Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Data

Bio-mimetic Hetero-Bimetallic Architecture of Ni(II) and Fe(II) for CO_2 Hydrogenation in Aqueous Media. A DFT Study.

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NOTE: All the given values are in '*hartrees*' unless mentioned otherwise.

1. **(I) Comparison of computed barrier height of NiFe1 (kcal mol^{-1}) at various DFT functionals using PBE-D3 optimized geometries.**

	PBE-D3	M06L	M06	PBE0-D3	B3LYP
NiFe	-2657.561533	-2659.23558	-2658.563632	-2657.628457	-2659.31116
NiFe1	-2658.720787	-2660.39972	-2659.720842	-2658.788741	-2660.470849
H_2	-1.163558	-1.169106	-1.168309	-1.165914	-1.177418
Barrier height	0.81	1.23	5.07	1.64	9.24

(II) Comparison of barrier height of NiFe1 (kcal mol^{-1}) computed by using two different basis sets LANL2DZ and SDD for Ni and Fe centers.

	PBE-D3/6-31+G(d,p)//LANL2DZ	PBE-D3/6-31+G(d,p)//SDD
NiFe	-2657.561533	-2659.689385
NiFe1	-2658.720787	-2660.847903
Barrier Height	0.81	1.27

2. **Optimized geometries of CO2 hydrogenation cycle.**
   (I) Model 1:

Name-CO2:G=-188.408473//H=-188.384108//SPE=-188.3987698

Angstroms

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.18037922
O	0.00000000	0.00000000	-1.18037922

Name-HCOOH:G=-189.574978//H=-189.546648//SPE=-189.5831106

Angstroms

Atom	X	Y	Z
C	0.12007422	0.37842142	0.00002373
H	0.02903271	1.48273467	0.00022663
O	1.18779078	-0.22381427	-0.00005317
O	-1.05658723	-0.28957466	0.00009812
H	-1.79910644	0.35384822	-0.00072863

Name-H2:G=-1.163558//H=-1.148747//SPE=-1.1619885

Angstroms

Atom	X	Y	Z
H	0.00000000	-0.00000000	0.37520468

H	0.00000000	0.00000000	-0.37520468

Name-HCOO-:G= -189.136888//H= -189.109070//SPE =-189.1327082

Angstroms

Atom	X	Y	Z
C	-0.00008000	0.34696600	0.00000000
H	0.00176400	1.46969800	0.00000000
O	-0.00008000	-0.22196800	1.14238000
O	-0.00008000	-0.22196800	-1.14238000

Name-NiFe:G= -2657.561533//H= -2657.471272//SPE =-2658.0149592

Angstroms

Atom	X	Y	Z
S	-0.44034190	-1.51884023	-1.74130495
Ni	-1.69375585	0.00026753	-0.79043753
Fe	1.10271352	0.00095411	-0.80131235
S	-0.44116245	1.52102659	-1.73954935
C	-1.05374818	-2.88540093	-0.62564246
C	-2.54728089	-2.66047437	-0.42417012
H	-0.50248705	-2.86732390	0.32533405
H	-0.87189983	-3.85299841	-1.11980467
C	-1.05589318	2.88647145	-0.62326453
C	-2.54921619	2.66008129	-0.42197221
H	-0.87493683	3.85442611	-1.11705219
H	-0.50459156	2.86860970	0.32768584
N	-2.78588035	-1.29879766	0.15998275
N	-2.78671635	1.29774443	0.16110564
H	-2.98005561	-3.43215386	0.24159992
H	-3.06880593	-2.70364901	-1.39321099
C	-4.17699581	-0.78020325	-0.05831760
C	-4.17752595	0.77839077	-0.05751061
H	-4.50403019	1.13790678	-1.04327574
H	-4.86098097	1.19512361	0.70395757
H	-4.50313425	-1.13892743	-1.04449522
H	-4.86027697	-1.19813429	0.70265616
C	-2.42177544	-1.28488622	1.61826573
C	-2.42246413	1.28287167	1.61930923
H	-1.33312993	1.41940673	1.69418980
H	-2.91380626	2.14907574	2.10227319
H	-2.91275462	-2.15170334	2.10050109
H	-1.33239394	-1.42094166	1.69309917
C	-2.85974805	-0.00140097	2.31968750
P	2.35721606	-1.38961893	0.33098076
P	2.35545739	1.39015517	0.33457393
C	2.23902085	0.00304394	-2.19548270
N	2.96851786	0.00411009	-3.15236985
H	-3.07075421	2.70354665	-1.39098984
H	-2.98265870	3.43088578	0.24437975
C	1.82840894	1.23104201	2.12909415
C	1.83176340	-1.23538340	2.12634146
N	1.06111489	-0.00342081	2.34908605

H	1.16937564	2.08891246	2.34585074
H	2.72384889	1.31075670	2.78971040
H	1.17552383	-2.09554803	2.34248065
H	2.72808999	-1.31347007	2.78590601
C	0.48501115	-0.00576107	3.69875311
H	-0.14256950	-0.90181970	3.83168283
H	-0.14356151	0.88918534	3.83437940
H	1.26706184	-0.00643584	4.49209903
C	4.11415820	0.77325107	0.33655259
C	4.11517143	-0.77084250	0.33288117
C	2.54458008	3.19868616	0.07407168
H	2.89058112	3.36652976	-0.95820345
H	3.28971499	3.60084489	0.78077364
H	1.58462542	3.71425862	0.22157107
C	2.54757495	-3.19710333	0.06452705
H	1.58853862	-3.71411170	0.21294273
H	3.29499926	-3.60079200	0.76792108
H	2.89090422	-3.36123932	-0.96923720
H	-2.42184682	-0.00172167	3.33061082
H	-3.95307106	-0.00174769	2.46129058
H	4.59428533	-1.16908711	-0.57602898
H	4.63594531	-1.19412117	1.20778897
H	4.63275884	1.19295695	1.21445959
H	4.59457284	1.17643125	-0.56949840

Name-NiFe1:G= -2658.720787//H= -2658.630821//SPE =-2659.1926516

Angstroms

Atom	X	Y	Z
S	0.59111877	1.54666122	-1.66268385
Ni	1.82867831	-0.00000380	-0.70323657
Fe	-0.96908236	-0.00011076	-0.68921357
S	0.59124118	-1.54683692	-1.66262639
C	1.20749279	2.89596724	-0.53529524
C	2.69203472	2.66201680	-0.29554181
H	0.62493153	2.89354118	0.39792495
H	1.04789351	3.86399885	-1.03716565
C	1.20779684	-2.89604784	-0.53521556
C	2.69230386	-2.66191765	-0.29544780
H	1.04832451	-3.86409753	-1.03709375
H	0.62523374	-2.89371088	0.39800355
N	2.90091546	1.29480115	0.28615154
N	2.90103026	-1.29466086	0.28620219
H	3.11964212	3.42476093	0.38412113
H	3.23633954	2.70258671	-1.25219929
C	4.29892504	0.77831346	0.11742482
C	4.29899656	-0.77804565	0.11746598
H	4.65947816	-1.13796599	-0.85611897
H	4.95415241	-1.19671897	0.90281913
H	4.65936320	1.13822048	-0.85618128
H	4.95404918	1.19708419	0.90275313

C	2.49122552	1.28607517	1.73352600
C	2.49132067	-1.28589774	1.73356352
H	1.40220521	-1.43861558	1.77371676
H	2.97805186	-2.14691056	2.23009529
H	2.97793050	2.14712865	2.23000605
H	1.40210872	1.43874151	1.77367241
C	2.88961139	0.00011579	2.45438575
P	-2.43824088	1.38448038	0.15803438
P	-2.43807826	-1.38467236	0.15843885
C	-1.85181569	-0.00015202	-2.32396195
N	-2.39149759	-0.00015165	-3.39326611
H	3.23663131	-2.70245985	-1.25209194
H	3.11997191	-3.42459386	0.38425318
C	-2.45455204	-1.22742702	2.03931606
C	-2.45447970	1.22806848	2.03895251
N	-1.78843488	0.00036546	2.48613203
H	-1.89941081	-2.08964617	2.44574226
H	-3.50872561	-1.29910076	2.38782373
H	-1.89916877	2.09038852	2.44494048
H	-3.50859249	1.30000601	2.38759141
C	-1.58772941	0.00058157	3.94224992
H	-1.01385783	0.89563448	4.23287005
H	-1.01384639	-0.89437606	4.23314017
H	-2.54702912	0.00066118	4.50332062
C	-4.13867950	-0.77367881	-0.30555030
C	-4.13880744	0.77304005	-0.30562420
C	-2.50649834	-3.19799047	-0.11824211
H	-2.57889054	-3.38634539	-1.20098124
H	-3.38574347	-3.62727368	0.39055293
H	-1.59022581	-3.66808560	0.26974269
C	-2.50693524	3.19764991	-0.11952927
H	-1.59064803	3.66802683	0.26808459
H	-3.38615123	3.62708958	0.38918038
H	-2.57949338	3.38544749	-1.20235497
H	0.18445023	-0.00016767	0.48210586
H	-0.54337364	0.00012624	0.94610644
H	2.39707280	0.00010040	3.44083727
H	3.97393113	0.00015862	2.65436961
H	-4.36501733	1.17428124	-1.30629320
H	-4.87109578	1.19181496	0.40478605
H	-4.87100758	-1.19251278	0.40478721
H	-4.36466010	-1.17504600	-1.30622017

Name-NiFe2:G= -2658.720595//H= -2658.556121//SPE =-2659.195704

Angstroms

Atom	X	Y	Z
S	-0.48667789	-1.54973520	-1.77742986
Ni	-1.68777527	0.00047914	-0.76527519
Fe	1.03440025	0.00079773	-0.76225688
S	-0.48698964	1.55282379	-1.77387734

C	-1.10665418	-2.88986498	-0.64131243
C	-2.58921311	-2.65903988	-0.39077918
H	-0.52742076	-2.87034917	0.29348396
H	-0.94599914	-3.86610224	-1.12742032
C	-1.10856872	2.89132611	-0.63670163
C	-2.59107160	2.65878357	-0.38754619
H	-0.94846016	3.86811396	-1.12186362
H	-0.53001384	2.87160544	0.29853846
N	-2.79401650	-1.29589714	0.19906807
N	-2.79472083	1.29478995	0.20064933
H	-3.01351575	-3.42626674	0.28709258
H	-3.13913906	-2.69424517	-1.34453794
C	-4.18931284	-0.77811142	0.02536258
C	-4.18974074	0.77639034	0.02658435
H	-4.54769276	1.13604284	-0.94804082
H	-4.85011282	1.19384418	0.80917836
H	-4.54689598	-1.13651768	-0.94985789
H	-4.84956377	-1.19704680	0.80728093
C	-2.39713488	-1.29247028	1.64809921
C	-2.39689769	1.28971997	1.64930255
H	-1.31011710	1.45497378	1.69434569
H	-2.89667874	2.14369147	2.14682171
H	-2.89773005	-2.14665911	2.14442824
H	-1.31051456	-1.45851358	1.69374068
C	-2.79194391	-0.00164569	2.36619343
P	2.33901171	-1.37646965	0.26873277
P	2.33785871	1.37674728	0.27211224
C	2.09506245	0.00327278	-2.30910062
N	2.76098136	0.00434716	-3.31033113
H	-3.14028402	2.69431775	-1.34169678
H	-3.01669489	3.42484470	0.29081963
C	2.05759813	1.25276766	2.14268162
C	2.05533185	-1.25946886	2.13903875
N	1.29565782	-0.00306375	2.44449285
H	1.43032602	2.09893695	2.46353425
H	2.99969954	1.25020651	2.71308619
H	1.42521874	-2.10542083	2.45499751
H	2.99613864	-1.26158381	2.71158484
C	0.70207054	-0.00448398	3.81225445
H	0.08258846	-0.90535696	3.92381019
H	0.08386235	0.89699094	3.92615525
H	1.51006012	-0.00596102	4.55824618
C	4.10248001	0.77411040	0.12636274
C	4.10323148	-0.77115440	0.12705983
C	2.49906848	3.19635764	0.04488883
H	2.72641750	3.38846731	-1.01581932
H	3.31639023	3.58912355	0.67268002
H	1.55849221	3.70273137	0.30766259
C	2.50317408	-3.19511467	0.03622845
H	1.56260717	-3.70356956	0.29498957
H	3.31944359	-3.58880307	0.66482101
H	2.73350084	-3.38348462	-1.02450506

H	-0.03918886	-0.00285274	0.41773657
H	-2.30584317	-0.00214108	3.35560426
H	-3.87734017	-0.00162345	2.56174142
H	4.49542129	-1.17307780	-0.82118104
H	4.70312566	-1.19271155	0.95072694
H	4.70428759	1.19707329	0.94789986
H	4.49133127	1.17555583	-0.82343341
H	0.52303056	-0.00145093	1.67311915

Name-NiFe3:G= -2847.115645//H= -2847.016787//SPE =-2847.5994969

Angstroms

Atom	X	Y	Z
S	-0.67676820	-1.21649982	-1.47222058
Ni	-2.09528980	0.11146562	-0.48540102
S	-0.69258524	1.74572352	-0.81484939
C	-1.45391479	-2.71089134	-0.67870156
C	-2.95584679	-2.53800056	-0.91168759
H	-1.19569701	-2.76379255	0.39067831
H	-1.08310138	-3.62106789	-1.17829785
C	-1.48010813	2.75321249	0.53705207
C	-2.98144348	2.68426248	0.24986911
H	-1.11653312	3.79199126	0.47379666
H	-1.22207714	2.34657138	1.52712624
N	-3.43691944	-1.28872918	-0.22676136
N	-3.45029960	1.25785605	0.33781668
H	-3.52201675	-3.41298849	-0.54015678
H	-3.15474925	-2.43129493	-1.98994371
C	-4.61605490	-0.61834420	-0.87217173
C	-4.62180353	0.91142943	-0.53710096
H	-4.50849103	1.48444815	-1.46822500
H	-5.56586778	1.22210598	-0.05277463
H	-4.50639114	-0.74922749	-1.95789762
H	-5.55459964	-1.11105153	-0.55837883
C	-3.71480568	-1.59518779	1.21517375
C	-3.72983415	0.92269272	1.77329385
H	-2.77536327	0.97531147	2.31363961
H	-4.40617799	1.70162454	2.17443930
H	-4.38212091	-2.47767480	1.24924357
H	-2.75833016	-1.86259483	1.68381299
C	-4.39074348	-0.44187241	1.95228817
P	2.75996763	-1.26136291	-0.65029889
P	2.73765651	1.43296275	-0.04614968
C	1.34326531	0.55075003	-2.32172553
N	1.48013556	0.82785010	-3.47964004
H	-3.18360735	3.04745898	-0.77038247
H	-3.55342077	3.31162528	0.95929412
C	3.57077073	1.00342690	1.58189687
C	3.70678379	-1.48787209	0.96262039
N	3.45177338	-0.43396315	2.00031695
H	3.09936375	1.59960927	2.37903342

H	4.63896598	1.27028313	1.51795832
H	3.40099829	-2.44469031	1.41402829
H	4.78693596	-1.52329169	0.74550615
C	4.31767245	-0.68077613	3.19772523
H	4.12929626	-1.70067181	3.56126579
H	4.05311892	0.04882851	3.97603218
H	5.37383232	-0.56747729	2.91233650
C	4.12151592	1.07711670	-1.25492894
C	4.08557559	-0.41953877	-1.65579361
C	2.63994810	3.25865717	0.07255635
H	2.27663301	3.64045103	-0.89458008
H	3.62777223	3.69355492	0.29714391
H	1.91966952	3.52927467	0.86038082
C	2.66201810	-2.98505139	-1.26668489
H	1.96375563	-3.55365952	-0.63258294
H	3.65512003	-3.46360601	-1.25808135
H	2.27262584	-2.95790710	-2.29656519
H	-4.38697264	-0.67999136	3.02901035
H	-5.45215262	-0.38311352	1.65751246
H	3.81890722	-0.54142065	-2.71622545
H	5.04936724	-0.92415178	-1.47933852
H	5.07936222	1.36054368	-0.78937239
H	3.95775552	1.72708985	-2.12850411
O	-1.05067715	-0.55917286	2.45945334
C	0.17583907	-0.49735883	2.24697577
H	0.51386109	0.15891436	1.35079533
Fe	1.05657420	0.14050269	-0.57021811
O	1.11847390	-1.01613660	2.93749023
H	2.42459889	-0.61424442	2.35340591

Name-NiFe4:G=-2657.979634//H=-2857.738721/SPE=-2658.3431114

Angstroms

Atom	X	Y	Z
S	-0.47333400	-1.49799700	-1.71305300
Ni	-1.72874400	-0.00026600	-0.75951400
Fe	1.06869300	-0.00011100	-0.78733200
S	-0.47347000	1.49690800	-1.71417400
C	-1.08846200	-2.88457100	-0.62599800
C	-2.58678100	-2.66594700	-0.43242300
H	-0.54412600	-2.90132600	0.32982500
H	-0.90658600	-3.84050100	-1.14188900
C	-1.08861500	2.88412100	-0.62796200
C	-2.58691400	2.66558400	-0.43418200
H	-0.90675200	3.83975300	-1.14440700
H	-0.54423900	2.90140100	0.32782300
N	-2.84295600	-1.30697500	0.16145000
N	-2.84300800	1.30699600	0.16058400
H	-3.02719200	-3.45239100	0.20948300
H	-3.09176200	-2.69928200	-1.41024700
C	-4.22963000	-0.78138200	-0.08276800

C	-4.22966700	0.78118400	-0.08325000
H	-4.53927600	1.14141000	-1.07418900
H	-4.93767600	1.19970600	0.65391300
H	-4.53917500	-1.14224000	-1.07349600
H	-4.93765200	-1.19948100	0.65462500
C	-2.50460200	-1.28984100	1.62182100
C	-2.50457700	1.29078700	1.62097400
H	-1.41387900	1.44408600	1.70200400
H	-2.99216200	2.15314600	2.11385500
H	-2.99225000	-2.15185900	2.11523500
H	-1.41392400	-1.44315700	1.70298700
C	-2.93854600	0.00070500	2.31763700
P	2.37206000	-1.39205600	0.26611400
P	2.37167900	1.39271700	0.26554300
C	2.30394500	-0.00104100	-2.13839100
N	3.09052600	-0.00184900	-3.03370800
H	-3.09194600	2.69826100	-1.41200400
H	-3.02732800	3.45242600	0.20723200
C	2.00122600	1.27217700	2.12514400
C	2.00101400	-1.27165200	2.12554600
N	1.22857800	0.00036900	2.42396000
H	1.36494300	2.11631300	2.43313000
H	2.90651800	1.27228500	2.75241000
H	1.36436100	-2.11562000	2.43323600
H	2.90603100	-1.27199000	2.75321300
C	0.67530800	0.00064700	3.82237600
H	0.06814200	-0.90250100	3.97224200
H	0.06805800	0.90380600	3.97183900
H	1.51032400	0.00084600	4.53603600
C	4.12670600	0.77280700	0.19074600
C	4.12693700	-0.77147800	0.19170500
C	2.52300400	3.19866800	-0.00826500
H	2.75921300	3.34230900	-1.07481700
H	3.33351200	3.62852000	0.60177400
H	1.58465000	3.72600700	0.21501600
C	2.52407500	-3.19786500	-0.00803300
H	1.58571800	-3.72548300	0.21458200
H	3.33438900	-3.62769600	0.60227700
H	2.76083900	-3.34104100	-1.07452800
H	-2.53008300	0.00104000	3.34138300
H	-4.03136000	0.00075500	2.45521600
H	4.54419000	-1.15747100	-0.75167800
H	4.71385100	-1.19773800	1.02120600
H	4.71407700	1.20029800	1.01929000
H	4.54312600	1.15774000	-0.75344100
H	0.43853000	0.00030300	1.73456800

