Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	0.000000	0.000000	2.538353
6	C	0.000000	1.208511	1.834708
6	C	0.000000	1.203886	0.438375
6	C	0.000000	0.000000	-0.279672
6	C	0.000000	-1.203886	0.438375
6	C	0.000000	-1.208511	1.834708
1	H	0.000000	0.000000	3.625646
1	H	0.000000	2.152062	2.376056
1	H	0.000000	2.133074	-0.123199
1	H	0.000000	-2.133074	-0.123199
1	H	0.000000	-2.152062	2.376056
6	C	0.000000	0.000000	-1.817696
8	O	0.000000	-1.130429	-2.378392
8	O	0.000000	1.130429	-2.378392

Sum of electronic and zero-point Energies= -420.246594

Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	1.353128	-0.040706	-0.002053
1	H	1.759564	0.638315	-0.761842
1	H	1.740820	-1.049887	-0.176874
1	H	1.730564	0.310396	0.968144
6	C	-0.199691	0.000080	-0.006939
8	O	-0.801510	-1.108240	0.001585
8	O	-0.717436	1.151357	0.001481

Sum of electronic and zero-point Energies= -228.553228

Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-5.178522	0.200061	-0.083928
7	N	-3.926782	0.125672	0.472270
7	N	-5.572454	-0.709832	-0.957431
1	H	-4.920717	-1.453735	-1.198756
1	H	-6.489559	-0.667858	-1.380378
7	N	3.949879	0.503321	-0.145100
6	C	5.192437	0.019065	0.177696
1	H	6.441411	-1.589850	0.070894
1	H	4.873565	-1.751642	-0.720479
7	N	5.543961	-1.201850	-0.187043
1	H	3.760866	1.464325	0.110754
1	H	-3.700567	0.826070	1.166734
6	C	1.669181	0.532836	-0.983089
6	C	1.224004	1.764126	-0.379152
6	C	0.598089	0.037530	-1.806736
6	C	-0.091676	2.024623	-0.850359
1	H	1.765249	2.384567	0.323536
6	C	-0.472281	0.964805	-1.728334
1	H	0.627093	-0.876383	-2.382535
1	H	-0.707506	2.866525	-0.564181
1	H	-1.429525	0.864759	-2.222726
6	C	-1.672604	-0.677968	0.900878
6	C	-1.222091	0.376137	1.775242
6	C	-0.603814	-1.634967	0.784551
6	C	0.094056	0.050614	2.201405
1	H	-1.761872	1.267916	2.066481
6	C	0.470959	-1.184683	1.592956
1	H	-0.636642	-2.535882	0.189077
1	H	0.711757	0.655174	2.851719
1	H	1.429012	-1.676342	1.698753
26	Fe	-0.002060	0.215606	0.143366
7	N	6.013662	0.814386	0.856751
7	N	-5.968836	1.202405	0.289476
1	H	5.733048	1.732968	1.171770
1	H	6.947627	0.512995	1.101230

1	H	-6.895899	1.306947	-0.102464
1	H	-5.659887	1.920210	0.931084
6	C	2.934047	-0.196895	-0.819183
6	C	-2.942865	-0.835302	0.180235
8	O	3.113457	-1.330672	-1.251973
8	O	-3.151383	-1.748721	-0.612223

Sum of electronic and zero-point Energies= -2286.370105

Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	0.080044	3.956006	-0.533095
7	N	-0.304363	2.854874	0.193441
7	N	0.000000	5.172198	-0.010406
1	H	-0.295847	5.253482	0.959191
1	H	0.282056	5.986767	-0.538014
7	N	0.304363	-2.854874	0.193441
6	C	-0.080044	-3.956006	-0.533095
1	H	-0.282056	-5.986767	-0.538014
1	H	0.295847	-5.253482	0.959191
7	N	0.000000	-5.172198	-0.010406
6	C	0.908016	0.798301	-4.518824
6	C	0.000000	0.000000	-3.808717
6	C	0.914155	0.792269	-5.913625
6	C	-0.908016	-0.798301	-4.518824
6	C	0.000000	0.000000	-6.613876
1	H	1.630399	1.404938	-6.454151
6	C	-0.914155	-0.792269	-5.913625
1	H	-1.618718	-1.408552	-3.970704
1	H	0.000000	0.000000	-7.700459
1	H	-1.630399	-1.404938	-6.454151
6	C	0.000000	0.000000	-2.300445
8	O	-0.520295	-0.991441	-1.702771
8	O	0.520295	0.991441	-1.702771
1	H	0.148028	-1.955495	-0.291140
1	H	-0.148028	1.955495	-0.291140
6	C	1.197279	-1.565439	2.046977
6	C	1.318981	-1.295089	3.452847
6	C	1.589480	-0.376731	1.333159
6	C	1.785803	0.037461	3.603121
1	H	1.080804	-1.991223	4.244775
6	C	1.956900	0.599118	2.302252

1	H	1.594530	-0.230782	0.261024
1	H	1.951341	0.548919	4.541921
1	H	2.282375	1.608158	2.085119
6	C	-1.197279	1.565439	2.046977
6	C	-1.318981	1.295089	3.452847
6	C	-1.589480	0.376731	1.333159
6	C	-1.785803	-0.037461	3.603121
1	H	-1.080804	1.991223	4.244775
6	C	-1.956900	-0.599118	2.302252
1	H	-1.594530	0.230782	0.261024
1	H	-1.951341	-0.548919	4.541921
1	H	-2.282375	-1.608158	2.085119
26	Fe	0.000000	0.000000	2.549829
1	H	1.618718	1.408552	-3.970704
7	N	-0.508713	-3.731422	-1.768758
7	N	0.508713	3.731422	-1.768758
1	H	-0.586073	-2.757352	-2.093831
1	H	-0.839433	-4.489523	-2.349229
1	H	0.839433	4.489523	-2.349229
1	H	0.586073	2.757352	-2.093831
6	C	0.760015	-2.866905	1.513181
6	C	-0.760015	2.866905	1.513181
8	O	0.801852	-3.896326	2.185359
8	O	-0.801852	3.896326	2.185359

