

## Supporting Information

# **H<sub>2</sub> activation by hydrogenase-inspired NiFe catalyst using frustrated Lewis pair: Effect of buffer and halide ion in the heterolytic H–H bond cleavage**

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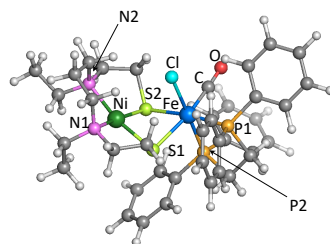
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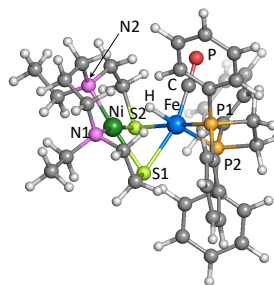
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(a) Complex 1



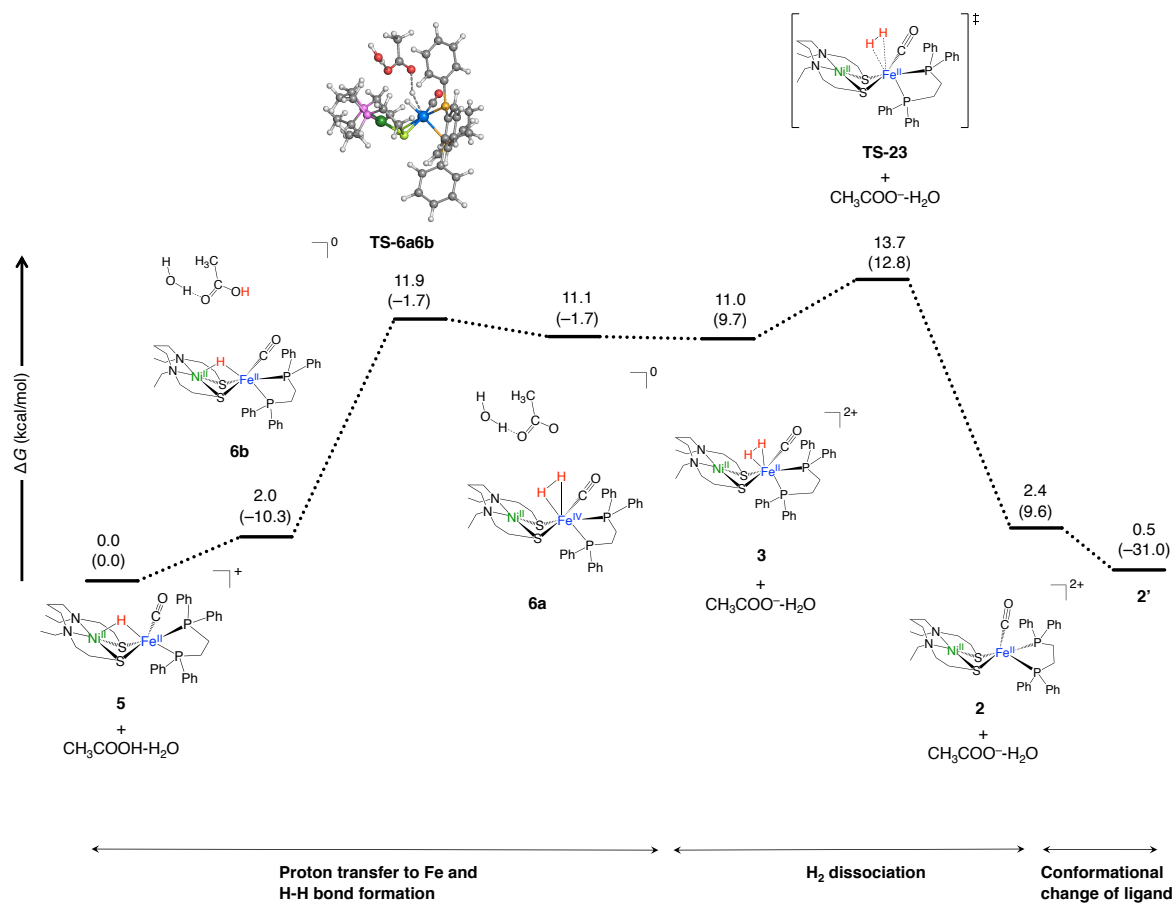
(b) Complex 5



	calc.		X-ray
Ni-Fe	3.23	0.04	3.27
Ni-N1	2.08	0.05	2.03
Ni-N2	2.07	0.05	2.02
Ni-S1	2.22	0.06	2.16
Ni-S2	2.18	0.00	2.18
Fe-S1	2.40	0.09	2.31
Fe-S2	2.33	0.00	2.33
Fe-P1	2.25	0.01	2.24
Fe-P2	2.24	0.00	2.24
Fe-C(O)	1.73	0.04	1.77
Fe-Cl	2.41	0.04	2.37
C-O	1.17	0.03	1.14

	calc.		X-ray
Ni-Fe	2.61	0.08	2.69
Ni-N1	2.02	0.02	2.00
Ni-N2	2.02	0.03	1.99
Ni-S1	2.26	0.09	2.17
Ni-S2	2.23	0.03	2.20
Fe-S1	2.42	0.08	2.34
Fe-S2	2.36	0.01	2.37
Fe-P1	2.18	0.00	2.18
Fe-P2	2.26	0.00	2.26
Fe-C(O)	1.71	0.03	1.74
Ni-H	1.78	0.26	2.04
Fe-H	1.56	0.09	1.47
C-O	1.18	0.02	1.16

**Fig. S1.** Key geometrical parameters of (a) complex **1** and (b) complex **5** in the optimised geometries.



**Figure S2.** Free energy profile of H<sub>2</sub> evolution reaction by NiFe complex.

**Table S1.** Imaginary frequencies ( $\text{cm}^{-1}$ ) of optimized transition states

label	frequency
<b>TS-23</b>	382.7
<b>TS-4a4b</b>	108.0
<b>TS-6a6b</b>	467.6
<b>TS-7a7b</b>	766.9
<b>TS-8a8b</b>	521.5
<b>TS-9a9b</b>	645.7

**Table S2.** Total electronic energy ( $E_{\text{SCF}}$ ), thermal correction to enthalpy ( $H_{\text{corr}}$ ), and thermal correction to free energy ( $G_{\text{corr}}$ ). All are given in a.u.

label	$E_{\text{SCF}}$	$H_{\text{corr}}$	$G_{\text{corr}}$	$\langle S^2 \rangle$
<b>1</b>	-3897.1897955	0.8209080	0.6892940	0.00
<b>15</b>	-3437.4782314	0.8246150	0.6943480	0.11
<b>2</b>	-3436.7390529	0.8183330	0.6905500	0.00
<b>3</b>	-3437.9179454	0.8355720	0.7064350	0.00
<b>31</b>	-3897.1631226	0.8197980	0.6863720	2.01
<b>35</b>	-3437.4718117	0.8243590	0.6932460	2.02
<b>35(Ni-H2O-X)</b>	-3973.6426546	0.8458280	0.7088430	2.00
<b>4a</b>	-4234.4225967	0.9202760	0.7690930	0.00
<b>4b</b>	-4234.4376760	0.9215130	0.7677840	0.00
<b>5</b>	-3437.4782314	0.8246150	0.6943480	0.11
<b>51</b>	-3897.1257335	0.8195910	0.6829450	6.06
<b>55</b>	-3437.4179964	0.8229840	0.6895190	6.07
<b>55(Ni-H2O-X)</b>	-3973.6110521	0.8456990	0.7042650	6.07
<b>55(Ni-H2O-Y)</b>	-3973.6231712	0.8460670	0.7060840	6.06
<b>6a</b>	-3743.1642504	0.9158190	0.7659510	0.00
<b>6b</b>	-3743.1794097	0.9171740	0.7666020	0.00
<b>71</b>	-3897.0925729	0.8179900	0.6754770	12.05
<b>75</b>	-3437.3686167	0.8217470	0.6833320	12.06
<b>75(Ni-H2O-X)</b>	-3973.5836375	0.8452880	0.7017410	12.06
<b>75(Ni-H2O-Y)</b>	-3973.5922735	0.8444260	0.6981190	12.06
<b>7a</b>	-4234.4132436	0.9207230	0.7674150	0.00
<b>7b</b>	-4234.4295300	0.9218870	0.7648650	0.00
<b>8a</b>	-3667.3774844	0.9174290	0.7733480	0.00
<b>8b</b>	-3667.3719187	0.9151970	0.7706770	0.00
<b>9a</b>	-3974.8509717	0.8646730	0.7275830	0.00
<b>9b</b>	-3974.8443979	0.8618810	0.7225820	0.00
<b>Cl</b>	-460.4240768	0.0023600	-0.0150230	0.00
<b>H2</b>	-1.1748220	0.0130320	-0.0018220	0.00
<b>H2O</b>	-76.4755123	0.0242290	0.0027470	0.00
<b>H2PO4</b>	-796.9341527	0.0949950	0.0455320	0.00
<b>HPO4</b>	-796.4669627	0.0827360	0.0359680	0.00
<b>NiFeSH</b>	-3437.1388471	0.8286030	0.7010180	0.00
<b>NiFeSH-H</b>	-3437.8949406	0.8342360	0.7040620	0.00

**Table S2 (Continue).** Total electronic energy ( $E_{\text{SCF}}$ ), thermal correction to enthalpy ( $H_{\text{corr}}$ ), and thermal correction to free energy ( $G_{\text{corr}}$ ). All are given in a.u.

label	$E_{\text{SCF}}$	$H_{\text{corr}}$	$G_{\text{corr}}$	$\langle S^2 \rangle$
<b>NiFe-OH</b>	-3512.7527141	0.8320850	0.7005720	0.00
<b>OH</b>	-75.9742634	0.0113790	-0.0082110	0.00
<b>TS-23</b>	-3437.9086835	0.8311430	0.7015710	0.00
<b>TS-4a4b</b>	-4234.4219852	0.9186120	0.7693810	0.00
<b>TS-6a6b</b>	-3743.1612580	0.9127450	0.7641500	0.00
<b>TS-7a7b</b>	-4234.4077183	0.9172080	0.7655550	0.00
<b>TS-8a8b</b>	-3667.3653792	0.9125190	0.7687670	0.00
<b>TS-9a9b</b>	-3974.8410658	0.8607440	0.7244550	0.00

## XYZ coordinate

<sup>1</sup>

Ni	2.524059	-0.112176	-0.181659
Fe	-0.692381	0.131543	-0.416119
S	0.899669	-0.416978	1.300481
S	1.179431	1.417400	-0.957015
P	-2.437166	-1.059534	0.363464
P	-1.384895	1.796103	0.919036
O	-2.178828	1.005471	-2.750161
N	3.523450	-1.759278	0.612651
N	3.719554	0.163065	-1.851412
C	-1.600536	0.666966	-1.785158
C	-3.445680	0.059207	1.470916
H	-4.149450	0.589344	0.794492
H	-4.046394	-0.531862	2.190654
C	-2.519784	1.049641	2.179611
H	-1.863684	0.526202	2.903981
H	-3.070569	1.829808	2.742474
C	-2.040567	-2.547308	1.373538
C	-2.021524	-2.520600	2.785435
H	-2.304216	-1.614164	3.340639
C	-1.627893	-3.662949	3.505992
H	-1.615426	-3.632305	4.606897
C	-1.250038	-4.835452	2.826864
H	-0.938742	-5.726480	3.394518
C	-1.274044	-4.866543	1.419783
H	-0.980693	-5.781629	0.881461
C	-1.666382	-3.730049	0.694918
H	-1.659152	-3.750184	-0.405806
C	-3.693932	-1.730462	-0.815103
C	-5.001954	-2.006970	-0.351479
H	-5.275487	-1.825954	0.699466
C	-5.967454	-2.526720	-1.229800
H	-6.984059	-2.734058	-0.859768
C	-5.637286	-2.784086	-2.573741
H	-6.396156	-3.191896	-3.260201
C	-4.334776	-2.524090	-3.034118
H	-4.066368	-2.730729	-4.082349
C	-3.365015	-1.999413	-2.160675
H	-2.339156	-1.818385	-2.515368
C	-2.348018	3.116993	0.063510
C	-1.823966	3.677789	-1.125546
H	-0.864716	3.318599	-1.530662
C	-2.522104	4.690027	-1.803274
H	-2.097399	5.120837	-2.723451
C	-3.761344	5.141651	-1.313953
H	-4.313773	5.929146	-1.850289
C	-4.293894	4.580649	-0.139807
H	-5.265745	4.925472	0.247049
C	-3.591003	3.577345	0.551265
H	-4.026592	3.160685	1.471434
C	-0.119728	2.725722	1.894046
C	0.293087	2.259612	3.164267
H	-0.184944	1.384371	3.626080
C	1.328762	2.909579	3.857668
H	1.634596	2.536568	4.847759
C	1.971029	4.024974	3.291562
H	2.785728	4.529435	3.834585
C	1.562287	4.497533	2.031285
H	2.051755	5.376255	1.582712
C	0.524287	3.854499	1.336224
H	0.217810	4.246252	0.355705

C	1.198835	-2.223043	1.444899
H	0.612749	-2.623273	2.294649
H	0.862467	-2.706739	0.507876
C	2.680734	-2.373884	1.702857
H	2.960569	-3.445904	1.809528
H	2.935697	-1.870549	2.655206
C	4.865363	-1.459681	1.215232
H	5.611782	-1.407381	0.402208
H	5.165017	-2.330761	1.840823
C	4.879067	-0.168669	2.026268
H	5.895775	0.008574	2.431787
H	4.596448	0.697994	1.392289
H	4.172048	-0.203152	2.879300
C	3.627234	-2.760290	-0.498238
H	2.586448	-3.022904	-0.778864
H	4.111842	-3.677674	-0.092549
C	4.374157	-2.306845	-1.751077
H	5.440238	-2.085387	-1.537199
H	4.392483	-3.184670	-2.430423
C	3.722713	-1.171528	-2.533894
H	4.227533	-1.066824	-3.519381
H	2.659810	-1.423703	-2.730911
C	5.086190	0.653999	-1.470982
H	5.492887	-0.026709	-0.707619
H	4.926034	1.626956	-0.965508
C	6.093565	0.791366	-2.613840
H	7.044051	1.183650	-2.197874
H	6.317708	-0.183998	-3.091297
H	5.756562	1.496630	-3.399815
C	3.102140	1.172333	-2.791764
H	3.459610	0.983096	-3.826829
H	3.467371	2.174096	-2.489331
C	1.589954	1.147878	-2.729430
H	1.154925	0.177142	-3.039006
H	1.143373	1.962678	-3.334740
Cl	0.054569	-1.752139	-1.717925
<sup>15</sup>			
Ni	1.598365	-1.260633	-0.913111
Fe	-0.405536	-0.164061	0.348129
S	0.196866	0.148448	-1.979476
S	-0.336596	-2.327336	-0.597157
P	-0.316589	1.882731	1.090693
P	-2.645202	0.091468	0.221644
O	-0.460269	-1.073133	3.095046
N	3.169891	-0.107826	-1.426513
N	2.548810	-2.714637	0.110844
C	-0.461435	-0.700793	1.972014
C	-1.950389	2.201651	1.960110
H	-1.867559	1.647606	2.919375
H	-2.067668	3.279651	2.190770
C	-3.119683	1.679919	1.112840
H	-3.379139	2.418118	0.328216
H	-4.032682	1.526026	1.722391
C	-0.160044	3.264170	-0.125737
C	-1.106770	3.365697	-1.174041
H	-1.929763	2.641231	-1.263067
C	-0.979339	4.364756	-2.152523
H	-1.724565	4.430770	-2.960745
C	0.106931	5.259814	-2.114911
H	0.212860	6.034067	-2.890990
C	1.062701	5.150923	-1.089750
H	1.923073	5.838009	-1.059577