Name-NiFe6:G= -2659.156846//H= -2659.065501//SPE =-2659.6394046

	Angstroms		
Atom	X	Y	Z
S	0.66559490	1.52511479	-1.32437362
Ni	1.98947096	-0.00670808	-0.51179541
Fe	-0.96089732	0.00100048	-0.43074392
S	0.65221618	-1.53230303	-1.31577627
C	1.38447172	2.86831269	-0.25039716
C	2.89458999	2.65681693	-0.24799014
H	0.95000463	2.85031481	0.76077692
H	1.13432091	3.83941572	-0.70697186
C	1.34951158	-2.86982579	-0.22130382
C	2.86229207	-2.67879831	-0.21651038
H	1.08779269	-3.84469275	-0.66316144
H	0.91284629	-2.82968967	0.78830501
N	3.21036387	1.28816021	0.28599682
N	3.19495336	-1.30776627	0.30141537
H	3.41601800	3.42917698	0.34951877
H	3.27187241	2.70893188	-1.28140764
C	4.55068455	0.76011534	-0.13696388
C	4.54165600	-0.80119202	-0.12725303
H	4.71266250	-1.17054267	-1.14802104
H	5.33665990	-1.22061629	0.51591326
H	4.72478468	1.11425703	-1.16260698
H	5.35135896	1.17837091	0.49989560
C	3.06051726	1.27928733	1.78134619
C	3.04785038	-1.28033648	1.79682911
H	1.97873663	-1.40768518	2.02694973
H	3.58605994	-2.14945082	2.22032900
H	3.60522364	2.14850624	2.19620182
H	1.99171693	1.41785009	2.00693318
C	3.58631522	0.00075709	2.42543713
P	-2.58846505	1.40637898	-0.02960457
P	-2.63180507	-1.36730675	-0.09953459
C	-1.52848768	0.01280838	-2.22122257
N	-1.88198950	0.01334381	-3.35506490
H	3.24245409	-2.74937696	-1.24779363
H	3.37100805	-3.45058125	0.39252738
C	-3.25336168	-1.29177512	1.69011592
C	-3.21710462	1.25064289	1.75395431
N	-2.76952344	-0.04416182	2.39907185
H	-2.86427692	-2.15275861	2.25505656
H	-4.35290001	-1.30389202	1.74990963
H	-2.80437586	2.07012333	2.36229174
H	-4.31600694	1.29217052	1.81509907
C	-3.11117509	-0.07550669	3.86694224
H	-2.66928309	0.80224102	4.35717481
H	-2.70562363	-0.99463379	4.31047518
H	-4.20356888	-0.05596292	3.97546378
C	-4.12611572	-0.70653685	-1.00123666
C	-4.09468294	0.84166747	-0.97239372
C	-2.59694328	-3.16692295	-0.43332148
H	-2.31616566	-3.29616112	-1.49075629

H	-3.57930388	-3.63446135	-0.25924875
H	-1.83869725	-3.65848534	0.19486412
C	-2.50626101	3.22193994	-0.25352045
H	-1.73705656	3.65482298	0.40384389
H	-3.47645397	3.70274057	-0.04984185
H	-2.22196099	3.41167090	-1.30066243
H	-0.24806717	0.41295688	0.95753200
H	-0.33576950	-0.47407279	0.97661639
H	3.30188985	0.00876562	3.48991681
H	4.68822547	-0.00464135	2.41750009
H	-3.99202295	1.24181622	-1.99271768
H	-5.00375456	1.27594455	-0.52594547
H	-5.04487389	-1.11957164	-0.55436480
H	-4.05695287	-1.07269746	-2.03674434
H	-1.73847349	-0.05511482	2.29124480

Name-NiFe7:G= -2848.298239//H= -2848.197683//SPE =-2848.7993808

Angstroms

Atom	X	Y	Z
S	0.64255506	-2.25625469	-0.88083138
Ni	1.94257119	-0.89338298	0.23533700
Fe	-0.94245359	-0.86196270	0.25484838
S	0.67182470	-1.16074836	2.00291995
C	1.27736070	-1.70681301	-2.54312478
C	2.77881254	-1.49715860	-2.39758891
H	0.74604833	-0.80092728	-2.87129789
H	1.06996283	-2.50832494	-3.27031660
C	1.34285162	0.35293067	2.85654816
C	2.84235057	0.38687371	2.58702302
H	1.14832729	0.25315184	3.93653567
H	0.82149244	1.25306548	2.49622526
N	3.04713320	-0.49453171	-1.31463199
N	3.08604605	0.41932788	1.10746020
H	3.23604047	-1.15351761	-3.34574041
H	3.26005898	-2.44273394	-2.10136162
C	4.43894063	-0.56570565	-0.75795659
C	4.46108871	-0.02086918	0.70215545
H	4.75306348	-0.83011044	1.38600806
H	5.17861565	0.81076653	0.82575694
H	4.72532065	-1.62663897	-0.75234603
H	5.14124633	-0.02401806	-1.41714944
C	2.71649674	0.88617316	-1.80955046
C	2.76841771	1.78916397	0.57586072
H	1.68222056	1.92928993	0.67046871
H	3.27292047	2.53450865	1.21932685
H	3.18354484	1.01605084	-2.80426208
H	1.62376560	0.94505624	-1.93003442
C	3.20913980	1.97979523	-0.87022137
P	-2.51613296	-0.75591187	-1.25141723
P	-2.52660094	0.18023468	1.33876741
C	-1.62477228	-2.48868412	0.86351383

N	-2.01587258	-3.54543041	1.26018600
H	3.31377676	-0.52673489	2.98264212
H	3.32105615	1.26385848	3.06444757
C	-2.97671136	1.86073534	0.62710210
C	-2.91250001	0.99652024	-1.80018234
N	-2.60210453	2.09106494	-0.81370938
H	-2.45414927	2.63616918	1.20861057
H	-4.06374064	2.01153510	0.73127179
H	-2.31948597	1.21758792	-2.70167913
H	-3.98337918	1.05105309	-2.05572226
C	-3.23074737	3.37247185	-1.28553284
H	-2.87781998	3.57689867	-2.30578813
H	-2.91753663	4.18248609	-0.61223094
H	-4.32418009	3.26266709	-1.27218203
C	-4.11170201	-0.75287127	1.03342185
C	-4.11895454	-1.24979715	-0.43376415
C	-2.48597514	0.54613799	3.13235364
H	-2.37181202	-0.40793579	3.67040738
H	-3.41797081	1.04330710	3.44792473
H	-1.62152937	1.19144928	3.35225973
C	-2.48659357	-1.62107278	-2.86609316
H	-1.62940060	-1.26319504	-3.45707858
H	-3.42342117	-1.43853719	-3.41820333
H	-2.37269012	-2.69992385	-2.67631573
H	2.80151345	2.94086635	-1.22395246
H	4.30613370	2.07072500	-0.92872633
H	-4.17652195	-2.34830058	-0.48310086
H	-4.95920556	-0.83342456	-1.01258530
H	-4.96742029	-0.09582316	1.25783277
H	-4.12768683	-1.59582918	1.74087035
H	-1.53589424	2.31291422	-0.85771041
O	1.01265016	4.79278356	-0.15258014
O	-0.16112651	3.08759890	-1.09320703
C	0.14466531	3.87295295	-0.12127677
H	-0.41079021	3.71456856	0.83875181
H	-0.25223084	0.61009618	0.16487639
H	-0.26712199	0.32008936	-0.64055753

Name-NiFe8:G= -2847.134425//H= -2847.036735//SPE =-2847.6211889

Angstroms

Atom	X	Y	Z
S	0.52182158	1.67838777	-1.17216091
Ni	2.01298605	0.18187414	-0.62794631
Fe	-1.04170037	0.00201788	-0.64735509
S	0.83046559	-1.34909921	-1.64932229
C	1.01116378	2.81369327	0.21556300
C	2.53561958	2.84303411	0.22162410
H	0.58867052	2.44447220	1.16272725
H	0.60542949	3.81911891	0.01597311
C	1.84910423	-2.75816541	-0.96671556
C	3.30385959	-2.30146669	-0.97660034

H	1.71983246	-3.62418345	-1.63640247
H	1.51099753	-3.05766032	0.03733383
N	3.07057570	1.45247531	0.40877595
N	3.45698968	-1.05131281	-0.16026900
H	2.92834102	3.50615016	1.01647687
H	2.90084262	3.21445351	-0.74896533
C	4.45211705	1.25436812	-0.14049147
C	4.67066287	-0.24311534	-0.51411430
H	4.80729066	-0.32851145	-1.60121960
H	5.56468253	-0.66627617	-0.01982329
H	4.52579965	1.86521752	-1.05074577
H	5.20673033	1.61965458	0.57968785
C	2.98732811	1.07000285	1.86190785
C	3.45543270	-1.39601260	1.29845714
H	2.47277691	-1.82064436	1.54072347
H	4.21470900	-2.18451103	1.46409531
H	3.39488636	1.90675185	2.46075448
H	1.92132319	0.95629880	2.11044289
C	3.76928875	-0.19881142	2.19228763
P	-2.74541796	1.31973958	-0.29942396
P	-2.62599823	-1.44012072	-0.17510613
C	-1.52625667	0.06004135	-2.41944470
N	-1.80932433	0.11221494	-3.58458452
H	3.61055892	-2.06385248	-2.00755043
H	3.97702550	-3.08873213	-0.58363031
C	-3.20262553	-1.22294410	1.61808256
C	-3.35568186	1.31169195	1.48047030
N	-2.83720170	0.11148603	2.22015947
H	-2.71704730	-1.99109415	2.24009432
H	-4.29550556	-1.34377208	1.69087579
H	-2.96368613	2.19928455	1.99985170
H	-4.45612028	1.31127748	1.53063253
C	-3.21155453	0.16151616	3.66963215
H	-2.85794117	1.11431371	4.08668964
H	-2.72581192	-0.67933133	4.18323043
H	-4.30466778	0.08657721	3.75724673
C	-4.16290565	-0.94618247	-1.10561247
C	-4.23264232	0.59939289	-1.17337620
C	-2.54625776	-3.27023750	-0.29103820
H	-2.31473466	-3.53381976	-1.33520243
H	-3.50344812	-3.72961170	0.00645276
H	-1.73608369	-3.63673157	0.35873169
C	-2.76873141	3.10850878	-0.69902068
H	-2.02414114	3.63132328	-0.07899735
H	-3.77045554	3.53107837	-0.51616456
H	-2.50490626	3.22701910	-1.76166442
H	3.53088110	-0.47993120	3.23150177
H	4.85145955	0.01210259	2.17185131
H	-4.19546135	0.95400531	-2.21450128
H	-5.14694955	0.99756607	-0.70464638
H	-5.04460460	-1.38525291	-0.61104334
H	-4.07901092	-1.38546017	-2.11237739

H	-1.78384476	0.17927206	2.13545699
O	0.32967163	-1.28848645	3.10762206
O	-0.33934399	-0.06155743	1.33304491
C	0.06016661	-1.16990291	1.88703680
H	0.12900987	-2.05056117	1.21172050

Name-NiFe9:G= -2847.838218//H= -2847.736889//SPE=-2848.3270148

Angstroms

Atom	X	Y	Z
S	0.49891282	-2.26858765	-1.06586123
Ni	1.78422933	-0.98798793	0.17054073
Fe	-1.03038538	-0.96101021	0.21994049
S	0.55583895	-1.44360556	1.93414627
C	1.14545981	-1.54226404	-2.65337284
C	2.65267324	-1.39232785	-2.50396768
H	0.64568147	-0.58182256	-2.85461153
H	0.90838525	-2.23321683	-3.47941811
C	1.25614662	-0.01619868	2.90204818
C	2.75603077	0.01694442	2.64302361
H	1.05558628	-0.18414956	3.97327078
H	0.75525459	0.91716746	2.60082955
N	2.95450522	-0.51127902	-1.32870961
N	3.00693290	0.16933897	1.17233485
H	3.11955132	-0.97108986	-3.41640631
H	3.10382337	-2.37797016	-2.30645364
C	4.32682034	-0.71990631	-0.76266669
C	4.35716747	-0.31326291	0.74014973
H	4.59134946	-1.19805770	1.34871841
H	5.12343534	0.45682326	0.94778198
H	4.54985531	-1.79236560	-0.85000270
H	5.07496859	-0.16529136	-1.35934284
C	2.73256133	0.92726642	-1.70126344
C	2.78231633	1.59748266	0.76927371
H	1.70402114	1.79243913	0.86411696
H	3.32088840	2.25001207	1.48319795
H	3.24403784	1.11824745	-2.66459356
H	1.65099577	1.06910191	-1.84765099
C	3.26478059	1.89426916	-0.64795957
P	-2.48858558	-0.52224399	-1.28913575
P	-2.44920952	0.20003965	1.32986858
C	-1.86757335	-2.59278884	0.67838052
N	-2.37027081	-3.64479009	0.97379148
H	3.20764362	-0.93597771	2.96195315
H	3.25318688	0.84011259	3.19362806
C	-2.67055930	1.98619031	0.76788028
C	-2.70081793	1.29855499	-1.72100425
N	-2.27373535	2.27722110	-0.65728387

H	-2.03664933	2.63314341	1.39485035
H	-3.72271199	2.28861626	0.89515898
H	-2.08380378	1.52328429	-2.60540777
H	-3.75641870	1.50018097	-1.96523444
C	-2.75683034	3.65045770	-1.03180532
H	-2.37690109	3.89415153	-2.03347132
H	-2.37229205	4.37308206	-0.29898439
H	-3.85586411	3.65254367	-1.02833975
C	-4.16247856	-0.45615409	0.93078175
C	-4.18279077	-0.87097819	-0.56147672
C	-2.48072964	0.46433847	3.15384470
H	-2.50395385	-0.52226357	3.64320125
H	-3.37015911	1.04408486	3.45300451
H	-1.56912023	0.99690857	3.46649610
C	-2.57294955	-1.23790722	-2.98483201
H	-1.67271938	-0.95447870	-3.55191584
H	-3.47335217	-0.88607358	-3.51588116
H	-2.60563856	-2.33480864	-2.89033001
H	2.92978309	2.90901427	-0.91643072
H	4.36702548	1.91785525	-0.67568073
H	-4.35578571	-1.95328270	-0.67293173
H	-4.95947775	-0.33869920	-1.13539178
H	-4.92267122	0.30762030	1.16465458
H	-4.33179537	-1.32210955	1.59043807
H	-1.20740026	2.36240437	-0.69117451
O	1.40334548	4.93076189	0.02768898
O	0.23610437	3.24590230	-0.96018613
C	0.53700856	4.00298833	0.02853498
H	-0.01738061	3.81882654	0.98575265
H	-0.22391721	0.33714475	-0.13891207

Name-NiFe10:G=-2658.262595//H=-2658.164616//SPE=-2658.7142401

Angstroms

Atom	X	Y	Z
S	-0.62723009	-1.55040857	-1.72511826
Ni	-1.77100021	0.00129062	-0.65524409
Fe	0.95188917	0.00166742	-0.82254346
S	-0.62714037	1.55804828	-1.71773127
C	-1.19423937	-2.88600489	-0.55669027
C	-2.66850689	-2.66225858	-0.25547240
H	-0.58067001	-2.85607121	0.35636337
H	-1.04659351	-3.86632181	-1.03964960
C	-1.19554954	2.88869304	-0.54437719
C	-2.66985251	2.66273537	-0.24496241
H	-1.04831614	3.87091842	-1.02356775
H	-0.58259914	2.85596571	0.36901690
N	-2.86070092	-1.29792706	0.33480785
N	-2.86131118	1.29604276	0.34003001
H	-3.06760260	-3.42942088	0.43812629

H	-3.24882865	-2.70374146	-1.19092661
C	-4.25749890	-0.77873067	0.18558089
C	-4.25781875	0.77673008	0.18860218
H	-4.63253384	1.13725887	-0.77944311
H	-4.90699109	1.19184667	0.98237764
H	-4.63231932	-1.13569196	-0.78374916
H	-4.90628310	-1.19716003	0.97793043
C	-2.43743860	-1.29514153	1.77492224
C	-2.43798809	1.28785587	1.78001300
H	-1.35087357	1.45272019	1.80268344
H	-2.92845843	2.14035969	2.28989038
H	-2.92764916	-2.14979095	2.28145184
H	-1.35027519	-1.45979117	1.79694827
C	-2.81584825	-0.00514403	2.50308572
P	2.32487892	-1.35122506	0.15369539
P	2.32511550	1.35006873	0.15951026
C	1.88732164	0.00654173	-2.46264922
N	2.45367652	0.01019471	-3.52638167
H	-3.24955494	2.70719533	-1.18065362
H	-3.06998788	3.42699961	0.45124572
C	2.37834711	1.22882185	2.04528966
C	2.37805110	-1.23728863	2.04002388
N	1.79907922	-0.00529516	2.58865457
H	1.80034798	2.08101962	2.44500885
H	3.44035851	1.37260193	2.35888937
H	1.79977253	-2.09099005	2.43615183
H	3.44000341	-1.38269535	2.35309383
C	1.91041439	-0.00838466	4.05109879
H	1.41393685	-0.90391025	4.46104448
H	1.41390590	0.88540874	4.46478525
H	2.96889779	-0.00908043	4.40140973
C	4.06245917	0.77339890	-0.25975324
C	4.06225116	-0.77311085	-0.26339245
C	2.44848982	3.17961369	-0.06729530
H	2.54681038	3.39325647	-1.14355674
H	3.32986122	3.57548797	0.46596571
H	1.54211432	3.67446057	0.31301926
C	2.44841962	-3.17998867	-0.07963485
H	1.54235990	-3.67630557	0.29952359
H	3.33015269	-3.57741506	0.45186066
H	2.54619455	-3.38999326	-1.15665460
H	-2.30496539	-0.00696864	3.48037811
H	-3.89649972	-0.00583139	2.72440394
H	4.30182625	-1.17432196	-1.26159771
H	4.78157940	-1.19737044	0.45786234
H	4.78158083	1.19400958	0.46384814
H	4.30269163	1.17921364	-1.25593186
H	0.04622196	-0.00136647	0.44681397

Name-NiFe11:G= -2846.674126//H= -2846.574349//SPE =-2847.1425713

	Angstroms		
Atom	X	Y	Z
S	-0.72618054	-1.58428196	-1.36722705
Ni	-2.04115826	-0.02698413	-0.59530918
S	-0.72700409	1.46182054	-1.50211477
C	-1.40363807	-2.86051847	-0.19192117
C	-2.92008584	-2.68639275	-0.21842652
H	-0.97714610	-2.71970156	0.81288236
H	-1.12255282	-3.86245886	-0.55569550
C	-1.40590570	2.82991815	-0.43649112
C	-2.92245262	2.65412714	-0.44451327
H	-1.12721136	3.79853574	-0.88308763
H	-0.97679169	2.77439908	0.57548824
N	-3.28358466	-1.29541409	0.21879848
N	-3.28536893	1.30453696	0.10771561
H	-3.42417330	-3.42701632	0.43180295
H	-3.29079790	-2.82083551	-1.24711591
C	-4.59229977	-0.79875768	-0.32316472
C	-4.59186740	0.76183458	-0.39355426
H	-4.68717501	1.07515348	-1.44256377
H	-5.43184375	1.20150845	0.17516626
H	-4.69455453	-1.20532624	-1.33898002
H	-5.42913367	-1.18494080	0.28736387
C	-3.24993427	-1.21581596	1.71808293
C	-3.25788382	1.35414494	1.60762261
H	-2.21733846	1.52886761	1.91533231
H	-3.86226147	2.22449262	1.92837197
H	-3.84623983	-2.05913315	2.11676225
H	-2.20585298	-1.35316448	2.03326920
C	-3.82071635	0.09291887	2.25747431
P	2.59752207	-1.39418856	-0.18704476
P	2.60436309	1.35489209	-0.32405835
C	1.46960204	-0.11402873	-2.48556651
N	1.75230693	-0.16508976	-3.65179054
H	-3.29525234	2.70300876	-1.47995892
H	-3.42446400	3.44641042	0.14351962
N	3.91504553	0.08016426	1.80849595
C	4.31381723	0.14998245	3.22328901
H	3.43829057	0.19203628	3.90954755
H	4.92863092	1.04963316	3.39108358
H	4.91560241	-0.73651978	3.48287856
C	4.12006358	0.70552452	-1.20289018
C	4.11581120	-0.84488013	-1.12489030
C	2.51547183	3.15083226	-0.69470587
H	2.18826094	3.27747014	-1.73867203
H	3.49734423	3.63025633	-0.54863601
H	1.77199267	3.61687830	-0.02857176
C	2.49779553	-3.21839651	-0.36676326
H	1.76129068	-3.60913454	0.35356785
H	3.48003949	-3.68380790	-0.18180796
H	2.15826753	-3.45350343	-1.38767278
H	-3.59682891	0.14015806	3.33614138