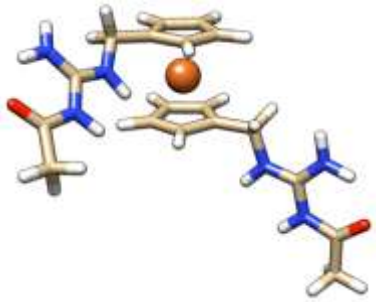
Sum of electronic and zero-point Energies= -2706.681917

Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-3.984035	1.325733	0.280364
7	N	-2.899406	0.615023	-0.173986
7	N	-5.191368	0.775993	0.300418
1	H	-5.272146	-0.200175	0.026915
1	H	-5.994323	1.289463	0.636933
7	N	2.903444	0.650406	0.176110
6	C	3.983737	1.363038	-0.285068
1	H	5.989966	1.326822	-0.665331
1	H	5.272316	-0.166400	-0.058394
7	N	5.189708	0.811522	-0.325255
6	C	-0.100323	4.684878	-0.044360
6	C	-0.021292	3.164471	0.010179
8	O	1.044013	2.594859	-0.367180
8	O	-1.040901	2.542433	0.437651
1	H	2.005102	1.162343	0.117147
1	H	-2.001417	1.123547	-0.096258
6	C	1.643329	-1.202238	1.107428
6	C	1.370354	-2.605574	1.252911
6	C	0.482161	-0.478284	1.559475
6	C	0.064728	-2.743824	1.793901
1	H	2.047088	-3.403668	0.981826
6	C	-0.478474	-1.437858	1.986271
1	H	0.342537	0.594406	1.560019
1	H	-0.443004	-3.677846	1.994300
1	H	-1.467420	-1.211424	2.362981
6	C	-1.627880	-1.227107	-1.107440
6	C	-1.340331	-2.628093	-1.244297
6	C	-0.474048	-0.494045	-1.563818
6	C	-0.032903	-2.756164	-1.783662
1	H	-2.008616	-3.431587	-0.968104
6	C	0.496810	-1.446012	-1.984467
1	H	-0.348779	0.580209	-1.575341
1	H	0.484557	-3.686114	-1.978001
1	H	1.483198	-1.211599	-2.362961

26	Fe	0.010284	-1.704216	0.001762
7	N	3.752797	2.614615	-0.662192
7	N	-3.753522	2.573206	0.669978
1	H	2.784940	2.966727	-0.640314
1	H	4.493969	3.186654	-1.042191
1	H	-4.496523	3.143248	1.049420
1	H	-2.780841	2.917311	0.666801
6	C	2.920988	-0.681990	0.589455
6	C	-2.911780	-0.714089	-0.597288
8	O	3.935126	-1.376909	0.533575
8	O	-3.925337	-1.410572	-0.556188
1	H	-0.315726	5.075220	0.956272
1	H	0.827239	5.125796	-0.414552
1	H	-0.930521	4.985793	-0.692875

Sum of electronic and zero-point Energies= -2514.995170



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	4.602814	0.615180	-0.369187
7	N	3.498151	0.197587	0.240274
7	N	4.833711	0.380151	-1.651872
7	N	5.527292	1.315580	0.371863
1	H	4.178633	-0.133285	-2.224113
1	H	5.701694	0.733275	-2.049954
7	N	-3.469408	0.086833	-0.125950
6	C	-4.462523	0.972055	-0.148801
7	N	-4.134274	2.306574	-0.089470
1	H	-6.432647	1.354507	-0.255684
1	H	-6.017409	-0.354189	-0.199845
7	N	-5.733384	0.614117	-0.242129
6	C	2.410738	-0.557433	-0.420672
6	C	-3.629552	-1.371657	-0.213163
1	H	-2.526483	0.412906	0.048987
1	H	3.374124	0.408315	1.222710
6	C	-2.325227	-2.025763	-0.566550
6	C	-1.855428	-3.266586	-0.029827
6	C	-1.397680	-1.609956	-1.577074
6	C	-0.646579	-3.611861	-0.701451
1	H	-2.333732	-3.832253	0.759443
6	C	-0.361667	-2.586819	-1.652454
1	H	-1.468516	-0.710480	-2.175348
1	H	-0.035701	-4.482161	-0.501171
1	H	0.499497	-2.546007	-2.306773
6	C	1.316119	-0.832175	0.564865
6	C	1.212981	-1.975053	1.424155
6	C	0.222585	0.042816	0.872577
6	C	0.055952	-1.813424	2.239180
1	H	1.884937	-2.823635	1.427047
6	C	-0.554449	-0.567694	1.901466
1	H	0.038408	1.001701	0.403915

1	H	-0.309956	-2.521688	2.970768
1	H	-1.451725	-0.161684	2.350995
26	Fe	-0.451473	-1.795816	0.242794
1	H	5.308821	1.461635	1.350856
1	H	-3.146058	2.530364	-0.074920
1	H	2.029961	0.036552	-1.258614
1	H	2.819423	-1.494175	-0.814614
1	H	-4.008683	-1.765020	0.736871
1	H	-4.369220	-1.588495	-0.993510
6	C	6.739655	1.850206	-0.089977
6	C	-5.027644	3.389564	-0.068143
6	C	-4.354233	4.733882	0.015414
1	H	-3.692994	4.885219	-0.844879
1	H	-5.120131	5.509077	0.026585
1	H	-3.746478	4.805056	0.923987
6	C	7.527525	2.575500	0.969100
1	H	6.944597	3.406728	1.380489
1	H	7.776411	1.898347	1.793436
1	H	8.444975	2.958735	0.522873
8	O	7.100174	1.725131	-1.250573
8	O	-6.237471	3.228782	-0.117922