C	0.930247	4.161825	-0.097694	H	4.520558	-4.872337	0.047393
H	1.692316	4.084217	0.692456	H	2.899339	-5.566307	0.408943
C	0.946554	2.272332	2.376986	C	1.597501	-3.171183	1.181045
C	0.815410	3.405236	3.213059	H	1.482227	-2.310813	1.865202
H	-0.048230	4.079913	3.105076	H	2.051751	-4.001253	1.766302
C	1.797307	3.685434	4.178839	C	0.242280	-3.572450	0.638455
H	1.687504	4.568516	4.828026	H	-0.501353	-3.630893	1.458910
C	2.918611	2.844584	4.314837	H	0.262336	-4.553456	0.121782
H	3.686982	3.069289	5.071476	H	1.142969	-0.301176	0.510214
C	3.054291	1.717609	3.484251	2			
H	3.927671	1.053754	3.584003	Ni	2.484791	0.020980	-0.957315
C	2.070317	1.430780	2.522500	Fe	-0.474481	0.066843	0.053637
H	2.159376	0.543462	1.874400	S	0.860530	1.485692	-1.178962
C	-3.591236	0.134229	-1.363771	S	0.821154	-1.403212	-1.194633
C	-3.139283	-0.671581	-2.434333	P	-1.878072	1.558220	0.914842
H	-2.241985	-1.295749	-2.308312	P	-1.976520	-1.417355	0.798944
C	-3.829396	-0.682884	-3.659102	O	1.084606	0.000225	2.459717
H	-3.466871	-1.318143	-4.482773	N	3.789931	1.591889	-0.510984
C	-4.971233	0.119454	-3.833067	N	3.734223	-1.546283	-0.477080
H	-5.508013	0.117197	-4.794928	C	0.442205	0.020954	1.474311
C	-5.427387	0.924253	-2.772373	C	-2.637156	0.807758	2.430958
H	-6.324983	1.550098	-2.899922	H	-1.860531	0.937375	3.212085
C	-4.746525	0.930015	-1.542287	H	-3.524205	1.396384	2.740108
H	-5.131287	1.554515	-0.721411	C	-2.950743	-0.685989	2.229873
C	-3.461519	-1.272664	1.159567	H	-4.022658	-0.853027	2.007037
C	-3.711967	-2.509881	0.521350	H	-2.703758	-1.269217	3.137853
H	-3.553611	-2.616659	-0.562946	C	-3.179984	1.750743	-0.359777
C	-4.164164	-3.613090	1.265242	C	-4.524766	1.392252	-0.114855
H	-4.357990	-4.570036	0.754886	H	-4.857063	1.090344	0.889020
C	-4.371147	-3.497200	2.652840	C	-5.453567	1.403893	-1.168904
H	-4.725342	-4.363078	3.234222	H	-6.496750	1.110277	-0.974993
C	-4.123259	-2.269220	3.292661	C	-5.054367	1.780547	-2.464109
H	-4.282516	-2.168801	4.378170	H	-5.785289	1.777446	-3.287599
C	-3.666623	-1.163033	2.553883	C	-3.719098	2.149403	-2.709405
H	-3.456028	-0.217775	3.078219	H	-3.400548	2.441065	-3.722093
C	1.456308	1.441853	-2.369342	C	-2.780751	2.121720	-1.666793
H	1.721628	1.301876	-3.436843	H	-1.728462	2.376267	-1.869000
H	1.006699	2.446524	-2.271247	C	-1.280524	3.216760	1.403830
C	2.648926	1.300201	-1.456469	C	-1.600986	4.370497	0.656106
H	3.460987	2.004602	-1.744624	H	-2.297597	4.310727	-0.193589
H	2.348558	1.544458	-0.417953	C	-1.021270	5.606360	0.992163
C	3.586790	-0.603046	-2.787958	H	-1.272996	6.501715	0.402570
H	2.667045	-0.698355	-3.396781	C	-0.126941	5.699880	2.073403
H	3.959971	-1.634428	-2.645801	H	0.329534	6.668792	2.329599
C	4.628866	0.236072	-3.529717	C	0.182645	4.553467	2.828795
H	4.849943	-0.259214	-4.497216	H	0.881414	4.620340	3.677138
H	4.263145	1.258213	-3.755230	C	-0.386409	3.314139	2.496413
H	5.584369	0.319451	-2.973738	H	-0.108163	2.420985	3.077571
C	4.304725	-0.123584	-0.456098	C	-1.365786	-3.043500	1.370305
H	3.951800	0.418199	0.444109	C	-1.512749	-4.202200	0.578080
H	5.144676	0.469496	-0.877922	H	-2.091982	-4.166570	-0.357456
C	4.789178	-1.506183	-0.039676	C	-0.902333	-5.403844	0.978618
H	5.698676	-1.359394	0.578639	H	-1.017995	-6.305625	0.357340
H	5.113084	-2.113986	-0.909419	C	-0.142073	-5.452642	2.160951
C	3.774259	-2.242686	0.822793	H	0.341617	-6.393589	2.466696
H	4.250541	-3.110242	1.328387	C	0.000465	-4.298084	2.954118
C	3.421352	-1.558893	1.621861	H	0.595263	-4.332008	3.880165
C	2.844221	-3.792323	-0.898662	C	-0.607640	-3.094838	2.562824
H	3.474838	-3.331305	-1.682461	H	-0.472768	-2.189703	3.176285
H	1.885156	-4.039088	-1.393244	C	-3.200969	-1.754070	-0.528059
C	3.510183	-5.062356	-0.367284	C	-2.948031	-1.292077	-1.837193
H	3.626429	-5.772929	-1.210987	H	-2.010908	-0.760926	-2.066557



C -3.907744 -1.477117 -2.846269  
 H -3.712690 -1.095153 -3.859932  
 C -5.117622 -2.130975 -2.553555  
 H -5.873420 -2.268551 -3.342602  
 C -5.366292 -2.606483 -1.251815  
 H -6.311199 -3.123789 -1.022906  
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H	4.654430	-0.781022	-3.558286	H	-4.916761	5.301283	-2.260793
H	3.045866	-1.406848	-3.100823	C	-4.815072	4.027909	-0.496528
C	4.954028	0.779110	-1.256302	H	-5.847124	4.245236	-0.179224
H	5.335366	0.084526	-0.488936	C	-4.024089	3.157389	0.274486
H	4.586476	1.670621	-0.709936	H	-4.455178	2.715142	1.184614
C	6.082631	1.151609	-2.218047	C	-0.565457	2.846943	1.857134
H	6.888802	1.646014	-1.638646	C	-0.214963	2.516398	3.187188
H	6.523511	0.260397	-2.708509	H	-0.609468	1.609414	3.666053
H	5.753761	1.858811	-3.006005	C	0.653243	3.345604	3.918625
C	3.097292	1.178298	-2.812504	H	0.911579	3.078490	4.955379
H	3.511429	1.064234	-3.835863	C	1.189037	4.505784	3.332063
H	3.374515	2.188969	-2.452856	H	1.871337	5.151861	3.906710
C	1.587265	1.048181	-2.816948	C	0.844515	4.840308	2.010007
H	1.239114	0.062171	-3.183515	H	1.252816	5.750461	1.543292
H	1.102900	1.847116	-3.413857	C	-0.027089	4.018604	1.275737
H	-0.814563	-1.317972	-1.324216	H	-0.287483	4.303484	0.246494
H	-0.180158	-0.859384	-1.680712	C	1.294414	-2.011373	1.754846
<sup>31</sup> Ni	2.374617	-0.032080	-0.215699	H	0.829101	-2.428817	2.668969
Fe	-0.610889	0.121872	-0.332068	H	0.903451	-2.560160	0.880470
S	0.826525	-0.230838	1.587007	C	2.805361	-2.131862	1.864650
S	1.042027	1.704797	-1.010682	H	3.089953	-3.204881	1.953613
P	-2.239027	-1.272714	0.350846	H	3.127563	-1.640531	2.802689
P	-1.623560	1.717766	0.851077	C	4.848833	-0.968267	1.324616
O	-2.079981	0.671747	-2.773963	H	5.599140	-0.869067	0.519814
N	3.583793	-1.512773	0.733868	H	5.267348	-1.725124	2.027391
N	3.654800	0.311628	-1.928311	C	4.650736	0.372596	2.024365
C	-1.501867	0.458524	-1.773582	H	5.619373	0.735140	2.424145
C	-3.476385	-0.256109	1.312794	H	4.263587	1.142509	1.322563
H	-4.173873	0.162692	0.556621	H	3.934806	0.304058	2.867848
H	-4.062603	-0.897539	2.000608	C	3.871823	-2.539179	-0.316960
C	-2.743785	0.864832	2.056552	H	2.897082	-2.983395	-0.600297
H	-2.081399	0.448997	2.841921	H	4.483517	-3.351729	0.141001
H	-3.434226	1.578391	2.548857	C	4.599050	-2.045805	-1.578924
C	-1.810808	-2.688235	1.448643	H	5.616687	-1.681347	-1.325616
C	-1.862385	-2.578224	2.855757	H	4.771174	-2.955141	-2.192969
H	-2.216708	-1.655532	3.338523	C	3.894514	-1.045000	-2.505850
C	-1.443761	-3.651258	3.662140	H	4.497283	-0.948835	-3.437699
H	-1.488116	-3.555752	4.758436	H	2.904543	-1.440337	-2.806945
C	-0.965857	-4.836571	3.074123	C	4.911444	0.993930	-1.483352
H	-0.634047	-5.673205	3.708900	H	5.352876	0.406773	-0.663227
C	-0.915991	-4.950725	1.672539	H	4.591470	1.956546	-1.036138
H	-0.545934	-5.876763	1.205139	C	5.974948	1.220374	-2.560908
C	-1.337274	-3.883952	0.862144	H	6.815043	1.793851	-2.118174
H	-1.286472	-3.979372	-0.233824	H	6.389677	0.264498	-2.941060
C	-3.241688	-2.111638	-0.951912	H	5.591489	1.799761	-3.425229
C	-4.592706	-2.450214	-0.709207	C	2.964484	1.205537	-2.924063
H	-5.071166	-2.200405	0.250253	H	3.214188	0.882191	-3.958537
C	-5.339111	-3.120001	-1.693613	H	3.379841	2.224873	-2.799962
H	-6.393175	-3.373345	-1.498473	C	1.450544	1.283127	-2.766706
C	-4.743469	-3.468944	-2.920117	H	0.966124	0.319416	-3.009809
H	-5.330936	-3.995337	-3.688889	H	1.043086	2.066345	-3.437331
C	-3.396465	-3.144950	-3.160555	Cl	0.737879	-1.557125	-1.364761
H	-2.922427	-3.418075	-4.116501	<sup>35</sup> Ni	1.534050	-1.229280	-0.996617
C	-2.647859	-2.465940	-2.183125	Fe	-0.392639	-0.197767	0.253172
H	-1.594072	-2.214086	-2.377339	S	0.120825	0.366017	-2.038093
C	-2.701298	2.859666	-0.122181	S	-0.499467	-2.347627	-0.719232
C	-2.188311	3.447251	-1.302903	P	-0.208416	1.815048	1.140089
H	-1.164844	3.208684	-1.634483	P	-2.622948	0.139974	0.252970
C	-2.977185	4.327427	-2.060898	O	-0.457969	-1.228016	2.962901
H	-2.560652	4.781391	-2.973722	N	3.186593	-0.048121	-1.446241
C	-4.294390	4.618201	-1.661530	N	2.469008	-2.808685	0.013448

C	-0.454533	-0.823297	1.855312	H	4.275931	1.368478	-3.741781
C	-1.807063	2.120139	2.074275	H	5.577750	0.371690	-3.004424
H	-1.723734	1.500598	2.992406	C	4.308581	-0.176795	-0.474359
H	-1.876827	3.182879	2.381210	H	3.980051	0.334385	0.452894
C	-3.011573	1.701345	1.222247	H	5.189912	0.389321	-0.851820
H	-3.246523	2.487662	0.477955	C	4.721687	-1.606918	-0.126632
H	-3.922041	1.555820	1.837078	H	5.648913	-1.530198	0.478787
C	-0.041089	3.291714	0.047791	H	5.010855	-2.180475	-1.031649
C	-0.997604	3.494267	-0.976989	C	3.705374	-2.371485	0.721529
H	-1.825672	2.785116	-1.123785	H	4.193699	-3.253713	1.194057
C	-0.868410	4.577387	-1.861445	H	3.369506	-1.715959	1.551799
H	-1.618414	4.723295	-2.654612	C	2.726347	-3.825329	-1.054670
C	0.226299	5.456113	-1.751884	H	3.397719	-3.348474	-1.796094
H	0.332836	6.296995	-2.455141	H	1.764459	-3.986452	-1.583009
C	1.189236	5.248466	-0.748877	C	3.310638	-5.164532	-0.600361
H	2.054729	5.924192	-0.662820	H	3.445374	-5.815049	-1.488514
C	1.057709	4.173315	0.148622	H	4.302890	-5.048900	-0.118683
H	1.825407	4.017881	0.921587	H	2.639954	-5.697746	0.103713
C	1.085689	2.038147	2.434407	C	1.493568	-3.275512	1.039284
C	1.016966	3.105182	3.360488	H	1.414312	-2.452733	1.772853
H	0.194610	3.835904	3.309811	H	1.895378	-4.157930	1.588344
C	2.008007	3.245727	4.347124	C	0.106949	-3.605914	0.492338
H	1.946932	4.077910	5.066129	H	-0.609632	-3.682722	1.335535
C	3.075547	2.329999	4.417151	H	0.095768	-4.575832	-0.046248
H	3.850394	2.445145	5.191542	H	1.184530	-0.348746	0.391780
C	3.149395	1.268990	3.497076	<sup>35</sup> (Ni-H2O-X)			
H	3.979943	0.546882	3.542421	Ni	2.369019	-0.645562	-0.455695
C	2.156264	1.122605	2.514197	Fe	-0.896914	0.181636	-0.626914
H	2.200598	0.286017	1.798947	S	0.544145	-0.909805	0.998820
C	-3.565583	0.289733	-1.324428	S	1.152277	1.129312	-1.388461
C	-3.148551	-0.473325	-2.438405	P	-2.740670	-0.667770	0.342375
H	-2.271482	-1.132275	-2.353729	P	-0.935074	1.785951	0.965023
C	-3.853635	-0.401366	-3.652079	O	-2.343243	1.806456	-2.547687
H	-3.518684	-1.002041	-4.512432	N	3.377258	-2.113856	0.694696
C	-4.975613	0.438618	-3.768471	N	3.908121	-0.068083	-1.802881
H	-5.523629	0.499983	-4.721967	C	-1.774451	1.157935	-1.749101
C	-5.398904	1.197216	-2.661421	C	-3.302894	0.536400	1.651679
H	-6.281525	1.851075	-2.743464	H	-3.920755	1.285472	1.112094
C	-4.701752	1.122540	-1.442561	H	-3.951271	0.035920	2.398991
H	-5.059198	1.713166	-0.585240	C	-2.079377	1.188255	2.296920
C	-3.490210	-1.223804	1.144205	H	-1.493731	0.438912	2.865944
C	-3.875715	-2.391557	0.447148	H	-2.343398	2.005664	2.997442
H	-3.768613	-2.444844	-0.646982	C	-2.524436	-2.288730	1.193263
C	-4.402032	-3.491476	1.146384	C	-2.343357	-2.397338	2.589327
H	-4.702664	-4.394553	0.591762	H	-2.372459	-1.508171	3.236259
C	-4.547145	-3.439842	2.545288	C	-2.119385	-3.656515	3.175336
H	-4.959482	-4.303013	3.091243	H	-1.978972	-3.730051	4.265322
C	-4.163959	-2.280111	3.243011	C	-2.076048	-4.814277	2.377296
H	-4.274727	-2.230627	4.337858	H	-1.899388	-5.797952	2.840224
C	-3.634856	-1.177410	2.549270	C	-2.259111	-4.709607	0.985789
H	-3.322249	-0.287650	3.117405	H	-2.227399	-5.611258	0.353861
C	1.480184	1.595752	-2.295101	C	-2.480758	-3.454892	0.395140
H	1.742406	1.511027	-3.369867	H	-2.606573	-3.374447	-0.695325
H	1.108376	2.624721	-2.137885	C	-4.289833	-0.968193	-0.619020
C	2.686850	1.355932	-1.405890	C	-5.455705	-1.334892	0.095341
H	3.498886	2.070544	-1.674518	H	-5.419587	-1.458916	1.189742
H	2.412754	1.560312	-0.351575	C	-6.663842	-1.553570	-0.585999
C	3.562403	-0.503061	-2.824552	H	-7.566014	-1.835568	-0.020359
H	2.628365	-0.545514	-3.422378	C	-6.719620	-1.417252	-1.986446
H	3.903676	-1.552379	-2.729917	H	-7.667174	-1.591543	-2.520500
C	4.616954	0.329710	-3.556563	C	-5.561251	-1.066198	-2.700748
H	4.818155	-0.136147	-4.542862	H	-5.595249	-0.967797	-3.797340