H	-4.92038040	0.08627906	2.17283665
H	4.05468280	-1.29464669	-2.12841811
H	5.01319360	-1.24065744	-0.62282034
H	5.01935659	1.14368021	-0.74101545
H	4.06303057	1.05234271	-2.24650446
O	-0.02103381	-0.98877591	2.76404070
C	0.03041763	0.14377439	2.20926249
H	0.06535082	0.13094854	1.04587767
Fe	0.96352878	-0.03572399	-0.74389875
O	0.00727812	1.29604896	2.72540918
C	3.17035568	-1.17319955	1.58336679
H	2.27536615	-1.27486049	2.23198340
H	3.85061349	-2.01240222	1.81367701
C	3.19498967	1.31805361	1.45413010
H	3.89769672	2.16105873	1.57982867
H	2.31435819	1.51590823	2.09999751

Name-TS12:G= -2658.721708//H= -2658.632236//SPE =-2659.1912338

Angstroms

Atom	X	Y	Z
S	-0.49129764	-1.55824554	-1.71000653
Ni	-1.73296377	-0.00278833	-0.77092650
Fe	1.04003261	-0.01183698	-0.70481592
S	-0.48084638	1.53383002	-1.72870681
C	-1.13578167	-2.89683287	-0.58547984
C	-2.62363443	-2.65804048	-0.37415749
H	-0.57422491	-2.88417853	0.36059668
H	-0.96817720	-3.87127002	-1.07236442
C	-1.11170307	2.88688597	-0.61338387
C	-2.60140011	2.66324240	-0.39662406
H	-0.93737336	3.85609084	-1.10835520
H	-0.54773640	2.87733331	0.33144820
N	-2.83644967	-1.28860441	0.19877482
N	-2.82648232	1.30065067	0.18803738
H	-3.06636101	-3.41742603	0.30016973
H	-3.15062681	-2.69994079	-1.34049983
C	-4.22856176	-0.76751491	0.00377571
C	-4.22244630	0.78869620	-0.00380941
H	-4.56410633	1.14519795	-0.98546831
H	-4.89120435	1.21288805	0.76747935
H	-4.57399880	-1.13074388	-0.97409086
H	-4.89971848	-1.17940349	0.77958967
C	-2.45154546	-1.27457451	1.65190527
C	-2.44488399	1.29690052	1.64212433
H	-1.35620342	1.44521861	1.69994638
H	-2.93757696	2.16117800	2.12765455
H	-2.94596389	-2.13326443	2.14550173
H	-1.36303492	-1.42542877	1.70843929
C	-2.86219054	0.01486333	2.35953895
P	2.39302375	-1.39464962	0.28998137

P	2.41413178	1.38220477	0.24252934
C	2.04520775	-0.03121207	-2.26487074
N	2.67798146	-0.04079214	-3.28512711
H	-3.13017968	2.70253906	-1.36208325
H	-3.03538542	3.43227502	0.27244422
C	2.13342968	1.27430289	2.11381617
C	2.13250538	-1.19949815	2.15918042
N	1.38276523	0.04256818	2.41142090
H	1.51368740	2.13558586	2.41175830
H	3.09751637	1.31525267	2.65465274
H	1.52000106	-2.04798722	2.50457739
H	3.10429261	-1.21351253	2.68734027
C	0.68237516	0.06673444	3.70685592
H	0.04821239	-0.82958185	3.78743941
H	0.04638086	0.96404785	3.75312650
H	1.39371663	0.08335443	4.55339872
C	4.16036540	0.74731436	0.05496757
C	4.14738018	-0.79822861	0.06624326
C	2.56838479	3.18741188	-0.06015635
H	2.78659981	3.34162084	-1.12878514
H	3.38789086	3.60747231	0.54668690
H	1.62562680	3.69536075	0.19223595
C	2.51772181	-3.21406387	0.06657263
H	1.57422203	-3.69778614	0.36004244
H	3.34355162	-3.61650259	0.67676747
H	2.71315804	-3.42061344	-0.99763403
H	-0.08183309	0.00380056	0.48551573
H	0.52811792	0.02167492	1.22225564
H	-2.39299740	0.01724752	3.35710255
H	-3.95087388	0.01833473	2.53466801
H	4.50314570	-1.20962342	-0.89208455
H	4.77376434	-1.21735398	0.87142508
H	4.78089647	1.16772852	0.86403795
H	4.53986442	1.13849576	-0.90275933

Name-TS23: G= -2847.097309//H= -2846.999793//SPE =-2847.5785483

Angstroms

Atom	X	Y	Z
S	0.51177308	2.00338689	-0.46365287
Ni	1.95331400	0.36747535	-0.54871373
S	0.64150514	-0.68551815	-1.94557815
C	1.20191613	2.61895240	1.15030302
C	2.71771397	2.63349459	0.97147693
H	0.87787307	1.96941694	1.97843663
H	0.82362939	3.63805236	1.33567638
C	1.52553368	-2.30290370	-1.68115954
C	3.01629557	-1.97966264	-1.71495188
H	1.26227555	-2.98361091	-2.50783022
H	1.21450966	-2.76863497	-0.73501866

N	3.20323063	1.24244305	0.67754155
N	3.35009859	-1.00597430	-0.62124649
H	3.23345226	3.02906120	1.86759695
H	2.98147618	3.27120234	0.11262416
C	4.47589084	1.18467086	-0.11361284
C	4.56250199	-0.16385852	-0.89542769
H	4.56974566	0.04525443	-1.97420009
H	5.48169309	-0.72660510	-0.64839161
H	4.44609544	2.01612660	-0.83175995
H	5.34738987	1.33466564	0.55004806
C	3.32673577	0.48075477	1.96498897
C	3.49284096	-1.74286280	0.67768616
H	2.51171468	-2.16764300	0.92830031
H	4.19173304	-2.58620878	0.51665339
H	3.90548529	1.10260251	2.67484693
H	2.31326026	0.35310655	2.36822357
C	4.02940825	-0.86434577	1.80440707
P	-2.78548558	1.36214958	0.27849855
P	-2.67034289	-1.21496302	-0.71105365
C	-1.58133012	1.05314299	-2.20168203
N	-1.85130363	1.55872434	-3.25587973
H	3.27133051	-1.50332816	-2.67511911
H	3.63423790	-2.89190114	-1.60458481
C	-3.27128278	-1.72736928	1.01191161
C	-3.37578634	0.62476055	1.91371184
N	-2.79228872	-0.74970270	2.04987429
H	-2.83021860	-2.70358810	1.26408377
H	-4.36903858	-1.79066165	1.06614577
H	-2.98510268	1.22849225	2.74685645
H	-4.47259038	0.55746723	1.97744667
C	-2.91113327	-1.28987846	3.43884885
H	-2.46707384	-0.56474993	4.13441694
H	-2.37354451	-2.24712192	3.49139851
H	-3.97532308	-1.43914842	3.66911100
C	-4.21247486	-0.39383099	-1.37080591
C	-4.28854403	1.04328378	-0.79538426
C	-2.56097509	-2.84366501	-1.55057830
H	-2.35333831	-2.66726974	-2.61780906
H	-3.50014147	-3.41170860	-1.44428741
H	-1.72618882	-3.41366869	-1.11260122
C	-2.82477030	3.16257169	0.62987160
H	-2.05066818	3.40453420	1.37469731
H	-3.81604031	3.46509923	1.00567104
H	-2.60423960	3.69922389	-0.30640424
H	3.91841386	-1.41827245	2.75127912
H	5.11208225	-0.70555816	1.66752953
H	-4.26954813	1.79502791	-1.59948044
H	-5.19841240	1.20458381	-0.19429095
H	-5.09475414	-0.99945342	-1.10592822
H	-4.12182195	-0.37829549	-2.46850353
O	0.48795577	-0.94365621	2.87630487
C	0.19582009	-1.65102531	1.95065306

H	-0.53957004	-0.43463350	0.81790035
Fe	-1.10671709	0.28265552	-0.56941078
O	0.06380525	-2.68365024	1.35496704
H	-1.77436424	-0.59726247	1.78821157

Name-TS71:G=-2848.289993//H=-2848.014352//SPE=-2848.79409276

Angstroms

Atom	X	Y	Z
S	0.68603000	-2.21654000	-1.05654000
Ni	1.91597000	-0.92456000	0.21424000
Fe	-0.93966000	-0.92819000	0.16707000
S	0.61042000	-1.38925000	1.91544000
C	1.39757000	-1.54975000	-2.64411000
C	2.88509000	-1.32604000	-2.40805000
H	0.87005000	-0.63280000	-2.94684000
H	1.24372000	-2.30780000	-3.42898000
C	1.18497000	0.08135000	2.90472000
C	2.68942000	0.20117000	2.69301000
H	0.95967000	-0.10574000	3.96706000
H	0.63538000	0.98239000	2.59068000
N	3.08023000	-0.39228000	-1.24924000
N	2.98785000	0.34581000	1.22931000
H	3.38261000	-0.91383000	-3.30753000
H	3.36905000	-2.28088000	-2.14852000
C	4.44526000	-0.48274000	-0.63209000
C	4.39128000	-0.03161000	0.85797000
H	4.67706000	-0.87447000	1.50298000
H	5.07831000	0.80881000	1.06577000
H	4.74548000	-1.53875000	-0.67850000
H	5.16966000	0.10776000	-1.22209000
C	2.75691000	1.01494000	-1.66918000
C	2.66408000	1.74404000	0.78465000
H	1.57301000	1.86824000	0.84943000
H	3.13524000	2.44647000	1.49793000
H	3.29306000	1.22011000	-2.61536000
H	1.67533000	1.06427000	-1.86872000
C	3.16266000	2.04931000	-0.62487000
P	-2.39350000	-0.52981000	-1.42674000
P	-2.59733000	-0.07655000	1.28466000
C	-1.67788000	-2.59204000	0.57078000
N	-2.12244000	-3.66009000	0.87064000
H	3.19093000	-0.71385000	3.04566000
H	3.10805000	1.06452000	3.24593000
C	-2.71714000	1.75857000	1.02330000
C	-2.91021000	1.28290000	-1.54769000
N	-2.53765000	2.20628000	-0.41315000
H	-1.90755000	2.23910000	1.59637000
H	-3.68621000	2.12634000	1.39782000
H	-2.42904000	1.71319000	-2.44005000
H	-4.00282000	1.32473000	-1.68718000

C	-3.23943000	3.52020000	-0.60769000
H	-2.98850000	3.90585000	-1.60542000
H	-2.88445000	4.21913000	0.16243000
H	-4.32409000	3.36719000	-0.51527000
C	-4.22875000	-0.67879000	0.56557000
C	-4.00315000	-1.24656000	-0.85251000
C	-2.76861000	-0.20869000	3.10446000
H	-2.54314000	-1.24645000	3.39487000
H	-3.79330000	0.05169000	3.41533000
H	-2.04614000	0.46715000	3.58877000
C	-2.19726000	-0.97254000	-3.19324000
H	-1.35788000	-0.40393000	-3.62176000
H	-3.12392000	-0.75211000	-3.74824000
H	-1.97310000	-2.04916000	-3.25468000
H	2.74014000	3.02116000	-0.92754000
H	4.25763000	2.17657000	-0.62103000
H	-3.88523000	-2.33990000	-0.83188000
H	-4.82100000	-0.98856000	-1.54478000
H	-4.91458000	0.18470000	0.54412000
H	-4.65132000	-1.43013000	1.25159000
H	-1.24764000	2.66119000	-0.54434000
O	1.08594000	4.91350000	-0.19280000
O	-0.13481000	3.13810000	-0.92100000
C	0.17393000	4.04834000	-0.06327000
H	-0.42603000	4.05806000	0.88256000
H	-0.34714000	0.56860000	0.34697000
H	-0.13347000	0.35699000	-0.45309000

Name-TS910:G=-2847.830525//H=-2847.734074//SPE=-2848.3233153

Angstroms

Atom	X	Y	Z
S	0.52541000	-2.16712000	-1.11793000
Ni	1.81129000	-0.90173000	0.13393000
Fe	-0.99803000	-0.87333000	0.18813000
S	0.59035000	-1.39138000	1.89286000
C	1.16988000	-1.41671000	-2.69542000
C	2.67736000	-1.26867000	-2.54601000
H	0.66991000	-0.45313000	-2.88048000
H	0.93147000	-2.09472000	-3.53172000
C	1.28426000	0.02524000	2.88175000
C	2.78320000	0.07224000	2.61976000
H	1.09024000	-0.16121000	3.95120000
H	0.77329000	0.95844000	2.59642000
N	2.98042000	-0.40368000	-1.35901000
N	3.03255000	0.24388000	1.15092000
H	3.14272000	-0.83458000	-3.45317000
H	3.12917000	-2.25684000	-2.36325000
C	4.35234000	-0.62103000	-0.79526000
C	4.38303000	-0.23243000	0.71224000
H	4.61804000	-1.12432000	1.31002000

H	5.14892000	0.53550000	0.92894000
H	4.57367000	-1.69277000	-0.89511000
H	5.10147000	-0.06042000	-1.38511000
C	2.76115000	1.03995000	-1.71329000
C	2.80608000	1.67679000	0.76567000
H	1.72694000	1.86828000	0.86017000
H	3.34172000	2.32097000	1.48926000
H	3.27548000	1.24243000	-2.67277000
H	1.68028000	1.18556000	-1.86105000
C	3.29211000	1.99228000	-0.64627000
P	-2.45154000	-0.41084000	-1.31725000
P	-2.40585000	0.29344000	1.31386000
C	-1.84978000	-2.50439000	0.62151000
N	-2.36362000	-3.55651000	0.89659000
H	3.24083000	-0.88182000	2.92648000
H	3.27594000	0.89135000	3.18027000
C	-2.61105000	2.08455000	0.75202000
C	-2.64148000	1.41111000	-1.74704000
N	-2.22096000	2.38236000	-0.67410000
H	-1.96465000	2.72245000	1.37490000
H	-3.65873000	2.39807000	0.89074000
H	-2.00964000	1.63353000	-2.62156000
H	-3.69144000	1.62220000	-2.00699000
C	-2.70941000	3.75657000	-1.03849000
H	-2.33101000	4.00867000	-2.03875000
H	-2.32685000	4.47568000	-0.30116000
H	-3.80845000	3.75468000	-1.03429000
C	-4.12446000	-0.34597000	0.90182000
C	-4.15178000	-0.73907000	-0.59480000
C	-2.44574000	0.54290000	3.15563000
H	-1.57179000	0.05224000	3.60880000
H	-3.36139000	0.08940000	3.56753000
H	-2.42933000	1.61330000	3.41421000
C	-2.54155000	-1.12402000	-3.01355000
H	-1.64024000	-0.84588000	-3.58147000
H	-3.44022000	-0.76587000	-3.54331000
H	-2.58127000	-2.22078000	-2.92000000
H	2.95922000	3.01087000	-0.90196000
H	4.39444000	2.01490000	-0.67112000
H	-4.34463000	-1.81649000	-0.72069000
H	-4.91793000	-0.18552000	-1.16260000
H	-4.88079000	0.41650000	1.15256000
H	-4.29287000	-1.22170000	1.54842000
H	-0.94107000	2.62659000	-0.75705000
O	1.38699000	4.84623000	0.07414000
O	0.21636000	3.16492000	-0.91509000
C	0.52010000	3.91913000	0.07515000
H	-0.03166000	3.73268000	1.03322000
H	-0.18039000	0.42185000	-0.15811000

Name-TS1011:G=-2846.657193//H=-2846.514253//SPE=-2847.10382308

Angstroms

Atom	X	Y	Z
S	0.56903000	2.04578000	-0.28658000
Ni	1.99700000	0.40123000	-0.48147000
S	0.68355000	-0.52442000	-1.96788000
C	1.23520000	2.50785000	1.39397000
C	2.75259000	2.51411000	1.23817000
H	0.88612000	1.79303000	2.15572000
H	0.87088000	3.51398000	1.65960000
C	1.57071000	-2.16500000	-1.82714000
C	3.05942000	-1.83030000	-1.84913000
H	1.30529000	-2.77551000	-2.70607000
H	1.31790000	-2.72550000	-0.90961000
N	3.23789000	1.15143000	0.83213000
N	3.39294000	-0.96150000	-0.67022000
H	3.25981000	2.82847000	2.17018000
H	3.03002000	3.21962000	0.43852000
C	4.51324000	1.17050000	0.03954000
C	4.60455000	-0.09705000	-0.86552000
H	4.61313000	0.21225000	-1.92006000
H	5.52395000	-0.67935000	-0.67152000
H	4.47999000	2.06458000	-0.59879000
H	5.38271000	1.26316000	0.71574000
C	3.38328000	0.27410000	2.04767000
C	3.54552000	-1.81502000	0.55498000
H	2.56784000	-2.26360000	0.77810000
H	4.24686000	-2.63469000	0.30601000
H	3.97158000	0.84058000	2.79505000
H	2.40206000	0.05118000	2.49528000
C	4.10038000	-1.03943000	1.74676000
P	-2.73897000	1.36787000	0.40580000
P	-2.67948000	-1.10446000	-0.82274000
C	-1.54645000	1.26606000	-2.09425000
N	-1.81197000	1.86524000	-3.09894000
H	3.30898000	-1.26937000	-2.76389000
H	3.67991000	-2.74709000	-1.82441000
N	-3.77706000	-0.78538000	1.67095000
C	-4.08357000	-1.60998000	2.86876000
H	-4.05310000	-0.97523000	3.76686000
H	-3.33785000	-2.41694000	2.98452000
H	-5.08752000	-2.05550000	2.78105000
C	-4.20566000	-0.20250000	-1.40859000
C	-4.26358000	1.16142000	-0.66816000
C	-2.54464000	-2.65532000	-1.79488000
H	-2.32085000	-2.38950000	-2.84040000
H	-3.48163000	-3.23413000	-1.74974000
H	-1.71159000	-3.25568000	-1.39526000
C	-2.77212000	3.12170000	0.94366000
H	-1.98011000	3.29224000	1.68991000
H	-3.75508000	3.37038000	1.37501000
H	-2.57893000	3.75779000	0.06505000

H	4.01691000	-1.67829000	2.64154000
H	5.17831000	-0.85848000	1.60006000
H	-4.25122000	1.99898000	-1.38298000
H	-5.16292000	1.26348000	-0.03916000
H	-5.08958000	-0.82952000	-1.20741000
H	-4.11926000	-0.06029000	-2.49751000
O	0.67330000	-1.40870000	2.94059000
C	0.23848000	-1.83522000	1.84761000
H	-0.48348000	-0.51030000	0.77645000
Fe	-1.08180000	0.37661000	-0.56271000
O	0.25547000	-2.92960000	1.24606000
C	-3.28645000	-1.79214000	0.83523000
H	-4.01826000	-2.58522000	0.64954000
H	-2.36706000	-2.25207000	1.22212000
C	-3.20830000	0.43045000	1.93447000
H	-2.26016000	0.32595000	2.53833000
H	-3.94387000	0.96017000	2.55411000

(II) Model 2

Name-NiFe:G= -2541.045914//H= -2540.959516//SPE =-2541.4377756

Angstroms

Atom	X	Y	Z
S	-0.78988963	-1.54215856	-1.53858297
Ni	-1.94404719	0.00000429	-0.50457891
Fe	0.83613168	0.00000730	-0.76942097
S	-0.78987755	1.54216692	-1.53857342
C	-1.25447310	-2.87111589	-0.30059956
C	-2.71708262	-2.66854722	0.07222595
H	-0.61834936	-2.78087710	0.59409178
H	-1.09004193	-3.85807723	-0.76062700
C	-1.25444265	2.87111018	-0.30056819
C	-2.71706519	2.66856470	0.07222055
H	-1.08997741	3.85807781	-0.76057013
H	-0.61833385	2.78083250	0.59413047
N	-2.85955397	-1.28507108	0.60798589
N	-2.85958990	1.28507966	0.60794409
H	-3.04018102	-3.41174904	0.82512006
H	-3.36886817	-2.75548657	-0.81164884
C	-4.25044220	-0.77748158	0.80690220
C	-4.25049718	0.77747768	0.80661638
H	-4.85431802	1.14679887	-0.03529890
H	-4.67191144	1.18846272	1.73944800
H	-4.85452858	-1.14714180	-0.03467213
H	-4.67151023	-1.18815813	1.74002331
P	2.15222583	-1.39032912	0.29080009