Sum of electronic and zero-point Energies= -2443.500582

Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	0.000000	3.960086	0.175565
7	N	-0.402714	2.866387	0.812102
7	N	-0.086850	5.176001	0.702395
7	N	0.525348	3.790733	-1.086124
1	H	-0.426543	5.323703	1.641603
1	H	0.288694	5.949896	0.158136
7	N	0.402714	-2.866387	0.812102
6	C	0.000000	-3.960086	0.175565
7	N	-0.525348	-3.790733	-1.086124
1	H	-0.288694	-5.949896	0.158136
1	H	0.426543	-5.323703	1.641603
7	N	0.086850	-5.176001	0.702395
6	C	-1.066490	2.884921	2.118198
6	C	1.066490	-2.884921	2.118198
6	C	-0.578381	1.061647	-4.099419
6	C	0.000000	0.000000	-3.390151
6	C	-0.587680	1.057529	-5.494963
6	C	0.578381	-1.061647	-4.099419
6	C	0.000000	0.000000	-6.195162
1	H	-1.052203	1.877548	-6.035684
6	C	0.587680	-1.057529	-5.494963
1	H	1.035993	-1.877283	-3.548236
1	H	0.000000	0.000000	-7.281707
1	H	1.052203	-1.877548	-6.035684
6	C	0.000000	0.000000	-1.880622
8	O	0.049333	-1.119517	-1.291073
8	O	-0.049333	1.119517	-1.291073
1	H	0.315317	-1.981985	0.293241
1	H	-0.315317	1.981985	0.293241
6	C	1.321140	-1.498055	2.637073
6	C	1.398387	-1.161757	4.027187
6	C	1.640999	-0.319214	1.888563

6	C	1.754523	0.215297	4.134989
1	H	1.203756	-1.838104	4.849938
6	C	1.897393	0.736959	2.814324
1	H	1.652748	-0.228296	0.810150
1	H	1.867083	0.771274	5.056508
1	H	2.140321	1.759261	2.555404
6	C	-1.321140	1.498055	2.637073
6	C	-1.398387	1.161757	4.027187
6	C	-1.640999	0.319214	1.888563
6	C	-1.754523	-0.215297	4.134989
1	H	-1.203756	1.838104	4.849938
6	C	-1.897393	-0.736959	2.814324
1	H	-1.652748	0.228296	0.810150
1	H	-1.867083	-0.771274	5.056508
1	H	-2.140321	-1.759261	2.555404
26	Fe	0.000000	0.000000	3.088075
1	H	-1.035993	1.877283	-3.548236
1	H	0.466679	2.824011	-1.447675
1	H	-0.466679	-2.824011	-1.447675
1	H	-0.442908	3.428181	2.837597
1	H	-2.018065	3.428449	2.026496
1	H	0.442908	-3.428181	2.837597
1	H	2.018065	-3.428449	2.026496
6	C	1.086203	4.784948	-1.881442
6	C	-1.086203	-4.784948	-1.881442
6	C	-1.658773	-4.282570	-3.183265
1	H	-0.997102	-3.559594	-3.669093
1	H	-1.832797	-5.131836	-3.844662
1	H	-2.614753	-3.781974	-2.988362
6	C	1.658773	4.282570	-3.183265
1	H	2.614753	3.781974	-2.988362
1	H	0.997102	3.559594	-3.669093
1	H	1.832797	5.131836	-3.844662
8	O	1.132303	5.961274	-1.536569
8	O	-1.132303	-5.961274	-1.536569

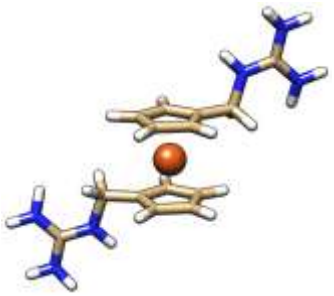
Sum of electronic and zero-point Energies= -2863.808333

Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	3.872070	0.597699	0.362957
7	N	2.771989	-0.122514	0.554923
7	N	5.077794	0.179956	0.731923
7	N	3.723973	1.824611	-0.242762
1	H	5.221089	-0.729761	1.144976
1	H	5.868000	0.786905	0.524062
7	N	-2.770527	-0.131184	-0.550200
6	C	-3.862040	0.601437	-0.354900
7	N	-3.697100	1.820765	0.260534
1	H	-5.854816	0.817074	-0.516044
1	H	-5.227303	-0.703910	-1.146220
7	N	-5.072180	0.202428	-0.729943
6	C	2.780376	-1.420143	1.236488
6	C	-2.786789	-1.423681	-1.240984
6	C	-0.013542	2.346459	-0.022862
8	O	-0.994463	1.733470	0.500664
8	O	1.014709	1.763849	-0.478734
1	H	-1.884429	0.275655	-0.217106
1	H	1.888501	0.299872	0.231111
6	C	-1.411405	-2.005141	-1.402566
6	C	-1.136498	-3.410353	-1.449022
6	C	-0.185324	-1.315028	-1.669721
6	C	0.249775	-3.585748	-1.734074
1	H	-1.859820	-4.198608	-1.282113
6	C	0.838039	-2.291977	-1.863119
1	H	-0.037484	-0.242666	-1.679272
1	H	0.767827	-4.532945	-1.808904
1	H	1.882414	-2.083236	-2.055951
6	C	1.403815	-1.998854	1.396373
6	C	1.129350	-3.404104	1.448183
6	C	0.177837	-1.307870	1.660666
6	C	-0.256909	-3.578744	1.733626

1	H	1.852933	-4.192839	1.284642
6	C	-0.845269	-2.284507	1.857500
1	H	0.028540	-0.235567	1.661602
1	H	-0.774762	-4.525759	1.812124
1	H	-1.889855	-2.075158	2.048690
26	Fe	-0.003486	-2.508171	-0.002313
1	H	2.742121	2.083922	-0.451533
1	H	-2.708311	2.064243	0.467781
1	H	3.406902	-2.124558	0.675878
1	H	3.234860	-1.290250	2.229532
1	H	-3.416428	-2.129469	-0.685566
1	H	-3.240229	-1.284282	-2.233119
6	C	4.747342	2.710781	-0.560785
6	C	-4.709070	2.713321	0.595216
6	C	-4.217360	3.969798	1.270423
1	H	-3.553848	4.527450	0.600476
1	H	-5.074850	4.590425	1.530879
1	H	-3.650168	3.726881	2.175213
6	C	4.271978	3.986753	-1.210414
1	H	3.656082	3.772587	-2.089902
1	H	3.661334	4.562901	-0.506073
1	H	5.138932	4.579061	-1.503538
8	O	5.927978	2.474822	-0.324957
8	O	-5.893040	2.495394	0.357831
6	C	-0.101520	3.864833	-0.112983
1	H	-0.915796	4.139704	-0.793726
1	H	-0.347526	4.280662	0.869432
1	H	0.828458	4.305808	-0.476957

