.204	5.157	-1.243
H	8.150	5.958	-0.526
C	7.939	7.930	3.867
H	8.689	7.573	4.541
H	7.093	8.274	4.425
N	6.231	6.686	2.467
H	5.499	7.399	2.615
C	7.517	6.818	2.954
C	6.173	5.592	1.682
H	5.282	5.221	1.203
N	7.371	5.012	1.631
C	8.216	5.767	2.416
H	9.253	5.506	2.524
C	13.858	-2.292	-0.008
H	14.586	-2.502	0.748
H	14.231	-1.530	-0.661
C	12.576	-1.815	0.644

C	11.496	-1.389	-0.142
H	11.577	-1.444	-1.217
C	10.336	-0.877	0.417
H	9.527	-0.536	-0.220
C	10.244	-0.760	1.803
O	9.091	-0.169	2.314
H	9.280	0.238	3.199
C	12.434	-1.733	2.033
H	13.241	-2.075	2.674
C	11.278	-1.211	2.620
H	11.200	-1.137	3.700
C	13.036	1.879	0.069
H	12.899	0.836	-0.128
H	13.857	2.010	0.743
N	11.678	2.577	2.054
H	12.471	2.390	2.693
C	11.790	2.439	0.685
C	10.425	2.959	2.364
H	10.061	3.114	3.368
N	9.706	3.098	1.245
C	10.557	2.778	0.195
H	10.230	2.808	-0.825
C	4.344	1.400	-0.682
C	3.066	-0.136	-2.059
H	2.912	-1.112	-2.502
C	4.127	0.109	-1.214
H	4.810	-0.700	-0.986
C	2.164	0.899	-2.366
O	1.149	0.594	-3.192
H	0.635	1.392	-3.402
C	3.429	2.427	-1.001
H	3.570	3.413	-0.577
C	2.346	2.183	-1.822
H	1.630	2.971	-2.032
C	5.549	1.721	0.055
O	5.826	2.947	0.323
C	6.487	0.735	0.507
H	6.415	-0.323	0.284
H	6.372	1.029	2.013
O	7.806	1.237	0.536
H	8.356	0.728	1.231
O	7.177	2.753	2.638
O	6.716	1.526	2.944
Fe	7.697	3.159	0.981

Model ^{1}A2

E=-3130.468924 au ZPE=0.5555867853 au

C	8.888	6.378	-3.389
H	8.377	7.246	-3.030
H	8.632	6.213	-4.415
N	8.451	3.891	-3.041
H	8.749	3.593	-3.982
C	8.484	5.190	-2.577
C	8.137	3.079	-2.010
H	8.065	2.006	-2.097
N	7.957	3.789	-0.896
C	8.158	5.107	-1.248
H	8.084	5.905	-0.529
C	7.851	7.864	3.858
H	8.602	7.495	4.525
H	7.010	8.208	4.423
N	6.147	6.678	2.393
H	5.431	7.411	2.524
C	7.417	6.763	2.935
C	6.078	5.579	1.617
H	5.196	5.253	1.091
N	7.254	4.949	1.622
C	8.093	5.680	2.435
H	9.113	5.378	2.589
C	13.817	-2.275	0.016
H	14.531	-2.480	0.786
H	14.199	-1.512	-0.629
C	12.519	-1.805	0.642
C	11.463	-1.369	-0.171
H	11.578	-1.410	-1.243
C	10.286	-0.865	0.357
H	9.501	-0.515	-0.304
C	10.157	-0.765	1.739
O	8.975	-0.184	2.228
H	9.138	0.247	3.112
C	12.336	-1.737	2.026
H	13.124	-2.084	2.688
C	11.163	-1.220	2.586
H	11.056	-1.154	3.664
C	12.998	1.880	0.092
H	12.871	0.835	-0.102
H	13.817	2.020	0.766
N	11.629	2.564	2.076
H	12.421	2.383	2.716

C	11.745	2.431	0.706
C	10.368	2.930	2.381
H	9.998	3.079	3.383
N	9.648	3.060	1.263
C	10.508	2.753	0.216
H	10.187	2.782	-0.807
C	4.353	1.316	-0.721
C	3.062	-0.189	-2.122
H	2.908	-1.158	-2.581
C	4.134	0.041	-1.287
H	4.808	-0.780	-1.075
C	2.154	0.848	-2.397
O	1.127	0.555	-3.216
H	0.616	1.358	-3.411
C	3.433	2.344	-1.005
H	3.573	3.322	-0.560
C	2.342	2.117	-1.825
H	1.624	2.910	-2.009
C	5.556	1.606	0.041
O	5.799	2.815	0.487
C	6.586	0.674	0.222
H	6.545	-0.391	0.033
H	5.519	3.025	2.451
O	7.775	1.197	0.552
H	8.336	0.611	1.257
O	7.322	2.546	2.712
O	6.098	2.993	3.244
Fe	7.625	3.111	1.011