C	-4.349030	-0.842387	-2.021769	H	0.825207	-2.052164	-1.946389
H	-3.444085	-0.593529	-2.591679	4a			
C	-1.607448	3.415101	0.406466	Ni	-1.415521	-1.871570	0.576177
C	-1.059336	4.017412	-0.750493	Fe	0.794214	0.176693	-0.636057
H	-0.269122	3.499554	-1.318401	S	0.209494	-0.696216	1.514733
C	-1.529338	5.264211	-1.193219	S	-0.018668	-1.958763	-1.076503
H	-1.089283	5.722498	-2.092893	P	1.710937	2.095837	0.078578
C	-2.564304	5.916974	-0.498765	P	2.898394	-0.653303	-0.619505
H	-2.938117	6.891439	-0.850616	O	1.080311	0.953625	-3.424453
C	-3.123609	5.316759	0.643021	N	-2.633486	-1.482911	2.208752
H	-3.938667	5.817551	1.188957	N	-2.836075	-2.766679	-0.630898
C	-2.646941	4.074306	1.099059	C	0.991855	0.635285	-2.299824
H	-3.097783	3.630306	1.998768	C	3.585264	2.012653	-0.100194
C	0.607126	2.279202	1.869413	H	3.930527	2.954897	-0.569180
C	0.849618	1.851630	3.194904	H	4.004839	1.980337	0.923855
H	0.129140	1.213148	3.724568	C	4.017897	0.796251	-0.923260
C	2.025061	2.235485	3.862739	H	5.075101	0.513461	-0.742124
H	2.194538	1.894951	4.896061	H	3.903903	0.988200	-2.011256
C	2.985141	3.029437	3.212810	C	1.443696	2.511848	1.850034
H	3.911957	3.315858	3.734150	C	2.127665	1.773143	2.843412
C	2.756288	3.451742	1.891189	H	2.849762	0.991130	2.562756
H	3.499646	4.075635	1.370510	C	1.867774	2.013756	4.202556
C	1.572657	3.089475	1.226474	H	2.404289	1.432809	4.968864
H	1.410017	3.446390	0.200603	C	0.918739	2.982893	4.581016
C	0.855488	-2.726161	0.958362	H	0.712830	3.166556	5.647184
H	0.202827	-3.230448	1.698795	C	0.228275	3.708908	3.593466
H	0.606466	-3.126838	-0.040157	H	-0.523634	4.460607	3.880423
C	2.322977	-2.977611	1.357286	C	0.484750	3.475046	2.231372
H	2.564327	-4.046330	1.171340	H	-0.079943	4.033504	1.471310
H	2.407535	-2.825715	2.451631	C	1.212377	3.635539	-0.802084
C	4.245561	-1.494537	1.748462	C	1.900777	4.840590	-0.521428
H	5.164200	-1.128189	1.253183	H	2.722342	4.854578	0.213104
H	4.572277	-2.294635	2.453432	C	1.528514	6.031882	-1.163169
C	3.600709	-0.336532	2.497161	H	2.068542	6.964846	-0.937734
H	4.320263	0.073790	3.234378	C	0.465181	6.033920	-2.087496
H	3.319107	0.485326	1.805265	H	0.171812	6.969431	-2.589118
H	2.681208	-0.633129	3.037738	C	-0.230657	4.842607	-2.354606
C	4.225377	-2.931957	-0.230828	H	-1.086429	4.836934	-3.045943
H	3.536590	-3.498445	-0.884309	C	0.136588	3.645571	-1.711622
H	4.792912	-3.675221	0.377296	H	-0.444071	2.734413	-1.910743
C	5.229445	-2.156063	-1.100859	C	3.428835	-1.871747	-1.900388
H	5.944725	-1.586097	-0.472102	C	2.693644	-2.080160	-3.087014
H	5.850589	-2.929118	-1.601220	H	1.749595	-1.548274	-3.266972
C	4.691665	-1.264960	-2.226879	C	3.161859	-2.980953	-4.059705
H	5.548853	-0.941143	-2.859820	H	2.576253	-3.138769	-4.978883
H	4.044247	-1.864852	-2.898211	C	4.365356	-3.679377	-3.857437
C	4.705563	0.898806	-0.978165	H	4.727850	-4.387413	-4.619285
H	4.931913	0.413980	-0.009419	C	5.104006	-3.473490	-2.677539
H	4.018917	1.738023	-0.742774	H	6.048063	-4.016203	-2.512335
C	6.003962	1.412363	-1.603536	C	4.638623	-2.577121	-1.701072
H	6.437731	2.191935	-0.944287	H	5.220441	-2.427858	-0.777540
H	6.760086	0.608249	-1.711212	C	3.421126	-1.466337	0.940998
H	5.838683	1.869174	-2.601172	C	4.398787	-0.929387	1.804093
C	3.307586	0.628466	-3.002860	H	4.934870	-0.004188	1.546247
H	3.696941	0.165864	-3.933581	C	4.704033	-1.583684	3.012421
H	3.656898	1.680059	-3.007221	H	5.467296	-1.157092	3.681952
C	1.768455	0.630270	-3.051492	C	4.045460	-2.776163	3.359906
H	1.344544	-0.356987	-3.313919	H	4.287815	-3.284538	4.306417
H	1.430975	1.356098	-3.819145	C	3.079536	-3.322444	2.493191
Cl	-1.007530	-1.617312	-2.195786	H	2.562284	-4.258324	2.756719
O	1.807942	-2.204094	-1.746376	C	2.764282	-2.669274	1.292212
H	2.233491	-2.195223	-2.627401	H	2.002321	-3.098924	0.621020

C	-0.967260	0.387121	2.436723	H	3.622397	2.672015	0.742842
H	-0.398632	0.979921	3.177395	C	3.824530	1.463240	-1.074977
H	-1.480949	1.074468	1.733529	H	4.925324	1.425080	-0.941621
C	-1.901802	-0.562297	3.152247	H	3.620436	1.581236	-2.160588
H	-2.648215	-0.000513	3.757046	C	1.050729	2.693727	1.752191
H	-1.316323	-1.189073	3.852510	C	1.886925	2.103232	2.728377
C	-3.039800	-2.691555	3.000496	H	2.723079	1.452654	2.427923
H	-3.889842	-3.175533	2.486575	C	1.639984	2.319644	4.094100
H	-3.439291	-2.343310	3.979813	H	2.297276	1.854071	4.845247
C	-1.902751	-3.689096	3.191881	C	0.551892	3.116756	4.499708
H	-2.263859	-4.563079	3.770815	H	0.356504	3.281120	5.571086
H	-1.524742	-4.048607	2.211709	C	-0.288567	3.695696	3.531408
H	-1.046072	-3.247138	3.739200	H	-1.147501	4.312646	3.839216
C	-3.823687	-0.744397	1.676793	C	-0.043826	3.484786	2.163030
H	-3.445772	0.203342	1.243877	H	-0.719687	3.927315	1.417372
H	-4.479442	-0.481101	2.538336	C	0.529448	3.709938	-0.889158
C	-4.650669	-1.465261	0.614429	C	0.997818	5.021018	-0.629151
H	-5.139797	-2.375693	1.018381	H	1.817769	5.184609	0.088630
H	-5.476209	-0.771131	0.356800	C	0.409684	6.124555	-1.267166
C	-3.933519	-1.750842	-0.700338	H	0.780099	7.139732	-1.054488
H	-4.673950	-2.066882	-1.465050	C	-0.653632	5.934200	-2.172308
H	-3.479906	-0.812777	-1.076948	H	-1.116757	6.800150	-2.670700
C	-3.278090	-4.097963	-0.099386	C	-1.132330	4.636643	-2.421706
H	-3.586479	-3.960616	0.948211	H	-1.984152	4.476469	-3.099621
H	-2.371205	-4.734345	-0.077876	C	-0.547091	3.529711	-1.778366
C	-4.407247	-4.782948	-0.871597	H	-0.950455	2.527746	-1.963502
H	-4.635405	-5.748777	-0.376192	C	3.787230	-1.316131	-1.908148
H	-5.337712	-4.179962	-0.870493	C	3.085955	-1.638706	-3.090671
H	-4.135042	-5.002845	-1.923338	H	2.078490	-1.235327	-3.265068
C	-2.290138	-2.976147	-2.024179	C	3.669879	-2.477961	-4.056046
H	-3.130346	-3.006719	-2.750611	H	3.110628	-2.724307	-4.972482
H	-1.794403	-3.967598	-2.040394	C	4.957300	-3.005222	-3.848852
C	-1.295092	-1.901499	-2.405519	H	5.411512	-3.667128	-4.603174
H	-1.737509	-0.885146	-2.423157	C	5.662499	-2.686511	-2.673281
H	-0.811398	-2.118073	-3.379710	H	6.672026	-3.094371	-2.505757
H	-0.780555	0.627684	-0.987747	C	5.081550	-1.848017	-1.706354
H	-0.508068	1.030044	-0.256408	H	5.639868	-1.607389	-0.787495
P	-3.045448	2.062952	-1.010817	C	3.795163	-0.763436	0.905641
O	-2.212869	2.386779	0.290905	C	4.725278	-0.019620	1.662191
O	-4.500019	1.610413	-0.683996	H	5.089922	0.955699	1.306658
O	-3.165992	3.531762	-1.824805	C	5.199964	-0.521911	2.888917
O	-2.296392	1.109349	-1.999946	H	5.922750	0.068248	3.474234
H	-2.886017	4.245577	-1.184075	C	4.761142	-1.771357	3.361520
O	-5.906336	0.086440	-2.338000	H	5.135388	-2.161079	4.321356
H	-6.451926	-0.403824	-1.693515	C	3.843822	-2.524213	2.603198
H	-5.343195	0.670761	-1.729657	H	3.497545	-3.505049	2.965631
O	-2.115347	5.000155	0.303724	C	3.358035	-2.020347	1.386726
H	-1.279047	5.201236	-0.163197	H	2.631073	-2.608504	0.801527
H	-2.066774	3.986606	0.425702	C	-0.938500	0.214854	2.426606
4b				H	-0.466514	0.902776	3.153330
Ni	-1.069847	-2.097526	0.597998	H	-1.546414	0.804175	1.714053
Fe	0.812900	0.214644	-0.647254	C	-1.729016	-0.840769	3.165529
S	0.380693	-0.693030	1.514238	H	-2.545618	-0.381578	3.766575
S	0.328998	-2.011888	-1.060187	H	-1.056417	-1.364500	3.872265
P	1.320210	2.278002	-0.024727	C	-2.538959	-3.117239	3.053168
P	3.037503	-0.172305	-0.662796	H	-3.316913	-3.727035	2.558760
O	0.642982	0.925107	-3.451305	H	-2.971627	-2.818727	4.035038
N	-2.324868	-1.873030	2.241922	C	-1.266852	-3.936724	3.239765
N	-2.356665	-3.200549	-0.580012	H	-1.488895	-4.843408	3.838362
C	0.750872	0.649326	-2.307210	H	-0.854758	-4.254036	2.258849
C	3.173850	2.590414	-0.266637	H	-0.475283	-3.365232	3.764766
H	3.307759	3.569896	-0.766473	C	-3.622572	-1.329726	1.725028

H	-3.401829	-0.330763	1.299608
H	-4.303883	-1.174996	2.593365
C	-4.337079	-2.169456	0.668554
H	-4.682490	-3.140725	1.079147
H	-5.258102	-1.609214	0.408601
C	-3.591354	-2.357092	-0.648026
H	-4.283913	-2.783740	-1.403617
H	-3.284798	-1.365890	-1.035184
C	-2.599226	-4.575151	-0.030272
H	-2.910710	-4.473049	1.020415
H	-1.610418	-5.075136	-0.015482
C	-3.627621	-5.423256	-0.781446
H	-3.710920	-6.406144	-0.274133
H	-4.634551	-4.959006	-0.775279
H	-3.338396	-5.614270	-1.834302
C	-1.800081	-3.350664	-1.975939
H	-2.633542	-3.505682	-2.694490
H	-1.173232	-4.264917	-1.985029
C	-0.955579	-2.161418	-2.376733
H	-1.534997	-1.221402	-2.428048
H	-0.457128	-2.328063	-3.353353
H	-1.767778	0.636787	-1.335341
H	-0.656627	0.579990	-0.506992
P	-3.631949	1.668484	-0.791368
O	-2.839732	2.065968	0.478516
O	-4.937850	0.882407	-0.617600
O	-3.934945	3.031198	-1.664569
O	-2.648317	0.806801	-1.809172
H	-3.622108	3.817171	-1.107662
O	-5.950352	-0.990322	-2.271748
H	-6.385887	-1.561012	-1.609363
H	-5.536305	-0.286553	-1.688811
O	-2.956622	4.713709	0.212813
H	-2.106772	4.981105	-0.193548
H	-2.783867	3.762723	0.501850
S			
Ni	1.598365	-1.260633	-0.913111
Fe	-0.405536	-0.164061	0.348129
S	0.196866	0.148448	-1.979476
S	-0.336596	-2.327336	-0.597157
P	-0.316589	1.882731	1.090693
P	-2.645202	0.091468	0.221644
O	-0.460269	-1.073133	3.095046
N	3.169891	-0.107826	-1.426513
N	2.548810	-2.714637	0.110844
C	-0.461435	-0.700793	1.972014
C	-1.950389	2.201651	1.960110
H	-1.867559	1.647606	2.919375
H	-2.067668	3.279651	2.190770
C	-3.119683	1.679919	1.112840
H	-3.379139	2.418118	0.328216
H	-4.032682	1.526026	1.722391
C	-0.160044	3.264170	-0.125737
C	-1.106770	3.365697	-1.174041
H	-1.929763	2.641231	-1.263067
C	-0.979339	4.364756	-2.152523
H	-1.724565	4.430770	-2.960745
C	0.106931	5.259814	-2.114911
H	0.212860	6.034067	-2.890990
C	1.062701	5.150923	-1.089750
H	1.923073	5.838009	-1.059577
C	0.930247	4.161825	-0.097694