Sum of electronic and zero-point Energies= -2672.123596

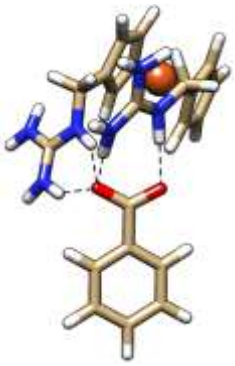


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-5.513380	0.096321	-0.652171
7	N	-4.292996	-0.418990	-0.486347
7	N	-5.673828	1.420146	-0.780958
1	H	-4.897331	2.014409	-1.032976
1	H	-6.596590	1.816680	-0.890510
7	N	4.293206	0.417971	-0.486870
6	C	5.513267	-0.098334	-0.651993
1	H	6.595207	-1.819728	-0.888782
1	H	4.895834	-2.016216	-1.031500
7	N	5.672739	-1.422379	-0.779731
6	C	-3.051952	0.371795	-0.365463
6	C	3.051698	-0.371984	-0.365350
1	H	4.195271	1.425044	-0.511140
1	H	-4.194405	-1.426023	-0.509574
6	C	1.936464	0.507369	0.113628
6	C	1.611657	0.796117	1.480271
6	C	1.053550	1.277323	-0.713768
6	C	0.529592	1.723280	1.492253
1	H	2.094106	0.363812	2.347686
6	C	0.184408	2.019521	0.138156
1	H	1.041238	1.274278	-1.796387
1	H	0.039999	2.116778	2.373480
1	H	-0.611846	2.677229	-0.185752
6	C	-1.936409	-0.506562	0.114614
6	C	-1.611398	-0.793360	1.481614
6	C	-1.053546	-1.277613	-0.711817
6	C	-0.529275	-1.720437	1.494760
1	H	-2.093772	-0.359882	2.348488
6	C	-0.184254	-2.018567	0.141036
1	H	-1.041371	-1.276102	-1.794440
1	H	-0.039535	-2.112661	2.376473
1	H	0.611994	-2.676687	-0.182047

26	Fe	0.000051	0.000727	0.496134
1	H	-2.798960	0.811702	-1.337491
1	H	-3.229961	1.184773	0.345589
1	H	2.798632	-0.812800	-1.336946
1	H	3.229191	-1.184307	0.346585
7	N	6.584432	0.708179	-0.679972
7	N	-6.583964	-0.710978	-0.679616
1	H	6.524958	1.656395	-0.336268
1	H	7.513168	0.327277	-0.794394
1	H	-7.512943	-0.330832	-0.794550
1	H	-6.523878	-1.658889	-0.335182

Sum of electronic and zero-point Energies= -2138.263865

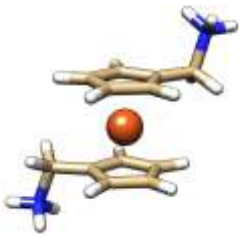


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	0.061266	-2.226395	2.475466
7	N	0.345348	-2.072779	1.176623
7	N	0.918555	-2.847602	3.309536
1	H	1.563041	-3.538365	2.953117
1	H	0.676107	-2.942168	4.286155
6	C	1.574210	-2.556422	0.546050
6	C	-4.964744	0.497770	0.082232
6	C	-4.015123	-0.338426	-0.521430
6	C	-6.193143	0.733515	-0.536281
6	C	-4.317051	-0.940140	-1.751638
6	C	-6.481888	0.138262	-1.767395
1	H	-6.925037	1.379011	-0.058371
6	C	-5.540919	-0.699241	-2.374507
1	H	-3.580339	-1.592583	-2.208369
1	H	-7.437277	0.323909	-2.250851
1	H	-5.763160	-1.164342	-3.331154
6	C	-2.687174	-0.609739	0.140287
8	O	-1.960555	-1.520354	-0.331721
8	O	-2.373267	0.104811	1.162507
1	H	-0.467173	-1.843944	0.568837
6	C	2.419666	2.077069	-0.685601
6	C	3.684204	1.873899	-1.317305
6	C	2.428051	1.382327	0.566734
6	C	4.480047	1.055942	-0.460576
1	H	3.973915	2.250528	-2.289848
6	C	3.704258	0.745826	0.698024
1	H	5.481596	0.701552	-0.667688
1	H	4.019689	0.132619	1.533273
6	C	1.927497	-1.796156	-0.707748
6	C	3.194994	-1.895420	-1.366335
6	C	1.077177	-0.993640	-1.532140

6	C	3.124080	-1.163020	-2.588681
1	H	4.059688	-2.428646	-0.990964
6	C	1.815854	-0.604772	-2.687541
1	H	0.048550	-0.734989	-1.320638
1	H	3.931486	-1.031170	-3.297492
1	H	1.451851	0.028852	-3.486225
26	Fe	2.763848	0.072611	-0.988893
1	H	-4.738207	0.948995	1.042829
1	H	2.395947	-2.472136	1.263540
1	H	1.468190	-3.622861	0.295949
7	N	-1.072249	-1.702129	2.954138
1	H	-1.334930	-1.847987	3.918123
1	H	-1.611500	-1.031982	2.386382
1	H	1.588288	2.631807	-1.101861
6	C	1.390965	1.417103	1.660652
1	H	1.392157	0.467390	2.200557
1	H	1.655762	2.188620	2.395112
7	N	0.017902	1.657465	1.218254
6	C	-0.581354	2.853413	1.191833
7	N	0.136031	3.987574	1.282292
7	N	-1.916070	2.897726	1.123990
1	H	-0.625432	0.862463	1.141124
1	H	-0.330771	4.882651	1.233930
1	H	1.119859	3.984822	1.052581
1	H	-2.392487	3.746098	0.854167
1	H	-2.421132	2.005987	1.104325

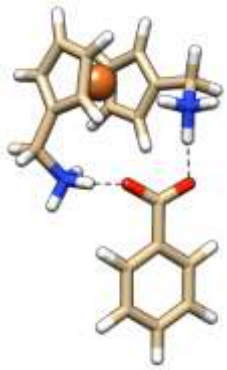
Sum of electronic and zero-point Energies= -2558.561817