Model ^{1}TS2

E=-3130.466703 au ZPE=0.5615801553 au

C	8.917	6.430	-3.420
H	8.408	7.301	-3.062
H	8.661	6.264	-4.446
N	8.469	3.949	-3.075
H	8.759	3.649	-4.018
C	8.509	5.246	-2.607
C	8.168	3.136	-2.041
H	8.092	2.063	-2.125
N	8.009	3.845	-0.925
C	8.202	5.162	-1.274
H	8.135	5.957	-0.549
C	7.867	7.852	3.863
H	8.621	7.484	4.527
H	7.030	8.200	4.432
N	6.158	6.679	2.401
H	5.449	7.421	2.526
C	7.425	6.748	2.947
C	6.079	5.581	1.624
H	5.198	5.278	1.081
N	7.242	4.929	1.640
C	8.088	5.653	2.453
H	9.105	5.343	2.606
C	13.828	-2.283	0.014
H	14.540	-2.490	0.785
H	14.212	-1.519	-0.630
C	12.530	-1.812	0.639
C	11.472	-1.384	-0.177
H	11.587	-1.432	-1.248
C	10.295	-0.880	0.349
H	9.505	-0.541	-0.312
C	10.165	-0.771	1.731
O	8.987	-0.182	2.210
H	9.147	0.247	3.094
C	12.347	-1.738	2.023
H	13.136	-2.080	2.686
C	11.172	-1.220	2.579
H	11.065	-1.149	3.657
C	12.993	1.873	0.092
H	12.874	0.828	-0.104
H	13.808	2.018	0.770
N	11.610	2.554	2.069
H	12.399	2.379	2.714
C	11.734	2.414	0.701
C	10.344	2.913	2.366
H	9.973	3.066	3.367
N	9.627	3.031	1.244
C	10.497	2.724	0.204
H	10.183	2.746	-0.821
C	4.313	1.329	-0.623
C	3.098	-0.213	-2.050
H	2.978	-1.187	-2.510
C	4.137	0.042	-1.178
H	4.838	-0.755	-0.952
C	2.183	0.806	-2.366
O	1.187	0.494	-3.217
H	0.670	1.288	-3.430
C	3.392	2.343	-0.961

H	3.511	3.331	-0.536
C	2.331	2.087	-1.807
H	1.608	2.867	-2.025
C	5.505	1.680	0.120
O	5.816	2.923	0.309
C	6.488	0.738	0.544
H	6.315	-0.323	0.690
H	5.416	3.175	2.431
O	7.758	1.154	0.476
H	8.343	0.634	1.192
O	7.049	2.249	2.460
O	5.989	2.860	3.159
Fe	7.604	3.121	0.924

Model ^{1}A3

E=-3130.513930 au ZPE=0.5669586703 au

C	8.960	6.524	-3.458
H	8.471	7.406	-3.101
H	8.713	6.371	-4.488
N	8.429	4.056	-3.136
H	8.724	3.752	-4.075
C	8.509	5.347	-2.658
C	8.085	3.245	-2.112
H	7.970	2.176	-2.201
N	7.937	3.954	-0.993
C	8.183	5.266	-1.329
H	8.135	6.057	-0.599
C	7.972	7.922	3.908
H	8.738	7.546	4.554
H	7.153	8.280	4.497
N	6.209	6.763	2.511
H	5.510	7.511	2.657
C	7.496	6.824	3.006
C	6.106	5.683	1.710
H	5.211	5.401	1.179
N	7.270	5.031	1.667
C	8.143	5.741	2.465
H	9.167	5.434	2.572
C	13.751	-2.239	-0.013
H	14.481	-2.426	0.746
H	14.107	-1.473	-0.670
C	12.454	-1.789	0.633
C	11.371	-1.373	-0.154
H	11.462	-1.414	-1.229
C	10.200	-0.881	0.404
H	9.387	-0.551	-0.235
C	10.097	-0.774	1.789
O	8.933	-0.206	2.306
H	9.141	0.245	3.164
C	12.302	-1.718	2.022
H	13.111	-2.051	2.665
C	11.135	-1.217	2.607
H	11.052	-1.153	3.687
C	12.947	1.849	0.042
H	12.819	0.808	-0.172
H	13.748	1.974	0.740
N	11.558	2.571	1.993
H	12.342	2.405	2.645
C	11.681	2.397	0.631
C	10.294	2.952	2.276
H	9.927	3.133	3.273
N	9.579	3.050	1.152
C	10.446	2.705	0.123
H	10.130	2.704	-0.903
C	4.281	1.488	-0.647
C	3.289	-0.278	-1.975
H	3.219	-1.313	-2.286
C	4.163	0.120	-0.983
H	4.788	-0.625	-0.499
C	2.462	0.672	-2.604
O	1.613	0.227	-3.548
H	1.106	0.970	-3.912
C	3.455	2.432	-1.302
H	3.527	3.477	-1.025
C	2.542	2.031	-2.251
H	1.889	2.756	-2.723
C	5.293	1.978	0.240
O	5.628	3.188	0.276
C	6.193	1.117	1.146
H	5.806	0.141	1.445
H	5.107	3.140	2.607
O	7.443	1.087	0.513
H	8.082	0.619	1.143
O	6.520	1.907	2.323
O	5.310	2.279	3.020
Fe	7.589	3.274	0.818