P	2.15222255	1.39033429	0.29082207
C	1.87759033	-0.00000872	-2.23528989
N	2.54591041	0.00000016	-3.23615805
H	-3.36882686	2.75553890	-0.81166872
H	-3.04016947	3.41175552	0.82512246
C	1.67573650	1.22862108	2.10073082
C	1.67574132	-1.22865984	2.10071109
N	0.89525978	-0.00002179	2.32407085
H	1.03621081	2.09429567	2.34039402
H	2.58701068	1.28587214	2.74000647
H	1.03621825	-2.09434070	2.34035849
H	2.58701445	-1.28591765	2.73998712
C	0.31763838	-0.00003656	3.67436567
H	-0.31326539	-0.89432075	3.80430091
H	-0.31327416	0.89423902	3.80431666
H	1.09543499	-0.00004017	4.47040858
C	3.90796002	0.77137263	0.22987055
C	3.90796157	-0.77136267	0.22985949
C	2.34560871	3.19599747	0.01185432
H	2.66432641	3.35025608	-1.03130114
H	3.11498330	3.59640864	0.69310568
H	1.39677465	3.72472434	0.18033353
C	2.34561202	-3.19597708	0.01174318
H	1.39680186	-3.72472621	0.18028388
H	3.11505513	-3.59641205	0.69290260
H	2.66423378	-3.35017791	-1.03145039
H	4.35457124	-1.17256113	-0.69431243
H	4.45885703	-1.19352830	1.08672118
H	4.45885573	1.19352654	1.08673782
H	4.35456856	1.17258436	-0.69429616
H	-2.35851244	-1.24677665	1.51030042
H	-2.35866127	1.24676333	1.51032213

Name-NiFe10:G= -2541.741641//H= -2541.652440//SPE =-2542.1371685

Angstroms

Atom	X	Y	Z
S	1.02090771	1.63651512	-1.44727293
Ni	1.96911833	0.00768240	-0.30884697
S	1.00335933	-1.50757578	-1.58228509
C	1.46842330	2.90529847	-0.14973899
C	2.89143978	2.63982431	0.32036987
H	0.76327420	2.81757096	0.69279132
H	1.37220163	3.91271696	-0.58721121
C	1.41731182	-2.90594678	-0.41612517
C	2.80268269	-2.67959472	0.17341750
H	1.37508175	-3.85519442	-0.97474048
H	0.66400871	-2.93896029	0.38882110
N	2.93237567	1.24755094	0.84345427
N	2.78092837	-1.35014800	0.84117051
H	3.20730327	3.35804429	1.10182351

H	3.60075626	2.70423001	-0.52137509
C	4.27342672	0.62576327	1.00068673
C	4.07226480	-0.84348783	1.41514288
H	4.90518786	-1.45864010	1.04198823
H	4.03659203	-0.94558629	2.51216452
H	4.76824963	0.68643282	0.01858439
H	4.89177052	1.16916894	1.74028779
P	-2.07413894	1.36690913	0.19397654
P	-2.10796803	-1.33068541	0.02393513
C	-1.45966605	0.12158738	-2.48234105
N	-1.94770204	0.16110972	-3.58400292
H	3.57089463	-2.64834215	-0.61616243
H	3.06888245	-3.47559983	0.89673961
C	-2.24051320	-1.33295809	1.90850556
C	-2.21472560	1.12110606	2.06314670
N	-1.65541513	-0.14766474	2.54905396
H	-1.70008828	-2.22364647	2.27541798
H	-3.31747212	-1.46645161	2.17060953
H	-1.66133613	1.94628019	2.54508712
H	-3.29080098	1.23880561	2.33607344
C	-1.82316743	-0.23709288	4.00463659
H	-1.33016752	0.62185483	4.48998408
H	-1.35557201	-1.16380689	4.37735620
H	-2.89389097	-0.24144604	4.31498343
C	-3.81341512	-0.69670228	-0.44071640
C	-3.79228178	0.84584193	-0.35026396
C	-2.26551248	-3.13602680	-0.34039261
H	-2.34527425	-3.26728048	-1.43144683
H	-3.17056070	-3.54273154	0.14262118
H	-1.38352892	-3.68491989	0.02175460
C	-2.17521580	3.20936748	0.07878992
H	-1.29167292	3.67524825	0.54011277
H	-3.08433664	3.57451338	0.58688863
H	-2.21401653	3.49254672	-0.98516230
H	-3.97049584	1.31006984	-1.33407376
H	-4.54423778	1.23904442	0.35537206
H	-4.57216146	-1.14892157	0.22065864
H	-4.01031669	-1.03855472	-1.46990431
Fe	-0.66001630	0.05736189	-0.77661104
H	2.09413762	-1.40866829	1.60660365
H	2.44308552	1.23432279	1.75162910
H	0.12532780	0.01718626	0.57714319

Name-NiFe1:G= -2542.204244//H= -2542.119544//SPE =-2542.6140193

Angstroms

Atom	X	Y	Z
S	-0.99333157	-1.57421793	-1.35248886
Ni	-2.13180172	-0.00003370	-0.32738631
Fe	0.65710818	0.00010057	-0.59757638
S	-0.99349692	1.57436793	-1.35232684

C	-1.43627591	-2.86764680	-0.07736032
C	-2.89494771	-2.67675197	0.31419250
H	-0.77229986	-2.75367203	0.79540738
H	-1.26940573	-3.86380486	-0.51744837
C	-1.43667782	2.86765937	-0.07713824
C	-2.89533832	2.67653139	0.31433771
H	-1.26992064	3.86386563	-0.51716045
H	-0.77273162	2.75372461	0.79565404
N	-3.04841626	-1.27624660	0.79961236
N	-3.04861878	1.27597747	0.79967506
H	-3.20113298	-3.39356749	1.09945614
H	-3.55698440	-2.80471714	-0.55719868
C	-4.44119528	-0.77719671	0.99462467
C	-4.44133102	0.77670744	0.99456375
H	-5.04053656	1.14901455	0.15057737
H	-4.86388587	1.18891808	1.92690377
H	-5.04044585	-1.14966858	0.15074340
H	-4.86356237	-1.18940861	1.92704851
P	2.23377376	-1.38473897	0.03282137
P	2.23352377	1.38496127	0.03340803
C	1.31021330	0.00032024	-2.33375301
N	1.70045591	0.00046890	-3.46602157
H	-3.55735552	2.80444398	-0.55707643
H	-3.20166731	3.39325845	1.09962616
C	2.53468671	1.22794517	1.88829690
C	2.53496656	-1.22847199	1.88776705
N	1.95099017	-0.00044973	2.44276668
H	2.04770903	2.09074503	2.37371216
H	3.63020719	1.30375750	2.07012778
H	2.04820362	-2.09159282	2.37282746
H	3.63050907	-1.30409788	2.06953559
C	2.05144967	-0.00074921	3.91110269
H	1.55121009	-0.89610495	4.31434551
H	1.55103851	0.89434339	4.31471677
H	3.10620448	-0.00071871	4.26199875
C	3.84476933	0.77396582	-0.68278840
C	3.84491526	-0.77316356	-0.68311287
C	2.26025235	3.19816654	-0.25150923
H	2.17302663	3.38554945	-1.33339992
H	3.20521808	3.62645377	0.12212322
H	1.41126183	3.66825962	0.26717428
C	2.26070235	-3.19780787	-0.25292730
H	1.41175665	-3.66822281	0.26553907
H	3.20571258	-3.62617228	0.12050326
H	2.17348616	-3.38469738	-1.33490415
H	-0.34442906	0.00005298	0.72667493
H	0.43846005	-0.00036218	1.07614053
H	3.91467253	-1.17263182	-1.70708584
H	4.67727221	-1.19215631	-0.09363695
H	4.67706889	1.19287582	-0.09317190
H	3.91441466	1.17387517	-1.70659814
H	-2.54270879	-1.20724457	1.69708360

H	-2.54295139	1.20699942	1.69717107

Name-NiFe9:G=//H=//SPE=

	Angstroms		
Atom	X	Y	Z
S	-0.96679706	1.49772567	-1.57377626
Ni	-2.14255489	0.57093282	0.01524536
S	-0.93054706	1.49526190	1.57377859
C	-1.44400583	0.19026422	-2.82345671
C	-2.93676867	-0.07566671	-2.65181842
H	-0.84879251	-0.71908680	-2.64106409
H	-1.21742165	0.56803151	-3.83331931
C	-1.37855756	0.18946360	2.83693066
C	-2.87514382	-0.07499405	2.70034672
H	-1.12716853	0.56543020	3.84113517
H	-0.79278588	-0.72368036	2.63801228
N	-3.16501515	-0.47492767	-1.23882700
N	-3.13383768	-0.48540531	1.29325192
H	-3.28204064	-0.87025543	-3.33973515
H	-3.52116104	0.83783856	-2.84922188
C	-4.56714520	-0.48209264	-0.73627318
C	-4.54913395	-0.49493559	0.82007790
H	-5.03180615	0.41384290	1.20932617
H	-5.07931253	-1.37180293	1.23022206
H	-5.05421812	0.43545523	-1.09893872
H	-5.11245792	-1.34930564	-1.14740086
P	2.25982190	0.22059780	-1.40407510
P	2.31678344	0.29443735	1.35584878
C	1.27197238	2.54448596	-0.03346485
N	1.60242039	3.69795555	-0.04638675
H	-3.45576343	0.83910134	2.90303276
H	-3.20595127	-0.86499571	3.40004074
C	2.82576473	-1.51625715	1.31615102
C	2.75587867	-1.59216978	-1.27548214
N	2.52097090	-2.26928317	0.05080814
H	2.29350610	-2.04516231	2.12215507
H	3.91001399	-1.57747214	1.50820040
H	2.17331868	-2.16100452	-2.01676749
H	3.82710682	-1.67439608	-1.52385436
C	3.25196589	-3.58283883	0.07005479
H	2.94482775	-4.16461830	-0.81003315
H	2.97845479	-4.12106551	0.98883469
H	4.33469518	-3.39402932	0.04467561
C	3.87038896	1.09274549	0.69822388
C	3.83570296	1.05475991	-0.85009756
C	2.33656525	0.60432486	3.16288700
H	2.16524668	1.68004200	3.32556539
H	3.30776869	0.31401885	3.59603066
H	1.52683173	0.03278393	3.64211341
C	2.23436446	0.41337620	-3.22824129

H	1.41910942	-0.19311324	-3.65157363
H	3.19804661	0.09753181	-3.66048480
H	2.05520075	1.47494348	-3.46077190
H	3.82218343	2.07061115	-1.27598662
H	4.69610893	0.51405287	-1.27570962
H	4.74778848	0.56824470	1.11072219
H	3.88030460	2.12808275	1.07174248
O	-2.02995226	-2.91770811	-0.11344329
C	-0.80259690	-2.61581755	-0.01281852
H	-0.53725913	-1.52031304	-0.03241314
Fe	0.68622736	0.83265474	-0.00877911
O	0.17039423	-3.43260260	0.11122385
H	1.47885826	-2.58595532	0.09042252
H	-2.74338871	-1.43458349	1.15363537
H	-2.76260503	-1.42141965	-1.08613253

Name-NiFe8:G= -2730.625485//H= -2730.529413//SPE =-2731.0493648

Angstroms

Atom	X	Y	Z
S	0.83313676	1.41061215	-1.52237112
Ni	2.18506552	0.06005825	-0.45223317
Fe	-0.73727558	-0.11168172	-0.60644619
S	1.13369881	-1.70235156	-1.19949431
C	1.19891078	2.87383118	-0.42649445
C	2.68467633	2.85543936	-0.08627028
H	0.58651227	2.79299513	0.48584099
H	0.92451872	3.79438265	-0.96591406
C	2.01929663	-2.89738488	-0.06380226
C	3.46239377	-2.42857933	0.08302203
H	1.97520038	-3.89609579	-0.52720114
H	1.51673530	-2.95374369	0.91539045
N	2.98559392	1.53152361	0.52643034
N	3.44245867	-1.01761204	0.55792627
H	2.94472132	3.67315931	0.61252489
H	3.30149794	2.95821488	-0.99355386
C	4.42013515	1.21654293	0.83598286
C	4.71065222	-0.24579679	0.44314814
H	5.02509874	-0.30634582	-0.61061275
H	5.50651590	-0.68335170	1.07332574
H	5.07227452	1.89439111	0.26535582
H	4.59918027	1.38800584	1.90991924
P	-2.50569354	1.15588581	-0.56738246
P	-2.23274817	-1.48747658	0.19233071
C	-1.19317949	-0.50125367	-2.34204295
N	-1.46278297	-0.73243977	-3.48839675
H	3.97761429	-2.44479129	-0.89108087
H	4.02503388	-3.06551110	0.79165813
C	-2.86346900	-0.90435738	1.87890714
C	-3.11585667	1.52997298	1.17407130

N	-2.57142442	0.54536528	2.17024007
H	-2.35315608	-1.48742996	2.66119443
H	-3.95078077	-1.06146011	1.96199905
H	-2.74701692	2.52212040	1.47629312
H	-4.21634096	1.51519083	1.22570416
C	-2.98760516	0.90311042	3.56433704
H	-2.68304420	1.93966604	3.76370205
H	-2.48739333	0.22060992	4.26486747
H	-4.07911791	0.80254991	3.64538168
C	-3.77858753	-1.32023269	-0.83384687
C	-3.94684935	0.16681378	-1.23342683
C	-2.02583995	-3.28483843	0.49983501
H	-1.78297491	-3.77039540	-0.45848961
H	-2.94842563	-3.72326209	0.91509377
H	-1.19060441	-3.43762621	1.20112123
C	-2.63663703	2.79808745	-1.37085182
H	-1.90504173	3.48437038	-0.91728781
H	-3.65492040	3.20474881	-1.25642739
H	-2.40306976	2.67526860	-2.44014106
H	-3.94062242	0.28838038	-2.32749189
H	-4.88220191	0.60041825	-0.84375539
H	-4.64187191	-1.70230267	-0.26519096
H	-3.64056081	-1.95745027	-1.72167051
H	-1.52235154	0.63829994	2.08685104
O	1.41329703	-0.03296291	2.97288408
O	-0.05123799	0.45456709	1.32079491
C	0.62917855	-0.37876163	2.05328795
H	0.46523876	-1.45901295	1.84496039
H	3.13395570	-1.01433973	1.54432581
H	2.45328052	1.47787948	1.41109302

NiFe8B, complex is similar to NiFe8 in which oxygen and hydrogen of formate anion are attached with Fe and Ni, respectively.

Name-NiFe8B:G= -2730.622452//H= -2730.526653//SPE =-2731.0463124

Angstroms

Atom	X	Y	Z
S	-1.01081714	-1.49842326	-1.19261461
Ni	-2.34048753	0.00290394	-0.33619954
Fe	0.72006196	0.03719971	-0.55436488
S	-1.05913245	1.63473465	-1.00921948
C	-1.59056172	-2.81199585	-0.00047533
C	-3.11408130	-2.71975749	0.06168303
H	-1.14020224	-2.64294622	0.99234475
H	-1.26537112	-3.79713479	-0.37231815
C	-1.75671404	2.81526534	0.25976326
C	-3.27435929	2.63925980	0.23892477

H	-1.46872683	3.84223535	-0.01829916
H	-1.34521316	2.59181186	1.25832458
N	-3.45471552	-1.33896764	0.50665865
N	-3.56272415	1.21422986	0.56862264
H	-3.53633131	-3.46800689	0.75826398
H	-3.55811485	-2.87470749	-0.93502164
C	-4.87541570	-0.87980183	0.39668901
C	-4.90229824	0.66478738	0.21631181
H	-5.08111275	0.92081343	-0.83889785
H	-5.69578143	1.12984630	0.82812118
H	-5.32407733	-1.36357284	-0.48319818
H	-5.43700233	-1.19743187	1.29103956
P	2.44100738	-1.31843326	-0.51783487
P	2.38445100	1.43292293	-0.23745128
C	0.95114298	0.18618808	-2.37042931
N	1.06351137	0.27076829	-3.56207644
H	-3.67817848	2.84302676	-0.76651780
H	-3.77188252	3.31172341	0.96218220
C	3.24225002	1.16506389	1.42301252
C	3.30335191	-1.36461373	1.16073372
N	2.95242274	-0.18327186	2.01987535
H	2.85834395	1.91244419	2.13430255
H	4.33330879	1.28623353	1.32188649
H	2.96462011	-2.26023367	1.70408707
H	4.39778753	-1.40659452	1.03611187
C	3.55740151	-0.30853917	3.38026917
H	3.23916381	-1.26431972	3.81882712
H	3.20062403	0.52523474	4.00076612
H	4.65312122	-0.27545457	3.29206820
C	3.75676717	0.97184101	-1.41442491
C	3.79116853	-0.56926986	-1.56755477
C	2.28090734	3.26361676	-0.29786263
H	1.92083948	3.55601471	-1.29681969
H	3.26850779	3.71754791	-0.11264701
H	1.56068475	3.60922905	0.45999769
C	2.41484574	-3.09820792	-0.96213592
H	1.73013531	-3.63160666	-0.28455130
H	3.42661925	-3.53036443	-0.89069152
H	2.04442910	-3.18926175	-1.99532593
H	3.59548598	-0.87007777	-2.60840528
H	4.75908629	-0.99815638	-1.26080864
H	4.70912709	1.37551098	-1.03371762
H	3.53423873	1.46182224	-2.37500551
H	1.87556198	-0.22421504	2.08611740
O	-0.39993045	-0.19518410	3.59413357
O	0.44037695	-0.19936740	1.49927711
C	-0.52292969	-0.05974067	2.34976110
H	-1.51205470	0.19070219	1.90746113
H	-3.17842138	-1.27495857	1.49870772
H	-3.41174151	1.10054327	1.58288755

Name-NiFe2:G= -2542.204975//H= -2542.116848//SPE =-2542.6157599

Angstroms

Atom	X	Y	Z
S	0.89087512	1.51991433	-1.55725842
Ni	1.96381926	-0.00835284	-0.39539267
Fe	-0.72686823	-0.04234621	-0.68761755
S	0.90700995	-1.62424413	-1.45123456
C	1.35335749	2.88832320	-0.37270074
C	2.78673961	2.67926585	0.09577178
H	0.66298857	2.86754888	0.48730771
H	1.24134235	3.85484824	-0.89005684
C	1.41018709	-2.89311878	-0.17440153
C	2.86756484	-2.65222321	0.19205393
H	1.26304177	-3.90022307	-0.59736789
H	0.76359797	-2.78374695	0.71215621
N	2.85270448	1.32576250	0.71103194
N	2.97073134	-1.25631645	0.69911717
H	3.08972302	3.45498965	0.82573038
H	3.48954203	2.69912903	-0.75284376
C	4.20013386	0.82587636	1.14140394
C	4.33366692	-0.66608245	0.77095375
H	4.77724293	-0.77549600	-0.23089746
H	4.97026462	-1.20596461	1.49643212
H	4.97878522	1.40985499	0.62837555
H	4.31109221	0.98378584	2.22664211
P	-2.17859533	1.36025776	0.08134018
P	-2.14237641	-1.39090562	0.23056883
C	-1.56835009	-0.10346347	-2.36115591
N	-2.09108679	-0.14011361	-3.44319775
H	3.51506769	-2.73548192	-0.69623247
H	3.22308757	-3.36978264	0.95618561
C	-2.12733792	-1.15439993	2.11319604
C	-2.15262171	1.34740653	1.97656522
N	-1.41935825	0.12563487	2.44240611
H	-1.55070602	-1.97427925	2.56826078
H	-3.14197195	-1.12928087	2.54025825
H	-1.58974262	2.22482327	2.33059300
H	-3.16439111	1.35219937	2.41126355
C	-0.99266212	0.20705187	3.86813745
H	-0.39371320	1.11910616	4.00178561
H	-0.38620535	-0.67953603	4.10174289
H	-1.88069718	0.23914066	4.51569053
C	-3.87574072	-0.83360408	-0.19142393
C	-3.89779350	0.70925570	-0.26908120
C	-2.24402451	-3.22356818	0.09695636
H	-2.31579964	-3.48716577	-0.97011854
H	-3.13691636	-3.59469206	0.62750422
H	-1.34351564	-3.68998339	0.52279017
C	-2.33397314	3.15890646	-0.27506890
H	-1.43312417	3.69611127	0.05576245
H	-3.21926574	3.57399739	0.23505765

H	-2.44769514	3.28278848	-1.36382116
H	0.18649074	0.00079471	0.63403866
H	-4.16107513	1.05670590	-1.28120176
H	-4.61050669	1.15805765	0.44257330
H	-4.58036099	-1.22985953	0.55859501
H	-4.12160629	-1.28796847	-1.16514375
H	-0.55685531	0.09636793	1.76792170
H	2.53528209	-1.22757276	1.63404477
H	2.24083721	1.34213294	1.54053549