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
7	N	-0.944908	4.231225	-0.796445
7	N	0.944908	-4.231225	-0.796445
6	C	0.000000	3.045765	-0.619444
6	C	0.000000	-3.045765	-0.619444
1	H	1.387240	-4.492250	0.091219
1	H	-1.387240	4.492250	0.091219
6	C	0.746623	-1.851648	-0.128794
6	C	0.981262	-1.501809	1.244413
6	C	1.408138	-0.873753	-0.946547
6	C	1.769529	-0.316228	1.267482
1	H	0.602685	-2.036590	2.106221
6	C	2.032682	0.069843	-0.082063
1	H	1.411014	-0.851760	-2.028908
1	H	2.088191	0.216100	2.153814
1	H	2.590581	0.942705	-0.395026
6	C	-0.746623	1.851648	-0.128794
6	C	-0.981262	1.501809	1.244413
6	C	-1.408138	0.873753	-0.946547
6	C	-1.769529	0.316228	1.267482
1	H	-0.602685	2.036590	2.106221
6	C	-2.032682	-0.069843	-0.082063
1	H	-1.411014	0.851760	-2.028908
1	H	-2.088191	-0.216100	2.153814
1	H	-2.590581	-0.942705	-0.395026
26	Fe	0.000000	0.000000	0.258660
1	H	0.454896	2.881813	-1.596872
1	H	0.766072	3.378803	0.081484
1	H	-0.454896	-2.881813	-1.596872
1	H	-0.766072	-3.378803	0.081484
1	H	-0.450239	5.057326	-1.150770
1	H	-1.696247	4.011615	-1.458903
1	H	0.450239	-5.057326	-1.150770
1	H	1.696247	-4.011615	-1.458903

Sum of electronic and zero-point Energies= -1840.657730



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
7	N	0.425045	2.358697	-1.510830
7	N	-0.514024	-2.143440	0.651257
6	C	1.469730	2.874252	-0.562698
6	C	0.667213	-2.886063	0.082089
6	C	-4.516584	1.150369	0.451814
6	C	-3.682583	0.226110	-0.193327
6	C	-5.816882	0.796502	0.811317
6	C	-4.174487	-1.054225	-0.482631
6	C	-6.299374	-0.483475	0.521494
1	H	-6.454901	1.517158	1.315808
6	C	-5.476706	-1.407823	-0.128630
1	H	-3.529250	-1.761510	-0.993577
1	H	-7.313300	-0.758584	0.799545
1	H	-5.850677	-2.401515	-0.360164
6	C	-2.274383	0.605602	-0.581758
8	O	-1.503452	-0.298812	-1.033279
8	O	-1.936866	1.820356	-0.433890
1	H	-0.961688	-1.466815	-0.045612
1	H	-0.525568	2.110060	-1.030259
6	C	1.750655	-1.977415	-0.415875
6	C	3.125658	-2.044892	-0.019000
6	C	1.657299	-1.030477	-1.487188
6	C	3.869810	-1.145261	-0.833975
1	H	3.521110	-2.667793	0.773264
6	C	2.963171	-0.517679	-1.740066
1	H	0.739962	-0.766620	-1.997207
1	H	4.931093	-0.948574	-0.757580
1	H	3.222865	0.229495	-2.479109
6	C	1.896972	1.847795	0.443732

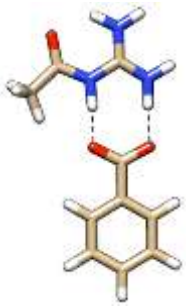
6	C	3.249874	1.627536	0.858782
6	C	1.055572	1.023613	1.256929
6	C	3.242264	0.671559	1.915107
1	H	4.124516	2.095448	0.425229
6	C	1.887796	0.295757	2.159136
1	H	-0.023696	0.986828	1.193762
1	H	4.113281	0.275348	2.420071
1	H	1.556406	-0.418429	2.902565
26	Fe	2.421818	-0.129060	0.210022
1	H	-4.131597	2.141543	0.667228
1	H	2.321451	3.207132	-1.158692
1	H	1.031988	3.749171	-0.073033
1	H	1.039373	-3.542424	0.870245
1	H	0.271630	-3.507092	-0.725570
1	H	0.227418	3.052372	-2.237873
1	H	0.756526	1.510987	-1.977312
1	H	-1.235954	-2.798263	0.967618
1	H	-0.222949	-1.592230	1.462940

Sum of electronic and zero-point Energies= -2260.954897

Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-1.245539	0.105821	-0.000029
8	O	-1.262406	1.326433	-0.000214
6	C	-2.475937	-0.761901	-0.000029
7	N	-0.040233	-0.617552	0.000393
6	C	1.228599	-0.094593	0.000051
7	C	1.401965	1.215836	0.000161
7	C	2.251337	-0.944008	0.000112
1	H	-0.114898	-1.628182	-0.000108
1	H	2.325788	1.626995	-0.000435
1	H	0.572645	1.806034	0.000104
1	H	3.207321	-0.613296	-0.000793
1	H	2.114432	-1.945774	-0.001549
1	H	-2.491920	-1.406100	0.885995
1	H	-3.356839	-0.120339	-0.000469
1	H	-2.491501	-1.406694	-0.885651

Sum of electronic and zero-point Energies= -358.381432



Standard orientation:

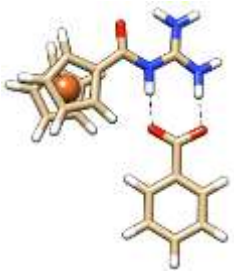
Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	3.274804	1.282314	-0.024884
8	O	4.504313	1.259314	-0.057921
6	C	2.495006	2.576274	-0.000101
7	N	2.491392	0.139713	0.006273
6	C	2.958774	-1.152132	0.009925
7	N	4.268030	-1.388666	-0.004164
7	N	2.056260	-2.120650	0.030805
1	H	1.437340	0.260410	0.028544
1	H	4.629548	-2.331869	-0.010790
1	H	4.891114	-0.584575	-0.028129
1	H	2.362339	-3.084732	0.030068
1	H	1.020421	-1.919068	0.025296
1	H	2.677202	3.072880	0.959560
1	H	2.878410	3.231521	-0.787194
1	H	1.421725	2.425830	-0.125858
6	C	-4.266993	1.492980	0.014535
6	C	-2.900893	1.209286	0.028658
6	C	-2.449035	-0.117077	0.006506
6	C	-3.388504	-1.156405	-0.030427
6	C	-4.755273	-0.875778	-0.044855
6	C	-5.197571	0.450312	-0.022466
1	H	-4.606843	2.525320	0.032133
1	H	-2.167922	2.008675	0.057210
1	H	-3.031430	-2.180910	-0.047602
1	H	-5.475761	-1.689164	-0.073531
1	H	-6.261997	0.669992	-0.033628
6	C	-0.965480	-0.423833	0.021844
8	O	-0.171001	0.565583	0.052613
8	O	-0.622428	-1.641489	0.004197