Model ^{1}TS3'

E=-3130.504130 au ZPE=-3130.504130 au

C	8.967	6.497	-3.488
H	8.467	7.372	-3.128
H	8.722	6.344	-4.518
N	8.469	4.017	-3.164
H	8.759	3.716	-4.106
C	8.531	5.312	-2.692
C	8.145	3.204	-2.135
H	8.047	2.133	-2.221
N	7.993	3.915	-1.019
C	8.213	5.231	-1.361
H	8.157	6.023	-0.634
C	7.978	7.964	3.884
H	8.736	7.603	4.547
H	7.143	8.315	4.454
N	6.245	6.737	2.504
H	5.521	7.460	2.656
C	7.535	6.854	2.981
C	6.175	5.654	1.705
H	5.282	5.315	1.205
N	7.369	5.056	1.641
C	8.221	5.802	2.431
H	9.259	5.538	2.523
C	13.771	-2.229	-0.023
H	14.522	-2.418	0.715
H	14.114	-1.470	-0.695
C	12.498	-1.764	0.658
C	11.392	-1.339	-0.092
H	11.440	-1.386	-1.171
C	10.250	-0.826	0.509
H	9.420	-0.480	-0.097
C	10.202	-0.712	1.897
O	9.071	-0.124	2.458
H	9.317	0.323	3.308
C	12.399	-1.687	2.051
H	13.227	-2.030	2.665
C	11.262	-1.168	2.677
H	11.218	-1.097	3.759
C	13.058	1.870	-0.008
H	12.917	0.830	-0.218
H	13.869	1.989	0.680
N	11.699	2.619	1.955
H	12.486	2.440	2.603
C	11.806	2.432	0.594
C	10.450	3.035	2.245
H	10.095	3.222	3.245
N	9.728	3.143	1.126
C	10.576	2.770	0.093
H	10.246	2.769	-0.928
C	4.336	1.484	-0.642
C	3.206	-0.174	-2.005
H	3.073	-1.191	-2.351
C	4.138	0.140	-1.037
H	4.735	-0.659	-0.613
C	2.404	0.838	-2.561
O	1.507	0.467	-3.491
H	1.018	1.242	-3.813
C	3.526	2.489	-1.219
H	3.652	3.514	-0.896
C	2.561	2.173	-2.150
H	1.922	2.950	-2.557
C	5.409	1.881	0.224
O	5.807	3.067	0.308
C	6.253	0.893	1.041
H	6.095	-0.165	0.825
H	5.643	2.776	3.100
O	7.603	1.237	0.729
H	8.212	0.749	1.370
O	6.053	1.038	2.445
O	5.070	2.058	2.775
Fe	7.737	3.297	0.815

Model ^{1}A4'

E=-3130.529514 au ZPE=0.5650352558 au

C	8.950	6.480	-3.454
H	8.453	7.356	-3.092
H	8.698	6.326	-4.482
N	8.453	4.002	-3.126
H	8.741	3.699	-4.067
C	8.519	5.296	-2.653
C	8.134	3.191	-2.092
H	8.031	2.120	-2.179
N	7.988	3.898	-0.974
C	8.210	5.212	-1.320
H	8.158	6.006	-0.593
C	8.011	7.952	3.900

H	8.769	7.583	4.558
H	7.183	8.309	4.475
N	6.260	6.748	2.525
H	5.543	7.474	2.683
C	7.553	6.849	2.998
C	6.179	5.668	1.720
H	5.276	5.332	1.239
N	7.363	5.063	1.646
C	8.226	5.795	2.434
H	9.262	5.520	2.518
C	13.825	-2.272	-0.020
H	14.566	-2.470	0.726
H	14.180	-1.510	-0.682
C	12.547	-1.805	0.649
C	11.441	-1.412	-0.120
H	11.499	-1.487	-1.196
C	10.290	-0.899	0.457
H	9.459	-0.585	-0.166
C	10.232	-0.748	1.841
O	9.087	-0.158	2.373
H	9.319	0.309	3.211
C	12.436	-1.694	2.039
H	13.262	-2.014	2.667
C	11.289	-1.170	2.643
H	11.233	-1.073	3.722
C	13.037	1.819	-0.024
H	12.891	0.783	-0.249
H	13.850	1.923	0.664
N	11.734	2.665	1.934
H	12.545	2.547	2.565
C	11.789	2.378	0.589
C	10.483	3.067	2.241
H	10.170	3.325	3.236
N	9.709	3.068	1.155
C	10.527	2.638	0.119
H	10.162	2.552	-0.888
C	4.333	1.467	-0.562
C	3.274	-0.203	-1.967
H	3.183	-1.217	-2.336
C	4.189	0.126	-0.985
H	4.817	-0.659	-0.577
C	2.438	0.790	-2.507
O	1.561	0.409	-3.454
H	1.054	1.175	-3.768
C	3.488	2.454	-1.121
H	3.575	3.478	-0.781
C	2.539	2.121	-2.063
H	1.873	2.881	-2.458
C	5.402	1.895	0.300
O	5.742	3.095	0.398
C	6.324	0.940	1.080
H	6.018	-0.111	1.080
H	7.716	2.229	3.318
O	7.607	1.153	0.538
H	8.257	0.690	1.146
O	6.322	1.233	2.476
O	7.023	2.519	2.696
Fe	7.685	3.259	0.885