Name-TS12:G= -2542.205522//H= -2542.117478//SPE =-2542.6114511

Angstroms

Atom	X	Y	Z
S	-0.87284472	-1.53953132	-1.48286641
Ni	-2.01483424	0.00524107	-0.41971735
Fe	0.73888028	0.02490852	-0.63589442
S	-0.88604781	1.60462876	-1.41746565
C	-1.34416121	-2.87621771	-0.26422960
C	-2.79976631	-2.68248793	0.13763889
H	-0.68480663	-2.80787843	0.61756805
H	-1.19089507	-3.85706423	-0.74220727
C	-1.39035993	2.87696986	-0.14338105
C	-2.86019938	2.66158264	0.18920548
H	-1.21682824	3.88222605	-0.56011480
H	-0.76241298	2.75413743	0.75504420
N	-2.92532431	-1.30352151	0.68492235
N	-3.00500006	1.26067341	0.67285415
H	-3.11292224	-3.43047739	0.89118318
H	-3.46669721	-2.76100781	-0.73594410
C	-4.30247322	-0.81237905	1.01205844
C	-4.38506680	0.70784067	0.73277369
H	-4.83976479	0.89132076	-0.25274368
H	-4.98958944	1.22844666	1.49751273
H	-5.02269881	-1.34668890	0.37522931
H	-4.53201316	-1.04807964	2.06434717
P	2.22545717	-1.37736576	0.10707152
P	2.20210955	1.39832509	0.20306046
C	1.53942612	0.06326871	-2.30976553
N	2.03774015	0.08468816	-3.40194757
H	-3.48741756	2.77275773	-0.71024739
H	-3.21440867	3.37499860	0.95736370
C	2.17425216	1.17451252	2.08671337
C	2.19136219	-1.29350915	2.00093802
N	1.46464421	-0.07717720	2.40661949
H	1.60709136	2.01401333	2.51941961
H	3.20333548	1.18267647	2.49069133
H	1.63507287	-2.17004903	2.37037072
H	3.21940520	-1.31652743	2.40723090
C	0.92615633	-0.12898314	3.77717434
H	0.30674783	-1.03325649	3.88311985

H	0.29881619	0.75975218	3.94816832
H	1.73389160	-0.15236064	4.53134724
C	3.91616567	0.81401156	-0.24598690
C	3.93000703	-0.73021668	-0.29751354
C	2.29355144	3.22265394	0.00421570
H	2.36666439	3.45510695	-1.06992349
H	3.18164082	3.61684272	0.52600677
H	1.38738280	3.69261597	0.41424792
C	2.35182788	-3.17865144	-0.23288852
H	1.44667833	-3.69456362	0.12007502
H	3.23730037	-3.59915262	0.27242920
H	2.44887932	-3.32248221	-1.32073459
H	-0.22928814	0.00277728	0.69731765
H	4.17499662	-1.09572560	-1.30779172
H	4.65508306	-1.16782306	0.40888727
H	4.63469589	1.21730722	0.48715025
H	4.15233641	1.25008624	-1.23026829
H	0.47953901	-0.04208897	1.35737026
H	-2.57346767	1.20753894	1.60907080
H	-2.36184769	-1.27070752	1.54864246

Name-TS23: G= -2730.581595//H= -2730.497974//SPE =-2731.0114372

Angstroms

Atom	X	Y	Z
S	-0.96372651	1.40069947	1.57073740
Ni	-2.10233222	-0.12184030	0.48979570
S	-0.81730419	-1.72612975	1.23389176
C	-1.70058830	2.80734970	0.58781959
C	-3.18927198	2.52268141	0.42490243
H	-1.20029552	2.88487715	-0.38927617
H	-1.53463882	3.74310165	1.14612997
C	-1.32003268	-2.91538362	-0.11278046
C	-2.82433362	-2.77555198	-0.31710585
H	-1.05456988	-3.93704260	0.20363484
H	-0.76789830	-2.67518779	-1.03634475
N	-3.32890420	1.19720053	-0.24334722
N	-3.09173682	-1.34813716	-0.64574285
H	-3.69347337	3.30794816	-0.16918438
H	-3.68352832	2.45578600	1.40799677
C	-4.64793749	0.51497158	-0.12789050
C	-4.52099367	-0.90131391	-0.73041590
H	-5.15012568	-1.60449090	-0.16467806
H	-4.84262515	-0.92252832	-1.78461764
H	-4.87841511	0.45567356	0.94718407
H	-5.44625055	1.09485217	-0.62644410
P	2.28584490	1.42112608	0.17607512
P	2.44685587	-1.33717089	0.21855636
C	1.29756713	-0.12524707	2.45725243
N	1.60586629	-0.18954879	3.61531534
H	-3.37173266	-3.02085052	0.60748519

H	-3.18644089	-3.43522682	-1.12861339
C	2.96280415	-1.24514981	-1.59564633
C	2.80045275	1.26922521	-1.64134041
N	2.32467989	-0.03678564	-2.21337941
H	2.57500027	-2.12723366	-2.12763756
H	4.05419788	-1.17841297	-1.72372630
H	2.30970594	2.07026310	-2.21400505
H	3.89197012	1.33490018	-1.77112376
C	2.38147267	-0.05661481	-3.70718537
H	1.81340740	0.80245365	-4.09126167
H	1.93603277	-0.99612676	-4.06215562
H	3.43219253	0.01146557	-4.02134885
C	3.97040402	-0.61816385	1.03770211
C	3.87492282	0.92840058	1.02466061
C	2.54133065	-3.13978353	0.54882458
H	2.35471971	-3.30331767	1.62197170
H	3.53723025	-3.53075727	0.28266494
H	1.76753628	-3.66057526	-0.03579360
C	2.16581267	3.24379293	0.35756228
H	1.31317980	3.60660006	-0.23779373
H	3.09398736	3.73540244	0.02191750
H	1.98664326	3.47444797	1.41948343
H	3.82703165	1.33346826	2.04802376
H	4.72864483	1.39732188	0.50808248
H	4.86715713	-0.98555224	0.51228237
H	3.99201003	-1.00688560	2.06754698
O	-1.10431873	-0.43168115	-2.85616713
C	-0.71212017	0.61419371	-2.40917910
H	0.12274748	0.06403269	-0.87383872
Fe	0.76646396	-0.04276628	0.67279139
O	-0.51595168	1.79724254	-2.39903854
H	1.32058253	-0.10005829	-1.86663601
H	-2.64746849	-1.16857623	-1.55953070
H	-3.10740244	1.32720351	-1.24214455

Name-TS1011:G=

	Angstroms		
Atom	X	Y	Z
S	1.32243141	-1.74088413	-1.06115276
Ni	2.38267377	-0.19157025	0.09031011
S	1.27125143	-0.71505960	1.91449736
C	1.89888786	-1.02509652	-2.68857842
C	3.37050858	-0.65215279	-2.56194211
H	1.29608851	-0.13312662	-2.92105300
H	1.74341392	-1.77376771	-3.48314545
C	1.75998864	0.86479464	2.78489988
C	3.21486088	1.17869345	2.46422497
H	1.61635165	0.73034094	3.86955420
H	1.10343431	1.68394292	2.44369240
N	3.49153745	0.31337273	-1.43275638

N	3.33286332	1.26088959	0.98303592
H	3.76039507	-0.20273053	-3.49566884
H	3.98167770	-1.53649738	-2.31819865
C	4.84283441	0.49687055	-0.84154591
C	4.71454406	1.39105778	0.41053254
H	5.44496899	1.06624949	1.16680983
H	4.90953101	2.45118237	0.17814887
H	5.20108970	-0.50403614	-0.55371352
H	5.55211680	0.92485156	-1.57495013
P	-1.66561299	0.11055384	-1.46952146
P	-1.68941656	0.90167933	1.12345011
C	-1.23253119	-1.96995755	0.60882139
N	-1.81055742	-2.97980577	0.92314310
H	3.87754749	0.36926435	2.81163092
H	3.53993898	2.12718710	2.93508692
N	-2.22574827	2.81322505	-0.87095410
C	-2.10548312	4.21335515	-1.29877274
H	-1.04635716	4.54216410	-1.39934970
H	-2.59918231	4.87159180	-0.56445820
H	-2.59973336	4.34885723	-2.27522228
C	-3.42717381	0.37184650	0.65645154
C	-3.41870767	-0.06373380	-0.82968038
C	-1.80892368	1.17290734	2.94809613
H	-1.77949903	0.19612967	3.45647376
H	-2.75310633	1.68742529	3.19418834
H	-0.96337596	1.78265269	3.30173017
C	-1.71901142	-0.66162026	-3.14710890
H	-0.82246254	-0.37913496	-3.71990711
H	-2.61816774	-0.33416623	-3.69593087
H	-1.73395789	-1.75708908	-3.03228966
H	-3.69884067	-1.12418034	-0.94276616
H	-4.10467368	0.53828450	-1.44874687
H	-4.14214721	1.18770276	0.85541612
H	-3.67826603	-0.47378130	1.31752692
O	1.55448071	2.09435346	-1.88024240
C	1.32050573	2.30261552	-0.71443999
H	0.68594805	0.94193734	-0.28419054
Fe	-0.30326907	-0.40809381	0.12138779
O	1.37999326	2.91245657	0.32916439
C	-1.65029313	1.93595585	-1.90852057
H	-0.59391048	2.18611012	-2.14163393
H	-2.23919127	2.08472588	-2.83166893
C	-1.66286662	2.66412533	0.48449224
H	-2.26468883	3.29807918	1.16054703
H	-0.60151877	2.99904306	0.56060478
H	3.14892454	1.22378292	-1.77085195
H	2.78706360	2.08517105	0.69018044

3. Optimized geometries of complexes involved in splitting of CO_3^{2-}, HCO_3^-, HCO_3H with their computed thermodynamic data.

Name-CO_3^{2-}: G= -263.852919//H= -263.823735//SPE =-263.840367

Angstroms

Atom	X	Y	Z
C	0.00000000	0.00000000	-0.00160500
O	0.00000000	0.00000000	1.31557000
O	0.00000000	1.14010800	-0.65718300
O	0.00000000	-1.14010800	-0.65718300

Name-HCO_3^-: G= -264.320533//H= -264.290198//SPE =-264.3201271

Angstroms

Atom	X	Y	Z
C	-0.13024400	0.04980300	-0.00006500
O	-1.16804400	-0.67610600	0.00003200
O	-0.03898900	1.31700400	0.00000800
O	1.07935000	-0.67626400	-0.00002100
H	1.80292900	-0.01589500	0.00024100

Name-HCO_3H: G= -264.755925//H= -264.725056//SPE =-264.7670189

Angstroms

Atom	X	Y	Z
C	0.04392500	0.12191400	-0.00004100
O	0.62028900	1.20653600	0.00007200
O	-1.30111600	0.02842000	-0.00012200
H	-1.57907700	-0.91343100	0.00075400
O	0.64333900	-1.09301400	0.00003400
H	1.61543100	-0.95359200	-0.00037500

Name-H_2O: G=-76.359441//H= -76.337974//SPE =-76.3623209

Angstroms

Atom	X	Y	Z
O	0.00000000	0.00000000	0.12037000
H	0.00000000	0.76754500	-0.48148200
H	0.00000000	-0.76754500	-0.48148200

Name-NiFe16: G= -2921.402683//H= -2921.301231//SPE =-2921.8637091

Angstroms

Atom	X	Y	Z

S	-0.85549700	-0.53368000	-2.08779100
Ni	-2.08852600	0.39076400	-0.53393000
Fe	0.93216400	0.37459000	-0.63796000
S	-0.73063200	2.10398700	-0.48742400
C	-1.66053100	-2.20246100	-1.88998600
C	-3.15233400	-1.96171000	-1.69026200
H	-1.20334800	-2.74100400	-1.04580800
H	-1.48933200	-2.78496500	-2.81064800
C	-1.31556300	2.65506700	1.18840000
C	-2.83395400	2.51676000	1.19199100
H	-1.02393800	3.70791600	1.33727700
H	-0.83743800	2.04670700	1.97217400
N	-3.36892500	-1.08869300	-0.49064700
N	-3.21027700	1.09343500	0.90567600
H	-3.70720400	-2.91293800	-1.56432800
H	-3.56378400	-1.43174000	-2.56413900
C	-4.68741700	-0.37509300	-0.49088100
C	-4.59392300	0.93183900	0.35308900
H	-4.78164800	1.79636600	-0.29912000
H	-5.33864700	0.95238500	1.17052900
H	-4.91256100	-0.11572600	-1.53503700
H	-5.48550700	-1.04810000	-0.12548200
C	-3.18865300	-1.89517500	0.76221800
C	-3.01169200	0.26126100	2.14198100
H	-1.92942800	0.20381300	2.33154800
H	-3.49014200	0.78730000	2.99087600
H	-3.80088700	-2.81369700	0.67010400
H	-2.13099700	-2.19300100	0.81623600
C	-3.61092700	-1.13697200	2.01783900
P	2.58485600	-1.02756400	-0.89383500
P	2.57080100	1.38067300	0.38669200
C	1.39669700	1.21566000	-2.20280600
N	1.66649600	1.77611700	-3.23357800
H	-3.26546500	3.14250100	0.39446700
H	-3.27378700	2.83192000	2.15878300
N	3.98105100	-0.74771400	1.54346600
C	4.41183700	-1.40995400	2.78393200
H	3.55256000	-1.78151500	3.38771700
H	4.98941100	-0.70315100	3.40263800
H	5.05951000	-2.26895100	2.54147700
C	4.07444200	1.31602700	-0.72283000
C	4.07193800	-0.04533500	-1.46908300
C	2.46972200	3.11214100	1.00361500
H	2.10753600	3.75806900	0.18835200
H	3.45633300	3.46345200	1.34914700
H	1.75057400	3.15572000	1.83746000
C	2.50542500	-2.50212000	-1.99337700
H	1.73951800	-3.19210200	-1.60490900
H	3.47975400	-3.01561100	-2.04936500
H	2.20202400	-2.16765300	-2.99836200
H	-3.28291700	-1.72240600	2.89277200
H	-4.71097300	-1.08427700	2.07722200

H	3.97108200	0.09642700	-2.55652900
H	4.99031000	-0.62515600	-1.28013600
H	4.98420800	1.46033000	-0.11773600
H	3.99211700	2.15898200	-1.42709600
O	0.20658400	-2.66710400	1.00151700
O	0.25995300	-0.38304700	1.17258800
O	-0.05922200	-1.63511000	3.00721000
C	0.13986100	-1.58004700	1.71272900
C	3.28652100	-1.73909600	0.69487000
H	2.45749900	-2.25469700	1.22080100
H	4.02667900	-2.50728500	0.40601900
C	3.18262100	0.44322200	1.88869300
H	3.82685800	1.12292100	2.47390100
H	2.28637600	0.20287000	2.50104500

Name-NiFe14:G= -2921.503743//H= -2921.758483//SPE =-2922.3340528

Angstroms

Atom	X	Y	Z
S	-0.79273700	-0.18478300	-2.10129200
Ni	-2.08711700	0.47261300	-0.46535500
Fe	0.95007200	0.49518500	-0.56408600
S	-0.73835200	2.15132400	-0.11157000
C	-1.54915200	-1.88598800	-2.15508200
C	-3.05514000	-1.69778500	-2.00012400
H	-1.11382000	-2.51519200	-1.36423100
H	-1.31906100	-2.34023000	-3.13304400
C	-1.39999000	2.46481200	1.60250000
C	-2.91597600	2.32088700	1.51268100
H	-1.12981100	3.49195100	1.89823500
H	-0.95729400	1.77439000	2.33745400
N	-3.34961400	-0.99844700	-0.70364400
N	-3.27541600	0.95360300	1.00887600
H	-3.59115800	-2.66651800	-2.03040100
H	-3.43785800	-1.06408300	-2.81591600
C	-4.66599400	-0.27991600	-0.67944200
C	-4.62615500	0.88286100	0.35991700
H	-4.78083900	1.83697500	-0.16294600
H	-5.41453700	0.78129300	1.12833200
H	-4.82141700	0.14047500	-1.68301800
H	-5.48642300	-0.99195600	-0.47307100
C	-3.25072100	-1.98120500	0.42656300
C	-3.14944700	-0.05034500	2.11977300
H	-2.08296200	-0.13691300	2.37287800
H	-3.68173300	0.34869500	3.00467000
H	-3.86598100	-2.86403900	0.16594000
H	-2.20400900	-2.30731200	0.49065200
C	-3.73460100	-1.41297600	1.75739400
P	2.60330300	-0.85331500	-1.07127100
P	2.60447300	1.31620300	0.60682700

C	1.41811200	1.60021400	-1.93617900
N	1.68802200	2.33617500	-2.84678800
H	-3.31196900	3.05401800	0.79214000
H	-3.39991500	2.49856900	2.49292600
N	3.99732400	-0.98399000	1.38403200
C	4.43263900	-1.84837200	2.49197200
H	3.57330100	-2.29876600	3.03870600
H	5.03087200	-1.26161300	3.20839600
H	5.06049900	-2.66548100	2.10031100
C	4.09645900	1.41804000	-0.51673800
C	4.08744100	0.20167900	-1.48129500
C	2.51520000	2.93609800	1.46865800
H	2.15659600	3.69114100	0.75139700
H	3.50487900	3.22857800	1.85663400
H	1.79634700	2.86632900	2.30056200
C	2.48383000	-2.13666600	-2.37961500
H	1.73219400	-2.88257400	-2.07510600
H	3.45586400	-2.62970900	-2.54575900
H	2.14599800	-1.65227100	-3.30932200
H	-3.45159800	-2.12369600	2.55145900
H	-4.83603400	-1.36208200	1.76742700
H	3.98447100	0.52357900	-2.52937500
H	5.00210600	-0.40676900	-1.39324400
H	5.01035700	1.45754900	0.09722600
H	4.01112000	2.36604800	-1.07083500
O	0.14997900	-2.90607400	0.62296000
O	0.22274200	-0.68705100	1.07956700
O	-0.05872900	-2.16167700	2.77936800
C	0.09829100	-2.03790800	1.53034100
C	3.27687500	-1.80960400	0.39516600
H	2.43569600	-2.37804400	0.83990700
H	3.99285300	-2.54750300	-0.00863500
C	3.22932300	0.14768900	1.93260700
H	3.90095600	0.72210100	2.59485300
H	2.35781200	-0.17617900	2.54440400
H	0.17258300	-0.12878800	1.88194900

Name-NiFe17:G= -2733.098274//H= -2733.339512//SPE =-2733.8965121

Angstroms

Atom	X	Y	Z
S	0.70070000	1.54230000	-1.44068100
Ni	1.98162100	-0.00000700	-0.55773600
Fe	-0.99177900	-0.00013900	-0.60423700
S	0.70074800	-1.54233100	-1.44072800
C	1.36034100	2.86006700	-0.30979900
C	2.87078600	2.66950600	-0.22389700
H	0.86916500	2.77850600	0.67336600
H	1.12200400	3.84905500	-0.73567700
C	1.36038900	-2.86008600	-0.30982700

C	2.87083000	-2.66949700	-0.22383300
H	1.12209800	-3.84908200	-0.73571400
H	0.86915500	-2.77854100	0.67331000
N	3.17565300	1.29733100	0.29996000
N	3.17567400	-1.29730000	0.30000100
H	3.34595100	3.43160500	0.42530300
H	3.31105300	2.74999700	-1.23065500
C	4.52798500	0.78022400	-0.08996200
C	4.52799500	-0.78017600	-0.08994200
H	4.72571400	-1.14105900	-1.10907700
H	5.30573800	-1.19480100	0.57848700
H	4.72571000	1.14108400	-1.10910400
H	5.30571600	1.19488000	0.57846100
C	2.99178500	1.28099200	1.78971600
C	2.99181900	-1.28091600	1.78975500
H	1.91738700	-1.41023800	1.98865300
H	3.53500200	-2.14752100	2.21380300
H	3.53493700	2.14763100	2.21373100
H	1.91734400	1.41029500	1.98858700
C	3.50741500	0.00005600	2.43761000
P	-2.59172100	1.36384600	-0.04453900
P	-2.59180600	-1.36392000	-0.04433100
C	-1.58006800	-0.00005100	-2.35343300
N	-1.93172600	0.00000500	-3.50592700
H	3.31116000	-2.75000900	-1.23056100
H	3.34596700	-3.43157200	0.42541500
N	-2.64676300	0.00026600	2.42386800
C	-3.04485300	0.00040300	3.83795800
H	-2.63874900	0.89526800	4.33771700
H	-2.63907100	-0.89455900	4.33780200
H	-4.15098200	0.00061000	3.96281200
C	-4.16362500	-0.77490800	-0.87491200
C	-4.16368500	0.77468400	-0.87480800
C	-2.59205200	-3.18633800	-0.30930000
H	-2.44716500	-3.38322000	-1.38349900
H	-3.54437300	-3.63370700	0.02247500
H	-1.75759900	-3.63559700	0.25206400
C	-2.59184900	3.18615500	-0.31018500
H	-1.75726300	3.63555100	0.25087500
H	-3.54407500	3.63374100	0.02157000
H	-2.44711400	3.38259300	-1.38448400
H	3.18633800	0.00006800	3.49256500
H	4.61006500	0.00007100	2.45343900
H	-4.15954200	1.17364500	-1.90132600
H	-5.03580300	1.19413000	-0.34570000
H	-5.03583300	-1.19450000	-0.34606400
H	-4.15918100	-1.17373100	-1.90148100
O	-0.13261900	-0.00036000	1.24339500
H	-0.90493700	-0.00006400	1.86210600
C	-3.09543200	1.24171600	1.77191300
H	-2.62398700	2.08797900	2.30104400
H	-4.20011000	1.37814800	1.83685400