Sum of electronic and zero-point Energies= -778.676315

Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-3.684643	-0.299284	-0.280308
7	N	-2.447777	0.262574	-0.452043
7	N	-4.135322	-0.555018	0.936442
1	H	-3.538937	-0.306306	1.723643
1	H	-5.035812	-0.990608	1.083712
1	H	-2.178456	0.475229	-1.404137
6	C	3.157210	-0.991951	0.449418
6	C	2.810407	-1.259267	-0.909693
6	C	2.064826	-1.401705	1.273885
6	C	1.502807	-1.833937	-0.927546
1	H	3.420759	-1.039510	-1.775922
6	C	1.044503	-1.922125	0.422069
1	H	2.012013	-1.314216	2.351156
1	H	0.949661	-2.132158	-1.808494
1	H	0.079105	-2.292925	0.742406
6	C	-0.252111	1.132099	0.101141
6	C	0.281100	1.220515	-1.238254
6	C	0.757354	1.623018	1.004718
6	C	1.581778	1.786707	-1.147155
1	H	-0.200564	0.919461	-2.159653
6	C	1.872477	2.034501	0.229312
1	H	0.657440	1.676099	2.079433
1	H	2.246936	1.969378	-1.980498
1	H	2.797532	2.439172	0.617780
26	Fe	1.456947	0.032949	-0.068063
7	N	-4.403090	-0.568028	-1.367791
1	H	-5.325086	-0.977372	-1.296521
1	H	-4.041620	-0.413720	-2.299019
6	C	-1.530581	0.594678	0.566488
8	O	-1.816076	0.448998	1.752838
1	H	4.077582	-0.537384	0.792336

Sum of electronic and zero-point Energies= -1968.455906



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.118140	3.468346	-0.302936
7	N	-0.458655	2.222100	0.167157
7	N	-1.048514	4.407540	-0.463382
1	H	-2.003515	4.172915	-0.202858
1	H	-0.794144	5.345243	-0.739788
1	H	0.319194	1.516745	0.139255
6	C	-3.535723	-2.414108	-1.104091
6	C	-2.172272	-2.836433	-1.157684
6	C	-3.605302	-1.078215	-1.605932
6	C	-1.397436	-1.762575	-1.694172
1	H	-1.790416	-3.794590	-0.829790
6	C	-2.283600	-0.677948	-1.970755
1	H	-4.498039	-0.471027	-1.680081
1	H	-0.325568	-1.760740	-1.842126
1	H	-1.998926	0.290101	-2.363053
6	C	-1.898558	0.489311	1.118276
6	C	-0.923036	-0.547119	1.346721
6	C	-3.186049	-0.029647	1.504795
6	C	-1.609163	-1.672999	1.878343
1	H	0.135233	-0.481947	1.131528
6	C	-2.999510	-1.355804	1.976233
1	H	-4.118937	0.512513	1.445722
1	H	-1.154976	-2.620158	2.139123
1	H	-3.780141	-2.020113	2.323224
26	Fe	-2.358544	-1.169759	0.024290
7	N	1.154944	3.689342	-0.595140
1	H	1.420952	4.599736	-0.947203
1	H	1.926746	2.997751	-0.390577
6	C	-1.740410	1.847868	0.577468
8	O	-2.703014	2.620037	0.512404
1	H	-4.367013	-2.997030	-0.728951
6	C	6.264074	-0.875607	0.089262

6	C	5.915429	-2.229170	0.120982
6	C	4.568002	-2.600316	0.091230
6	C	3.574900	-1.621887	0.031037
6	C	3.915370	-0.262856	-0.000811
6	C	5.268980	0.100268	0.027273
1	H	7.310514	-0.582462	0.112116
1	H	6.689609	-2.990570	0.168371
1	H	4.292546	-3.651538	0.114854
1	H	2.526311	-1.899484	0.007020
1	H	5.524987	1.154320	0.001143
6	C	2.841907	0.803996	-0.066911
8	O	1.631276	0.419402	-0.074950
8	O	3.221302	2.009382	-0.112439

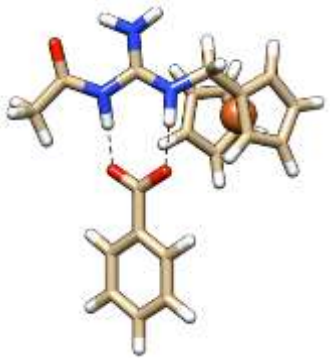
Sum of electronic and zero-point Energies= -2388.750374

Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	3.100972	-0.364201	-0.014417
7	N	1.914925	0.233381	-0.013684
7	N	3.228163	-1.682537	-0.018122
1	H	2.423065	-2.292168	-0.017327
1	H	4.170318	-2.067928	-0.017324
6	C	0.617460	-0.480601	-0.008357
1	H	1.878204	1.245382	-0.007349
6	C	-4.323569	-0.409263	-0.770045
6	C	-4.391852	-0.328591	0.654711
6	C	-3.324459	-1.371718	-1.110656
6	C	-3.435162	-1.241260	1.195126
1	H	-5.042136	0.322586	1.224504
6	C	-2.775182	-1.885214	0.104168
1	H	-3.025341	-1.651128	-2.112635
1	H	-3.233275	-1.403754	2.246033
1	H	-1.987969	-2.624099	0.184250
6	C	-0.505019	0.509875	-0.009848
6	C	-1.107165	1.108630	1.147097
6	C	-1.116486	1.093553	-1.169393
6	C	-2.091208	2.038318	0.701133
1	H	-0.864301	0.876127	2.176259
6	C	-2.096977	2.028935	-0.727724
1	H	-0.881921	0.847365	-2.197297
1	H	-2.737166	2.631523	1.335260
1	H	-2.747703	2.613906	-1.364604
26	Fe	-2.506105	0.149293	0.000985
1	H	0.566539	-1.121678	-0.895303
1	H	0.570319	-1.115214	0.883437
7	N	4.225942	0.428725	-0.011297
1	H	4.072047	1.430192	-0.008025
1	H	-4.913160	0.170147	-1.468757
6	C	6.568851	1.109416	0.035448
1	H	6.468595	1.684773	0.962649
1	H	7.568634	0.678835	-0.017134
1	H	6.419207	1.795652	-0.804635
6	C	5.559078	-0.007964	0.003805

