Electronic Supplementary Material for PCCP

How are the Ready and Unready states of Nickel-Iron Hydrogenase activated by H_2? A density functional theory study.

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Supplementary Information

Optimized Cartesian coordinates (Å) for all species studied in this paper and their absolute energies (Hartree) with Zero point correction. Imaginary frequencies (cm^{-1}) for the transition states are given in parentheses.

1. ***-4899.432678***

H	2.149108	-4.311625	-1.017135
H	2.248211	2.484738	2.587157
H	2.666095	1.551289	-2.438518
H	2.481435	1.745526	-0.663275
C	1.531645	-3.397125	-0.923310
S	2.036853	-2.532477	0.625454
H	1.332867	2.587861	-1.781738
H	-1.575914	-2.416974	2.257194
H	0.464177	-3.676063	-0.904863
H	1.709556	-2.751870	-1.800725
C	-1.912911	-1.510651	1.724342
S	-1.134724	-1.483380	0.056897
H	-3.008648	-1.504991	1.605606
H	-1.615967	-0.602253	2.271157
H	0.288764	1.755010	0.932175
C	2.061087	1.463854	2.970738
S	2.712879	0.160239	1.830250
C	1.935740	1.679473	-1.619187
S	0.836928	0.195842	-1.586881
Fe	-1.302305	0.746506	-0.671687
C	-1.112641	2.599051	-1.018760
N	-0.918351	3.760142	-1.214898
C	-2.954909	1.030392	0.224471
N	-4.001655	1.172301	0.777419
C	-2.139780	0.483610	-2.150233
O	-2.721698	0.315275	-3.173619
Ni	0.912439	-0.608225	0.680533
O	-0.229012	0.933908	1.086531
H	0.973799	1.339653	3.109530
H	2.563497	1.365063	3.951520

2. ***-4900.596435***

C	-2.540532	2.507453	1.340125
Fe	-0.757298	1.915536	1.584743
C	-0.117715	3.705500	1.618513
N	0.313613	4.816169	1.661515
N	-3.670866	2.825220	1.126551
C	-0.909929	1.930292	3.297787
O	-1.024604	1.948180	4.481151
O	-0.488246	1.776814	-0.459221
Ni	0.309316	-0.011610	-0.337890
S	-0.394648	-0.688180	-2.394706

C	-0.864679	0.856111	-3.298596
S	-1.330263	-0.396446	1.382318
C	-2.932890	-0.605622	0.487971
S	1.401972	1.006433	1.421570
C	2.378032	2.224640	0.446434
S	1.582082	-1.839825	-0.400432
C	1.820877	-2.379571	1.346178
H	-1.957943	1.024715	-3.287483
H	-0.373102	1.730607	-2.839991
H	-0.537793	0.769426	-4.351820
H	2.418813	-1.650926	1.919809
H	0.845393	-2.503280	1.846845
H	2.345019	-3.354812	1.330300
H	2.631601	3.077122	1.097296
H	3.288448	1.727130	0.069170
H	1.761867	2.593839	-0.388008
H	-2.724058	-0.799905	-0.577268
H	-3.458047	-1.477781	0.917814
H	-3.549349	0.300796	0.604476
H	1.544302	-1.248586	-4.496876
H	-1.408363	1.684139	-0.791628
H	1.923587	-1.325974	-5.147362

3. ***-4900.572388*** ***(177.23i)***

C	-2.530975	3.132596	1.916394
Fe	-1.007573	2.006229	1.672734
S	0.810945	0.544228	1.337885
C	2.081085	1.550772	0.468661
N	-3.499384	3.808797	2.069469
C	0.136167	3.424603	2.246654
N	0.889728	4.302084	2.535766
C	-1.241531	1.377509	3.281176
O	-1.414626	0.976543	4.382962
O	-0.862020	2.730767	-0.168111
Ni	-0.268785	-0.619197	-0.289459
S	-1.508932	-1.804005	-1.811103
C	-0.636160	-1.469850	-3.398750
S	-2.169746	0.204749	0.727005
C	-3.238447	0.981044	-0.551139
S	1.228072	-2.246661	-0.543395
C	2.833091	-1.915671	0.317829
H	-0.673371	-0.397177	-3.663975
H	0.420152	-1.786406	-3.334387
H	-1.135719	-2.047951	-4.200572
H	3.516309	-1.307678	-0.304299
H	2.670896	-1.396208	1.278313
H	3.321986	-2.888318	0.515534
H	2.561662	2.198284	1.220188
H	2.822672	0.888849	-0.008627

H	1.583917	2.186045	-0.281398
H	-3.424587	0.240177	-1.345843
H	-4.174525	1.286160	-0.053099
H	-2.718950	1.875298	-0.933203
H	-0.096098	0.792399	-1.559435
H	-0.418464	3.600255	-0.061192
H	-0.295351	1.480291	-1.176571