C	-3.09575700	-1.24113600	1.77203700
H	-4.20049200	-1.37718200	1.83683800
H	-2.62470200	-2.08746900	2.30140600

Name-NiFe18:G=-2733.198073//H=-2733.805924//SPE=-2734.3769589

Angstroms

Atom	X	Y	Z
S	0.73282000	1.50303900	-1.40757500
Ni	2.04564200	0.00375600	-0.50350500
Fe	-0.94204700	-0.02441800	-0.63429100
S	0.77260800	-1.55423000	-1.36049300
C	1.33491800	2.84385000	-0.26667300
C	2.85042100	2.69324700	-0.17458900
H	0.84022000	2.75388000	0.71303300
H	1.07121500	3.82323900	-0.69863500
C	1.45511600	-2.86469000	-0.22457600
C	2.96371700	-2.64277700	-0.15723000
H	1.23177800	-3.85461900	-0.65530400
H	0.97569100	-2.80781100	0.76594500
N	3.19353200	1.33086000	0.35419800
N	3.25264900	-1.26526900	0.36505900
H	3.29853000	3.47080000	0.47434700
H	3.29306800	2.78383600	-1.17939200
C	4.55844500	0.84332700	-0.03427300
C	4.59118100	-0.71815200	-0.03796700
H	4.78582000	-1.07312100	-1.05969100
H	5.38317900	-1.11698900	0.62278400
H	4.74988200	1.21049800	-1.05221900
H	5.32521800	1.27298700	0.63647500
C	3.00550700	1.31024900	1.84436200
C	3.08960200	-1.25267300	1.85683300
H	2.02845600	-1.43330700	2.07804900
H	3.67442300	-2.09550600	2.27246100
H	3.52011200	2.19410500	2.26745300
H	1.92818900	1.40780500	2.04303200
C	3.56261100	0.04879000	2.49622300
P	-2.56487400	1.35233000	-0.14544700
P	-2.54336000	-1.39101900	-0.04179000
C	-1.50966500	-0.07282100	-2.36840600
N	-1.84064200	-0.10554300	-3.52327900
H	3.39359100	-2.71497500	-1.16892200
H	3.45679200	-3.39836300	0.48522000
N	-3.75054600	0.05751300	2.04924700
C	-4.07547200	0.11029900	3.48210900

H	-3.16362000	0.14746500	4.12066200
H	-4.65978200	-0.78091700	3.76354500
H	-4.68246000	1.00606800	3.69235400
C	-4.11195300	-0.83981700	-0.89092500
C	-4.12358200	0.71048600	-0.95053400
C	-2.46109500	-3.21558100	-0.24178100
H	-2.16268800	-3.44120300	-1.27759100
H	-3.43695400	-3.68000200	-0.02322600
H	-1.69830500	-3.61859100	0.44350300
C	-2.51341300	3.15458200	-0.49972700
H	-1.75945900	3.63117700	0.14709500
H	-3.49854500	3.61656400	-0.32176500
H	-2.21949800	3.29443300	-1.55192400
H	3.24578400	0.04362000	3.55225600
H	4.66448400	0.08422600	2.50811900
H	-4.11732700	1.06988800	-1.99155800
H	-5.00030300	1.14242600	-0.44150100
H	-4.98277700	-1.24496100	-0.35054700
H	-4.09889400	-1.27856600	-1.90123100
O	-0.05379000	0.00490800	1.29526200
C	-3.06936500	1.30214100	1.66035100
H	-2.17079100	1.52377200	2.28436000
H	-3.77121900	2.13846000	1.82693700
C	-3.02573600	-1.19238800	1.76188200
H	-3.69354000	-2.03374200	2.01782000
H	-2.10725400	-1.30714300	2.38182900
H	-0.10782100	-0.88055300	1.70579300
H	-0.46535000	0.60356000	1.94864000

Name-TS1417:G=-2921.496042//H=-2921.223735//SPE=-2922.2312120

Angstroms

Atom	X	Y	Z
S	0.76344300	2.17399300	0.32497400
Ni	2.11491300	0.59660100	-0.36675900
Fe	-1.00040800	0.65912600	-0.43464200
S	0.80232600	0.27038200	-2.08426100
C	1.44428000	2.14304400	2.05808400
C	2.95998300	2.02480100	1.93783700
H	1.00112300	1.31317000	2.63148100
H	1.17419200	3.08845500	2.55783700
C	1.56994400	-1.38134500	-2.48621600
C	3.07667100	-1.23539600	-2.29369700
H	1.34701400	-1.62207500	-3.53917800
H	1.13611900	-2.17176500	-1.85486200
N	3.31599400	0.78566600	1.16809400
N	3.38003900	-0.80624400	-0.88800900
H	3.44712300	1.99600900	2.93222900
H	3.35611400	2.88940200	1.38208300

C	4.66196200	0.84413500	0.50557700
C	4.69858900	-0.10644300	-0.73111800
H	4.85996000	0.48859400	-1.64127600
H	5.51713800	-0.84650800	-0.65793200
H	4.80887300	1.88058800	0.16964000
H	5.45828400	0.60468200	1.23421000
C	3.20916100	-0.41185300	2.07112400
C	3.28559200	-1.98616800	0.03744400
H	2.23543300	-2.31243500	0.04800000
H	3.89180100	-2.80799900	-0.39116900
H	3.75921500	-0.18569000	3.00507300
H	2.14676300	-0.54789500	2.32775900
C	3.78562200	-1.67974200	1.44844700
P	-2.63394200	1.18839800	0.90459900
P	-2.65198200	-0.52236300	-1.22536100
C	-1.43458700	2.05545500	-1.55313600
N	-1.67146200	2.97852300	-2.28982800
H	3.46007000	-0.45388300	-2.96894800
H	3.60838300	-2.18127000	-2.51885100
N	-4.01464700	-1.24298800	1.13735300
C	-4.43759400	-2.34144800	2.01904300
H	-3.57387700	-2.90851900	2.43525500
H	-5.07387900	-3.04568200	1.45764600
H	-5.02413600	-1.93818000	2.86086900
C	-4.14419500	0.59932900	-1.35693400
C	-4.15091800	1.54826400	-0.12866900
C	-2.58231800	-1.46606300	-2.80663200
H	-2.29862800	-0.77761500	-3.61870400
H	-3.55655500	-1.92867100	-3.03750500
H	-1.81087900	-2.24902300	-2.72198300
C	-2.55194400	2.54802600	2.14496600
H	-1.79897000	2.29914200	2.90991200
H	-3.53157600	2.69929900	2.62860600
H	-2.24524700	3.47490100	1.63495800
H	3.51457100	-2.53053900	2.09594300
H	4.88733100	-1.63159900	1.45123300
H	-4.09661600	2.60450700	-0.43788600
H	-5.05350200	1.42044700	0.49072800
H	-5.06363300	-0.00544900	-1.42381900
H	-4.03866200	1.16575900	-2.29594400
O	0.09219600	-3.12041000	2.28346000
O	-0.34059600	-0.83715800	0.83611000
O	-0.14706000	-3.54586000	-0.02248300
C	-0.05597000	-3.16107700	1.10206800
C	-3.23875200	-0.26472200	1.92399300
H	-2.34880400	-0.71658600	2.41568700
H	-3.90020200	0.12824000	2.71660900
C	-3.30082500	-1.81151900	-0.02386800
H	-4.01167700	-2.45296900	-0.57480300
H	-2.44573300	-2.44847600	0.28015900
H	0.61867700	-0.71392600	0.66706300

Name-TS18:G= -2733.197363//H= -2733.023735//SPE =-2733.840367

Angstroms

Atom	X	Y	Z
S	0.75587714	1.49883140	-1.60740117
Ni	2.06869914	-0.00045160	-0.70333117
Fe	-0.91898986	-0.02862560	-0.83411717
S	0.79566514	-1.55843760	-1.56031917
C	1.35797514	2.83964240	-0.46649917
C	2.87347814	2.68903940	-0.37441517
H	0.86327714	2.74967240	0.51320683
H	1.09427214	3.81903140	-0.89846117
C	1.47817314	-2.86889760	-0.42440217
C	2.98677414	-2.64698460	-0.35705617
H	1.25483514	-3.85882660	-0.85513017
H	0.99874814	-2.81201860	0.56611883
N	3.21658914	1.32665240	0.15437183
N	3.27570614	-1.26947660	0.16523283
H	3.32158714	3.46659240	0.27452083
H	3.31612514	2.77962840	-1.37921817
C	4.58150214	0.83911940	-0.23409917
C	4.61423814	-0.72235960	-0.23779317
H	4.80887714	-1.07732860	-1.25951717
H	5.40623614	-1.12119660	0.42295783
H	4.77293914	1.20629040	-1.25204517
H	5.34827514	1.26877940	0.43664883
C	3.02856414	1.30604140	1.64453583
C	3.11265914	-1.25688060	1.65700683
H	2.05151314	-1.43751460	1.87822283
H	3.69748014	-2.09971360	2.07263483
H	3.54316914	2.18989740	2.06762683
H	1.95124614	1.40359740	1.84320583
C	3.58566814	0.04458240	2.29639683
P	-2.54181686	1.34812240	-0.34527317
P	-2.52030286	-1.39522660	-0.24161617
C	-1.48660786	-0.07702860	-2.56823217
N	-1.81758486	-0.10975060	-3.72310517
H	3.41664814	-2.71918260	-1.36874817
H	3.47984914	-3.40257060	0.28539383
N	-3.72748886	0.05330540	1.84942083
C	-4.05241486	0.10609140	3.28228283
H	-3.14056286	0.14325740	3.92083583
H	-4.63672486	-0.78512460	3.56371883
H	-4.65940286	1.00186040	3.49252783
C	-4.08889586	-0.84402460	-1.09075117
C	-4.10052486	0.70627840	-1.15036017
C	-2.43803786	-3.21978860	-0.44160717
H	-2.13963086	-3.44541060	-1.47741717
H	-3.41389686	-3.68420960	-0.22305217

H	-1.67524786	-3.62279860	0.24367683
C	-2.49035586	3.15037440	-0.69955317
H	-1.73640186	3.62696940	-0.05273117
H	-3.47548786	3.61235640	-0.52159117
H	-2.19644086	3.29022540	-1.75175017
H	3.26884114	0.03941240	3.35242983
H	4.68754114	0.08001840	2.30829283
H	-4.09426986	1.06568040	-2.19138417
H	-4.97724586	1.13821840	-0.64132717
H	-4.95971986	-1.24916860	-0.55037317
H	-4.07583686	-1.28277360	-2.10105717
O	-0.07684714	0.00911560	1.49508817
C	-3.04630786	1.29793340	1.46052483
H	-2.14773386	1.51956440	2.08453383
H	-3.74816186	2.13425240	1.62711083
C	-3.00267886	-1.19659560	1.56205583
H	-3.67048286	-2.03794960	1.81799383
H	-2.08419686	-1.31135060	2.18200283
H	-0.13087814	-0.87634540	1.90561917
H	-0.48840714	0.60776760	2.14846617

Name-NiFe15:G=-2921.865157//H=-2921.762188//SPE=-2922.3375238

Angstroms

Atom	X	Y	Z
S	-0.83795403	-0.48282843	-2.07816113
Ni	-2.08609979	0.41410262	-0.52249261
Fe	0.94510709	0.40371151	-0.62801039
S	-0.71621866	2.11441018	-0.42804467
C	-1.66663067	-2.14640446	-1.93828863
C	-3.15846029	-1.88499783	-1.75989629
H	-1.23584295	-2.71826087	-1.10310916
H	-1.48772433	-2.70312866	-2.87313495
C	-1.29144942	2.61370733	1.26725608
C	-2.81192390	2.49756080	1.26239508
H	-0.98427542	3.65587105	1.45428372
H	-0.82324788	1.97043964	2.02843044
N	-3.38583110	-1.04713082	-0.53648554
N	-3.20938716	1.09010684	0.92574758
H	-3.73044674	-2.83049742	-1.67665156
H	-3.54384926	-1.32048324	-2.62381928
C	-4.68962833	-0.30595849	-0.54066437
C	-4.58930690	0.96786480	0.35278554
H	-4.75834487	1.85836091	-0.26868985
H	-5.34257287	0.96848183	1.16225477
H	-4.88525874	-0.00465659	-1.57945108
H	-5.50883264	-0.97489030	-0.21701934
C	-3.25553522	-1.89845785	0.69171880
C	-3.03619037	0.21587368	2.13664139

H	-1.95717584	0.13649497	2.33512794
H	-3.51161563	0.72396585	2.99776726
H	-3.90186671	-2.78829544	0.56168594
H	-2.21371572	-2.24193415	0.74578603
C	-3.66383580	-1.16510361	1.96719778
P	2.60332428	-0.98950913	-0.92878967
P	2.58111636	1.38070887	0.43807631
C	1.41467249	1.28263700	-2.16243416
N	1.68534354	1.87308720	-3.17456128
H	-3.23248506	3.15724733	0.48681143
H	-3.24849249	2.78480998	2.23890864
N	3.97910060	-0.79449162	1.52373671
C	4.41026563	-1.49817650	2.74112665
H	3.55081023	-1.89706705	3.32693870
H	4.98022982	-0.81026407	3.38715064
H	5.06461563	-2.34317449	2.46979151
C	4.08694864	1.35293951	-0.66620251
C	4.09119588	0.01644687	-1.45572161
C	2.47534944	3.08595744	1.11886801
H	2.10965723	3.76096351	0.32925719
H	3.46276902	3.42497704	1.47385665
H	1.75935593	3.09653523	1.95638588
C	2.52475859	-2.41781188	-2.08436037
H	1.75315960	-3.12041454	-1.73173879
H	3.49793504	-2.93152449	-2.15317880
H	2.23114043	-2.04098811	-3.07718349
H	-3.35691198	-1.78313379	2.82721827
H	-4.76249505	-1.08742722	2.02077751
H	3.99760808	0.19335131	-2.53855805
H	5.00868160	-0.56807384	-1.27866303
H	4.99377680	1.48037730	-0.05324159
H	4.00415800	2.21785726	-1.34315580
O	0.17717932	-2.63541582	0.81111324
O	0.25686768	-0.40934818	1.16835985
C	0.09807864	-1.55891757	1.68872567
C	3.29438871	-1.75752362	0.63860880
H	2.47416135	-2.30078367	1.14989222
H	4.03825978	-2.51197971	0.32464708
C	3.17556193	0.38066955	1.90646047
H	3.81290135	1.03699930	2.52479269
H	2.27550125	0.11766024	2.50360457
H	0.04936632	-3.44397498	1.34943149
O	-0.13091023	-1.80035469	2.91133816

Name-NiFe13:G=-2922.297531//H=-2922.185922//SPE=-2922.7753945

Angstroms

Atom	X	Y	Z
S	-0.78966252	0.14659126	2.08231704
Ni	-2.09151364	-0.49331382	0.44995180
Fe	0.96114600	-0.51134174	0.54750985
S	-0.72528619	-2.14460814	0.05261115
C	-1.57633520	1.83122817	2.20616483

C	-3.07950264	1.61852913	2.05240232
H	-1.16039006	2.50668882	1.44589946
H	-1.35068365	2.24662105	3.20207058
C	-1.39221752	-2.43523630	-1.66475274
C	-2.90912549	-2.31239081	-1.55768087
H	-1.11218924	-3.45434644	-1.97818380
H	-0.96404339	-1.72882017	-2.39292028
N	-3.37315802	0.95108022	0.73849380
N	-3.28370690	-0.96074370	-1.02212458
H	-3.63198685	2.57616598	2.11512182
H	-3.44439351	0.95479572	2.85210653
C	-4.67953546	0.21365954	0.70512425
C	-4.63029243	-0.92445480	-0.36065550
H	-4.76622447	-1.89197032	0.14217091
H	-5.42581700	-0.81826905	-1.12084860
H	-4.82272893	-0.23184589	1.69954912
H	-5.51073021	0.91880237	0.52043229
C	-3.30087482	1.96278119	-0.36660444
C	-3.18126844	0.07095418	-2.10965425
H	-2.11895773	0.17217901	-2.37538406
H	-3.72026896	-0.31230180	-2.99734728
H	-3.93264396	2.82635926	-0.08226556
H	-2.26302797	2.31421554	-0.42440468
C	-3.77962577	1.41810907	-1.70927057
P	2.61902331	0.82640295	1.09215034
P	2.62340976	-1.32169840	-0.62374085
C	1.41583203	-1.63980792	1.89626726
N	1.67251159	-2.39605778	2.79280151
H	-3.28840878	-3.06548999	-0.84882853
H	-3.39898285	-2.47733143	-2.53700989
N	4.03544412	0.98178462	-1.34701580
C	4.50471024	1.85616442	-2.43308324
H	3.66286925	2.32827784	-2.98864188
H	5.10694367	1.27082013	-3.14704285
H	5.13748452	2.65710351	-2.01697104
C	4.10431177	-1.44290743	0.51119575
C	4.09189460	-0.24254676	1.49562096
C	2.52825550	-2.92741167	-1.50808501
H	2.15382073	-3.68853614	-0.80554621
H	3.52007373	-3.22340909	-1.88752981
H	1.82038657	-2.83857898	-2.34747413
C	2.48746898	2.09060842	2.41591672
H	1.73241099	2.83652357	2.12021658
H	3.45634852	2.58645423	2.59122013
H	2.15031540	1.59109827	3.33778227
H	-3.51108792	2.15125056	-2.48775752
H	-4.88021190	1.35286749	-1.71471674
H	3.97647973	-0.58124136	2.53702590
H	5.01008207	0.36284869	1.42661712
H	5.02203467	-1.47390722	-0.09722039
H	4.01366918	-2.39931608	1.04959443
O	0.15289639	2.84865025	-0.49177181

O	0.24589532	0.75133322	-1.14401228
C	0.06075271	2.03167804	-1.54522895
C	3.30738577	1.79912455	-0.35976150
H	2.47878762	2.37926688	-0.81344282
H	4.01996716	2.53073724	0.06073443
C	3.26673429	-0.13408144	-1.92466974
H	3.94283738	-0.70372478	-2.58634708
H	2.40754531	0.20607499	-2.54534942
H	0.17946873	0.18880337	-1.94594208
H	0.01815160	3.76813819	-0.80973681
O	-0.16387600	2.35400769	-2.70960171

4. Optimized geometries of CN substituted complexes with their corresponding thermodynamic energies.

Name-NiFeF:G= -2664.568453//H= -2664.477856//SPE =-2665.0137534

Angstroms

Atom	X	Y	Z
S	-0.49035467	-1.53360655	-1.79543436
Ni	-1.65720794	0.00000780	-0.75957974
Fe	1.09632838	0.00001340	-0.91992188
S	-0.49036088	1.53365430	-1.79539603
C	-1.03999725	-2.89496911	-0.64553092
C	-2.51442594	-2.66406807	-0.34271626
H	-0.42914545	-2.88423507	0.26872640
H	-0.89759387	-3.86416817	-1.14998751
C	-1.04003451	2.89498501	-0.64546756
C	-2.51446482	2.66406306	-0.34268353
H	-0.89763186	3.86419828	-1.14989701
H	-0.42920610	2.88423545	0.26880437
N	-2.70946175	-1.30093641	0.25193660
N	-2.70948427	1.30092235	0.25195320
H	-2.90663479	-3.43277242	0.35105809
H	-3.09844847	-2.70584497	-1.27540091
C	-4.10768663	-0.77881858	0.10224153
C	-4.10769996	0.77878322	0.10224546
H	-4.48276821	1.13690055	-0.86649507
H	-4.75447646	1.19582891	0.89513633
H	-4.48275446	-1.13693724	-0.86649875
H	-4.75445119	-1.19587960	0.89513416
C	-2.27532749	-1.28667353	1.69077407
C	-2.27535549	1.28665147	1.69079133
H	-1.18387061	1.42841312	1.71635650
H	-2.74691069	2.15000813	2.19848259
H	-2.74685947	-2.15004795	2.19845691
H	-1.18383930	-1.42840908	1.71633295
C	-2.67481260	-0.00002042	2.41143029
P	2.39257053	-1.39121840	0.16770266