8	O	5.849485	-1.194829	-0.001521

Sum of electronic and zero-point Energies= -2047.020642

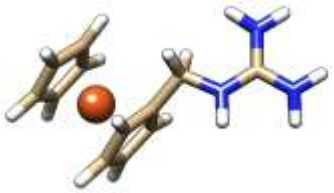


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.460904	2.810745	-0.681330
7	N	-0.700090	1.589809	-1.138225
7	N	-1.319330	3.825620	-0.801226
1	H	-2.081844	3.784913	-1.461472
1	H	-0.999106	4.729179	-0.455647
6	C	-1.963929	1.174552	-1.754218
1	H	0.116881	0.932660	-1.175953
6	C	-1.401448	-2.017052	1.938430
6	C	-2.811266	-2.122590	2.143241
6	C	-1.080758	-0.636481	1.759588
6	C	-3.363818	-0.806484	2.091918
1	H	-3.366247	-3.040017	2.292820
6	C	-2.294883	0.110857	1.854205
1	H	-0.096611	-0.228942	1.565085
1	H	-4.410682	-0.551002	2.196195
1	H	-2.391002	1.183704	1.746565
6	C	-2.309506	-0.262763	-1.466008
6	C	-3.641434	-0.738385	-1.234968
6	C	-1.440124	-1.400916	-1.479577
6	C	-3.592440	-2.157703	-1.097793
1	H	-4.527801	-0.119921	-1.165402
6	C	-2.231946	-2.565036	-1.245044
1	H	-0.365002	-1.368818	-1.602754
1	H	-4.434806	-2.806146	-0.893975
1	H	-1.859006	-3.578499	-1.168257
26	Fe	-2.418295	-1.252892	0.323505
1	H	-2.768873	1.806299	-1.368796
1	H	-1.909086	1.338676	-2.839881
7	N	0.729721	2.999609	-0.016569
1	H	1.283698	2.126133	0.207440
1	H	-0.701752	-2.842465	1.903349

6	C	2.581798	4.128531	1.092359
1	H	2.952402	3.104853	1.166710
1	H	3.285191	4.728502	0.505277
1	H	2.521249	4.575994	2.089051
6	C	1.221640	4.211925	0.439505
8	O	0.614325	5.276092	0.326110
6	C	4.505024	-3.008667	-1.159047
6	C	5.351911	-3.045960	-0.047237
6	C	5.199499	-2.104884	0.975405
6	C	4.204377	-1.131165	0.885447
6	C	3.349298	-1.088694	-0.224369
6	C	3.509647	-2.034953	-1.245894
1	H	4.621482	-3.737865	-1.956584
1	H	6.127195	-3.804577	0.021656
1	H	5.856360	-2.130641	1.840982
1	H	4.076195	-0.394672	1.671770
1	H	2.846681	-1.992849	-2.103720
6	C	2.270204	-0.032437	-0.322062
8	O	1.519755	-0.046895	-1.341843
8	O	2.181221	0.803401	0.632138

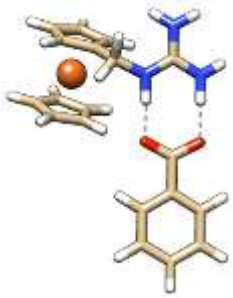
Sum of electronic and zero-point Energies= -2467.312961



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	4.104877	-0.251091	-0.004700
7	N	2.908707	0.299571	-0.222265
7	N	4.225898	-1.580815	0.107774
1	H	3.516723	-2.198431	-0.260070
1	H	5.121199	-1.998474	0.319217
6	C	1.626099	-0.432995	-0.236421
1	H	2.876723	1.287140	-0.441266
6	C	-3.384965	-0.389921	-0.624050
6	C	-3.307704	-0.460191	0.800882
6	C	-2.414160	-1.287981	-1.163811
6	C	-2.289378	-1.402141	1.142110
1	H	-3.904274	0.112351	1.499346
6	C	-1.736816	-1.913026	-0.072094
1	H	-2.216020	-1.454456	-2.214827
1	H	-1.979869	-1.669864	2.144184
1	H	-0.936181	-2.637463	-0.151393
6	C	0.487170	0.530521	-0.095266
6	C	-0.049808	1.033378	1.135968
6	C	-0.208785	1.179530	-1.168920
6	C	-1.076931	1.970416	0.821315
1	H	0.263377	0.734915	2.128536
6	C	-1.175793	2.060330	-0.601338
1	H	-0.038274	1.009520	-2.224604
1	H	-1.690293	2.504025	1.535789
1	H	-1.876856	2.673631	-1.152432
26	Fe	-1.505251	0.127241	0.016058
1	H	1.533714	-0.998084	-1.171399
1	H	1.632497	-1.143288	0.596117
7	N	5.185761	0.531036	0.121904
1	H	6.108464	0.133151	0.223982
1	H	5.090743	1.522300	0.291611
1	H	-4.050535	0.245251	-1.194254