4. ***-4900.590293***

C	-2.361886	2.451043	2.013796
N	-3.453593	2.819083	2.318343
Fe	-0.632150	1.824377	1.517053
S	-1.432080	-0.241343	0.759741
C	-2.934126	0.123265	-0.237067
S	1.417165	0.875431	0.765416
Ni	0.412927	-0.480523	-0.791616
S	1.337249	-2.441044	-0.091667
C	1.336385	-2.410497	1.749533
C	0.165311	3.524224	1.841445
N	0.697159	4.591484	1.898519
C	-0.372489	1.301057	3.124234
O	-0.204440	0.969736	4.251348
O	-0.985940	2.586866	-0.447884
C	2.406784	2.150180	-0.129747
S	-0.208406	-1.550834	-2.655702
C	-0.702972	-0.311615	-3.938719
H	-1.537813	0.318781	-3.585705
H	0.135715	0.349281	-4.221039
H	-1.036847	-0.859351	-4.841832
H	1.814732	-3.337109	2.121214
H	1.893394	-1.540014	2.138267
H	0.304144	-2.364965	2.139478
H	2.637102	2.971619	0.568504
H	3.336552	1.677152	-0.490192
H	1.863130	2.554974	-0.999959
H	-3.184415	-0.779398	-0.819417
H	-3.754099	0.394992	0.448204
H	-2.754864	0.968192	-0.919972
H	0.101247	0.748172	-1.610420
H	-0.384865	3.365415	-0.378887
H	-0.485957	1.871359	-0.978443

5. ***-4900.622597***

C	9.235073	5.241452	3.981318
Fe	7.548785	5.809781	3.333413
O	6.793663	5.388638	5.367083
N	10.274332	4.839685	4.398747
S	6.878916	3.664880	2.683524

Ni	4.769563	4.181082	3.372797
S	4.287040	2.047216	3.766110
C	3.678520	1.576836	2.085835
S	5.360746	6.169957	2.580788
C	4.578677	7.611079	3.441119
C	7.795672	7.543033	4.035771
N	7.839891	8.591637	4.601160
C	8.269782	6.235435	1.840945
O	8.783890	6.540353	0.822405
C	7.605201	2.523181	3.941738
S	2.786374	4.779627	4.219906
C	1.829823	5.561520	2.847953
H	2.954054	2.326813	1.736098
H	4.558124	1.580840	1.426412
H	3.227877	0.571760	2.116218
H	2.342704	6.453843	2.455467
H	1.665377	4.857410	2.015790
H	0.847716	5.863621	3.252262
H	4.055952	8.221250	2.686121
H	3.857146	7.251751	4.194593
H	5.375008	8.210104	3.910740
H	7.239724	1.496809	3.772697
H	8.698165	2.568642	3.819267
H	7.352985	2.863152	4.956831
H	7.208912	6.189600	5.771723
H	5.832610	5.602975	5.282368
H	3.035894	2.278235	4.301284

6. ***-4900.582916 (-74.96i)***

C	-2.308604	2.379688	1.949262
Fe	-0.570684	1.707791	1.558689
O	-1.288436	3.367193	-0.581392
N	-3.402807	2.837082	2.088652
S	-1.419146	-0.322324	0.805944
Ni	0.377878	-0.620386	-0.687320
S	-0.052619	-1.549655	-2.663957
C	-0.568449	-0.252350	-3.879162
S	1.430861	0.837115	0.740058
C	2.181463	2.172344	-0.292155
C	0.215089	3.409137	1.900918
N	0.684127	4.501625	2.012810
C	-0.333652	1.196969	3.153735
O	-0.177963	0.866977	4.283583
C	-2.851672	0.115413	-0.267027
S	1.309351	-2.581208	0.075602
C	1.349870	-2.433104	1.912279
H	-1.466113	0.288516	-3.532858
H	0.232167	0.488536	-4.049218
H	-0.803979	-0.744569	-4.843249

H	1.836036	-3.329787	2.343249
H	1.916729	-1.539375	2.229579
H	0.328126	-2.356993	2.326139
H	2.517255	2.992574	0.363231
H	3.038977	1.736329	-0.833371
H	1.447566	2.552539	-1.019254
H	-3.162440	-0.801538	-0.795795
H	-3.673833	0.508090	0.353653
H	-2.546399	0.872482	-1.006606
H	-0.048543	0.593160	-1.395756
H	-2.072753	3.289590	0.015979
H	-0.655284	3.876200	-0.017822

7. ***-4900.618372***

C	-2.434304	1.449059	0.298498
Fe	-0.612001	1.198936	0.750070
C	-0.218392	2.481120	-0.583569
N	-0.029783	3.304722	-1.426693
N	-3.567707	1.651321	-0.015406
C	-0.667837	2.405563	1.993326
O	-0.706258	3.225863	2.851203
S	-0.975759	-0.720771	1.958511
Ni	0.181105	-1.155831	0.042719
S	0.363313	-1.661552	-2.114619
C	-0.570268	-0.406174	-3.103954
S	1.597328	0.497515	0.978644
C	2.579640	1.106595	-0.457365
C	-2.640375	-1.406564	1.560101
S	0.975541	-3.185770	0.565746
C	1.717756	-3.029350	2.247582
O	-3.028220	3.947238	-2.082788
H	-1.648812	-0.438817	-2.880819
H	-0.211954	0.615143	-2.898409
H	-0.417065	-0.635190	-4.175666
H	2.133201	-4.015110	2.534362
H	2.530252	-2.282903	2.251858
H	0.963974	-2.723808	2.993268
H	3.623571	0.769139	-0.327439
H	2.167063	0.685294	-1.385821
H	2.530503	2.205932	-0.504363
H	-2.633435	-2.482720	1.803506
H	-3.402817	-0.880065	2.158662
H	-2.863249	-1.254720	0.494472
H	-0.627761	0.097818	-0.545033
H	-2.047914	3.853804	-1.986442
H	-3.348099	3.249782	-1.457950