H	1.692316	4.084217	0.692456
C	0.946554	2.272332	2.376986
C	0.815410	3.405236	3.213059
H	-0.048230	4.079913	3.105076
C	1.797307	3.685434	4.178839
H	1.687504	4.568516	4.828026
C	2.918611	2.844584	4.314837
H	3.686982	3.069289	5.071476
C	3.054291	1.717609	3.484251
H	3.927671	1.053754	3.584003
C	2.070317	1.430780	2.522500
H	2.159376	0.543462	1.874400
C	-3.591236	0.134229	-1.363771
C	-3.139283	-0.671581	-2.434333
H	-2.241985	-1.295749	-2.308312
C	-3.829396	-0.682884	-3.659102
H	-3.466871	-1.318143	-4.482773
C	-4.971233	0.119454	-3.833067
H	-5.508013	0.117197	-4.794928
C	-5.427387	0.924253	-2.772373
H	-6.324983	1.550098	-2.899922
C	-4.746525	0.930015	-1.542287
H	-5.131287	1.554515	-0.721411
C	-3.461519	-1.272664	1.159567
C	-3.711967	-2.509881	0.521350
H	-3.553611	-2.616659	-0.562946
C	-4.164164	-3.613090	1.265242
H	-4.357990	-4.570036	0.754886
C	-4.371147	-3.497200	2.652840
H	-4.725342	-4.363078	3.234222
C	-4.123259	-2.269220	3.292661
H	-4.282516	-2.168801	4.378170
C	-3.666623	-1.163033	2.553883
H	-3.456028	-0.217775	3.078219
C	1.456308	1.441853	-2.369342
H	1.721628	1.301876	-3.436843
H	1.006699	2.446524	-2.271247
C	2.648926	1.300201	-1.456469
H	3.460987	2.004602	-1.744624
H	2.348558	1.544458	-0.417953
C	3.586790	-0.603046	-2.787958
H	2.667045	-0.698355	-3.396781
H	3.959971	-1.634428	-2.645801
C	4.628866	0.236072	-3.529717
H	4.849943	-0.259214	-4.497216
H	4.263145	1.258213	-3.755230
H	5.584369	0.319451	-2.973738
C	4.304725	-0.123584	-0.456098
H	3.951800	0.418199	0.444109
H	5.144676	0.469496	-0.877922
C	4.789178	-1.506183	-0.039676
H	5.698676	-1.359394	0.578639
H	5.113084	-2.113986	-0.909419
C	3.774259	-2.242686	0.822793
H	4.250541	-3.110242	1.328387
H	3.421352	-1.558893	1.621861
C	2.844221	-3.792323	-0.898662
H	3.474838	-3.331305	-1.682461
H	1.885156	-4.039088	-1.393244
C	3.510183	-5.062356	-0.367284
H	3.626429	-5.772929	-1.210987
H	4.520558	-4.872337	0.047393

H	2.899339	-5.566307	0.408943	H	1.088308	3.139493	4.849066
C	1.597501	-3.171183	1.181045	C	1.200193	4.636586	3.269217
H	1.482227	-2.310813	1.865202	H	1.910671	5.278424	3.813524
H	2.051751	-4.001253	1.766302	C	0.743539	5.010444	1.991600
C	0.242280	-3.572450	0.638455	H	1.091784	5.948404	1.530760
H	-0.501353	-3.630893	1.458910	C	-0.161167	4.193000	1.294280
H	0.262336	-4.553456	0.121782	H	-0.505393	4.501439	0.295198
H	1.142969	-0.301176	0.510214	C	1.307563	-2.071784	1.710883
<sup>51</sup>				H	0.829477	-2.492666	2.617018
Ni	2.350219	-0.117747	-0.275920	H	0.934871	-2.616583	0.825805
Fe	-0.549066	0.060428	-0.396099	C	2.818667	-2.177669	1.848373
S	0.826217	-0.295355	1.536698	H	3.114778	-3.249278	1.893954
S	1.050883	1.661539	-1.108393	H	3.110386	-1.730615	2.817975
P	-2.308619	-1.275457	0.387787	C	4.792454	-0.844587	1.439186
P	-1.658926	1.839589	0.875728	H	5.579625	-0.667515	0.684375
O	-1.954816	0.451687	-2.932575	H	5.231583	-1.573892	2.158301
N	3.619589	-1.494332	0.766833	C	4.438409	0.463324	2.140168
N	3.689995	0.308908	-1.920156	H	5.346759	0.892690	2.609454
C	-1.400911	0.278825	-1.914021	H	4.037871	1.212698	1.423738
C	-3.494972	-0.179100	1.316365	H	3.674792	0.322552	2.930918
H	-4.175889	0.237366	0.543846	C	4.070169	-2.494345	-0.252660
H	-4.104147	-0.798315	2.005703	H	3.159868	-3.020975	-0.600455
C	-2.769171	0.950804	2.062102	H	4.719731	-3.246139	0.253929
H	-2.108668	0.544448	2.853847	C	4.836002	-1.939877	-1.465105
H	-3.486467	1.638619	2.553855	H	5.793005	-1.475326	-1.147741
C	-1.861740	-2.641420	1.532855	H	5.141454	-2.832128	-2.052114
C	-1.879999	-2.461944	2.933991	C	4.104334	-1.023425	-2.455230
H	-2.212420	-1.513099	3.379281	H	4.761212	-0.876327	-3.342174
C	-1.459951	-3.501799	3.781196	H	3.180182	-1.517013	-2.814038
H	-1.479830	-3.353096	4.872198	C	4.834145	1.112732	-1.380788
C	-1.012465	-4.721475	3.240645	H	5.233373	0.594232	-0.495606
H	-0.678887	-5.531784	3.907687	H	4.393376	2.059047	-1.007588
C	-0.993034	-4.902169	1.845582	C	5.979907	1.389795	-2.357614
H	-0.644679	-5.854016	1.414983	H	6.720712	2.052569	-1.865439
C	-1.414144	-3.868617	0.993086	H	6.508435	0.459807	-2.650191
H	-1.384048	-4.017492	-0.097403	H	5.637649	1.897271	-3.282614
C	-3.316384	-2.135507	-0.887829	C	3.001603	1.124545	-2.986011
C	-4.693508	-2.384116	-0.690733	H	3.258353	0.725793	-3.991014
H	-5.202538	-2.043104	0.223836	H	3.404914	2.154922	-2.942653
C	-5.425872	-3.080753	-1.667522	C	1.484584	1.193342	-2.848422
H	-6.500406	-3.265929	-1.511780	H	1.020623	0.211281	-3.053823
C	-4.790910	-3.543510	-2.835163	H	1.071565	1.944694	-3.551015
H	-5.368835	-4.090087	-3.597001	Cl	0.962856	-1.788925	-1.480232
C	-3.417622	-3.308472	-3.027283	<sup>55</sup>			
H	-2.914266	-3.670585	-3.937446	Ni	1.440145	-1.592740	-0.794152
C	-2.681440	-2.602985	-2.060180	Fe	-0.193851	-0.007631	0.221851
H	-1.606134	-2.416574	-2.212773	S	0.612098	0.178602	-2.048145
C	-2.755864	2.914392	-0.140136	S	-0.797291	-2.403872	-0.897238
C	-2.264767	3.381102	-1.383181	P	-0.133399	2.340834	0.751524
H	-1.246242	3.108938	-1.704098	P	-2.538476	0.275746	0.142631
C	-3.067374	4.186187	-2.208583	O	-0.298021	-0.569586	3.090653
H	-2.669207	4.547460	-3.169832	N	3.361505	-0.745062	-0.976370
C	-4.376461	4.517133	-1.814031	N	1.893697	-3.294370	0.333553
H	-5.009952	5.139663	-2.465433	C	-0.278804	-0.376415	1.928348
C	-4.875460	4.046861	-0.585430	C	-1.824367	2.700051	1.464313
H	-5.900392	4.300672	-0.271595	H	-1.775813	2.288418	2.494914
C	-4.070768	3.253953	0.251740	H	-1.982003	3.795042	1.541182
H	-4.479502	2.905163	1.212128	C	-2.946393	2.036491	0.653685
C	-0.626842	2.986168	1.869736	H	-3.116908	2.578696	-0.298606
C	-0.163082	2.614830	3.155256	H	-3.907640	2.043305	1.207973
H	-0.496213	1.677976	3.625257	C	0.128746	3.544916	-0.608999
C	0.740808	3.439197	3.847613	C	-0.647762	3.390386	-1.785154

H	-1.421116	2.610021	-1.844855	H	3.277635	-4.013806	1.791944
C	-0.410664	4.206483	-2.902333	H	2.686853	-2.345757	2.017844
H	-1.022379	4.075675	-3.808963	C	2.154654	-4.351404	-0.695362
C	0.614715	5.171191	-2.872951	H	3.014397	-4.007126	-1.303216
H	0.806292	5.801694	-3.755479	H	1.284401	-4.349507	-1.383009
C	1.398804	5.319122	-1.714509	C	2.412936	-5.766065	-0.172429
H	2.207350	6.066756	-1.685471	H	2.587838	-6.439294	-1.036389
C	1.160816	4.511487	-0.587838	H	3.310422	-5.818342	0.476947
H	1.792100	4.630060	0.305985	H	1.548011	-6.168049	0.393208
C	1.016993	2.831312	2.096477	C	0.690285	-3.586211	1.168597
C	0.886544	4.060972	2.783102	H	0.595805	-2.742458	1.876536
H	0.090064	4.769485	2.505556	H	0.859935	-4.502224	1.780004
C	1.780356	4.386417	3.817676	C	-0.604772	-3.726827	0.375220
H	1.674485	5.345066	4.349661	H	-1.459593	-3.681263	1.082494
C	2.808882	3.492387	4.172895	H	-0.659613	-4.707561	-0.142189
H	3.508211	3.752005	4.983314	H	1.184302	-0.791392	0.606767
C	2.940147	2.266422	3.496162	<sup>55</sup> (Ni-H <sub>2</sub> O-X)			
H	3.739324	1.560880	3.772624	Ni	2.373520	-0.664237	-0.447511
C	2.044635	1.934551	2.464802	Fe	-0.858463	-0.014959	-0.763463
H	2.132969	0.965601	1.946824	S	0.529216	-0.926655	0.996798
C	-3.519083	0.080288	-1.401468	S	1.159386	1.071909	-1.470138
C	-2.870690	0.177437	-2.650508	P	-2.793145	-0.644315	0.436306
H	-1.777620	0.308852	-2.688927	P	-0.837604	1.935911	0.980096
C	-3.616431	0.102143	-3.840180	O	-2.341525	1.338875	-2.892965
H	-3.101409	0.177541	-4.810949	N	3.393178	-2.058955	0.777172
C	-5.011093	-0.073937	-3.790051	N	3.931934	-0.095087	-1.788360
H	-5.593916	-0.137708	-4.722588	C	-1.764247	0.794961	-2.029158
C	-5.661403	-0.169647	-2.545076	C	-3.203580	0.664455	1.696195
H	-6.753594	-0.306030	-2.500726	H	-3.806567	1.415560	1.142557
C	-4.921714	-0.090115	-1.352595	H	-3.854164	0.226079	2.480404
H	-5.438728	-0.165111	-0.382880	C	-1.956637	1.309873	2.313561
C	-3.378884	-0.814201	1.361148	H	-1.358439	0.559112	2.868733
C	-3.743506	-2.128200	0.984772	H	-2.233731	2.110103	3.030070
H	-3.604212	-2.458585	-0.056327	C	-2.577915	-2.224224	1.354537
C	-4.271437	-3.016488	1.936168	C	-2.311368	-2.262409	2.740975
H	-4.552549	-4.036470	1.629759	H	-2.285777	-1.340408	3.340005
C	-4.440667	-2.606507	3.272361	C	-2.068859	-3.493579	3.376111
H	-4.853156	-3.304871	4.017539	H	-1.861553	-3.513216	4.457631
C	-4.083025	-1.299984	3.650407	C	-2.089315	-4.690922	2.637777
H	-4.214799	-0.968924	4.692667	H	-1.894760	-5.652195	3.138895
C	-3.552754	-0.406345	2.702657	C	-2.357056	-4.654436	1.256599
H	-3.266792	0.606381	3.025072	H	-2.373735	-5.587091	0.670857
C	2.165665	1.173706	-2.109326	C	-2.597545	-3.428541	0.615120
H	2.576268	1.053324	-3.132835	H	-2.777711	-3.402529	-0.470294
H	1.934385	2.248214	-1.966705	C	-4.377022	-0.895393	-0.471896
C	3.150929	0.731368	-1.039237	C	-5.607828	-0.840815	0.223713
H	4.122250	1.259527	-1.176062	H	-5.633835	-0.647715	1.307192
H	2.751869	1.031829	-0.051064	C	-6.814964	-1.041030	-0.466472
C	3.892640	-1.314564	-2.254608	H	-7.769138	-0.992028	0.081619
H	3.099994	-1.186777	-3.020485	C	-6.805852	-1.305979	-1.848989
H	3.986245	-2.407323	-2.101666	H	-7.754393	-1.462915	-2.386548
C	5.217032	-0.742291	-2.765032	C	-5.583395	-1.374477	-2.539771
H	5.502005	-1.277774	-3.693794	H	-5.568303	-1.588997	-3.620054
H	5.142362	0.336279	-3.011605	C	-4.371512	-1.169419	-1.856202
H	6.042203	-0.877642	-2.036400	H	-3.414703	-1.244461	-2.394096
C	4.224374	-1.038973	0.202067	C	-1.629084	3.465256	0.325866
H	3.797743	-0.461733	1.048567	C	-1.265025	3.893300	-0.972427
H	5.246161	-0.633482	0.024057	H	-0.523523	3.315936	-1.548463
C	4.313628	-2.509524	0.610668	C	-1.845110	5.046170	-1.528528
H	5.112762	-2.576281	1.378210	H	-1.548800	5.372582	-2.537980
H	4.662429	-3.147679	-0.227541	C	-2.809137	5.770629	-0.804056
C	3.043969	-3.067438	1.253715	H	-3.271444	6.668582	-1.243612



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 H -3.941403 5.903981 1.053256  
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 O 1.862372 -2.254589 -1.697005  
 H 2.287113 -2.258266 -2.578289  
 H 0.866817 -2.226563 -1.903646  
<sup>55</sup>(Ni-H<sub>2</sub>O-Y)  
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 Fe -0.716413 -0.036866 -0.572590  
 S 0.692122 -0.514758 1.308988  
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C	5.117324	-0.605570	2.100983
H	6.100467	-0.724110	2.600150
H	5.134736	0.337698	1.524694
H	4.347775	-0.509224	2.893954
C	3.451786	-2.852518	-0.514023
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H	3.840614	-3.834068	-0.151816
C	4.219603	-2.442948	-1.772759
H	5.296304	-2.273168	-1.564050
H	4.194723	-3.327785	-2.443364
C	3.625272	-1.290291	-2.579010
H	4.127745	-1.243570	-3.571973
H	2.552652	-1.504668	-2.764497
C	5.063563	0.485484	-1.550021
H	5.403350	-0.181648	-0.739193
H	4.954759	1.487737	-1.091125
C	6.107685	0.515609	-2.667822
H	7.070573	0.872987	-2.248393
H	6.286698	-0.489693	-3.100731
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C	3.101741	1.060016	-2.893139
H	3.498409	0.882859	-3.918763
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C	1.577920	1.042440	-2.931895
H	1.165784	0.049926	-3.203838
H	1.207354	1.793557	-3.657962
Cl	0.045659	-2.053627	-1.820912
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Ni	-1.228533	-1.724160	0.901441
Fe	0.524717	0.048399	-0.464132
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S	0.555616	-2.315010	-0.257836
P	0.736947	2.269022	-0.475110
P	2.828751	0.038380	-0.470339
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H	4.299229	1.736675	-1.522983
C	1.082605	3.160126	1.103681
C	1.880741	2.539482	2.092205
H	2.229377	1.503861	1.965139
C	2.216805	3.227092	3.269268
H	2.835761	2.726707	4.030055
C	1.757105	4.540242	3.474722
H	2.012357	5.076484	4.402220
C	0.969325	5.166298	2.491978
H	0.609368	6.195984	2.643870
C	0.635654	4.485175	1.308442
H	0.025385	4.992571	0.546182
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H	-3.885251	4.046281	-0.560674
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C	3.767532	-0.475271	1.030533
C	3.330034	-1.587499	1.786308
H	2.434441	-2.149705	1.484384
C	4.038913	-1.994020	2.929135
H	3.684270	-2.862613	3.505653
C	5.187586	-1.292718	3.334788
H	5.738780	-1.606757	4.235056
C	5.632830	-0.189984	2.583643
H	6.536805	0.360074	2.888773
C	4.931968	0.217617	1.435826
H	5.310455	1.076500	0.862486
C	3.485648	-1.036781	-1.813762
C	3.713203	-2.411895	-1.577594
H	3.608847	-2.831709	-0.566292
C	4.090872	-3.255660	-2.636207
H	4.268335	-4.324774	-2.440321
C	4.247058	-2.738044	-3.934686
H	4.543193	-3.401316	-4.762509
C	4.028626	-1.368858	-4.171518
H	4.152960	-0.954587	-5.184340
C	3.645830	-0.519631	-3.119418
H	3.460483	0.544484	-3.330864
C	-0.949693	0.760204	2.701802
H	-0.811241	0.587428	3.788135
H	-0.687747	1.814527	2.487980
C	-2.356926	0.461672	2.234821
H	-3.101772	0.946792	2.903622
H	-2.513334	0.868840	1.218911
C	-2.393076	-1.770985	3.421211
H	-1.301354	-1.786396	3.602244
H	-2.682881	-2.819913	3.214785
C	-3.110910	-1.245454	4.665217
H	-2.838134	-1.896582	5.520597
H	-2.800629	-0.212334	4.921298
H	-4.214825	-1.267416	4.570978
C	-4.074670	-1.144238	1.721597
H	-4.290882	-0.310670	1.030404
H	-4.707070	-0.976347	2.618077
C	-4.444782	-2.458033	1.050883
H	-5.539343	-2.431899	0.871380
H	-4.267105	-3.330744	1.712686
C	-3.762304	-2.613391	-0.300507
H	-4.271010	-3.386966	-0.913721
H	-3.827605	-1.653489	-0.849769
C	-2.087514	-4.320715	0.386620
H	-2.407007	-4.246550	1.444363
H	-0.995706	-4.493526	0.419722
C	-2.784695	-5.491126	-0.305417
H	-2.473872	-6.427131	0.201743
H	-3.889327	-5.429639	-0.241971
H	-2.496044	-5.578875	-1.372572
C	-1.762718	-2.829459	-1.622786
H	-1.944993	-1.781197	-1.935493
H	-2.331417	-3.489987	-2.313685
C	-0.280905	-3.132745	-1.685681