Model ^{1}TS4'

E=-3130.510004 au ZPE=0.5642942460 au

C	8.936	6.467	-3.446
H	8.432	7.371	-3.098
H	8.697	6.338	-4.505
N	8.456	3.988	-3.077
H	8.765	3.673	-4.008
C	8.485	5.297	-2.633
C	8.089	3.200	-2.045
H	7.994	2.127	-2.115
N	7.873	3.932	-0.950
C	8.106	5.242	-1.319
H	8.008	6.054	-0.617
C	8.031	7.995	3.922
H	8.808	7.622	4.593
H	7.202	8.391	4.517
N	6.277	6.785	2.557
H	5.559	7.512	2.714
C	7.571	6.887	3.028
C	6.190	5.703	1.759
H	5.286	5.355	1.286
N	7.377	5.104	1.686
C	8.244	5.832	2.470
H	9.280	5.552	2.549
C	13.808	-2.261	-0.016
H	14.572	-2.470	0.739
H	14.192	-1.492	-0.697
C	12.525	-1.787	0.642
C	11.426	-1.394	-0.136

H	11.490	-1.475	-1.211
C	10.272	-0.875	0.431
H	9.446	-0.560	-0.199
C	10.202	-0.717	1.814
O	9.054	-0.125	2.331
H	9.272	0.343	3.173
C	12.406	-1.666	2.030
H	13.228	-1.982	2.666
C	11.254	-1.138	2.623
H	11.192	-1.036	3.702
C	13.138	1.796	-0.067
H	13.035	0.736	-0.312
H	13.983	1.885	0.622
N	11.907	2.642	1.934
H	12.743	2.541	2.539
C	11.908	2.340	0.591
C	10.672	3.047	2.288
H	10.402	3.313	3.294
N	9.853	3.033	1.237
C	10.624	2.593	0.173
H	10.216	2.502	-0.819
C	4.289	1.405	-0.604
C	3.321	-0.274	-2.059
H	3.266	-1.286	-2.441
C	4.210	0.072	-1.057
H	4.859	-0.696	-0.647
C	2.457	0.696	-2.596
O	1.602	0.300	-3.560
H	1.079	1.058	-3.865
C	3.419	2.369	-1.162
H	3.462	3.386	-0.794
C	2.505	2.022	-2.134
H	1.822	2.765	-2.530
C	5.261	1.878	0.357
O	5.443	3.086	0.572
C	6.240	0.947	1.119
H	5.985	-0.120	1.076
H	7.597	2.411	3.372
O	7.527	1.217	0.553
H	8.192	0.737	1.135
O	6.266	1.178	2.491
O	6.979	2.670	2.663
Fe	7.666	3.272	0.998

Model ^{1}A7

E=-3130.639140 au ZPE=0.5692427303 au

C	8.994	6.580	-3.483
H	8.506	7.485	-3.118
H	8.747	6.470	-4.542
N	8.411	4.127	-3.203
H	8.697	3.833	-4.147
C	8.527	5.403	-2.694
C	8.044	3.305	-2.196
H	7.887	2.244	-2.323
N	7.919	3.988	-1.059
C	8.204	5.299	-1.364
H	8.177	6.072	-0.613
C	7.921	7.759	3.856
H	8.707	7.385	4.515
H	7.097	8.144	4.465
N	6.151	6.536	2.510
H	5.445	7.273	2.650
C	7.450	6.644	2.968
C	6.053	5.428	1.742
H	5.145	5.088	1.271
N	7.232	4.812	1.677
C	8.109	5.563	2.436
H	9.142	5.283	2.528
C	13.592	-2.121	-0.015
H	14.425	-2.248	0.683
H	13.879	-1.359	-0.749
C	12.348	-1.698	0.750
C	11.173	-1.282	0.102
H	11.128	-1.311	-0.980
C	10.076	-0.795	0.812
H	9.183	-0.466	0.289
C	10.145	-0.699	2.200
O	9.072	-0.141	2.901
H	9.430	0.305	3.715
C	12.359	-1.642	2.149
H	13.240	-1.983	2.686
C	11.276	-1.151	2.877
H	11.324	-1.093	3.960
C	13.045	1.886	-0.029
H	12.986	0.817	-0.252
H	13.837	2.013	0.713
N	11.589	2.507	1.900
H	12.357	2.330	2.570