8. ***-4824.178135***

C	-2.422871	1.413617	0.326986
N	-1.309757	1.161958	0.672642
Fe	-4.213679	1.763991	-0.215003
S	-6.456864	2.378644	-0.395017
C	-6.580217	4.143594	-0.914257
C	-3.612111	3.280454	-1.190606
N	-3.257880	4.229185	-1.820661
C	-4.058569	0.746970	-1.605236
O	-3.953106	0.044448	-2.559233
S	-5.114121	0.331036	1.341952
C	-3.866734	-0.066264	2.641034
Ni	-5.629827	2.498670	1.823455
S	-7.325027	2.151924	3.254257
C	-8.452817	0.943901	2.433298
S	-5.261434	4.484731	2.763235
C	-3.621782	5.120233	2.182803
H	-2.796428	4.478837	2.532892
H	-3.575768	5.161436	1.082497
H	-3.485595	6.139641	2.592524
H	-9.301801	0.742174	3.115757
H	-8.843517	1.351637	1.485234
H	-7.933402	-0.004489	2.212429
H	-7.650811	4.394897	-1.023442
H	-6.125309	4.780651	-0.141264
H	-6.042765	4.291846	-1.864040
H	-4.408099	-0.392347	3.545754
H	-3.203852	-0.867941	2.274313
H	-3.253743	0.820843	2.853582
H	-4.233167	2.831523	1.114759

9. ***-4899.986052***

C	1.849480	-3.315812	-0.712786
S	1.608153	-2.881087	1.065683
Ni	0.729070	-0.812719	0.923365
O	-0.226605	0.862698	1.158132
Fe	-1.341102	0.767696	-0.603748
C	-2.197748	0.623228	-2.082707
O	-2.800557	0.538681	-3.106469
S	-1.190812	-1.473931	0.019922
C	-2.184220	-1.674192	1.560504
S	0.738819	0.273578	-1.804014
C	1.796193	1.786447	-1.779705
C	-1.100821	2.636561	-0.830732
N	-0.877251	3.806432	-0.919065
C	-2.952585	1.074960	0.363901
N	-3.970955	1.245617	0.962192
S	2.646274	-0.157581	1.824548
C	2.421285	1.501961	2.643188

H	2.493295	-4.214467	-0.780889
H	2.589815	2.267719	1.869879
H	2.670045	1.616522	-2.437858
H	2.177957	2.015521	-0.764402
H	1.232583	2.667375	-2.128629
H	-1.867334	-2.605947	2.061378
H	0.874510	-3.523934	-1.185338
H	2.316978	-2.475055	-1.251478
H	-3.253037	-1.715345	1.290607
H	-2.026103	-0.801155	2.210983
H	0.330044	1.630308	0.898050
H	1.388826	1.591265	3.016403
H	3.160155	1.637443	3.452240
H	2.565430	-0.873625	2.986657

10. ***-4974.592576***

S	-1.534447	2.058873	1.115818
S	1.236949	1.412046	-0.653298
S	-1.324498	-0.596661	2.495620
S	-0.729020	-0.817960	-1.275531
Fe	1.621047	-0.832342	-1.285738
C	1.734664	-2.703932	-1.612463
N	1.787578	-3.871757	-1.844078
C	3.485431	-0.728959	-0.980261
N	4.639533	-0.632810	-0.686596
C	1.817743	-0.513897	-2.963499
O	1.963100	-0.294266	-4.122085
Ni	-0.163970	0.304603	0.787984
O	1.180601	-1.142994	0.722247
O	2.313799	-0.936717	1.666594
H	3.066775	-0.908215	1.012420
C	-1.281043	-2.496746	-0.762590
H	-2.342088	-2.437202	-0.467160
H	-1.140925	-3.192411	-1.605859
H	-0.675623	-2.845044	0.085588
C	-0.277446	-1.955457	3.174883
H	0.476864	-1.571534	3.883137
H	-0.935875	-2.675795	3.697134
H	0.255620	-2.466893	2.357564
C	-1.885655	2.762967	-0.552137
H	-0.971061	3.150231	-1.033065
H	-2.329147	1.997203	-1.211601
H	-2.611454	3.589527	-0.424380
C	2.550845	2.000679	0.496665
H	3.530115	1.928502	-0.004410
H	2.322322	3.046080	0.767240
H	2.563165	1.371032	1.400777