H	0.163636	-2.758876	-2.628347	C	-5.134515	0.690330	-0.941006
H	-0.054389	-4.214614	-1.603164	H	-5.435121	1.326505	-0.094589
H	-1.099967	-0.267829	-0.339019	C	-3.436625	-1.387295	1.667536
C	-4.657961	1.428534	-2.903443	C	-3.768877	-2.646752	1.116226
H	-5.170713	2.083436	-2.172460	H	-3.799076	-2.786071	0.024863
H	-4.458466	1.981379	-3.841592	C	-4.067214	-3.732091	1.958060
H	-5.344345	0.585569	-3.137468	H	-4.325337	-4.707374	1.515655
C	-3.369757	0.844369	-2.316404	C	-4.040736	-3.574474	3.356153
O	-3.368470	0.598140	-1.054641	H	-4.274799	-4.426416	4.013843
O	-2.402997	0.589593	-3.089075	C	-3.717482	-2.322053	3.909417
H	-0.988976	0.564732	-0.638578	H	-3.697588	-2.188086	5.002664
O	-5.018573	1.969396	0.500279	C	-3.412002	-1.234158	3.072741
H	-5.881965	1.569017	0.278763	H	-3.139099	-0.268508	3.525803
H	-4.395235	1.461777	-0.117504	C	0.978749	1.149408	-2.533624
6b				H	0.991683	1.125465	-3.642152
Ni	1.212835	-1.567308	-1.111853	H	0.625227	2.152026	-2.221126
Fe	-0.552665	-0.197619	0.368687	C	2.331695	0.855362	-1.928903
S	-0.245460	-0.129254	-1.998760	H	3.121568	1.488613	-2.385868
S	-0.674376	-2.436680	-0.338915	H	2.314588	1.087997	-0.846796
P	-0.581485	1.965274	0.781578	C	2.706992	-1.111373	-3.449762
P	-2.815419	-0.039411	0.573701	H	1.662721	-1.086574	-3.815003
O	-0.253257	-0.891817	3.166520	H	2.980449	-2.182684	-3.392893
N	2.702261	-0.598777	-2.031713	C	3.624465	-0.377780	-4.429394
N	2.218372	-3.057040	-0.234292	H	3.516165	-0.849061	-5.427601
C	-0.390182	-0.580381	2.035961	H	3.353220	0.692186	-4.535495
C	-1.936996	2.178534	2.061464	H	4.694229	-0.442097	-4.146355
H	-1.624674	1.641866	2.980436	C	4.045744	-0.742474	-1.394889
H	-2.066186	3.252771	2.305013	H	4.011591	-0.149719	-0.462786
C	-3.214610	1.571228	1.461717	H	4.802163	-0.257565	-2.047622
H	-3.628185	2.256659	0.694257	C	4.457738	-2.166589	-1.050140
H	-4.003434	1.413110	2.223620	H	5.513660	-2.126329	-0.711527
C	-1.229055	3.157649	-0.491359	H	4.450767	-2.836308	-1.934692
C	-1.970855	2.690962	-1.597011	C	3.638252	-2.735531	0.100898
H	-2.054007	1.610165	-1.785707	H	4.121953	-3.647883	0.510563
C	-2.600248	3.594009	-2.471478	H	3.604145	-1.993130	0.921957
H	-3.175267	3.207451	-3.327488	C	2.119022	-4.215625	-1.196158
C	-2.494822	4.977952	-2.250394	H	2.586685	-3.881178	-2.142183
H	-2.984407	5.687803	-2.935727	H	1.046484	-4.355207	-1.428407
C	-1.762690	5.453463	-1.145882	C	2.733950	-5.536934	-0.734125
H	-1.679704	6.536369	-0.961860	H	2.548775	-6.298500	-1.518944
C	-1.139020	4.551807	-0.267193	H	3.830707	-5.471919	-0.587676
H	-0.583617	4.940718	0.600523	H	2.274453	-5.908481	0.204241
C	0.901072	2.812689	1.460229	C	1.516408	-3.318684	1.071738
C	1.189622	2.760561	2.842312	H	1.638992	-2.399382	1.672696
H	0.526421	2.215647	3.531775	H	2.022771	-4.145388	1.617992
C	2.335921	3.400140	3.346664	C	0.041571	-3.612111	0.892188
H	2.552868	3.354530	4.425246	H	-0.501621	-3.497897	1.851573
C	3.201489	4.093480	2.480884	H	-0.150248	-4.634022	0.507378
H	4.096575	4.594637	2.881418	H	1.020158	-0.335149	0.287780
C	2.931446	4.126180	1.101694	C	4.424007	0.676039	3.516881
H	3.622947	4.627359	0.408752	H	5.125427	1.529106	3.505877
C	1.794403	3.479687	0.590637	H	3.742535	0.739092	4.386352
H	1.597832	3.504021	-0.492870	H	5.002604	-0.268180	3.607824
C	-3.956146	-0.088130	-0.876849	C	3.650294	0.632243	2.228650
C	-3.613608	-0.910021	-1.974961	O	3.988748	1.210942	1.196835
H	-2.702010	-1.524618	-1.937158	O	2.560878	-0.146855	2.299968
C	-4.429702	-0.947190	-3.118998	H	2.044649	-0.128555	1.432398
H	-4.149587	-1.592265	-3.966725	O	4.832117	2.692970	-1.057256
C	-5.591445	-0.157506	-3.182948	H	5.474271	3.307657	-0.651512
H	-6.225772	-0.177959	-4.083187	H	4.506811	2.191762	-0.273739
C	-5.942935	0.657081	-2.090282	<sup>71</sup>			
H	-6.856260	1.271634	-2.129853	Ni	2.611405	0.048767	-0.080602

Fe	-0.493550	-0.041902	-0.570670	C	2.769518	-2.352145	1.771641
S	0.923250	-0.362249	1.500128	H	3.018830	-3.436054	1.850047
S	1.271389	1.737542	-1.032947	H	3.047204	-1.883825	2.735747
P	-2.496962	-1.196768	0.399958	C	4.959879	-1.461762	1.295568
P	-1.500078	1.849261	0.950809	H	5.705806	-1.404570	0.481919
O	-1.769496	0.916566	-3.294225	H	5.262371	-2.337964	1.914679
N	3.616370	-1.737906	0.696773	C	4.989607	-0.176271	2.116856
N	3.887424	0.254290	-1.824117	H	6.001744	-0.022310	2.542676
C	-1.451696	0.697497	-2.206732	H	4.749352	0.709317	1.488604
C	-3.453186	-0.055798	1.520456	H	4.265444	-0.198772	2.955851
H	-4.188069	0.452561	0.861006	C	3.698652	-2.700803	-0.444280
H	-4.030692	-0.640682	2.265602	H	2.653039	-2.924805	-0.740844
C	-2.534830	0.964085	2.208071	H	4.150014	-3.650548	-0.071830
H	-1.810275	0.447408	2.870535	C	4.470865	-2.240012	-1.682524
H	-3.107031	1.677806	2.836025	H	5.538400	-2.046706	-1.448314
C	-2.040626	-2.660410	1.412793	H	4.485117	-3.114070	-2.367417
C	-2.001465	-2.630944	2.824206	C	3.870675	-1.086133	-2.485457
H	-2.326695	-1.740001	3.381910	H	4.399764	-1.016532	-3.463052
C	-1.531838	-3.748640	3.538503	H	2.807658	-1.312844	-2.709132
H	-1.504503	-3.715890	4.639192	C	5.248420	0.700069	-1.391225
C	-1.096474	-4.898614	2.855506	H	5.603097	0.010252	-0.608779
H	-0.725417	-5.769103	3.418946	H	5.104162	1.680709	-0.893457
C	-1.135857	-4.931162	1.448235	C	6.308031	0.801110	-2.491214
H	-0.795493	-5.827113	0.905386	H	7.257383	1.159014	-2.042647
C	-1.601912	-3.819149	0.729680	H	6.513994	-0.182715	-2.959983
H	-1.607237	-3.841673	-0.371942	H	6.025775	1.514736	-3.291427
C	-3.772402	-1.862537	-0.751154	C	3.326998	1.270982	-2.772755
C	-5.093830	-2.112779	-0.313657	H	3.683478	1.057878	-3.805714
H	-5.383338	-1.915535	0.730438	H	3.732053	2.260631	-2.481068
C	-6.046810	-2.623699	-1.210654	C	1.809047	1.338528	-2.753742
H	-7.074929	-2.813345	-0.863586	H	1.344498	0.379473	-3.060050
C	-5.689878	-2.896117	-2.545375	H	1.457205	2.131333	-3.443881
H	-6.439608	-3.298057	-3.245168	Cl	0.230421	-1.853060	-1.860077
C	-4.375058	-2.656235	-2.981950				
H	-4.089444	-2.870236	-4.024019	Ni	1.656748	-1.305373	-0.732800
C	-3.418607	-2.137430	-2.090291	Fe	-0.235001	-0.229461	0.259780
H	-2.386891	-1.957495	-2.430720	S	0.338205	0.176471	-2.126292
C	-2.620356	3.004164	0.061167	S	-0.348922	-2.612748	-0.508188
C	-2.164688	3.545243	-1.165685	P	-0.406953	2.182914	0.918796
H	-1.156878	3.291253	-1.534733	P	-2.731530	0.023549	0.130525
C	-2.984534	4.409738	-1.910332	O	-0.069732	-0.927482	3.279143
H	-2.615218	4.827825	-2.859919	N	3.323856	-0.152454	-1.292745
C	-4.274129	4.729833	-1.448262	N	2.641901	-2.871031	0.285943
H	-4.921759	5.399260	-2.036072	C	-0.392336	-0.574229	2.217885
C	-4.735711	4.189640	-0.233693	C	-2.112350	2.361159	1.662778
H	-5.744359	4.437120	0.133319	H	-2.020838	1.867531	2.654159
C	-3.914709	3.334695	0.522738	H	-2.343896	3.431246	1.839608
H	-4.293810	2.931731	1.474050	C	-3.215142	1.702774	0.814408
C	-0.354854	2.918955	1.911098	H	-3.448034	2.329684	-0.070005
C	0.118175	2.517114	3.183466	H	-4.153020	1.610971	1.399629
H	-0.257176	1.600427	3.660232	C	-0.266810	3.457945	-0.392919
C	1.085036	3.284675	3.856149	C	-1.103578	3.357313	-1.533022
H	1.439149	2.960401	4.847558	H	-1.860120	2.562001	-1.607291
C	1.596278	4.457414	3.271432	C	-0.941092	4.242228	-2.610524
H	2.355479	5.055434	3.799702	H	-1.598512	4.152001	-3.489527
C	1.126979	4.864635	2.008924	C	0.069871	5.222227	-2.580075
H	1.513882	5.784985	1.543562	H	0.203242	5.905658	-3.433257
C	0.161748	4.102184	1.330958	C	0.913391	5.317030	-1.458863
H	-0.188858	4.438482	0.344102	H	1.711266	6.075857	-1.429475
C	1.279097	-2.169886	1.558566	C	0.748089	4.442468	-0.369573
H	0.720383	-2.628507	2.397751	H	1.422129	4.521973	0.497075
H	0.925668	-2.632153	0.617115	C	0.737637	2.708891	2.252293

C	0.498598	3.848405	3.054795	H	1.519445	-2.471899	1.997833
H	-0.398945	4.465474	2.890935	H	2.108509	-4.154846	1.924550
C	1.415263	4.201572	4.060014	C	0.319269	-3.779505	0.762252
H	1.225518	5.088199	4.685350	H	-0.402665	-3.860537	1.600614
C	2.574068	3.427941	4.266353	H	0.386952	-4.778942	0.285516
H	3.290474	3.710635	5.053769	H	1.496909	-0.487132	0.691977
C	2.815056	2.294060	3.469485	<sup>75</sup> (Ni-H2O-X)			
H	3.717782	1.683654	3.629446	Ni	2.323768	-0.656712	-0.481260
C	1.898324	1.931825	2.467532	Fe	-0.782731	0.007688	-0.916017
H	2.065765	1.030901	1.850591	S	0.493295	-1.001794	0.956797
C	-3.680131	-0.140324	-1.434985	S	1.249643	1.101227	-1.735186
C	-3.102509	-0.872991	-2.495363	P	-2.911789	-0.644933	0.444283
H	-2.102111	-1.315489	-2.371357	P	-0.751487	1.860610	0.919955
C	-3.801122	-1.037783	-3.704729	O	-3.040296	1.482716	-2.512291
H	-3.343159	-1.611503	-4.525773	N	3.375750	-2.054719	0.862662
C	-5.075595	-0.465766	-3.865559	N	4.029259	-0.144236	-1.733058
H	-5.620056	-0.589158	-4.815034	C	-2.158925	0.995484	-1.942081
C	-5.656198	0.264793	-2.810958	C	-3.184261	0.679207	1.715641
H	-6.656693	0.709347	-2.932205	H	-3.753647	1.469391	1.179871
C	-4.966563	0.424137	-1.597045	H	-3.830095	0.309327	2.538952
H	-5.438771	0.984876	-0.775312	C	-1.866910	1.241628	2.270944
C	-3.496189	-1.214018	1.251871	H	-1.285332	0.447850	2.783051
C	-3.871519	-2.479770	0.744518	H	-2.064973	2.040434	3.015101
H	-3.813255	-2.680754	-0.336674	C	-2.646926	-2.233454	1.330826
C	-4.316883	-3.487800	1.615766	C	-2.495619	-2.316233	2.731968
H	-4.611774	-4.467556	1.207601	H	-2.589966	-1.421767	3.365796
C	-4.385860	-3.249853	3.001896	C	-2.217630	-3.556048	3.336723
H	-4.732990	-4.042732	3.682928	H	-2.099412	-3.610496	4.430592
C	-4.009743	-1.994269	3.512121	C	-2.094748	-4.718499	2.554287
H	-4.061338	-1.798435	4.594908	H	-1.877078	-5.686280	3.032860
C	-3.563622	-0.980208	2.645563	C	-2.240258	-4.636555	1.156346
H	-3.264058	-0.008704	3.068050	H	-2.133114	-5.539642	0.534833
C	1.680781	1.420916	-2.377939	C	-2.505197	-3.400920	0.544722
H	2.031748	1.319327	-3.425304	H	-2.574622	-3.334804	-0.552307
H	1.260944	2.440424	-2.275161	C	-4.543774	-0.864688	-0.376727
C	2.817178	1.249736	-1.383098	C	-5.763560	-0.545494	0.262631
H	3.649606	1.944672	-1.640201	H	-5.773943	-0.146837	1.288726
H	2.461096	1.523837	-0.369472	C	-6.981905	-0.745770	-0.409583
C	3.763175	-0.698652	-2.615019	H	-7.928711	-0.495132	0.094773
H	2.859626	-0.764112	-3.254589	C	-6.994717	-1.268861	-1.716280
H	4.078993	-1.745045	-2.442222	H	-7.952247	-1.426036	-2.237637
C	4.871607	0.069802	-3.336760	C	-5.782713	-1.586965	-2.355548
H	5.101477	-0.446897	-4.291020	H	-5.786163	-1.991086	-3.380264
H	4.572601	1.108599	-3.583883	C	-4.560148	-1.380359	-1.693267
H	5.809121	0.108214	-2.745523	H	-3.608238	-1.614135	-2.198181
C	4.392042	-0.195253	-0.256201	C	-1.525112	3.428779	0.326562
H	3.981641	0.325998	0.633476	C	-1.171405	3.887404	-0.963955
H	5.264295	0.404213	-0.602079	H	-0.459457	3.305503	-1.572890
C	4.858028	-1.590732	0.159509	C	-1.728387	5.072098	-1.475066
H	5.755771	-1.446839	0.796282	H	-1.441418	5.420354	-2.479926
H	5.211372	-2.180231	-0.711934	C	-2.658509	5.800604	-0.711369
C	3.852763	-2.376436	1.000383	H	-3.103895	6.723445	-1.115441
H	4.363961	-3.232819	1.495299	C	-3.022217	5.344075	0.569114
H	3.479658	-1.716778	1.811120	H	-3.751673	5.909365	1.170740
C	2.939567	-3.915831	-0.742078	C	-2.456064	4.167308	1.090842
H	3.659815	-3.471095	-1.455658	H	-2.747118	3.833216	2.098518
H	2.004774	-4.073420	-1.318262	C	0.765928	2.439168	1.795420
C	3.474977	-5.252704	-0.224780	C	0.985532	2.219749	3.174399
H	3.676426	-5.914701	-1.091655	H	0.235155	1.706405	3.792899
H	4.426049	-5.137274	0.333982	C	2.177640	2.656460	3.779541
H	2.746586	-5.773426	0.429256	H	2.334383	2.477865	4.855049
C	1.666557	-3.330893	1.318296	C	3.167428	3.304683	3.020586