C	11.752	2.392	0.536
C	10.314	2.860	2.163
H	9.914	2.995	3.155
N	9.631	2.999	1.023
C	10.527	2.710	0.004
H	10.229	2.758	-1.027
C	4.221	1.409	-0.921
C	3.093	-0.243	-2.276
H	2.908	-1.268	-2.572
C	3.951	0.064	-1.238
H	4.441	-0.727	-0.682
C	2.442	0.787	-2.971
O	1.601	0.415	-3.959
H	1.173	1.200	-4.338
C	3.585	2.436	-1.641
H	3.783	3.469	-1.383
C	2.684	2.130	-2.645
H	2.173	2.922	-3.181
C	5.204	1.751	0.091
O	5.724	2.877	0.177
C	6.127	1.030	2.201
H	6.277	0.032	2.616
H	4.390	1.452	2.908
O	7.358	1.673	2.107
H	8.094	1.022	2.325
O	5.571	0.727	0.888
O	5.282	1.836	2.911
Fe	7.650	3.150	0.717

Model ^{1}TS7

E=-3130.631667 au ZPE=0.5682478973 au

C	8.986	6.571	-3.477
H	8.498	7.477	-3.117
H	8.742	6.458	-4.536
N	8.396	4.118	-3.194
H	8.688	3.823	-4.137
C	8.514	5.396	-2.688
C	8.014	3.301	-2.190
H	7.855	2.240	-2.315
N	7.880	3.987	-1.055
C	8.176	5.296	-1.361
H	8.147	6.072	-0.612
C	7.919	7.767	3.861
H	8.703	7.390	4.522
H	7.095	8.154	4.468
N	6.151	6.560	2.501
H	5.450	7.305	2.637
C	7.446	6.654	2.972
C	6.050	5.457	1.728
H	5.146	5.135	1.237
N	7.223	4.826	1.676
C	8.099	5.567	2.446
H	9.129	5.278	2.547
C	13.608	-2.128	-0.016
H	14.441	-2.258	0.681
H	13.896	-1.366	-0.750
C	12.365	-1.703	0.748
C	11.191	-1.288	0.099
H	11.146	-1.319	-0.983
C	10.094	-0.801	0.808
H	9.201	-0.471	0.285
C	10.164	-0.703	2.197
O	9.090	-0.145	2.895
H	9.443	0.302	3.710
C	12.377	-1.647	2.147
H	13.256	-1.989	2.685
C	11.293	-1.155	2.875
H	11.340	-1.096	3.958
C	13.032	1.889	-0.031
H	12.971	0.820	-0.252
H	13.822	2.016	0.714
N	11.574	2.515	1.894
H	12.340	2.332	2.565
C	11.739	2.400	0.530
C	10.300	2.869	2.156
H	9.900	3.001	3.148
N	9.618	3.011	1.015
C	10.515	2.723	-0.003
H	10.218	2.773	-1.035
C	4.224	1.378	-0.893
C	3.103	-0.256	-2.274
H	2.914	-1.276	-2.582
C	3.952	0.037	-1.226
H	4.432	-0.761	-0.671
C	2.459	0.784	-2.964
O	1.622	0.424	-3.957
H	1.195	1.212	-4.331
C	3.597	2.416	-1.609

H	3.792	3.446	-1.336
C	2.704	2.124	-2.623
H	2.198	2.923	-3.154
C	5.171	1.716	0.151
O	5.663	2.855	0.282
C	6.144	0.961	2.226
H	6.374	-0.026	2.626
H	4.632	2.132	2.603
O	7.373	1.632	2.042
H	8.125	1.009	2.286
O	5.517	0.691	0.954
O	5.315	1.636	3.075
Fe	7.632	3.151	0.731