11. ***-4975.157506***

C	1.854514	-2.702563	-0.951792
N	1.852147	-1.643067	-0.403731
Fe	1.872500	-4.381913	-1.835608
C	0.355871	-4.900719	-0.824744
N	-0.536661	-5.275156	-0.122002
C	0.941517	-3.764877	-3.131712
O	0.300134	-3.325339	-4.034238
O	3.204666	-5.158974	-0.421196
O	2.576219	-5.809845	0.797080
Ni	4.037932	-6.585171	-1.378755
S	4.961520	-8.462045	-2.227778
C	5.389261	-7.941758	-3.947593
S	2.252948	-6.567199	-2.678900
C	1.190613	-7.794137	-1.798489
S	3.900796	-3.896066	-2.953771
C	4.156542	-2.065580	-2.966847
S	5.976489	-6.239805	-0.329895
C	5.709954	-4.916441	0.935059
H	1.619562	-5.586740	0.613556
H	5.158452	-1.859725	-3.391287
H	3.395469	-1.567455	-3.594421
H	4.083426	-1.645234	-1.951457
H	4.816550	-5.138246	1.534958
H	6.617224	-4.798879	1.553832
H	5.505381	-4.002109	0.359908
H	4.486323	-7.578920	-4.466908
H	6.138119	-7.131351	-3.944838
H	5.801815	-8.812346	-4.492949
H	0.155120	-7.691706	-2.164229
H	1.586874	-8.801451	-2.012757
H	1.199184	-7.602972	-0.714979
H	6.001585	-7.292676	0.544275

12. ***-4975.152496 (-66.89i)***

C	3.087796	7.526967	4.225447
Fe	3.320882	5.739309	3.615793
S	5.390769	6.197605	2.549905
C	6.108896	7.659977	3.418261
N	2.948438	8.657033	4.580197
C	1.835607	5.176718	4.642755
N	0.954518	4.794574	5.354519
C	2.344929	6.067171	2.239629
O	1.664731	6.301298	1.290754
O	4.679320	5.372556	5.132152
O	4.122378	4.763237	6.403465
Ni	5.890628	4.161380	3.845357
S	7.708782	4.916302	4.882461

C	7.328684	4.495454	6.643171
S	3.959674	3.560984	2.972411
C	3.347910	2.384981	4.250736
S	6.866531	2.134875	3.511013
C	7.146878	2.160930	1.681141
H	3.152512	4.913955	6.239689
H	7.168718	7.767048	3.121622
H	5.541422	8.563642	3.143842
H	6.033301	7.521191	4.506873
H	6.429072	5.074426	6.900075
H	7.085973	3.424118	6.710502
H	8.179033	4.757750	7.297533
H	6.182515	2.295413	1.161336
H	7.817819	2.987456	1.384706
H	7.598768	1.200288	1.362973
H	2.253610	2.295895	4.145327
H	3.851151	1.416564	4.090921
H	3.582693	2.783413	5.250981
H	8.469305	3.793088	4.620171

13. ***-4975.154844***

C	1.311780	-2.464715	-1.376482
N	1.203794	-1.313005	-1.085372
Fe	1.519294	-4.266682	-1.939385
C	-0.044649	-4.798055	-1.019926
N	-0.995926	-5.154871	-0.391153
C	0.619000	-3.919372	-3.377140
O	-0.014596	-3.659099	-4.351395
O	2.672879	-4.713746	-0.344112
O	2.063961	-4.520837	1.024190
Ni	4.219287	-5.955364	-2.178006
S	4.918865	-8.143700	-2.018475
C	5.534211	-8.246011	-3.757839
S	2.113143	-6.458597	-2.680884
C	1.629740	-7.527462	-1.263584
S	3.639026	-3.920795	-2.924124
C	4.413486	-2.624747	-1.867744
S	6.200127	-5.340104	-1.271424
C	5.593377	-5.430633	0.478944
H	1.106209	-4.593677	0.783093
H	5.508063	-2.604604	-2.016147
H	3.966812	-1.658464	-2.152665
H	4.142202	-2.836026	-0.820576
H	4.631021	-4.883938	0.504340
H	5.395827	-6.487244	0.718697
H	6.346802	-5.003299	1.162772
H	4.689066	-8.137719	-4.459113
H	6.267545	-7.447608	-3.978953
H	6.017808	-9.228489	-3.923633

H	0.535061	-7.652784	-1.304809
H	2.152666	-8.494940	-1.339783
H	1.900924	-6.991727	-0.339622
H	6.583469	-6.682845	-1.349772

14. ***-4976.311771***

C	2.197076	-3.145239	-1.760234
N	1.928160	-2.010417	-1.511506
Fe	2.528041	-4.989998	-2.083427
S	2.575093	-7.319358	-2.555148
Ni	0.483781	-7.454346	-3.290305
S	0.757587	-9.518843	-4.266144
C	0.893977	-10.560236	-2.746517
S	0.190258	-5.517130	-2.202858
C	-0.397346	-4.299205	-3.458031
C	4.399791	-4.738561	-2.151505
N	5.578238	-4.572163	-2.253500
C	2.583921	-5.268462	-0.367155
O	2.642685	-5.421403	0.811475
O	2.436986	-4.751459	-4.045610
O	3.263277	-3.660314	-4.633440
C	3.650501	-7.448958	-4.039948
S	-1.665593	-7.884513	-3.845230
C	-2.933924	-6.801527	-2.997955
H	4.013139	-3.657976	-3.985678
H	-1.343778	-4.625176	-3.925345
H	-0.533277	-3.338949	-2.933702
H	0.416581	-4.191318	-4.197747
H	-3.840206	-7.389247	-2.771332
H	-2.496485	-6.363146	-2.086045
H	-3.194614	-5.991276	-3.695720
H	1.710206	-10.184619	-2.105675
H	-0.041345	-10.555976	-2.153135
H	1.111637	-11.604108	-3.042601
H	4.694204	-7.423309	-3.683626
H	3.425324	-8.385500	-4.574745
H	3.452857	-6.550332	-4.651155
H	-1.794933	-8.899847	-2.944846
H	1.360478	-5.690994	-5.939267
H	1.031245	-5.914420	-6.583757