H	4.103220	3.635529	3.497731
C	2.958102	3.519787	1.645668
H	3.727953	4.021854	1.038503
C	1.766375	3.093921	1.037026
H	1.617634	3.266775	-0.039640
C	0.909002	-2.792804	1.069849
H	0.228705	-3.274813	1.800823
H	0.750084	-3.272613	0.086974
C	2.351090	-2.917722	1.569206
H	2.674736	-3.980120	1.512485
H	2.363994	-2.644342	2.642550
C	4.193110	-1.338142	1.893168
H	5.114994	-0.973421	1.403119
H	4.525232	-2.078102	2.658844
C	3.484654	-0.158250	2.543038
H	4.163318	0.324682	3.274401
H	3.202355	0.605495	1.787530
H	2.556649	-0.452541	3.070103
C	4.261109	-2.915444	0.018785
H	3.598645	-3.508264	-0.640231
H	4.792764	-3.632621	0.688081
C	5.310345	-2.189923	-0.833945
H	5.993618	-1.584820	-0.202802
H	5.954582	-2.988351	-1.259620
C	4.828451	-1.369969	-2.032075
H	5.715363	-1.086402	-2.642873
H	4.206714	-2.011690	-2.689213
C	4.761257	0.860262	-0.891652
H	4.877432	0.437462	0.122904
H	4.070291	1.720935	-0.780940
C	6.125414	1.313904	-1.413633
H	6.508914	2.124419	-0.760553
H	6.870241	0.492413	-1.398776
H	6.069614	1.712968	-2.447450
C	3.581590	0.490568	-3.030218
H	4.089266	-0.007168	-3.882973
H	3.916852	1.546604	-3.038232
C	2.068098	0.466373	-3.259915
H	1.682375	-0.546360	-3.485180
H	1.816747	1.120610	-4.119378
Cl	-0.987606	-1.929076	-2.414910
O	1.857622	-2.302745	-1.719496
H	2.309946	-2.284145	-2.588036
H	0.875784	-2.223920	-1.962221
<sup>75</sup> (Ni-H <sub>2</sub> O-Y)			
Ni	2.540067	-0.025551	-0.131074
Fe	-0.681648	-0.059482	-0.685595
S	0.768120	-0.525870	1.340512
S	1.119589	1.587875	-1.205382
P	-2.669828	-1.087871	0.441555
P	-1.396415	1.869915	0.977174
O	-2.195232	0.920648	-3.232871
N	3.477046	-1.954953	0.585150
N	3.795615	0.118699	-1.879055
C	-1.804424	0.701591	-2.165285
C	-3.453387	0.110919	1.634624
H	-4.172134	0.701166	1.027178
H	-4.041521	-0.431180	2.403436
C	-2.408481	1.031256	2.285489
H	-1.685720	0.437740	2.882215
H	-2.880019	1.768292	2.967981
C	-2.260170	-2.596184	1.407851

C	-2.175808	-2.602554	2.817509
H	-2.437888	-1.709238	3.404180
C	-1.743892	-3.759475	3.492187
H	-1.679964	-3.753495	4.591877
C	-1.394810	-4.915550	2.770901
H	-1.055085	-5.817937	3.303129
C	-1.477809	-4.911999	1.365202
H	-1.201361	-5.811268	0.792239
C	-1.901090	-3.758937	0.685971
H	-1.932697	-3.753860	-0.415412
C	-4.055114	-1.637566	-0.641282
C	-5.392560	-1.692644	-0.186311
H	-5.645123	-1.410011	0.847616
C	-6.413346	-2.116763	-1.054547
H	-7.454000	-2.153674	-0.695057
C	-6.109108	-2.497607	-2.375519
H	-6.912550	-2.830146	-3.051751
C	-4.778627	-2.452749	-2.829257
H	-4.534465	-2.750521	-3.861312
C	-3.754491	-2.019325	-1.968469
H	-2.710992	-1.981061	-2.321699
C	-2.475427	3.150174	0.218105
C	-2.098751	3.652303	-1.051227
H	-1.170397	3.292367	-1.525922
C	-2.897178	4.607659	-1.702680
H	-2.589434	4.995546	-2.686537
C	-4.089219	5.055757	-1.104870
H	-4.720726	5.797271	-1.619207
C	-4.475107	4.551349	0.151006
H	-5.408440	4.897941	0.622404
C	-3.672842	3.606260	0.814567
H	-3.988787	3.229460	1.799385
C	-0.069488	2.788847	1.859533
C	0.451884	2.316973	3.087883
H	-0.004264	1.456686	3.597308
C	1.573053	2.934488	3.670457
H	1.964250	2.552180	4.626442
C	2.192372	4.028209	3.039008
H	3.075340	4.504229	3.493157
C	1.672637	4.511163	1.823207
H	2.143690	5.371181	1.321845
C	0.554489	3.896102	1.234554
H	0.170884	4.285477	0.279939
C	1.105683	-2.330328	1.405463
H	0.533033	-2.783425	2.238629
H	0.756226	-2.791400	0.461309
C	2.591423	-2.533214	1.645702
H	2.813041	-3.623586	1.742150
H	2.862622	-2.057627	2.608633
C	4.866532	-1.934436	1.142531
H	5.580226	-1.878085	0.299283
H	5.057319	-2.919062	1.632247
C	5.141499	-0.789349	2.109850
H	6.137344	-0.931050	2.576849
H	5.140717	0.182803	1.583209
H	4.391964	-0.735824	2.925563
C	3.413642	-2.855385	-0.606738
H	2.344533	-2.939200	-0.890910
H	3.755478	-3.872667	-0.298435
C	4.204903	-2.417487	-1.839861
H	5.287672	-2.314746	-1.619384
H	4.138869	-3.262118	-2.557817

C	3.674657	-1.194257	-2.584442
H	4.185974	-1.122542	-3.571675
H	2.594355	-1.343802	-2.788863
C	5.186534	0.444961	-1.440848
H	5.470880	-0.275733	-0.655747
H	5.122209	1.429923	-0.937887
C	6.258206	0.468205	-2.532969
H	7.230175	0.742382	-2.073640
H	6.386638	-0.522741	-3.014334
H	6.041188	1.213546	-3.324777
C	3.299123	1.193638	-2.795025
H	3.731163	1.050311	-3.811942
H	3.676993	2.160746	-2.405262
C	1.780335	1.256665	-2.888107
H	1.336770	0.312481	-3.264829
H	1.484233	2.075911	-3.574121
Cl	-0.010032	-1.856857	-2.013718
O	3.349011	1.555397	1.014894
H	3.049276	1.412014	1.941156
H	2.790410	2.313288	0.719068
7a			
Ni	-1.164637	2.174756	-0.162682
Fe	-0.323558	-1.008803	-0.514412
S	-0.389314	0.627812	1.218493
S	-1.957689	0.479339	-1.245962
P	1.055616	-2.443498	0.567610
P	-2.029606	-2.186068	0.399738
O	-0.244837	-2.688810	-2.891474
N	-0.157383	3.605785	0.941059
N	-1.898221	3.389852	-1.675365
C	-0.310216	-2.027867	-1.928156
C	0.035433	-3.700840	1.496042
H	0.580742	-4.663741	1.544992
H	-0.026495	-3.327247	2.535129
C	-1.354632	-3.848896	0.879972
H	-2.065231	-4.366410	1.556268
H	-1.315175	-4.410415	-0.077760
C	2.151800	-1.732258	1.863542
C	1.566641	-1.323566	3.087624
H	0.493520	-1.477078	3.280519
C	2.343913	-0.675473	4.061191
H	1.874397	-0.356387	5.004539
C	3.707586	-0.420157	3.824101
H	4.313757	0.099281	4.582500
C	4.290901	-0.825113	2.609997
H	5.351961	-0.620805	2.398576
C	3.519298	-1.480093	1.632685
H	4.000496	-1.761246	0.686488
C	2.110930	-3.378379	-0.617297
C	1.984469	-4.776198	-0.773990
H	1.297864	-5.359696	-0.143203
C	2.735148	-5.447054	-1.756309
H	2.624376	-6.536811	-1.871255
C	3.618355	-4.733497	-2.584914
H	4.206788	-5.262702	-3.351031
C	3.740123	-3.339676	-2.435525
H	4.427321	-2.770261	-3.081334
C	2.982116	-2.657315	-1.469947
H	3.079445	-1.559303	-1.382009
C	-3.519789	-2.591678	-0.600924
C	-3.582427	-2.378859	-1.993709
H	-2.744294	-1.913760	-2.530594

C	-4.732302	-2.750818	-2.712271
H	-4.773293	-2.575069	-3.798545
C	-5.823913	-3.336394	-2.047154
H	-6.724656	-3.623529	-2.612244
C	-5.766024	-3.550296	-0.657246
H	-6.618515	-4.007066	-0.130508
C	-4.621314	-3.177314	0.065894
H	-4.586478	-3.338552	1.155383
C	-2.733029	-1.379046	1.893889
C	-2.342391	-1.735181	3.202220
H	-1.701521	-2.609820	3.384033
C	-2.773238	-0.967159	4.298893
H	-2.461103	-1.253012	5.315560
C	-3.593891	0.157477	4.100691
H	-3.919127	0.762515	4.961432
C	-4.005449	0.501732	2.799999
H	-4.656516	1.374264	2.636129
C	-3.580008	-0.260971	1.701442
H	-3.900933	0.023239	0.687228
C	1.210838	1.535720	1.340359
H	1.869242	1.018351	2.062762
H	1.720415	1.549224	0.361235
C	0.840159	2.912885	1.846420
H	1.747853	3.545999	1.943274
H	0.393602	2.825445	2.855659
C	-1.093207	4.410321	1.797562
H	-1.567668	5.177499	1.159123
H	-0.484983	4.964992	2.547183
C	-2.171419	3.565257	2.468833
H	-2.813061	4.213382	3.099514
H	-2.813898	3.069316	1.711028
H	-1.748368	2.768554	3.112787
C	0.617985	4.481674	0.002925
H	1.385148	3.834082	-0.470016
H	1.157021	5.241610	0.613176
C	-0.183912	5.193629	-1.084760
H	-0.938021	5.882203	-0.650169
H	0.536817	5.851082	-1.614523
C	-0.808626	4.300004	-2.150249
H	-1.209405	4.934972	-2.970078
H	-0.029013	3.655108	-2.600342
C	-3.081549	4.122590	-1.104033
H	-2.755725	4.628459	-0.179519
H	-3.798722	3.336781	-0.793360
C	-3.750415	5.137975	-2.031407
H	-4.646390	5.544078	-1.519072
H	-3.084593	5.993316	-2.263902
H	-4.086393	4.685104	-2.986090
C	-2.359746	2.549071	-2.850786
H	-2.215246	3.113384	-3.795732
H	-3.447551	2.374168	-2.734230
C	-1.644212	1.210762	-2.908485
H	-0.553397	1.308563	-3.067833
H	-2.075657	0.548617	-3.686597
H	1.151946	-0.387642	-0.770603
H	0.625713	0.000937	-1.343509
O	1.578292	1.866450	-2.400977
H	0.935651	2.117703	-1.706118
H	2.283085	1.343450	-1.853798
P	4.572176	1.152820	-0.582977
O	3.207443	0.474480	-1.001375
O	4.965043	2.330035	-1.515469