Model ^{1}A8

E=-3130.633605 au ZPE=0.5682400269 au

C	8.973	6.560	-3.471
H	8.485	7.467	-3.111
H	8.729	6.447	-4.530
N	8.379	4.107	-3.188
H	8.673	3.811	-4.130
C	8.497	5.385	-2.682
C	7.988	3.292	-2.185
H	7.827	2.231	-2.310
N	7.848	3.980	-1.052
C	8.149	5.289	-1.358
H	8.119	6.065	-0.611
C	7.914	7.769	3.865
H	8.697	7.390	4.525
H	7.090	8.157	4.472
N	6.152	6.576	2.483
H	5.454	7.325	2.614
C	7.440	6.657	2.973
C	6.050	5.473	1.710
H	5.152	5.163	1.200
N	7.218	4.828	1.678
C	8.090	5.563	2.459
H	9.116	5.266	2.573
C	13.617	-2.133	-0.018
H	14.453	-2.265	0.675
H	13.902	-1.370	-0.752
C	12.377	-1.710	0.752
C	11.201	-1.293	0.109
H	11.152	-1.321	-0.974
C	10.106	-0.809	0.823
H	9.211	-0.478	0.305
C	10.182	-0.717	2.212
O	9.109	-0.162	2.918
H	9.468	0.296	3.725
C	12.395	-1.660	2.151
H	13.276	-2.004	2.684
C	11.314	-1.170	2.885
H	11.364	-1.115	3.967
C	13.026	1.891	-0.036
H	12.963	0.821	-0.256
H	13.815	2.016	0.711
N	11.569	2.521	1.886
H	12.334	2.336	2.558
C	11.734	2.406	0.523
C	10.296	2.879	2.148
H	9.896	3.009	3.140
N	9.616	3.023	1.006
C	10.512	2.734	-0.012
H	10.213	2.785	-1.043
C	4.231	1.379	-0.876
C	3.125	-0.246	-2.280
H	2.939	-1.265	-2.597
C	3.969	0.040	-1.226
H	4.450	-0.762	-0.678
C	2.478	0.798	-2.961
O	1.646	0.446	-3.962
H	1.214	1.236	-4.326
C	3.600	2.420	-1.581
H	3.783	3.448	-1.291
C	2.715	2.135	-2.605
H	2.206	2.937	-3.128
C	5.157	1.704	0.189
O	5.625	2.852	0.371
C	6.172	0.967	2.231
H	6.319	-0.013	2.674
H	5.290	2.609	2.682
O	7.424	1.561	1.984
H	8.165	0.943	2.287
O	5.526	0.672	0.960
O	5.384	1.717	3.049
Fe	7.630	3.144	0.735

Model ^{1}TS8

E=-3130.607857 au ZPE=0.5638701460 au

C	8.941	6.508	-3.449
H	8.446	7.410	-3.084
H	8.695	6.399	-4.508
N	8.358	4.048	-3.176
H	8.652	3.759	-4.120
C	8.475	5.325	-2.665
C	7.965	3.226	-2.179
H	7.798	2.167	-2.311
N	7.822	3.909	-1.042
C	8.125	5.221	-1.342
H	8.093	5.994	-0.592
C	7.919	7.784	3.879
H	8.701	7.405	4.540
H	7.094	8.171	4.484
N	6.174	6.605	2.463
H	5.475	7.354	2.587
C	7.450	6.673	2.985
C	6.078	5.501	1.692
H	5.187	5.195	1.167
N	7.239	4.844	1.691
C	8.100	5.570	2.489
H	9.121	5.265	2.624
C	13.603	-2.131	-0.027
H	14.438	-2.259	0.668
H	13.889	-1.369	-0.762
C	12.362	-1.706	0.741
C	11.187	-1.284	0.098
H	11.135	-1.318	-0.983
C	10.094	-0.787	0.811
H	9.197	-0.460	0.295
C	10.180	-0.688	2.197
O	9.121	-0.109	2.919
H	9.504	0.310	3.736
C	12.382	-1.652	2.140
H	13.261	-2.002	2.674
C	11.306	-1.150	2.873
H	11.360	-1.091	3.955
C	13.044	1.885	-0.056
H	12.984	0.816	-0.277
H	13.835	2.013	0.688
N	11.604	2.536	1.870
H	12.376	2.362	2.537
C	11.754	2.400	0.507
C	10.335	2.897	2.140
H	9.947	3.045	3.134
N	9.639	3.017	1.004
C	10.524	2.714	-0.019
H	10.213	2.747	-1.048
C	4.405	1.376	-0.904
C	3.246	-0.205	-2.318
H	3.050	-1.213	-2.663
C	4.157	0.053	-1.314
H	4.688	-0.755	-0.824
C	2.542	0.857	-2.909
O	1.667	0.535	-3.885
H	1.212	1.333	-4.198
C	3.693	2.433	-1.494
H	3.854	3.446	-1.148
C	2.764	2.179	-2.491
H	2.204	2.993	-2.937
C	5.361	1.614	0.167
O	5.607	2.853	0.561
C	6.342	1.306	2.681
H	6.301	0.303	3.089
H	5.341	2.706	1.986
O	7.541	1.806	2.434
H	8.251	1.048	2.478
O	5.953	0.649	0.737
O	5.351	2.093	2.850
Fe	7.644	3.144	0.778

Model ^{1}P

E=-3130.647515 au ZPE=0.5670300877 au

C	8.974	6.568	-3.474
H	8.492	7.470	-3.093
H	8.724	6.478	-4.534
N	8.417	4.108	-3.235
H	8.728	3.827	-4.176
C	8.497	5.380	-2.709
C	8.024	3.268	-2.258
H	7.893	2.206	-2.394
N	7.837	3.935	-1.118
C	8.120	5.256	-1.396
H	8.057	6.020	-0.639
C	8.029	7.737	3.886
H	8.827	7.368	4.533