P	2.39259527	1.39121234	0.16772421
H	-3.09847159	2.70584302	-1.27537780
H	-2.90669484	3.43275336	0.35109439
C	1.97563607	1.22947419	1.98877028
C	1.97555074	-1.22953188	1.98873816
N	1.21202854	-0.00000684	2.24730502
H	1.33799693	2.09192896	2.24815740
H	2.90718609	1.29651688	2.59914999
H	1.33783714	-2.09195134	2.24806076
H	2.90707433	-1.29667423	2.59914829
C	0.70715792	-0.00001122	3.62512593
H	0.08732034	-0.89554751	3.79300033
H	0.08737451	0.89555738	3.79302742
H	1.52988455	-0.00004763	4.37624788
C	4.14829336	0.77188588	0.04809630
C	4.14828414	-0.77190230	0.04815405
C	2.57980805	3.20609553	-0.07797497
H	2.86585635	3.38898511	-1.12596647
H	3.36608020	3.59735840	0.58963130
H	1.63268259	3.72480056	0.13105775
C	2.57979156	-3.20609923	-0.07800805
H	1.63263062	-3.72479371	0.13089305
H	3.36597288	-3.59738028	0.58969487
H	2.86597450	-3.38897730	-1.12596464
H	-2.18575355	-0.00002264	3.39845979
H	-3.75908024	-0.00003421	2.61131544
H	4.56196577	-1.17280246	-0.89124063
H	4.73195979	-1.19350163	0.88391361
H	4.73204446	1.19354362	0.88377382
H	4.56189728	1.17270893	-0.89136541
F	2.25602426	0.00003208	-2.46123506

Name-NiFeH:G= -2565.363622//H= -2565.276013//SPE =-2565.815279

Angstroms

Atom	X	Y	Z
S	-0.49747759	-1.51253496	-1.81910530
Ni	-1.65894797	0.00001692	-0.75493069
Fe	1.10344202	-0.00011795	-1.02702965
S	-0.49733818	1.51245859	-1.81910236
C	-1.00649276	-2.88800082	-0.65639962
C	-2.47183353	-2.66012935	-0.30284248
H	-0.36217528	-2.88571384	0.23508132
H	-0.88403316	-3.85299512	-1.17403733
C	-1.00617641	2.88794176	-0.65633734
C	-2.47155312	2.66023985	-0.30280430
H	-0.88358586	3.85294670	-1.17392429
H	-0.36187942	2.88552752	0.23516106
N	-2.65198252	-1.30084832	0.30435896
N	-2.65186442	1.30097330	0.30438369
H	-2.83932211	-3.43501823	0.39829971

H	-3.08581999	-2.69848036	-1.21642143
C	-4.05618362	-0.77996524	0.22265161
C	-4.05611060	0.78021915	0.22263417
H	-4.47646450	1.13894918	-0.72727192
H	-4.66609267	1.19593695	1.04527147
H	-4.47660345	-1.13867432	-0.72723326
H	-4.66617792	-1.19561285	1.04531434
C	-2.14623336	-1.28702096	1.71883154
C	-2.14619178	1.28711139	1.71887905
H	-1.05529049	1.43300260	1.68976723
H	-2.59271051	2.14973043	2.25061386
H	-2.59271794	-2.14965282	2.25057299
H	-1.05533106	-1.43290490	1.68965458
C	-2.50426562	0.00003643	2.45991899
P	2.46213540	-1.37357787	-0.05777326
P	2.46231556	1.37338149	-0.05809604
H	-3.08552821	2.69867637	-1.21638721
H	-2.83895200	3.43516655	0.39834276
C	2.16257043	1.23249941	1.79581108
C	2.16254625	-1.23206430	1.79612475
N	1.42933965	0.00026460	2.11792937
H	1.53131252	2.09121917	2.08370660
H	3.12889485	1.31861097	2.34884662
H	1.53132162	-2.09069498	2.08435581
H	3.12892095	-1.31799596	2.34909935
C	1.02613280	0.00044140	3.52732708
H	0.41923348	-0.89475131	3.74086496
H	0.41928981	0.89572000	3.74066229
H	1.89914118	0.00049529	4.22052650
C	4.22482068	0.77139238	-0.24460486
C	4.22471451	-0.77190006	-0.24452976
C	2.64549854	3.19227285	-0.30556630
H	2.91315210	3.37869984	-1.35789132
H	3.44235629	3.58635456	0.34798087
H	1.70181068	3.71089470	-0.08104306
C	2.64507067	-3.19258376	-0.30463300
H	1.70136686	-3.71102433	-0.07975300
H	3.44199437	-3.58651133	0.34892694
H	2.91252881	-3.37942938	-1.35693386
H	-1.95948875	0.00000755	3.41783617
H	-3.57570436	0.00004748	2.71959687
H	4.59967166	-1.17766403	-1.19850583
H	4.83981267	-1.19360436	0.56870264
H	4.83990061	1.19309088	0.56864458
H	4.59993980	1.17700827	-1.19858077
H	1.98224059	-0.00026433	-2.23312180

Name-NiFeNCS:G= -3055.581961//H= -3055.487049//SPE =-3056.0350702

Angstroms

Atom	X	Y	Z

S	0.28070533	-1.65235409	-1.54127115
Ni	1.71802053	-1.04199453	-0.00849915
Fe	-0.97283269	-0.34861281	-0.00128485
S	0.28094300	-1.68303214	1.51211908
C	1.15406581	-0.72297371	-2.90489782
C	2.65050260	-0.87612977	-2.66707488
H	0.84417132	0.33191271	-2.90492484
H	0.87103847	-1.17042838	-3.87101081
C	1.15321282	-0.77812173	2.89267826
C	2.65011723	-0.92310105	2.65301977
H	0.87123265	-1.24382866	3.85047401
H	0.84005481	0.27556967	2.91190172
N	3.01109972	-0.37224917	-1.30073937
N	3.01082444	-0.39485108	1.29568953
H	3.23447236	-0.32859144	-3.43220230
H	2.93027717	-1.94031708	-2.71018498
C	4.30840563	-0.92307560	-0.78598511
C	4.30833691	-0.93649168	0.77161695
H	4.38532694	-1.97481332	1.12262538
H	5.15546698	-0.36757794	1.19517632
H	4.38523066	-1.95527123	-1.15478119
H	5.15580387	-0.34722020	-1.19954612
C	3.00135028	1.13107626	-1.27165471
C	3.00290638	1.10863666	1.29356015
H	1.96120249	1.44031912	1.42308235
H	3.58914148	1.45492911	2.16604991
H	3.58494565	1.49422802	-2.13900261
H	1.95847121	1.46254244	-1.39203244
C	3.60025016	1.69349965	0.01553948
P	-1.89887209	1.08145149	-1.38369540
P	-1.89186223	1.06575924	1.40275828
H	2.93249866	-1.98719493	2.67840268
H	3.23219654	-0.38754463	3.42799790
C	-0.94781188	2.67684872	1.24758855
C	-0.95311254	2.68997087	-1.21938758
N	-0.15032528	2.70878726	0.01248949
H	-0.25347499	2.71797994	2.10442516
H	-1.65201770	3.53759178	1.33490892
H	-0.26230416	2.73770193	-2.07878625
H	-1.65634173	3.55253461	-1.29544400
C	0.73053391	3.88319261	0.01654220
H	1.37150851	3.86987464	-0.87976684
H	1.37412415	3.86206267	0.91077937
H	0.15822459	4.83879981	0.02162483
C	-3.60311660	1.47556400	0.78767720
C	-3.60677035	1.48488268	-0.75533307
C	-2.13433686	0.85365378	3.21177391
H	-2.69686248	-0.07811635	3.38080357
H	-2.70726192	1.70614800	3.61361977
H	-1.16517496	0.78944725	3.72698859
C	-2.15052382	0.88288710	-3.19278292
H	-1.18383108	0.82361818	-3.71313210

H	-2.72635358	1.73755208	-3.58574186
H	-2.71280330	-0.04829456	-3.36586943
H	3.42343795	2.78069234	0.02515414
H	4.69487119	1.56237783	0.01371396
H	-4.28324459	0.71406296	-1.15985318
H	-3.91142132	2.45961660	-1.17133454
H	-3.90621268	2.44509511	1.21683473
H	-4.27725664	0.69953402	1.18608193
C	-3.55025465	-1.96966427	-0.01187019
N	-2.49366870	-1.40962237	-0.00754706
S	-4.98896636	-2.76847332	-0.01815429

Name-NiFeOH: G= -2640.537383//H= -2640.446956//SPE =-2640.9943366

Angstroms

Atom	X	Y	Z
S	-0.48050393	-1.53266822	-1.78849068
Ni	-1.64545758	-0.00012368	-0.75887652
Fe	1.14794336	-0.00021761	-0.95764982
S	-0.48070674	1.53219665	-1.78916387
C	-1.03277808	-2.89267430	-0.63960282
C	-2.51252613	-2.66611430	-0.35542291
H	-0.43313635	-2.87644305	0.28214243
H	-0.88081162	-3.86344058	-1.13845810
C	-1.03303308	2.89246428	-0.64062705
C	-2.51276124	2.66590285	-0.35631763
H	-0.88114585	3.86311682	-1.13972869
H	-0.43338322	2.87650618	0.28112086
N	-2.72095225	-1.30270219	0.23323222
N	-2.72108204	1.30267784	0.23281188
H	-2.91001825	-3.43544129	0.33474416
H	-3.08392308	-2.71307340	-1.29569317
C	-4.11443220	-0.77928594	0.05280786
C	-4.11450141	0.77904749	0.05249456
H	-4.46857930	1.13644299	-0.92448376
H	-4.77979431	1.19497241	0.83072228
H	-4.46854149	-1.13710477	-0.92400401
H	-4.77963338	-1.19497641	0.83123654
C	-2.31895690	-1.28694275	1.68039462
C	-2.31916635	1.28746508	1.67999910
H	-1.22871881	1.42867893	1.72852874
H	-2.80143729	2.15016107	2.17898005
H	-2.80102392	-2.14957690	2.17967739
H	-1.22847733	-1.42789908	1.72891894
C	-2.73447406	0.00033555	2.39099997
P	2.39150216	-1.38595489	0.18309500
P	2.39160219	1.38624461	0.18233051
H	-3.08420263	2.71251289	-1.29657910

H	-2.91027444	3.43543470	0.33360690
C	1.90837353	1.23183860	1.98926700
C	1.90793611	-1.23111336	1.98984051
N	1.14749892	0.00055385	2.23832548
H	1.25645629	2.09141498	2.22148354
H	2.82105358	1.31373796	2.62627184
H	1.25561016	-2.09036788	2.22210087
H	2.82041537	-1.31318871	2.62711170
C	0.62847376	0.00095648	3.61089782
H	0.00684414	-0.89446739	3.77305679
H	0.00697997	0.89655976	3.77259403
H	1.44337284	0.00108193	4.37076599
C	4.15766339	0.77251282	0.16050755
C	4.15759895	-0.77213026	0.16135507
C	2.59376700	3.20161183	-0.05056422
H	2.95388161	3.38522647	-1.07530124
H	3.33010841	3.59337428	0.67143993
H	1.63346482	3.71888541	0.08990388
C	2.59398842	-3.20129582	-0.04965455
H	1.63394320	-3.71885009	0.09155989
H	3.33096955	-3.59277026	0.67185228
H	2.95341688	-3.38488827	-1.07463743
H	-2.26912181	0.00052073	3.38944296
H	-3.82332334	0.00027713	2.56473990
H	4.63093137	-1.17776063	-0.74846886
H	4.68869544	-1.19289211	1.03160423
H	4.68920737	1.19421738	1.03003174
H	4.63060208	1.17711888	-0.74998206
O	2.29150944	-0.00165939	-2.53492858
H	3.23732550	-0.00068074	-2.29718109

Name-NiFeP:G= -3230.590754//H= -3230.492807//SPE =-3231.0245879

Angstroms

Atom	X	Y	Z
S	-0.17607794	-1.60822901	-1.76421484
Ni	-1.44598481	-0.00007593	-0.95022005
Fe	1.31241369	-0.00010990	-0.77565265
S	-0.17599620	1.60789080	-1.76446720
C	-0.73701096	-3.03678443	-0.67978577
C	-2.26707322	-3.05476812	-0.54292280
H	-0.26599049	-2.93849438	0.31001634
H	-0.37967232	-3.96824470	-1.14809894
C	-0.73683997	3.03659234	-0.68018502
C	-2.26690786	3.05471851	-0.54337340
H	-0.37940995	3.96798492	-1.14856345
H	-0.26585795	2.93833957	0.30964154
H	-2.60171487	-3.84031100	0.15715098
H	-2.75898404	-3.20877384	-1.51826424
C	-4.48123233	-0.78291131	-0.25895666
C	-4.48121829	0.78296334	-0.25916001

H	-4.78088366	1.17117410	-1.24524944
H	-5.16604762	1.19415458	0.50026681
H	-4.78096089	-1.17137386	-1.24492788
H	-5.16603324	-1.19389015	0.50061092
C	-2.51288140	-1.31446298	1.88823227
C	-2.51297561	1.31484742	1.88800340
H	-1.43461594	1.46292257	2.06745506
H	-3.05028865	2.17322098	2.32766936
H	-3.05007222	-2.17281189	2.32809444
H	-1.43449033	-1.46238464	2.06763160
C	-3.02546172	0.00022764	2.51351464
P	2.54776914	-1.39021208	0.37889577
P	2.54793726	1.39023681	0.37843692
C	2.46425289	-0.00028963	-2.15405525
N	3.20597289	-0.00079881	-3.10199365
H	-2.75877012	3.20865870	-1.51874946
H	-2.60150398	3.84036825	0.15660199
C	1.97883753	1.23323048	2.16026326
C	1.97840637	-1.23262987	2.16058409
N	1.20228129	0.00046064	2.36572403
H	1.31601889	2.09240700	2.35859246
H	2.85771057	1.31227002	2.84246141
H	1.31522070	-2.09151919	2.35893184
H	2.85713226	-1.31189528	2.84294980
C	0.60748684	0.00072492	3.70823621
H	-0.02200779	-0.89446829	3.83599027
H	-0.02175413	0.89612998	3.83575688
H	1.37974450	0.00071774	4.51073522
C	4.30517974	0.77148913	0.41642571
C	4.30507547	-0.77160534	0.41690601
C	2.76138012	3.19806037	0.12742471
H	3.11617671	3.36719940	-0.90164839
H	3.50963349	3.58327241	0.84031635
H	1.81048552	3.72924056	0.27386233
C	2.76114675	-3.19814933	0.12861923
H	1.81019153	-3.72921957	0.27504948
H	3.50921382	-3.58312237	0.84183644
H	3.11617688	-3.36772628	-0.90030066
H	-2.74338488	0.00033229	3.58075202
H	-4.12937777	0.00018554	2.48706209
H	4.80256951	-1.17343245	-0.48058777
H	4.80681492	-1.19356924	1.30352910
H	4.80719269	1.19394673	1.30265894
H	4.80248731	1.17268911	-0.48145000
P	-2.73871803	-1.37003279	0.05544386
P	-2.73870228	1.37009244	0.05519168

Name-NiFePy:G= -2774.065563//H= -2773.970004//SPE =-2774.5780348
Angstroms

Atom	X	Y	Z
S	-0.29231574	-1.57220452	1.56301979
Ni	-1.73486109	-0.99895376	0.02324142
Fe	0.98700829	-0.31811778	0.00834488
S	-0.28869654	-1.65253124	-1.47893729
C	-1.17198382	-0.62211163	2.90835650
C	-2.66827925	-0.79701828	2.67812043
H	-0.87360029	0.43625240	2.88374192
H	-0.88247104	-1.04357301	3.88439657
C	-1.15923940	-0.77016273	-2.87468382
C	-2.65765916	-0.92403570	-2.64362097
H	-0.86890695	-1.24329036	-3.82659997
H	-0.85172174	0.28537408	-2.90311977
N	-3.03791600	-0.32282393	1.30415110
N	-3.03250566	-0.38448663	-1.29465875
H	-3.25735711	-0.24394406	3.43564866
H	-2.93377286	-1.86401379	2.74060546
C	-4.32484283	-0.90101958	0.79492533
C	-4.32151988	-0.93823156	-0.76374616
H	-4.38191328	-1.98306844	-1.09860030
H	-5.17818376	-0.38990083	-1.19583816
H	-4.38692813	-1.92874685	1.17902842
H	-5.18344132	-0.33288554	1.19658491
C	-3.04991842	1.17913631	1.25082605
C	-3.05003009	1.11777533	-1.31531529
H	-2.01472065	1.46484448	-1.45420276
H	-3.64419170	1.44130549	-2.19152220
H	-3.63961315	1.54907650	2.11144661
H	-2.01182345	1.52631886	1.36735539
C	-3.65500411	1.71341118	-0.04557860
P	1.89829182	1.14371742	1.36487761
P	1.89467106	1.08479973	-1.41289470
H	-2.92983437	-1.99111293	-2.65942673
H	-3.23926643	-0.40328448	-3.42925017
C	0.92040991	2.68411022	-1.28098266
C	0.91482875	2.73085336	1.17767873
N	0.11390563	2.72340166	-0.05364101
H	0.23285245	2.70556348	-2.14396217
H	1.61238835	3.55477904	-1.37448214
H	0.22265348	2.77525810	2.03633655
H	1.60079542	3.60863290	1.24482589
C	-0.78186148	3.88554528	-0.07723689
H	-1.42596530	3.87696441	0.81702643
H	-1.42246018	3.84419736	-0.97311375
H	-0.22197595	4.84867537	-0.09374486
C	3.59797810	1.55148361	-0.80766407
C	3.59728914	1.59429889	0.73494552
C	2.14067584	0.92941579	-3.23256422
H	2.81048399	0.08051807	-3.43870879
H	2.60032551	1.85417181	-3.62096912
H	1.17839147	0.76194521	-3.73797078
C	2.15066432	1.06025107	3.18842180

H	1.19049343	0.90543014	3.70171144
H	2.60466515	2.00244795	3.53983079
H	2.82667808	0.22430787	3.42489006
H	-3.49356595	2.80282581	-0.07155356
H	-4.74776921	1.56739402	-0.04209631
H	4.29609087	0.85453849	1.15820311
H	3.86874452	2.58781990	1.13018420
H	3.88177149	2.51823599	-1.25701768
H	4.28784090	0.78067444	-1.18808424
N	2.52804437	-1.49660699	0.03108663
C	3.18822272	-1.96018196	1.14891964
C	3.17490321	-2.01468505	-1.07056304
C	4.26021540	-2.78446521	0.76639312
H	2.84899970	-1.68921972	2.14830619
C	4.25109259	-2.82023325	-0.66106752
H	2.82463345	-1.79062192	-2.07776540
H	4.94898506	-3.29850352	1.44004924
H	4.93199009	-3.36680957	-1.31688202

Name-NiFeSCH3:G=-3002.637686//H=-3002.544232//SPE=-3003.119091

Angstroms

Atom	X	Y	Z
S	-0.29131493	-2.11642731	-0.72872658
Ni	-1.69304094	-0.44348282	-0.71826074
Fe	1.08014084	-0.21486642	-0.58038220
S	-0.44638295	0.55379887	-2.21129972
C	-0.94696514	-2.83097775	0.86781652
C	-2.46222122	-2.67605749	0.83696876
H	-0.50111021	-2.30938525	1.72793400
H	-0.66890890	-3.89596101	0.92065029
C	-1.24826393	2.21817240	-1.93912517
C	-2.74016287	1.97251426	-1.75068705
H	-1.07310899	2.84508694	-2.82836585
H	-0.79947698	2.71771974	-1.06767397
N	-2.82659876	-1.23225465	0.66184137
N	-2.96480649	1.03773053	-0.60025099
H	-2.92611092	-3.06973089	1.76246167
H	-2.87600889	-3.22855580	-0.02117186
C	-4.20553180	-1.02650286	0.10916106
C	-4.28839512	0.33308392	-0.64840990
H	-4.51026616	0.14313608	-1.70787353
H	-5.08293146	0.98641900	-0.24399312
H	-4.39069883	-1.84476332	-0.60089027
H	-4.95610534	-1.09891428	0.91750465
C	-2.63071431	-0.48113460	1.94844424
C	-2.77792810	1.75914761	0.70400242
H	-1.71383213	2.02816808	0.79091430
H	-3.36956426	2.69427625	0.66767485
H	-3.11402834	-1.05709387	2.76101456
H	-1.54905178	-0.43710150	2.14895005