15. ***-4976.297442 (508.23i)***

C	31.258256	42.182202	114.283091
S	31.168974	43.232501	112.761831
Ni	29.260966	44.509247	112.994397
S	30.087532	45.537393	114.762089
Fe	28.155612	46.815679	115.102560

O	28.248074	47.518735	113.164537
O	28.970202	48.801072	112.906949
S	27.205446	44.849040	114.111649
C	25.997754	45.493847	112.868890
S	28.294973	43.475873	111.297978
C	28.008485	41.733998	111.866637
C	31.406664	46.628211	114.074275
C	27.948075	46.195493	116.696962
O	27.794321	45.798972	117.805987
C	26.470374	47.701011	115.257356
N	25.391835	48.198657	115.357347
C	29.093048	48.323628	115.750127
N	29.717572	49.287187	116.080869
H	30.415023	41.468974	114.350558
H	31.238432	42.824658	115.180398
H	31.832588	47.209466	114.909714
H	30.971688	47.314372	113.331709
H	27.269871	41.802096	112.679781
H	28.967279	41.359029	112.261136
H	26.515726	46.136917	112.139106
H	25.251950	46.099369	113.408839
H	32.165166	45.976828	113.609357
H	32.205220	41.606767	114.276687
H	27.625352	41.094803	111.049888
H	25.509149	44.647066	112.352995
H	29.168359	49.061535	113.847412
H	28.864416	46.652617	112.481529
H	29.294390	45.911396	111.939613
H	29.409368	43.143145	110.569954

16. ***-4976.309520***

C	30.567958	42.260634	115.274441
S	30.924594	42.331774	113.466069
Ni	30.316914	44.337001	112.613257
S	29.981108	43.410076	110.664742
C	28.130211	43.485490	110.553745
S	30.448144	45.559556	114.456064
C	31.606216	46.913244	113.961521
S	27.412249	44.473583	114.141235
C	25.569748	44.546658	114.272185
Fe	28.293332	46.529608	114.843682
C	29.056683	48.238078	115.154117
N	29.523561	49.335621	115.235212
O	28.109851	46.930790	112.749725
O	28.650038	48.264638	112.261558
C	28.307279	46.070870	116.487129
O	28.290798	45.754048	117.631722
C	26.586697	47.324779	115.101710
N	25.517498	47.819295	115.282322

H	29.486966	42.378320	115.457139
H	31.099374	43.067583	115.806213
H	31.752931	47.578234	114.827436
H	31.195507	47.496372	113.123738
H	27.879799	44.510186	110.242383
H	27.704161	43.312302	111.556760
H	25.153481	45.344638	113.636724
H	25.256421	44.747008	115.310238
H	32.560613	46.447556	113.661912
H	30.905781	41.282161	115.665377
H	27.768997	42.758013	109.805206
H	25.167523	43.565726	113.952590
H	28.854219	48.670310	113.153104
H	28.841000	46.304961	112.407579
H	30.111227	45.643831	111.882816
H	30.022709	42.079488	111.035018

17. ***-4975.772191***

C	31.637054	42.559410	114.016811
S	31.036495	43.552547	112.580026
Ni	29.014329	44.314787	113.168975
S	29.685680	45.280406	115.057450
Fe	27.989396	46.871564	114.888019
C	26.511236	48.006195	114.538886
N	25.551628	48.667998	114.304211
S	28.149724	43.381032	111.332515
C	27.638679	41.753974	112.042013
C	31.305729	46.132970	114.817035
S	26.990142	44.996385	113.920364
C	25.919125	45.603134	112.541602
C	29.035858	48.321313	115.465221
N	29.754635	49.251796	115.664564
O	28.676476	47.299002	112.848177
O	29.440955	48.554088	112.611421
C	27.375380	46.599982	116.463681
O	26.948423	46.432761	117.551168
H	31.049967	41.635656	114.149093
H	31.588104	43.139158	114.953064
H	31.529607	46.651120	115.762796
H	31.253225	46.882907	114.014147
H	26.809506	41.960304	112.734289
H	28.484112	41.322472	112.598534
H	26.480782	46.285346	111.888013
H	25.094033	46.164055	113.006136
H	32.081128	45.389704	114.578533
H	32.687927	42.284606	113.818809
H	27.306483	41.079559	111.236693
H	25.526478	44.746868	111.967714
H	29.473213	48.905412	113.553181