H	7.207	8.105	4.508
N	6.276	6.573	2.486
H	5.578	7.321	2.629
C	7.561	6.631	2.986
C	6.171	5.483	1.698
H	5.269	5.205	1.178
N	7.329	4.820	1.662
C	8.201	5.538	2.457
H	9.227	5.235	2.565
C	13.490	-2.090	-0.012
H	14.327	-2.193	0.685
H	13.763	-1.332	-0.754
C	12.243	-1.679	0.757
C	11.057	-1.276	0.120
H	10.997	-1.320	-0.961
C	9.966	-0.774	0.835
H	9.072	-0.443	0.316
C	10.062	-0.653	2.219
O	9.011	-0.063	2.945
H	9.408	0.364	3.752
C	12.270	-1.607	2.155
H	13.157	-1.938	2.688
C	11.196	-1.103	2.890
H	11.259	-1.031	3.971
C	13.014	1.837	-0.066
H	12.978	0.771	-0.304
H	13.791	1.969	0.691
N	11.546	2.542	1.828
H	12.317	2.428	2.506
C	11.704	2.318	0.478
C	10.257	2.860	2.070
H	9.862	3.064	3.052
N	9.561	2.866	0.929
C	10.459	2.528	-0.066
H	10.150	2.457	-1.094
C	4.467	1.413	-1.161
C	3.313	-0.255	-2.474
H	3.241	-1.239	-2.922
C	4.421	0.133	-1.749
H	5.262	-0.535	-1.604
C	2.250	0.651	-2.658
O	1.221	0.241	-3.425
H	0.608	0.980	-3.568
C	3.377	2.295	-1.312
H	3.401	3.273	-0.847
C	2.279	1.921	-2.061
H	1.439	2.599	-2.173
C	5.640	1.827	-0.441
O	5.532	2.969	0.344
C	6.245	1.553	3.008
H	6.381	0.817	3.810
H	5.111	2.737	1.228
O	7.359	1.806	2.323
H	8.084	1.089	2.484
O	6.776	1.335	-0.467
O	5.180	2.094	2.781
Fe	7.575	3.087	0.659

Model ^{5}TS3

E=-3130.492209 au

C	8.950	6.502	-3.543
H	8.443	7.398	-3.183
H	8.748	6.409	-4.612
N	8.430	4.022	-3.278
H	8.772	3.730	-4.207
C	8.455	5.313	-2.790
C	8.010	3.200	-2.296
H	7.910	2.132	-2.413
N	7.749	3.894	-1.189
C	8.015	5.216	-1.497
H	7.890	6.004	-0.770
C	7.933	8.010	3.961
H	8.714	7.633	4.625
H	7.125	8.439	4.562
N	6.131	6.814	2.642
H	5.436	7.569	2.778
C	7.429	6.888	3.108
C	6.008	5.712	1.880
H	5.094	5.410	1.395
N	7.170	5.058	1.829
C	8.061	5.790	2.588
H	9.088	5.485	2.679
C	13.709	-2.192	-0.017
H	14.508	-2.361	0.711
H	14.047	-1.427	-0.727
C	12.443	-1.746	0.693
C	11.307	-1.339	-0.023
H	11.323	-1.382	-1.104

C	10.173	-0.850	0.616
H	9.315	-0.519	0.040
C	10.166	-0.741	2.006
O	9.042	-0.183	2.617
H	9.319	0.296	3.441
C	12.383	-1.673	2.089
H	13.236	-2.002	2.676
C	11.257	-1.179	2.752
H	11.244	-1.112	3.835
C	13.126	1.816	-0.087
H	13.058	0.753	-0.330
H	13.946	1.928	0.628
N	11.774	2.536	1.889
H	12.576	2.395	2.530
C	11.860	2.327	0.527
C	10.522	2.918	2.198
H	10.181	3.115	3.201
N	9.774	2.979	1.093
C	10.606	2.610	0.047
H	10.247	2.584	-0.968
C	4.316	1.379	-0.421
C	3.400	-0.203	-2.019
H	3.312	-1.201	-2.431
C	4.202	0.059	-0.927
H	4.749	-0.758	-0.468
C	2.649	0.835	-2.608
O	1.863	0.507	-3.646
H	1.371	1.285	-3.958
C	3.564	2.411	-1.039
H	3.617	3.414	-0.637
C	2.739	2.147	-2.110
H	2.147	2.942	-2.551
C	5.133	1.718	0.696
O	5.434	3.025	0.901
C	6.105	0.810	1.460
H	5.957	-0.266	1.318
H	5.038	2.928	1.932
O	7.418	1.180	1.100
H	8.087	0.672	1.669
O	5.832	1.193	2.786
O	4.509	1.806	2.551
Fe	7.707	3.307	0.820