O	4.282001	1.935574	0.894287	H	-3.645377	0.459921	5.462662
O	5.677828	0.082802	-0.326261	C	-3.560998	0.901829	3.329128
H	4.072868	1.257723	1.573023	H	-3.716453	1.984524	3.460161
O	7.643944	1.883145	-1.076282	C	-3.384177	0.376224	2.040497
H	6.791494	2.296348	-1.389204	H	-3.394825	1.053792	1.169973
H	7.209103	1.064462	-0.712769	C	1.476706	0.745031	1.426836
7b				H	1.848365	-0.042288	2.106454
Ni	-0.396121	2.378390	-0.035785	H	2.010089	0.656935	0.467678
Fe	-0.853411	-0.819732	-0.712785	C	1.625286	2.104332	2.074999
S	-0.327109	0.525783	1.159217	H	2.694045	2.331401	2.272836
S	-1.774986	1.235909	-1.259616	H	1.106415	2.094049	3.052884
P	0.052685	-2.690974	0.029839	C	0.417193	4.223185	2.155701
P	-2.799049	-1.561568	0.136245	H	0.302978	5.171331	1.598513
O	-1.196984	-1.874719	-3.389655	H	1.147750	4.431356	2.970307
N	1.026480	3.207846	1.231659	C	-0.933270	3.792627	2.721748
N	-0.537260	3.923527	-1.401374	H	-1.315354	4.576711	3.406742
C	-1.092713	-1.471781	-2.283866	H	-1.674370	3.642176	1.908316
C	-1.292219	-3.887777	0.601335	H	-0.869064	2.841315	3.286822
H	-1.068148	-4.904722	0.223409	C	2.134076	3.812219	0.424255
H	-1.229378	-3.928812	1.706622	H	2.681804	2.973138	-0.056362
C	-2.679062	-3.421829	0.141724	H	2.854885	4.286621	1.129308
H	-3.496354	-3.872768	0.741676	C	1.725033	4.841129	-0.629047
H	-2.854068	-3.689204	-0.922197	H	1.272158	5.736487	-0.154860
C	1.171542	-2.560174	1.495809	H	2.668347	5.202803	-1.089029
C	0.623816	-2.248949	2.763070	C	0.850425	4.341864	-1.775131
H	-0.466333	-2.156523	2.892135	H	0.788209	5.134632	-2.552732
C	1.469757	-2.014669	3.860537	H	1.320738	3.463888	-2.262193
H	1.031910	-1.765715	4.839842	C	-1.343005	5.024459	-0.770394
C	2.868433	-2.080870	3.706627	H	-0.890899	5.264142	0.206624
H	3.529432	-1.884802	4.565205	H	-2.334679	4.580805	-0.550864
C	3.417738	-2.393835	2.448688	C	-1.487127	6.304691	-1.594841
H	4.510096	-2.448653	2.308924	H	-2.156591	7.001691	-1.050494
C	2.573529	-2.633057	1.348305	H	-0.516206	6.820605	-1.737941
H	3.020894	-2.850913	0.368178	H	-1.935066	6.119734	-2.592220
C	1.114135	-3.628198	-1.159486	C	-1.248390	3.453620	-2.655598
C	1.390143	-5.000093	-0.956923	H	-0.847733	3.994601	-3.538769
H	0.937315	-5.543291	-0.112441	H	-2.317409	3.727536	-2.559209
C	2.266122	-5.681388	-1.818600	C	-1.137741	1.951318	-2.839009
H	2.471505	-6.750782	-1.652636	H	-0.095638	1.618025	-2.999285
C	2.885962	-4.998871	-2.882379	H	-1.765003	1.597343	-3.682685
H	3.575509	-5.534133	-3.554235	H	0.557606	-0.494233	-1.147409
C	2.627791	-3.631132	-3.079349	H	1.285607	0.438725	-1.830590
H	3.117721	-3.086489	-3.901703	O	2.060277	1.019101	-2.120643
C	1.745686	-2.948564	-2.223599	H	1.954546	1.771351	-1.498136
H	1.558407	-1.874957	-2.368798	H	3.153809	0.064056	-1.373458
C	-4.400850	-1.254029	-0.731780	P	5.007048	0.088622	-0.142061
C	-4.411199	-0.884664	-2.094245	O	3.738230	-0.624346	-0.905918
H	-3.464357	-0.748566	-2.636179	O	5.342114	1.430283	-0.813909
C	-5.630639	-0.685012	-2.765621	O	4.435340	0.516148	1.364983
H	-5.626208	-0.393568	-3.827836	O	6.076875	-1.000785	0.027724
C	-6.848762	-0.849440	-2.081835	H	4.120461	-0.280501	1.849527
H	-7.803327	-0.687388	-2.607213	O	8.095103	0.877973	-0.578618
C	-6.845134	-1.218218	-0.723297	H	7.257994	1.363843	-0.791047
H	-7.796241	-1.349688	-0.183252	H	7.665172	0.027355	-0.307609
C	-5.628102	-1.418475	-0.049572	8a			
H	-5.633018	-1.702146	1.015188	Ni	2.315705	-0.548064	0.157084
C	-3.172906	-1.011361	1.852520	Fe	-0.789428	0.236889	-0.691851
C	-3.141249	-1.862902	2.976082	S	0.400446	-0.449216	1.251601
H	-2.985672	-2.945848	2.857714	S	1.388229	0.919268	-1.128014
C	-3.310382	-1.330740	4.269313	P	-2.847504	-0.254690	0.120329
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H	-4.747557	1.299299	0.315223	C	3.436415	-3.220018	0.676104
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H	-4.304217	-2.535722	-4.113181	O	0.905492	-3.208682	-1.909165
C	-3.663882	-1.552337	-2.285894	H	1.464017	-3.962437	-1.632347
H	-2.620615	-1.475991	-2.621813	H	1.197390	-3.037399	-2.859480
C	-0.530133	3.800361	-0.797102	O	-1.597229	-3.755474	-1.030325
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H	0.649298	4.852853	-3.846815	H	1.330391	-1.952610	-4.752355
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C	-0.470616	2.600700	1.812588	P	-2.774390	-0.447236	0.091872
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C	0.682017	2.853723	4.375125	C	-1.420265	0.383276	-2.323121
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H	3.737707	2.231044	-3.251039	H	-2.401492	-1.749077	-2.595131
C	4.487357	1.245438	0.842152	C	-2.114971	3.289707	0.372543
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C	5.156382	-0.112268	1.040534	C	-2.114876	5.018186	-1.358765
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P	-1.380407	1.735817	1.034029	H	5.521115	-1.029949	0.586000
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C	1.215199	-4.910803	-1.373488	C	-6.027523	0.899132	2.684680
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C	1.635024	-3.782237	-0.651050	H	-6.325212	-0.073025	3.127122
H	1.651629	-3.814048	0.449289	H	-5.649658	1.552657	3.496477
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C	4.965946	-2.081522	0.535035	H	-3.358577	0.852872	3.935309
H	5.321302	-1.872228	-0.485994	H	-3.349111	2.112370	2.662937
C	5.854872	-2.628546	1.476112	C	-1.508031	1.009062	2.800053
H	6.898216	-2.831071	1.186551	H	-1.098273	0.008715	3.044792
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C	4.080148	-2.662171	3.143984	H	-0.860961	-1.501834	1.416437
H	3.729386	-2.891797	4.162640	OH			
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C	2.383817	3.087388	-0.095757	TS-23			
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Fe	-0.649353	0.144082	-0.349260	C	2.713083	-2.371485	1.597082
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S	1.127970	1.518158	-0.864372	H	2.997105	-1.894930	2.554655
P	-2.330654	-1.246479	0.250136	C	4.866498	-1.402368	1.072468
P	-1.589802	1.718097	0.887788	H	5.590629	-1.318405	0.242633
O	-2.159804	0.889952	-2.727297	H	5.195804	-2.281713	1.670129
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C	-3.574329	-0.188190	1.149473	H	4.184752	-0.194208	2.777360
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C	-1.954926	-2.664910	1.357311	H	4.321920	-3.047303	-2.608692
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H	-1.595983	-3.502102	4.670066	C	4.980404	0.779364	-1.565135
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H	-0.866137	-5.670173	3.630779	H	4.816212	1.729829	-1.020318
C	-1.165513	-4.964077	1.591433	C	5.944560	0.978063	-2.735532
H	-0.852175	-5.913187	1.129177	H	6.898942	1.377494	-2.335972
C	-1.554265	-3.889379	0.775546	H	6.174480	0.024999	-3.253282
H	-1.535732	-4.000978	-0.320330	H	5.566214	1.702385	-3.484337
C	-3.278573	-2.049383	-1.107700	C	2.947235	1.302711	-2.808997
C	-4.613665	-2.458450	-0.886853	H	3.247408	1.132504	-3.864511
H	-5.100028	-2.281691	0.084976	H	3.329660	2.297949	-2.507891
C	-5.328233	-3.102998	-1.910168	C	1.440370	1.287003	-2.672892
H	-6.370147	-3.413433	-1.733974	H	0.985147	0.333279	-3.001884
C	-4.715932	-3.354778	-3.152534	H	0.969318	2.121101	-3.230705
H	-5.279079	-3.862287	-3.951475	H	0.146782	-1.882163	-1.693190
C	-3.384769	-2.959088	-3.371543	H	0.801030	-1.499377	-1.461409
H	-2.898815	-3.155545	-4.340006	TS-4a4b			
C	-2.668124	-2.305430	-2.353929	Ni	-1.461056	-1.840987	0.568553
H	-1.627696	-1.993525	-2.534274	Fe	0.800455	0.162988	-0.632367
C	-2.460463	3.023322	-0.072694	S	0.187172	-0.702410	1.513247
C	-1.806185	3.625188	-1.173813	S	-0.064661	-1.949254	-1.082336
H	-0.792904	3.303707	-1.461396	P	1.758429	2.057049	0.084518
C	-2.445018	4.629746	-1.916399	P	2.882752	-0.716760	-0.612197
H	-1.921180	5.092646	-2.766973	O	1.102051	0.935630	-3.419968
C	-3.750361	5.032810	-1.580517	N	-2.674465	-1.430773	2.199404
H	-4.255113	5.815320	-2.168424	N	-2.895590	-2.710279	-0.639950
C	-4.410612	4.429581	-0.495921	C	1.005427	0.619764	-2.294389
H	-5.434563	4.735776	-0.230640	C	3.631430	1.930855	-0.083732
C	-3.771240	3.431290	0.260049	H	4.003148	2.865777	-0.547124
H	-4.307948	2.979960	1.106905	H	4.044475	1.884632	0.942482
C	-0.442400	2.607423	2.018521	C	4.037637	0.706866	-0.909408
C	-0.100250	2.043097	3.270192	H	5.087779	0.399481	-0.727118
H	-0.559990	1.104215	3.612161	H	3.929816	0.904546	-1.997049
C	0.844646	2.675394	4.094750	C	1.487678	2.482297	1.853050
H	1.097019	2.229383	5.069347	C	2.148182	1.732571	2.853903
C	1.468010	3.864683	3.676215	H	2.855363	0.934221	2.580676
H	2.213549	4.354396	4.322153	C	1.882137	1.982779	4.210202
C	1.133694	4.428016	2.431475	H	2.400423	1.393703	4.982832
H	1.612074	5.362338	2.098764	C	0.949577	2.971912	4.577920
C	0.183812	3.805793	1.604546	H	0.738913	3.163140	5.641829
H	-0.067959	4.268785	0.639565	C	0.281181	3.708148	3.582687
C	1.221568	-2.226905	1.400131	H	-0.457995	4.475403	3.861463
H	0.673423	-2.648488	2.264336	C	0.544442	3.465177	2.223516
H	0.855186	-2.706808	0.474759	H	-0.002251	4.031775	1.456133

C	1.303788	3.609835	-0.797941	C	-2.350050	-2.934883	-2.030956
C	2.024449	4.796437	-0.519623	H	-3.189211	-2.954940	-2.759053
H	2.843417	4.790678	0.217983	H	-1.870880	-3.934543	-2.041334
C	1.688486	5.994708	-1.168432	C	-1.336143	-1.878900	-2.415295
H	2.253524	6.913237	-0.944963	H	-1.762121	-0.856435	-2.440423
C	0.630012	6.022361	-2.097984	H	-0.853213	-2.109703	-3.386581
H	0.366229	6.963099	-2.606231	H	-0.812830	0.704301	-1.009021
C	-0.098937	4.850270	-2.361404	H	-0.474846	1.019080	-0.245302
H	-0.951083	4.865367	-3.057157	P	-2.989893	2.134505	-0.984494
C	0.231010	3.646893	-1.709996	O	-2.207390	2.481893	0.337454
H	-0.374215	2.751444	-1.905464	O	-4.459837	1.700159	-0.720030
C	3.393267	-1.946328	-1.891148	O	-3.053480	3.573557	-1.850715
C	2.659160	-2.134383	-3.081911	O	-2.202613	1.136193	-1.909710
H	1.730379	-1.577326	-3.265469	H	-2.759576	4.301047	-1.230144
C	3.108821	-3.045978	-4.053348	O	-5.885693	0.199937	-2.383068
H	2.524210	-3.187502	-4.975827	H	-6.437210	-0.283295	-1.738264
C	4.292629	-3.775830	-3.845653	H	-5.313816	0.773610	-1.774962
H	4.640572	-4.492277	-4.606433	O	-2.016674	5.087857	0.247086
C	5.030257	-3.590404	-2.661701	H	-1.153252	5.246333	-0.185554
H	5.959059	-4.157623	-2.492283	H	-2.005694	4.080611	0.414946
C	4.583225	-2.683116	-1.686681	TS-6a6b			
H	5.163807	-2.549887	-0.759896	Ni	-1.389627	-1.683375	0.769501
C	3.383509	-1.542007	0.949558	Fe	0.592844	0.072295	-0.549952
C	4.368039	-1.025380	1.817225	S	0.102162	-0.358084	1.742989
H	4.923931	-0.111331	1.561444	S	0.389365	-2.259957	-0.406277
C	4.654332	-1.685247	3.027175	P	0.875602	2.273551	-0.426829
H	5.423019	-1.274036	3.700149	P	2.873451	-0.031576	-0.340040
C	3.969974	-2.863952	3.371839	O	0.918356	0.022029	-3.439000
H	4.197581	-3.376955	4.319525	N	-2.793908	-0.974421	2.015473
C	2.996840	-3.390291	2.500808	N	-2.479710	-2.897918	-0.365917
H	2.459218	-4.315216	2.762335	C	0.812993	0.060543	-2.273603
C	2.700183	-2.730851	1.298422	C	2.496871	2.597265	-1.281663
H	1.931586	-3.144188	0.624409	H	2.360698	2.339375	-2.352426
C	-0.970420	0.404079	2.431815	H	2.765876	3.669939	-1.204444
H	-0.392607	0.986574	3.173559	C	3.550412	1.698228	-0.618942
H	-1.468872	1.101374	1.727869	H	3.811930	2.102047	0.379891
C	-1.926381	-0.525526	3.144926	H	4.487869	1.649259	-1.207021
H	-2.662524	0.051515	3.747997	C	1.118831	3.093659	1.211164
H	-1.355674	-1.164305	3.846534	C	1.837304	2.423375	2.228300
C	-3.107107	-2.630803	2.990280	H	2.195377	1.394050	2.080488
H	-3.966106	-3.097108	2.474967	C	2.076275	3.049857	3.461916
H	-3.501038	-2.274682	3.969032	H	2.633338	2.510451	4.243685
C	-1.991185	-3.651660	3.183300	C	1.597213	4.351131	3.697314
H	-2.372520	-4.520658	3.756752	H	1.775712	4.838961	4.668487
H	-1.615336	-4.014147	2.203395	C	0.887922	5.026654	2.688036
H	-1.128766	-3.228991	3.736824	H	0.512558	6.047186	2.863120
C	-3.848318	-0.668126	1.664866	C	0.651723	4.406076	1.448801
H	-3.449878	0.273315	1.236575	H	0.098733	4.950267	0.668259
H	-4.501768	-0.393612	2.524679	C	-0.434905	3.231369	-1.262726
C	-4.686707	-1.370189	0.598249	C	-0.270642	3.769717	-2.556243
H	-5.196945	-2.269703	1.000434	H	0.698308	3.706762	-3.074087
H	-5.496101	-0.658195	0.337664	C	-1.360489	4.387347	-3.196754
C	-3.972158	-1.672679	-0.714378	H	-1.230846	4.803470	-4.208186
H	-4.717093	-1.975554	-1.480075	C	-2.609146	4.468346	-2.554744
H	-3.499001	-0.744636	-1.091447	H	-3.462315	4.940074	-3.066720
C	-3.366309	-4.030971	-0.106542	C	-2.773269	3.932102	-1.263920
H	-3.679463	-3.883695	0.938271	H	-3.755753	3.941773	-0.767855
H	-2.471949	-4.684551	-0.076598	C	-1.692878	3.309692	-0.622580
C	-4.503590	-4.697318	-0.883190	H	-1.830698	2.868297	0.377158
H	-4.756088	-5.654541	-0.382886	C	3.653500	-0.635294	1.217084
H	-5.421042	-4.074748	-0.893625	C	3.097465	-1.754233	1.879071
H	-4.227943	-4.930466	-1.931151	H	2.209637	-2.257989	1.468743