H	29.375947	46.602073	112.692905
H	29.348815	42.920015	110.833612

18. ***-4975.159964***

C	30.878518	42.298127	113.819267
S	31.225262	43.602411	112.557502
Ni	29.582912	45.080099	112.893576
S	30.314134	45.805661	114.857639
C	31.468503	47.143928	114.324067
S	27.411679	44.481441	114.787160
Fe	28.169104	46.742825	115.030206
C	27.933048	46.586544	116.720673
O	27.751812	46.475467	117.891323
S	28.325858	44.289605	111.241364
C	29.174148	44.934978	109.724985
O	28.632808	46.785548	112.992623
O	27.450446	47.014391	112.072823
C	25.636512	44.384267	115.308299
C	26.432888	47.418246	114.739379
N	25.351031	47.806661	114.409371
C	28.838600	48.521825	115.228678
N	29.268947	49.620964	115.399285
H	29.875945	41.861501	113.673010
H	30.925656	42.726091	114.834775
H	31.686251	47.787915	115.191524
H	30.987965	47.756459	113.547205
H	29.348847	46.015742	109.836273
H	28.573961	44.730698	108.820376
H	25.019980	45.126278	114.774784
H	25.533570	44.565835	116.394012
H	32.388411	46.668646	113.941442
H	31.639611	41.499402	113.723035
H	30.139248	44.407331	109.665156
H	25.264996	43.365692	115.085899
H	26.739500	47.161982	112.763259
H	27.475633	45.394932	111.407871

19. ***-4975.160946 (592.22 i)***

C	30.893128	42.296979	113.762663
S	31.235790	43.629672	112.531047
Ni	29.556443	45.058395	112.849789
O	28.618953	46.703307	112.993730
O	27.353449	46.918055	111.963584
S	30.247859	45.758551	114.847300
Fe	28.112038	46.752282	114.959657
C	28.797594	48.535649	115.078930
N	29.240693	49.635880	115.200660
S	28.300705	44.365872	111.111857

C	29.250885	45.060040	109.684187
C	31.467341	47.059064	114.366923
S	27.337162	44.499120	114.824436
C	25.611832	44.408086	115.489910
C	27.893232	46.681593	116.665007
O	27.731643	46.625284	117.840973
C	26.373082	47.412971	114.655086
N	25.284023	47.778702	114.324157
H	29.928972	41.802695	113.554185
H	30.857719	42.715934	114.782165
H	31.700700	47.667865	115.255731
H	31.029708	47.713962	113.600119
H	29.434008	46.134343	109.843027
H	28.696298	44.908311	108.740557
H	24.964591	45.168181	115.021662
H	25.597458	44.560767	116.585126
H	32.370658	46.551437	113.987152
H	31.704144	41.545281	113.704902
H	30.214858	44.527325	109.639151
H	25.211429	43.399473	115.273040
H	26.639750	46.965803	112.666978
H	27.522877	45.643004	111.448024

20. ***-4975.235143***

C	8.112775	1.503476	5.442062
S	7.766932	2.633391	4.021644
Ni	6.067818	3.976668	4.535765
S	5.573546	3.848163	2.334115
C	4.760483	5.454823	1.951057
O	4.733499	5.116436	4.822879
O	3.094388	2.178974	4.195865
Fe	4.445367	5.560453	6.521478
C	5.525989	7.136823	6.514068
N	6.208343	8.109996	6.557092
S	6.330641	4.069539	6.786738
C	7.892778	5.035761	6.960158
C	4.181480	6.013701	8.259149
O	4.034228	6.342936	9.380200
S	3.217265	3.749687	7.333351
C	1.428677	4.182214	7.255268
C	2.936580	6.598885	5.991302
N	1.985455	7.241147	5.678464
H	7.607310	0.532789	5.288835
H	7.748879	1.935257	6.391124
H	8.047985	5.273142	8.027375
H	7.831993	5.975829	6.392667
H	4.341939	5.866754	2.887221
H	3.941982	5.286818	1.227413
H	1.136064	4.481096	6.238160

H	1.192052	5.008079	7.946316
H	8.725573	4.419321	6.582281
H	9.202383	1.325822	5.514333
H	5.483517	6.172160	1.522877
H	0.865876	3.281100	7.562371
H	3.217024	2.654488	5.054233
H	3.741905	2.643702	3.606821

21. ***-4898.657562***

C	30.837726	42.158827	114.800107
S	30.679869	42.722133	113.049991
Ni	29.400306	44.708379	113.228695
S	28.851299	44.296310	111.004915
C	28.052377	45.862315	110.457283
O	28.562026	46.358206	113.210255
Fe	28.415183	46.657957	115.112473
C	29.035021	48.451730	115.033615
N	29.441684	49.577431	115.022991
S	30.669021	45.724996	114.909857
C	31.539051	46.937710	113.830738
S	27.824743	44.251229	114.959210
C	26.299688	44.238910	113.928766
C	28.375449	46.699999	116.847921
O	28.359586	46.703309	118.049359
C	26.608604	47.243416	115.012043
N	25.468033	47.604745	114.988434
H	29.840468	41.976150	115.243114
H	31.341011	42.930368	115.413702
H	31.933391	47.770884	114.440110
H	30.790737	47.327628	113.120711
H	27.960007	46.492010	111.373807
H	27.047044	45.673915	110.027202
H	26.375065	45.075863	113.217863
H	25.410671	44.382731	114.570011
H	32.356474	46.425016	113.289360
H	31.430109	41.219059	114.845768
H	28.668553	46.392179	109.701090
H	26.237443	43.283700	113.376099