Model ^{5}A4

E=-3130.528679 au

C	8.939	6.490	-3.538
H	8.429	7.386	-3.178
H	8.737	6.397	-4.607
N	8.407	4.011	-3.282
H	8.743	3.724	-4.215
C	8.446	5.300	-2.786
C	7.983	3.187	-2.305
H	7.865	2.121	-2.431
N	7.733	3.877	-1.192
C	8.011	5.199	-1.492
H	7.897	5.984	-0.760
C	7.908	8.003	3.955
H	8.683	7.616	4.620
H	7.101	8.436	4.556
N	6.124	6.853	2.570
H	5.438	7.619	2.694
C	7.402	6.891	3.092
C	6.003	5.755	1.802
H	5.106	5.490	1.264
N	7.147	5.065	1.803
C	8.023	5.773	2.601
H	9.037	5.443	2.736
C	13.738	-2.204	-0.037
H	14.548	-2.375	0.677
H	14.064	-1.439	-0.752
C	12.487	-1.755	0.696
C	11.339	-1.339	0.004
H	11.331	-1.381	-1.078
C	10.224	-0.842	0.670
H	9.355	-0.502	0.114
C	10.249	-0.738	2.059
O	9.142	-0.176	2.701
H	9.444	0.308	3.515
C	12.458	-1.684	2.093
H	13.320	-2.023	2.661
C	11.352	-1.183	2.781
H	11.360	-1.117	3.864
C	13.131	1.830	-0.093
H	13.058	0.766	-0.335
H	13.951	1.939	0.622
N	11.781	2.559	1.881
H	12.583	2.415	2.522
C	11.866	2.348	0.520

C	10.531	2.947	2.189
H	10.191	3.143	3.193
N	9.783	3.010	1.084
C	10.614	2.636	0.039
H	10.255	2.611	-0.976
C	4.319	1.300	-0.290
C	3.476	-0.184	-2.013
H	3.420	-1.160	-2.480
C	4.250	0.028	-0.879
H	4.793	-0.810	-0.453
C	2.729	0.869	-2.563
O	1.974	0.592	-3.653
H	1.481	1.382	-3.925
C	3.585	2.350	-0.865
H	3.608	3.334	-0.415
C	2.795	2.142	-1.986
H	2.211	2.963	-2.393
C	5.077	1.543	0.968
O	5.488	2.918	1.046
C	6.227	0.678	1.501
H	6.213	-0.382	1.231
H	5.227	3.209	1.935
O	7.485	1.231	1.336
H	8.192	0.694	1.839
O	5.696	0.870	2.832
O	4.388	1.255	2.210
Fe	7.704	3.294	0.807

Model ^{5}TS4

E=-3130.452583 au

C	8.933	6.483	-3.528
H	8.424	7.379	-3.169
H	8.729	6.388	-4.597
N	8.412	4.003	-3.265
H	8.754	3.714	-4.195
C	8.440	5.294	-2.774
C	7.982	3.181	-2.288
H	7.875	2.114	-2.408
N	7.718	3.875	-1.180
C	7.994	5.196	-1.483
H	7.871	5.983	-0.755
C	7.908	8.005	3.954
H	8.684	7.619	4.619
H	7.100	8.436	4.553
N	6.118	6.842	2.588
H	5.431	7.607	2.714
C	7.403	6.890	3.093
C	5.993	5.739	1.828
H	5.088	5.459	1.312
N	7.141	5.056	1.817
C	8.024	5.774	2.598
H	9.042	5.449	2.721
C	13.759	-2.214	-0.039
H	14.569	-2.390	0.676
H	14.089	-1.448	-0.752
C	12.509	-1.762	0.693
C	11.362	-1.349	-0.003
H	11.356	-1.397	-1.084
C	10.246	-0.849	0.658
H	9.379	-0.512	0.100
C	10.270	-0.736	2.047
O	9.165	-0.166	2.679
H	9.461	0.314	3.497
C	12.478	-1.687	2.090
H	13.338	-2.026	2.660
C	11.371	-1.181	2.773
H	11.377	-1.110	3.856
C	13.125	1.830	-0.089
H	13.050	0.766	-0.328
H	13.943	1.941	0.627
N	11.773	2.562	1.882
H	12.575	2.418	2.524
C	11.859	2.351	0.522
C	10.523	2.951	2.190
H	10.181	3.146	3.193
N	9.775	3.014	1.084
C	10.607	2.640	0.040
H	10.250	2.613	-0.975
C	4.342	1.280	-0.240
C	3.470	-0.169	-1.975
H	3.397	-1.132	-2.466
C	4.240	0.007	-0.842
H	4.776	-0.840	-0.424
C	2.730	0.911	-2.502
O	1.980	0.661	-3.588
H	1.486	1.455	-3.856
C	3.594	2.352	-0.778
H	3.625	3.320	-0.297

C	2.800	2.177	-1.895
H	2.213	3.006	-2.277
C	5.084	1.487	1.042
O	5.486	2.878	1.148
C	6.259	0.656	1.563
H	6.221	-0.410	1.311
H	5.282	3.117	2.068
O	7.514	1.191	1.224
H	8.231	0.708	1.756
O	5.966	0.886	2.925
O	4.194	1.163	2.034
Fe	7.685	3.278	0.822