Sum of electronic and zero-point Energies= -1894.400895

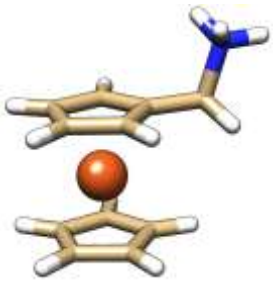


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.288155	3.183848	-0.056004
7	N	-0.353597	1.998925	0.552848
7	N	-1.355668	4.020657	-0.050161
1	H	-2.282968	3.625862	0.029087
1	H	-1.302006	4.872570	-0.591897
6	C	-1.452980	1.574536	1.413386
1	H	0.494143	1.386436	0.504602
6	C	-2.577789	-2.695031	-1.284203
6	C	-2.655700	-3.041492	0.099459
6	C	-1.405301	-1.901964	-1.474130
6	C	-1.529847	-2.462267	0.762088
1	H	-3.438644	-3.625933	0.565771
6	C	-0.755609	-1.756488	-0.209598
1	H	-1.075481	-1.470451	-2.410798
1	H	-1.312561	-2.530654	1.820586
1	H	0.150932	-1.194203	-0.018309
6	C	-2.588382	0.875916	0.700937
6	C	-3.585584	0.079917	1.351436
6	C	-2.940060	0.952709	-0.686086
6	C	-4.542281	-0.330848	0.374346
1	H	-3.599543	-0.174206	2.404149
6	C	-4.141229	0.204993	-0.886285
1	H	-2.375350	1.457828	-1.459056
1	H	-5.404980	-0.959199	0.555371
1	H	-4.644654	0.055063	-1.832717
26	Fe	-2.668469	-1.001323	-0.125154
1	H	-1.024907	0.908126	2.167620
1	H	-1.836123	2.448951	1.955964
7	N	0.858934	3.567211	-0.619683
1	H	0.868655	4.363692	-1.240552
1	H	1.702949	2.950005	-0.578141
1	H	-3.291430	-2.970825	-2.050178

6	C	6.462516	-0.555079	-0.490054
6	C	6.379920	-1.808306	0.124253
6	C	5.174874	-2.221276	0.700310
6	C	4.058585	-1.384595	0.661030
6	C	4.132258	-0.126738	0.047516
6	C	5.344896	0.279540	-0.525886
1	H	7.397449	-0.229653	-0.939179
1	H	7.249885	-2.459259	0.154174
1	H	5.106716	-3.194466	1.179849
1	H	3.118397	-1.693301	1.106063
1	H	5.394596	1.255967	-0.996474
6	C	2.921443	0.788411	0.008905
8	O	3.076047	1.926128	-0.520463
8	O	1.844952	0.345095	0.515275

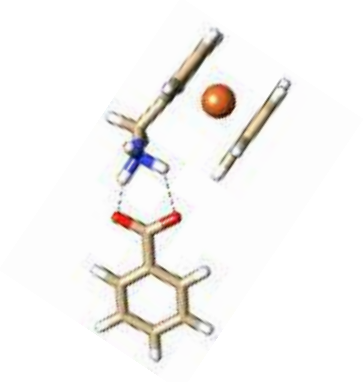
Sum of electronic and zero-point Energies= -2314.687937



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
7	N	-3.810457	-0.684867	0.000017
6	C	-2.339693	-1.099757	-0.000027
1	H	-4.034963	-0.120271	-0.825945
6	C	-1.460463	0.103108	-0.000022
6	C	-0.985265	0.805976	-1.159816
6	C	-0.985273	0.805939	1.159803
6	C	-0.217879	1.920085	-0.714265
1	H	-1.166180	0.522309	-2.188975
6	C	-0.217884	1.920067	0.714312
1	H	-1.166164	0.522177	2.188940
1	H	0.297468	2.628911	-1.349067
1	H	0.297457	2.628857	1.349162
6	C	2.490009	0.036004	0.714186
6	C	2.489948	0.035907	-0.714348
6	C	1.726581	-1.087391	1.156109
6	C	1.726476	-1.087578	-1.156042
1	H	2.968468	0.769492	-1.350225
6	C	1.254313	-1.781048	0.000107
1	H	1.526104	-1.355694	2.185308
1	H	1.525814	-1.355955	-2.185187
1	H	0.634723	-2.668813	0.000237
26	Fe	0.570065	0.156880	-0.000009
1	H	-2.207253	-1.717308	0.888978
1	H	-2.207277	-1.717292	-0.889043
1	H	-4.435558	-1.498514	0.000026
1	H	-4.034898	-0.120306	0.826023
1	H	2.968552	0.769714	1.349905

Sum of electronic and zero-point Energies= -1745.598548



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
7	N	-0.020008	-1.910950	-0.799420
6	C	0.843067	-2.206488	0.381482
1	H	0.321213	-2.351585	-1.655866
6	C	2.210857	-1.595665	0.300252
6	C	2.971080	-1.169354	1.438065
6	C	3.051206	-1.459833	-0.853441
6	C	4.264463	-0.770217	0.988781
1	H	2.614215	-1.148791	2.460118
6	C	4.312141	-0.944640	-0.427024
1	H	2.782385	-1.690943	-1.876709
1	H	5.059104	-0.377727	1.609817
1	H	5.149365	-0.708910	-1.071096
6	C	3.171940	2.095546	-0.943598
6	C	3.282655	2.313108	0.463862
6	C	1.847953	1.633757	-1.214467
6	C	2.027566	1.983880	1.061330
1	H	4.167902	2.649537	0.988169
6	C	1.138446	1.565184	0.024750
1	H	1.453580	1.372792	-2.188338
1	H	1.795704	2.029306	2.117737
1	H	0.110183	1.246587	0.145582
26	Fe	2.806719	0.354081	0.080153
1	H	0.305177	-1.837789	1.257921
1	H	0.901597	-3.296924	0.460175
1	H	-1.061886	-2.165856	-0.617356
1	H	-0.138152	-0.894936	-0.953367
1	H	3.958135	2.239386	-1.673631
6	C	-6.433979	-0.438491	0.528943
6	C	-6.666320	0.937400	0.441665
6	C	-5.623122	1.797403	0.085223

6	C	-4.354624	1.281878	-0.182563
6	C	-4.113059	-0.095845	-0.097661
6	C	-5.163977	-0.951038	0.260692
1	H	-7.242565	-1.110131	0.805913
1	H	-7.655247	1.337377	0.650228
1	H	-5.799752	2.867778	0.016557
1	H	-3.534387	1.935753	-0.460317
1	H	-4.970507	-2.016705	0.325317
6	C	-2.730654	-0.644583	-0.390709
8	O	-2.583833	-1.910546	-0.290946
8	O	-1.824236	0.173083	-0.711850

Sum of electronic and zero-point Energies= -2165.882066