22. ***-4899.823370***

C	30.793752	42.202155	115.110021
S	30.764329	42.807806	113.367288
Ni	29.446087	44.765041	113.483056
S	27.713869	44.233035	115.029686
C	26.298650	44.247706	113.852534
S	29.067635	44.382907	111.204284
C	28.302572	45.953977	110.623310
O	28.585964	46.400314	113.430065

Fe	28.258525	46.641087	115.318289
C	26.459474	47.206443	115.073087
N	25.320226	47.553214	114.956598
S	30.529838	45.744607	115.298695
C	31.493083	46.998296	114.354039
C	28.854620	48.443833	115.352765
N	29.242984	49.574218	115.413845
C	28.059047	46.627890	117.042828
O	27.933458	46.594430	118.236925
H	29.769347	41.983620	115.466757
H	31.227320	42.967791	115.781393
H	31.817068	47.810689	115.029248
H	30.821937	47.412716	113.583916
H	28.114791	46.558490	111.541189
H	27.346334	45.762065	110.095137
H	26.427276	45.120767	113.194740
H	25.347959	44.345061	114.408209
H	32.365566	46.507955	113.882756
H	31.403807	41.275473	115.178940
H	28.979388	46.510959	109.943025
H	26.311465	43.321143	113.250423
H	31.341884	44.674118	108.634751
H	30.914899	44.571437	109.264701

23. ***-4899.793374 (553.83i)***

C	7.801418	2.322870	5.487536
S	6.344272	2.169422	4.339881
Ni	4.566855	3.440350	5.024236
S	2.680610	4.276752	6.017409
C	1.642139	5.024643	4.697416
S	3.366097	2.165246	3.513525
C	3.051080	0.691215	4.579683
O	4.031205	6.955320	5.295022
Fe	3.736664	6.273002	6.973183
C	2.144503	7.295625	7.101193
N	1.121780	7.908366	7.197025
S	5.626227	4.654696	6.617967
C	6.801302	5.716803	5.677951
C	4.820012	7.658835	7.711784
N	5.520157	8.497126	8.198455
C	3.479570	5.620119	8.600370
O	3.303897	5.205122	9.708124
H	7.475656	2.743278	6.457023
H	8.594712	2.985601	5.083360
H	7.521397	6.157626	6.391146
H	6.190142	6.521731	5.220721
H	2.465304	0.976422	5.473857
H	4.015231	0.259432	4.908561
H	2.173168	5.927964	4.341729

H	0.682481	5.329813	5.151194
H	7.318320	5.113548	4.912662
H	8.249234	1.321307	5.660157
H	2.482306	-0.076065	4.010903
H	1.496365	4.279027	3.896338
H	4.522769	5.152504	3.858070
H	4.364147	5.858040	4.284498

24. -4899.838042

C	6.752755	2.009112	7.000863
S	6.091075	1.716549	5.302061
Ni	4.942240	3.616966	4.605170
S	6.111056	5.178985	5.802641
C	6.583938	6.575055	4.690162
S	3.189430	4.035722	6.243368
Fe	4.170345	6.079207	6.992444
C	4.668676	5.367504	8.489924
O	5.004232	4.913091	9.546100
S	3.946435	2.574586	2.793819
C	3.259706	0.992914	3.473090
C	1.702160	4.541009	5.276892
O	3.604470	6.959899	5.289875
C	2.567024	6.721969	7.795963
N	1.558542	7.092792	8.320142
C	5.080571	7.699047	7.450022
N	5.686570	8.685432	7.749051
H	7.228001	3.005138	7.064270
H	7.505925	1.234260	7.256279
H	7.309108	7.211130	5.228970
H	5.665527	7.161953	4.490403
H	2.398248	1.196449	4.137072
H	4.024471	0.458357	4.062888
H	1.789107	5.625614	5.072844
H	0.795842	4.347556	5.880964
H	7.032336	6.180100	3.760720
H	5.946358	1.975306	7.756120
H	2.915768	0.349731	2.634732
H	1.677399	3.961649	4.336526
H	4.496890	4.799360	3.837751
H	3.768011	6.212736	4.662908

25. -4900.008849

C	-2.940406	0.483354	-0.944054
S	-1.482115	0.617084	-2.068731
Ni	0.344172	1.098899	-0.947076
O	1.869754	2.090536	-0.133245
Fe	3.201505	1.306528	-1.530467
C	4.252532	0.634866	-2.733970