C	3.675914	-2.238199	3.064500	H	-0.999425	0.331388	-1.344602
H	3.231020	-3.110806	3.567824	O	-5.166997	2.160539	0.305649
C	4.809066	-1.606732	3.606301	H	-6.011029	2.081249	-0.180626
H	5.257403	-1.980982	4.540053	H	-4.551498	1.594288	-0.257124
C	5.370870	-0.496672	2.949573	TS-7a7b			
H	6.263333	-0.001494	3.363345	Ni	0.026753	-2.368684	-0.121152
C	4.801579	-0.012826	1.759248	Fe	0.829467	0.807286	-0.505458
H	5.266182	0.850287	1.259696	S	0.140931	-0.635001	1.255044
C	3.626157	-1.083732	-1.653264	S	1.550123	-1.291838	-1.213644
C	3.755870	-2.477866	-1.458693	P	0.256033	2.740641	0.486826
H	3.506437	-2.934768	-0.489675	P	2.879059	1.115632	0.383984
C	4.217396	-3.296050	-2.504034	O	1.464677	2.156326	-3.003485
H	4.318821	-4.380312	-2.339279	N	-1.558355	-3.106562	0.996278
C	4.552365	-2.734700	-3.749665	N	0.027573	-3.785876	-1.626649
H	4.914634	-3.378109	-4.566840	C	1.242725	1.620839	-1.983358
C	4.425642	-1.347817	-3.946461	C	1.723619	3.450376	1.395357
H	4.687101	-0.899368	-4.917843	H	1.677673	4.557154	1.395830
C	3.961557	-0.523693	-2.906872	H	1.603278	3.136662	2.449422
H	3.850345	0.556198	-3.088797	C	3.032629	2.921673	0.806387
C	-1.090769	0.795313	2.560028	H	3.896432	3.084640	1.483007
H	-0.946152	0.642620	3.648579	H	3.259726	3.407506	-0.166480
H	-0.820822	1.842642	2.325478	C	-1.077329	2.677892	1.759852
C	-2.504140	0.499231	2.106731	C	-0.773159	2.146135	3.037171
H	-3.240347	0.992253	2.780207	H	0.251341	1.828777	3.287399
H	-2.664670	0.896532	1.086504	C	-1.788236	1.972626	3.992660
C	-2.541749	-1.726771	3.302922	H	-1.537457	1.553046	4.979179
H	-1.448971	-1.741848	3.477400	C	-3.119046	2.311073	3.683555
H	-2.831435	-2.777160	3.101969	H	-3.916702	2.158193	4.426928
C	-3.250204	-1.195982	4.550405	C	-3.426514	2.838747	2.415805
H	-2.971779	-1.843169	5.407037	H	-4.464160	3.100461	2.152945
H	-2.937098	-0.161905	4.799529	C	-2.411277	3.027934	1.460194
H	-4.355002	-1.216687	4.465399	H	-2.680350	3.434001	0.475718
C	-4.232776	-1.105310	1.613769	C	-0.265669	3.979162	-0.775463
H	-4.458604	-0.271569	0.925178	C	0.427647	5.194656	-0.961158
H	-4.859605	-0.943302	2.515387	H	1.265539	5.477083	-0.307082
C	-4.600613	-2.421662	0.944846	C	0.062600	6.065458	-2.004290
H	-5.698278	-2.408760	0.783048	H	0.615896	7.007940	-2.140725
H	-4.402033	-3.292184	1.603877	C	-0.997052	5.736087	-2.866593
C	-3.938174	-2.574789	-0.417438	H	-1.280383	6.420514	-3.681651
H	-4.449294	-3.357249	-1.017427	C	-1.688802	4.523685	-2.688044
H	-4.027611	-1.619897	-0.970486	H	-2.518918	4.253771	-3.359703
C	-2.238091	-4.277211	0.200202	C	-1.320312	3.641509	-1.660079
H	-2.586441	-4.248043	1.251230	H	-1.867460	2.691387	-1.548618
H	-1.143205	-4.425583	0.255234	C	4.402793	0.767468	-0.590000
C	-2.886167	-5.440005	-0.551195	C	4.361159	0.493559	-1.972927
H	-2.578015	-6.384928	-0.059011	H	3.401001	0.444908	-2.504962
H	-3.993537	-5.400843	-0.530366	C	5.553489	0.267812	-2.683608
H	-2.554633	-5.492250	-1.608131	H	5.509847	0.049570	-3.762144
C	-1.948571	-2.721675	-1.764939	C	6.792099	0.314339	-2.019721
H	-2.132957	-1.664059	-2.035452	H	7.724370	0.133496	-2.577753
H	-2.523565	-3.359770	-2.472486	C	6.838759	0.587360	-0.639529
C	-0.464807	-3.012754	-1.862159	H	7.806022	0.623451	-0.114051
H	-0.040414	-2.588358	-2.792741	C	5.650329	0.810104	0.075119
H	-0.231977	-4.096326	-1.837704	H	5.692794	1.012733	1.157513
H	-1.012835	0.226833	-0.446952	C	3.139473	0.139321	1.921242
C	-4.172425	1.468005	-3.191581	C	2.988318	0.692260	3.210125
H	-4.873188	2.121652	-2.636450	H	2.853349	1.774357	3.349115
H	-3.704328	2.025253	-4.024886	C	3.007998	-0.143684	4.341865
H	-4.759129	0.625275	-3.617111	H	2.888047	0.298183	5.343562
C	-3.127036	0.889285	-2.246580	C	3.176109	-1.532410	4.197615
O	-3.477306	0.627943	-1.050977	H	3.178826	-2.183749	5.085680
O	-1.959995	0.648271	-2.704115	C	3.347596	-2.085881	2.914948

H	3.485184	-3.171593	2.792248	C	-1.504216	0.618306	-2.258813
C	3.331811	-1.256471	1.783068	C	-3.757584	1.166892	0.682178
H	3.451192	-1.701044	0.782374	H	-4.807795	1.079432	0.341547
C	-1.693561	-0.638562	1.409363	H	-3.768797	1.157214	1.789295
H	-2.007640	0.136792	2.130381	C	-3.105702	2.439963	0.138527
H	-2.156394	-0.408435	0.435264	H	-3.394179	3.344353	0.712564
C	-2.043797	-2.015798	1.924659	H	-3.384536	2.609031	-0.923335
H	-3.141895	-2.111273	2.060835	C	-2.764541	-1.416110	1.653734
H	-1.574490	-2.166824	2.915926	C	-2.298272	-0.834406	2.856711
C	-1.160802	-4.288380	1.833058	H	-2.050996	0.237252	2.900831
H	-1.159638	-5.184367	1.185939	C	-2.123108	-1.626863	4.003333
H	-1.958399	-4.458872	2.591190	H	-1.755065	-1.162510	4.931490
C	0.206075	-4.126436	2.492157	C	-2.404909	-3.005329	3.962583
H	0.431998	-5.022560	3.105007	H	-2.260727	-3.625537	4.861020
H	1.003502	-4.014642	1.727320	C	-2.871081	-3.587893	2.769917
H	0.255272	-3.236972	3.151951	H	-3.097243	-4.664949	2.730578
C	-2.690591	-3.443856	0.072960	C	-3.050939	-2.799181	1.619244
H	-3.059157	-2.486509	-0.352165	H	-3.420204	-3.267137	0.692882
H	-3.521684	-3.854975	0.690657	C	-4.044717	-1.265311	-0.937972
C	-2.380332	-4.427403	-1.053375	C	-5.348767	-1.496350	-0.436860
H	-2.095027	-5.421935	-0.651720	H	-5.619062	-1.167248	0.579697
H	-3.339193	-4.596270	-1.586552	C	-6.302487	-2.159936	-1.224527
C	-1.379456	-3.964594	-2.106463	H	-7.313470	-2.335696	-0.824446
H	-1.378079	-4.690020	-2.949160	C	-5.966244	-2.600109	-2.519231
H	-1.697636	-2.992306	-2.534353	H	-6.715869	-3.119187	-3.137193
C	0.625051	-5.046978	-1.065809	C	-4.671471	-2.379133	-3.018679
H	0.064382	-5.313429	-0.154721	H	-4.400020	-2.725233	-4.028398
H	1.646623	-4.773589	-0.734637	C	-3.712012	-1.717258	-2.230751
C	0.659919	-6.249431	-2.010344	H	-2.698864	-1.565844	-2.625388
H	1.178373	-7.084030	-1.495670	C	-0.750299	3.772229	-0.881738
H	-0.356965	-6.603384	-2.274617	C	-0.319569	3.700573	-2.223235
H	1.212832	-6.039331	-2.948073	H	-0.225895	2.730552	-2.729811
C	0.879708	-3.322625	-2.791657	C	0.004246	4.874957	-2.925995
H	0.487889	-3.754809	-3.736391	H	0.344565	4.805537	-3.971109
H	1.899703	-3.727570	-2.639883	C	-0.100133	6.128117	-2.297017
C	0.955905	-1.809450	-2.880251	H	0.157148	7.046172	-2.848599
H	-0.020389	-1.334731	-3.085955	C	-0.531035	6.206065	-0.959432
H	1.691049	-1.485080	-3.644708	H	-0.615881	7.184235	-0.460334
H	-0.716042	0.948428	-0.725315	C	-0.851903	5.035276	-0.252758
H	-0.734900	0.285126	-1.382734	H	-1.181816	5.105395	0.796220
O	-1.855746	-0.410188	-2.236351	C	-0.583766	2.641357	1.744500
H	-1.846469	-1.247562	-1.725798	C	-1.391050	2.743424	2.896325
H	-2.582225	0.184317	-1.701213	H	-2.486631	2.677107	2.826758
P	-4.775008	0.522589	-0.469791	C	-0.796804	2.939895	4.157248
O	-3.368754	1.072774	-0.948285	H	-1.435371	3.014775	5.051423
O	-5.140610	-0.827219	-1.150118	C	0.600019	3.046824	4.274805
O	-4.590202	0.080821	1.153715	H	1.060797	3.200581	5.263276
O	-5.853645	1.640672	-0.505118	C	1.408161	2.962544	3.125053
H	-4.197551	0.834833	1.646534	H	2.502437	3.049251	3.208262
O	-7.836776	-0.205576	-1.045435	C	0.821954	2.754375	1.867625
H	-6.998517	-0.721227	-1.193266	H	1.464925	2.672613	0.975799
H	-7.373149	0.647464	-0.819100	C	0.578426	-2.202391	1.558389
TS-8a8b				H	-0.288746	-2.557068	2.147952
Ni	2.337806	-0.440033	0.136673	H	0.634915	-2.768640	0.612160
Fe	-0.822394	0.205360	-0.723898	C	1.867762	-2.298691	2.352642
S	0.417974	-0.397182	1.212595	H	2.064050	-3.342037	2.681492
S	1.327329	0.902305	-1.234292	H	1.778968	-1.680714	3.267102
P	-2.825875	-0.379434	0.129063	C	4.035590	-1.161043	2.472389
P	-1.256791	2.274042	0.072705	H	5.010917	-1.124836	1.952032
O	-1.945922	0.871871	-3.318805	H	4.173782	-1.835099	3.348203
N	3.043794	-1.801179	1.544950	C	3.634451	0.243168	2.910078
N	3.911747	-0.517507	-1.199982	H	4.386467	0.641608	3.621036

H	3.579420	0.927925	2.037590
H	2.644961	0.262994	3.408291
C	3.643089	-2.989818	0.858244
H	2.810971	-3.509054	0.342742
H	4.035883	-3.676131	1.642569
C	4.741861	-2.698826	-0.159097
H	5.616762	-2.201665	0.308716
H	5.115650	-3.686269	-0.501780
C	4.282721	-1.952760	-1.405433
H	5.076152	-2.006652	-2.182495
H	3.383450	-2.450680	-1.817110
C	5.023822	0.317949	-0.632178
H	5.208808	-0.020310	0.402969
H	4.615424	1.345147	-0.552863
C	6.332873	0.308387	-1.422127
H	7.038254	1.022014	-0.949535
H	6.815454	-0.689783	-1.417134
H	6.192303	0.623427	-2.476163
C	3.484660	0.046442	-2.540567
H	3.986627	-0.509216	-3.360724
H	3.827855	1.098356	-2.597347
C	1.976634	-0.000209	-2.703223
H	1.582973	-1.033512	-2.683018
H	1.642166	0.500758	-3.634464
H	-0.883759	-1.903264	-1.145090
H	-0.301239	-1.119689	-1.369034
O	1.264856	-3.674870	-1.650826
H	1.601367	-4.581652	-1.505295
H	1.516891	-3.453132	-2.609375
O	-1.173846	-3.189806	-1.187128
H	-0.194516	-3.511854	-1.378387
H	-1.337074	-3.411000	-0.243871
O	1.983053	-3.068216	-4.128790
H	1.360343	-2.399339	-4.482632
H	2.818001	-2.562078	-4.038131
TS-9a9b			
Ni	2.294530	-0.805123	-0.035234
Fe	-0.713903	0.417830	-0.699201
S	0.453333	-0.517012	1.148638
S	1.519618	0.848118	-1.191623
P	-2.762653	0.099596	0.111535
P	-0.836342	2.485153	0.196734
O	-1.717601	1.254478	-3.294133
N	2.713876	-2.479549	1.105586
N	3.864582	-0.934744	-1.378714
C	-1.317991	0.946752	-2.231255
C	-3.487012	1.730895	0.713138
H	-4.530528	1.814937	0.351441
H	-3.525017	1.677086	1.818588
C	-2.643450	2.917865	0.238120
H	-2.814529	3.830842	0.844450
H	-2.868558	3.167877	-0.820599
C	-2.866833	-1.018910	1.570215
C	-2.391553	-0.568795	2.824376
H	-2.023347	0.461554	2.946137
C	-2.358945	-1.445966	3.921002
H	-1.984970	-1.087073	4.892653
C	-2.792219	-2.777851	3.774653
H	-2.762875	-3.465188	4.634756
C	-3.251552	-3.230980	2.524465
H	-3.573531	-4.276708	2.398630
C	-3.284480	-2.359608	1.421271

H	-3.597705	-2.739422	0.437483
C	-4.013762	-0.616082	-1.040246
C	-5.388109	-0.548303	-0.709669
H	-5.716441	-0.051384	0.217143
C	-6.347565	-1.134533	-1.550679
H	-7.414847	-1.074481	-1.285313
C	-5.945545	-1.802226	-2.723661
H	-6.699392	-2.262364	-3.381995
C	-4.580788	-1.888144	-3.046145
H	-4.256714	-2.424718	-3.951640
C	-3.616297	-1.300586	-2.208007
H	-2.551550	-1.404129	-2.454192
C	-0.075763	3.936699	-0.652820
C	0.257093	3.888553	-2.023693
H	0.103729	2.967589	-2.603358
C	0.793537	5.020721	-2.661478
H	1.053498	4.969998	-3.730504
C	1.003412	6.207880	-1.936855
H	1.428715	7.092267	-2.437086
C	0.671939	6.262004	-0.570300
H	0.833189	7.188905	0.002490
C	0.136866	5.132004	0.071363
H	-0.114471	5.180196	1.143038
C	-0.171168	2.629144	1.906067
C	-0.983692	2.853381	3.036983
H	-2.062914	3.037993	2.929170
C	-0.415828	2.843281	4.325298
H	-1.058830	3.016671	5.202494
C	0.961625	2.616195	4.492853
H	1.399752	2.603959	5.503293
C	1.779381	2.407503	3.365738
H	2.859122	2.226766	3.486974
C	1.217096	2.411720	2.080391
H	1.863677	2.232376	1.205416
C	0.206906	-2.337716	1.305996
H	-0.640604	-2.529817	1.991181
H	-0.036292	-2.796326	0.327602
C	1.493801	-2.844418	1.922505
H	1.466994	-3.947198	2.060282
H	1.607849	-2.397012	2.928405
C	3.853049	-2.259435	2.058623
H	4.799677	-2.363057	1.497776
H	3.847073	-3.086986	2.803656
C	3.802636	-0.895900	2.743112
H	4.659121	-0.797804	3.440537
H	3.861179	-0.075560	1.996658
H	2.869103	-0.747909	3.322007
C	2.983734	-3.614698	0.166066
H	2.035175	-3.799562	-0.381274
H	3.190332	-4.524524	0.774644
C	4.122569	-3.420231	-0.833058
H	5.094396	-3.289254	-0.313476
H	4.216792	-4.380233	-1.382303
C	3.924356	-2.339360	-1.890293
H	4.741757	-2.412430	-2.640835
H	2.980328	-2.517534	-2.444137
C	5.117686	-0.505463	-0.665784
H	5.211900	-1.107364	0.252829
H	4.931314	0.536180	-0.336786
C	6.414813	-0.600429	-1.470473
H	7.242728	-0.203301	-0.848319
H	6.668677	-1.647676	-1.731458

H	6.382237	-0.004013	-2.404527
C	3.637259	-0.006556	-2.554983
H	4.131997	-0.421164	-3.458552
H	4.131442	0.956698	-2.319405
C	2.162701	0.244888	-2.811784
H	1.613888	-0.660965	-3.125848
H	2.016547	1.037347	-3.573943
H	-0.985728	-1.068710	-1.023449
H	-0.257372	-1.364154	-1.666583
O	0.284064	-2.339386	-2.349740
H	-0.422195	-3.090657	-2.014483
H	1.074277	-2.508961	-1.787863
Cl	-1.642005	-4.145948	-1.310925