O	4.978402	0.192490	-3.551509
S	-0.462981	1.052112	1.163451
C	-0.786581	-0.683774	1.694586
S	1.331842	1.457976	-2.912272
C	0.915701	3.212744	-3.268498
S	2.153949	-0.671321	-0.886241
C	2.685791	-0.940443	0.851588
C	4.563143	1.165499	-0.222514
N	5.399499	1.046882	0.615012
C	3.756689	3.077357	-1.912116
N	3.992120	4.225029	-2.122039
H	-0.549207	-0.791992	2.763786
H	-0.191525	-1.376090	1.083618
H	-1.857653	-0.874896	1.538415
H	-2.989408	1.306001	-0.210029
H	-2.969944	-0.485089	-0.414586
H	-3.841462	0.543697	-1.579813
H	-0.157613	3.267998	-3.510068
H	1.524645	3.526204	-4.132060
H	1.167047	3.870334	-2.423854
H	2.081867	-1.743190	1.309519
H	2.617455	-0.006568	1.432490
H	3.748998	-1.228711	0.847109
H	1.871922	3.044952	-0.372995
H	0.798117	1.182812	1.668774

26. ***-4900.009370 (546.13i)***

C	-2.809355	0.053152	-1.069451
S	-1.502883	0.623788	-2.235743
Ni	0.261335	1.124103	-1.081699
S	-0.593172	1.365747	1.065745
C	-0.602651	-0.219610	2.006102
S	1.337973	1.610495	-2.978501
Fe	3.125369	1.286332	-1.528283
C	4.442221	0.972264	-0.205557
N	5.250427	0.740050	0.635625
S	1.949197	-0.672137	-1.052951
C	2.481742	-1.188660	0.629279
O	1.807353	2.092539	-0.087728
C	0.970622	3.403947	-3.157203
C	3.783454	3.045606	-1.778520
N	4.076151	4.192302	-1.904830
C	4.173119	0.625917	-2.731800
O	4.905084	0.185413	-3.544136
H	-0.187555	-0.055950	3.012706
H	-0.023356	-0.987200	1.477743
H	-1.650963	-0.544549	2.094039
H	-3.081843	0.830509	-0.336133
H	-2.494929	-0.859678	-0.536576

H	-3.699774	-0.191169	-1.676037
H	-0.033808	3.510367	-3.596645
H	1.737965	3.835853	-3.819482
H	1.024748	3.927746	-2.191960
H	1.893153	-2.068083	0.943524
H	2.380268	-0.365522	1.352357
H	3.551530	-1.447037	0.584758
H	1.895165	3.064130	-0.224012
H	0.830420	1.757618	1.022379

27. ***-4900.045782***

C	-2.775878	-0.401433	-1.134555
S	-1.744584	0.973456	-1.800690
Ni	0.241812	0.450499	-1.133452
O	2.443390	2.063300	0.205589
Fe	3.199597	1.212363	-1.629481
C	3.947603	0.615114	-3.062497
O	4.479927	0.215263	-4.032553
S	0.000849	0.147543	1.030124
C	-1.093064	1.520233	1.604838
S	1.245570	1.722718	-2.735395
C	0.774235	3.420622	-2.197616
S	2.080065	-0.823697	-1.302196
C	2.643818	-1.638260	0.244675
C	4.688100	0.705656	-0.557629
N	5.542800	0.392866	0.208712
C	3.968507	2.925053	-1.920135
N	4.427676	4.009403	-2.080548
H	-2.122093	1.393808	1.231880
H	-0.714115	2.495751	1.265036
H	-1.101293	1.498388	2.708723
H	-2.753486	-0.427021	-0.032795
H	-2.414928	-1.371155	-1.512563
H	-3.813341	-0.246163	-1.479834
H	-0.293904	3.580065	-2.415885
H	1.397010	4.123332	-2.774119
H	0.985434	3.554084	-1.126898
H	2.151064	-2.621103	0.318307
H	2.392262	-1.036309	1.133134
H	3.737891	-1.748298	0.188114
H	3.284213	2.064440	0.721429
H	1.828713	1.398573	0.650283

28. **-4900.036144**

C	-2.782775	-0.036001	-1.280788
S	-1.752471	1.497428	-1.291903
Ni	0.254934	0.561064	-0.935667
O	2.551977	2.166877	0.187340

Fe	3.303397	1.209271	-1.688824
C	4.024358	0.520969	-3.067452
O	4.548379	0.046716	-4.023255
S	-0.064264	-0.010927	1.188531
C	-1.355079	1.049951	1.976806
S	1.220945	1.562707	-2.720540
C	0.827221	3.349347	-2.483289
S	2.083520	-0.743022	-1.162435
C	2.722814	-1.512921	0.388024
C	4.808032	0.795262	-0.602110
N	5.683690	0.544600	0.170547
C	4.013261	2.912972	-2.156429
N	4.445066	3.978764	-2.470765
H	-2.371916	0.778235	1.645432
H	-1.197899	2.113857	1.738987
H	-1.283394	0.900192	3.071906
H	-2.743357	-0.543476	-0.299816
H	-2.438284	-0.750750	-2.049479
H	-3.832615	0.239721	-1.504898
H	-0.254576	3.485842	-2.651499
H	1.418587	3.928032	-3.211095
H	1.104860	3.665621	-1.467098
H	2.316534	-2.536313	0.466593
H	2.403133	-0.938564	1.274940
H	3.823061	-1.529746	0.335740
H	3.347915	1.898096	0.705521
H	1.808798	1.565287	0.498976