C	-3.22589505	0.92467835	1.90184406
P	2.23730314	-0.74898665	1.18672478
P	2.09766123	1.65990590	-0.14963174
H	-3.15565416	1.49323122	-2.65122648
H	-3.28541558	2.92060605	-1.57478117
C	1.32237314	2.34292004	1.42047146
C	1.47681490	0.19597225	2.62691211
N	0.61360185	1.29412599	2.16932011
H	0.58207460	3.10127150	1.11187690
H	2.10339050	2.85708001	2.03025399
H	0.84745813	-0.52325085	3.17902275
H	2.28474381	0.53974430	3.31634353
C	-0.09100231	1.88369697	3.31259185
H	-0.67551329	1.10605229	3.83085013
H	-0.78113851	2.66802327	2.96126822
H	0.60835887	2.34195440	4.04947428
C	3.86827975	1.34412184	0.36269388
C	3.95275835	-0.01829198	1.08085479
C	2.25109170	3.15314220	-1.21789995
H	2.78007747	2.87152421	-2.14231192
H	2.82597073	3.93537789	-0.69391914
H	1.25722494	3.54449929	-1.47952870
C	2.54818820	-2.40288448	1.94254296
H	1.59927802	-2.92093856	2.14399801
H	3.10341067	-2.28020244	2.88801787
H	3.14664914	-3.01128055	1.24781905
H	-2.92009652	1.45331775	2.81865168
H	-4.32649893	0.87139252	1.93508850
H	4.57289070	-0.73254412	0.51612429
H	4.37053502	0.06642035	2.09841350
H	4.20516273	2.17885352	1.00047599
H	4.47019062	1.34863292	-0.55947160
S	2.60006729	-0.83650395	-2.15267946
C	3.26767084	-2.48637048	-1.70190745
H	3.82097321	-2.87943585	-2.57328193
H	3.96695742	-2.43730695	-0.85041159
H	2.45332376	-3.18854150	-1.45576823

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Angstroms

Atom	X	Y	Z
S	0.21846158	2.16387270	-0.45934270
Ni	1.71318083	0.58287924	-0.66901793
Fe	-1.02876169	0.17255053	-0.51624261
S	0.48649648	-0.28915615	-2.25322515
C	0.86656547	2.71960582	1.20005750
C	2.38615219	2.65940078	1.12397677
H	0.47172075	2.07435036	1.99794086
H	0.52776678	3.75185751	1.38263868
C	1.37010555	-1.93312478	-2.18503501

C	2.85099395	-1.63074704	-1.99434170
H	1.20415580	-2.46200174	-3.13711943
H	0.96593941	-2.54806357	-1.36728691
N	2.82511578	1.26660727	0.77649740
N	3.05636271	-0.82740219	-0.74395559
H	2.84848801	2.96739268	2.08170585
H	2.75044592	3.32976045	0.32977722
C	4.20242298	1.20393947	0.18268027
C	4.33955598	-0.04946137	-0.73303768
H	4.52527533	0.27809222	-1.76561570
H	5.17613848	-0.70189855	-0.42423198
H	4.32924238	2.11038823	-0.42550416
H	4.96231520	1.22080434	0.98463276
C	2.69690112	0.36353857	1.97148433
C	2.93627909	-1.70538456	0.46967172
H	1.89025333	-2.04047081	0.53627494
H	3.57752149	-2.59379296	0.31366066
H	3.17078950	0.86819381	2.83488221
H	1.62386156	0.24217027	2.18764945
C	3.36302450	-0.99213431	1.75151946
P	-2.18536833	0.41239000	1.33534053
P	-1.96055055	-1.80610952	-0.32498312
H	3.22291411	-1.02986621	-2.83890991
H	3.44471424	-2.56383200	-1.94095579
C	-1.14323451	-2.63794600	1.14443954
C	-1.35238845	-0.67414142	2.61881352
N	-0.45610543	-1.65911103	1.99872670
H	-0.38565326	-3.33019935	0.73844429
H	-1.89867465	-3.24401722	1.69840673
H	-0.74101843	-0.00413254	3.24741237
H	-2.12874371	-1.14146741	3.26995273
C	0.31558127	-2.35431458	3.03572088
H	0.87757940	-1.61930881	3.63421321
H	1.03097636	-3.04822455	2.56561767
H	-0.33702895	-2.93899695	3.72355541
C	-3.73641654	-1.61475384	0.21438724
C	-3.86590057	-0.37124445	1.11830479
C	-2.05673641	-3.13602579	-1.59122762
H	-2.60097849	-2.74600336	-2.46609348
H	-2.59995197	-4.00438939	-1.18190252
H	-1.05009009	-3.44724688	-1.90508482
C	-2.56805506	1.94672354	2.27653507
H	-1.64497710	2.41887563	2.64243831
H	-3.21559234	1.69862883	3.13441288
H	-3.09465667	2.64801954	1.61069736
H	3.10364516	-1.64019404	2.60356129
H	4.45960182	-0.88206299	1.77482542
H	-4.51631379	0.39356993	0.66304338
H	-4.27233980	-0.61320763	2.11472758
H	-4.04841570	-2.54129581	0.72510652
H	-4.34008034	-1.51038636	-0.70130518
C	-3.35651623	2.24568558	-1.32009243

N	-3.92146470	3.19738343	-0.86733982
S	-2.60112497	0.91701968	-2.00572965

Name-TSF:G=-2854.101351//H=-2853.974252//SPE=-2854.61094959

Angstroms

Atom	X	Y	Z
S	0.53989504	1.95773366	-0.36693690
Ni	1.98143596	0.32182212	-0.45199775
S	0.66962710	-0.73117137	-1.84886218
C	1.23003809	2.57329917	1.24701900
C	2.74583593	2.58784136	1.06819291
H	0.90599504	1.92376371	2.07515261
H	0.85175135	3.59239914	1.43239236
C	1.55365565	-2.34855693	-1.58444356
C	3.04441753	-2.02531587	-1.61823590
H	1.29039752	-3.02926413	-2.41111425
H	1.24263162	-2.81428819	-0.63830268
N	3.23135259	1.19678982	0.77425753
N	3.37822055	-1.05162753	-0.52453051
H	3.26157422	2.98340797	1.96431293
H	3.00959815	3.22554911	0.20934013
C	4.50401280	1.13901763	-0.01689686
C	4.59062396	-0.20951175	-0.79871171
H	4.59786763	-0.00039880	-1.87748411
H	5.50981506	-0.77225833	-0.55167563
H	4.47421741	1.97047337	-0.73504398
H	5.37551183	1.28901241	0.64676404
C	3.35485774	0.43510155	2.06170495
C	3.52096292	-1.78851602	0.77440214
H	2.53983664	-2.21329623	1.02501629
H	4.21985501	-2.63186201	0.61336937
H	3.93360725	1.05694928	2.77156291
H	2.34138222	0.30745333	2.46493954
C	4.05753021	-0.90999899	1.90112305
P	-2.75736362	1.31649635	0.37521453
P	-2.64222093	-1.26061625	-0.61433767
H	3.29945248	-1.54898139	-2.57840313
H	3.66235986	-2.93755437	-1.50786883
C	-3.24316081	-1.77302251	1.10862759
C	-3.34766438	0.57910733	2.01042781
N	-2.76416676	-0.79535592	2.14659026
H	-2.80209664	-2.74924133	1.36079975
H	-4.34091662	-1.83631487	1.16286175
H	-2.95698072	1.18283902	2.84357243
H	-4.44446841	0.51181400	2.07416265
C	-2.88301130	-1.33553168	3.53556483
H	-2.43895188	-0.61040316	4.23113291
H	-2.34542254	-2.29277515	3.58811449
H	-3.94720112	-1.48480165	3.76582698
C	-4.18435289	-0.43948422	-1.27408994

C	-4.26042206	0.99763056	-0.69866828
C	-2.53285312	-2.88931824	-1.45386233
H	-2.32521634	-2.71292297	-2.52109309
H	-3.47201951	-3.45736182	-1.34757144
H	-1.69806686	-3.45932192	-1.01588524
C	-2.79664833	3.11691846	0.72658758
H	-2.02254622	3.35888097	1.47141329
H	-3.78791834	3.41944600	1.10238702
H	-2.57611764	3.65357067	-0.20968826
H	3.94653583	-1.46392568	2.84799510
H	5.14020421	-0.75121139	1.76424551
H	-4.24142617	1.74937468	-1.50276446
H	-5.17029044	1.15893058	-0.09757498
H	-5.06663217	-1.04510665	-1.00921224
H	-4.09369999	-0.42394871	-2.37178755
O	0.51607773	-0.98930943	2.97302085
C	0.22394206	-1.69667854	2.04736904
H	-0.51144807	-0.48028673	0.91461632
Fe	-1.07859512	0.23700229	-0.47269480
O	0.09192721	-2.72930347	1.45168302
H	-1.74624227	-0.64291570	1.88492755
F	-1.56911013	1.03330505	-2.15965551

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Angstroms

Atom	X	Y	Z
S	0.50084767	1.91280834	-1.04352027
Ni	1.89823397	0.26796637	-0.70336623
S	0.60356484	-1.04256724	-1.88545570
C	1.16765576	2.89014229	0.39806092
C	2.68645639	2.79225168	0.32972165
H	0.75683632	2.48911145	1.33822118
H	0.84499288	3.94004074	0.29754936
C	1.45368833	-2.58580774	-1.25986923
C	2.95104609	-2.30055341	-1.25543233
H	1.22500950	-3.41483138	-1.95022880
H	1.07004734	-2.85179718	-0.26304798
N	3.10002266	1.35141556	0.39951388
N	3.23638935	-1.12472413	-0.36736172
H	3.17654191	3.36115057	1.14406146
H	3.03667921	3.19530661	-0.63393658
C	4.44159743	1.07135157	-0.20699706
C	4.51502331	-0.41062145	-0.68841350
H	4.62839359	-0.42933626	-1.78136337
H	5.37362975	-0.94754148	-0.24356808
H	4.54875960	1.73653329	-1.07509659
H	5.24603773	1.31509190	0.51134789
C	3.03369082	0.88313133	1.82475763
C	3.21637894	-1.56852221	1.06450441
H	2.19382799	-1.89933208	1.28843849
H	3.88283315	-2.44769469	1.16162152

H	3.55862229	1.62644043	2.45594058
H	1.97399443	0.87214116	2.11691070
C	3.67826323	-0.48413375	2.03478094
P	-2.74307226	1.45353017	-0.32709799
P	-2.62961680	-1.26287366	-0.68250153
H	3.28010182	-2.03826932	-2.27366249
H	3.53812733	-3.17591985	-0.91381701
C	-3.43638252	-1.37601056	1.03692787
C	-3.54669413	1.11360590	1.35682358
N	-3.00516492	-0.19232922	1.85890516
H	-3.06613403	-2.27861717	1.54630083
H	-4.53680606	-1.39814714	0.99432614
H	-3.23341159	1.89361361	2.06767284
H	-4.64600597	1.05748297	1.31961050
C	-3.23898404	-0.39123964	3.31929167
H	-2.82262400	0.46891578	3.86178534
H	-2.73732297	-1.31696129	3.63603840
H	-4.32042911	-0.46811453	3.50148198
C	-4.06759102	-0.59640320	-1.68234528
C	-4.13448585	0.93756667	-1.47588004
C	-2.54812086	-3.04800487	-1.13417449
H	-2.22708002	-3.13002894	-2.18471790
H	-3.53066001	-3.53387199	-1.01131782
H	-1.80469333	-3.54823736	-0.49366936
C	-2.78879867	3.29462602	-0.37430640
H	-2.09697640	3.69529997	0.38325411
H	-3.80868554	3.66688867	-0.18099389
H	-2.45890021	3.62919447	-1.37036320
H	3.43815931	-0.81844560	3.05780530
H	4.77622929	-0.38963446	1.99364680
H	-3.97575484	1.47742203	-2.42359016
H	-5.10284234	1.26082619	-1.05772932
H	-5.00241126	-1.10056541	-1.38377739
H	-3.86396852	-0.85183926	-2.73523277
O	0.25674606	-0.45380455	3.18405138
C	-0.01849366	-1.31022695	2.39580064
H	-0.60187388	-0.16111592	0.89678750
Fe	-1.05791761	0.19031334	-0.68082912
O	-0.20084683	-2.39922271	1.93777086
H	-1.95091386	-0.11697849	1.63099439
H	-1.43770751	0.51368198	-2.13574788

Name-TSNCS:G=-3245.122175//H=-3245.012976//SPE=-3245.62387843

Angstroms

Atom	X	Y	Z
S	0.48756414	2.05040756	-0.56243361
Ni	1.92910507	0.41449602	-0.64749447
S	0.61729620	-0.63849748	-2.04435889
C	1.17770720	2.66597307	1.05152228
C	2.69350503	2.68051525	0.87269619

H	0.85366414	2.01643761	1.87965589
H	0.79942045	3.68507303	1.23689564
C	1.50132475	-2.25588303	-1.77994028
C	2.99208664	-1.93264197	-1.81373262
H	1.23806662	-2.93659024	-2.60661097
H	1.19030072	-2.72161430	-0.83379940
N	3.17902169	1.28946372	0.57876081
N	3.32588966	-0.95895363	-0.72002723
H	3.20924332	3.07608187	1.76881621
H	2.95726725	3.31822300	0.01384342
C	4.45168190	1.23169153	-0.21239358
C	4.53829306	-0.11683785	-0.99420843
H	4.54553673	0.09227509	-2.07298083
H	5.45748416	-0.67958444	-0.74717235
H	4.42188651	2.06314727	-0.93054069
H	5.32318093	1.38168630	0.45126732
C	3.30252684	0.52777544	1.86620823
C	3.46863202	-1.69584213	0.57890542
H	2.48750575	-2.12062233	0.82951957
H	4.16752411	-2.53918812	0.41787265
H	3.88127635	1.14962317	2.57606619
H	2.28905132	0.40012722	2.26944283
C	4.00519932	-0.81732510	1.70562633
P	-2.80969451	1.40917025	0.17971781
P	-2.69455183	-1.16794236	-0.80983439
H	3.24712158	-1.45630750	-2.77389985
H	3.61002896	-2.84488047	-1.70336555
C	-3.29549171	-1.68034861	0.91313087
C	-3.39999528	0.67178122	1.81493109
N	-2.81649765	-0.70268203	1.95109354
H	-2.85442754	-2.65656743	1.16530303
H	-4.39324751	-1.74364098	0.96736503
H	-3.00931161	1.27551292	2.64807571
H	-4.49679931	0.60448790	1.87866593
C	-2.93534220	-1.24285779	3.34006811
H	-2.49128278	-0.51772926	4.03563619
H	-2.39775344	-2.20010125	3.39261777
H	-3.99953202	-1.39212775	3.57033026
C	-4.23668379	-0.34681032	-1.46958665
C	-4.31275296	1.09030445	-0.89416500
C	-2.58518402	-2.79664435	-1.64935905
H	-2.37754724	-2.62024907	-2.71658980
H	-3.52435041	-3.36468793	-1.54306815
H	-1.75039776	-3.36664802	-1.21138196
C	-2.84897923	3.20959236	0.53109086
H	-2.07487712	3.45155486	1.27591657
H	-3.84024924	3.51211989	0.90689030
H	-2.62844853	3.74624456	-0.40518498
H	3.89420493	-1.37125178	2.65249838
H	5.08787331	-0.65853749	1.56874879
H	-4.29375706	1.84204858	-1.69826118
H	-5.22262133	1.25160448	-0.29307170

H	-5.11896307	-0.95243276	-1.20470896
H	-4.14603089	-0.33127482	-2.56728427
O	0.46374683	-0.89663554	2.77752413
C	0.17161116	-1.60400464	1.85187232
H	-0.57060665	-0.37897765	0.70241826
Fe	-1.13092602	0.32967619	-0.66819152
O	0.03959631	-2.63662958	1.25618630
H	-1.80198701	-0.54592422	1.68108016
N	-1.60240145	1.09507007	-2.28967205
C	-1.87149085	1.59899572	-3.34041742
S	-2.24182625	2.29252550	-4.78651013

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Angstroms

Atom	X	Y	Z
S	0.51451990	1.83693721	-0.99139809
Ni	1.94743849	0.22400178	-0.64302602
S	0.64947769	-1.15211580	-1.74603840
C	1.20152242	2.85549902	0.40285692
C	2.71931334	2.79750036	0.26810272
H	0.84928109	2.46507656	1.37071691
H	0.84511957	3.89406814	0.29795535
C	1.53254337	-2.65464683	-1.09213568
C	3.02555230	-2.34767566	-1.14941286
H	1.29457486	-3.51324052	-1.74210434
H	1.19036373	-2.89017058	-0.07320396
N	3.17582874	1.36975781	0.36432006
N	3.32592771	-1.13406009	-0.31863245
H	3.22799471	3.40668576	1.04037218
H	3.01534092	3.17775204	-0.72258273
C	4.48565429	1.09560820	-0.31060626
C	4.56982667	-0.40422438	-0.73221587
H	4.62865398	-0.46638029	-1.82779969
H	5.46271076	-0.90255019	-0.31094557
H	4.52414462	1.72482657	-1.21074766
H	5.32384815	1.38760920	0.34881326
C	3.21209688	0.95600680	1.80742107
C	3.38724884	-1.52147037	1.12938711
H	2.38304498	-1.85518328	1.42401933
H	4.07050779	-2.38785954	1.22465127
H	3.76709478	1.73027404	2.37191387
H	2.17619866	0.94290303	2.17156594
C	3.88996030	-0.39369544	2.02727190
P	-2.80475687	1.39200045	-0.23867912
P	-2.63297716	-1.34458337	-0.47583624
H	3.31627287	-2.12206326	-2.18772157
H	3.63454816	-3.20189391	-0.79436922

C	-3.37026820	-1.36451624	1.27290067
C	-3.49248989	1.14341381	1.50070528
N	-2.93136938	-0.14218897	2.03623079
H	-2.97701538	-2.24001626	1.81095895
H	-4.47094231	-1.39695633	1.26522721
H	-3.12866498	1.95240982	2.15263484
H	-4.59208078	1.09787755	1.53526947
C	-3.12672018	-0.29065247	3.51021378
H	-2.71824865	0.59904221	4.00863572
H	-2.59424095	-1.19229240	3.84495845
H	-4.20208538	-0.38473936	3.71683349
C	-4.11374479	-0.76480393	-1.45892900
C	-4.24228700	0.76674051	-1.27454024
C	-2.51716234	-3.15208966	-0.81365404
H	-2.24442224	-3.29065817	-1.87210152
H	-3.47590845	-3.65862573	-0.61198859
H	-1.72675443	-3.58740992	-0.18213343
C	-2.89297576	3.22189977	-0.40676867
H	-2.17276878	3.68701085	0.28455719
H	-3.91041217	3.58824557	-0.19062355
H	-2.61903890	3.48728513	-1.43996202
H	3.71942014	-0.69130420	3.07526137
H	4.98161922	-0.28634599	1.91323036
H	-4.18953340	1.28997789	-2.24175988
H	-5.18675723	1.05143635	-0.78147983
H	-5.01676273	-1.30834898	-1.13347598
H	-3.91771605	-1.02353880	-2.51210781
O	0.33266833	-0.16047863	3.04515180
C	0.07459058	-1.07193775	2.30817577
H	-0.57257635	-0.12352931	0.87064343
Fe	-1.08635728	0.14887400	-0.64370979
O	-0.05612672	-2.21251642	1.96592387
H	-1.90075145	-0.05872467	1.79196856
O	-1.48274976	0.58644207	-2.62394893
H	-1.53400698	-0.29969334	-3.03026064

Name-TSP: G= -3420.133991//H= -3420.029853//SPE =-3420.5961943

Angstroms

Atom	X	Y	Z
S	0.21053256	1.70535461	-1.44309622
Ni	1.43442267	0.04684108	-0.60240556
S	0.28956064	-1.57148630	-1.60896304
C	0.75573536	3.03652794	-0.25146906
C	2.28841342	3.14959173	-0.25997625
H	0.37898471	2.79676424	0.75491533
H	0.29799065	3.98618772	-0.57740428
C	0.93372621	-3.01334167	-0.61229600
C	2.47018599	-3.02112103	-0.62576500
H	0.53926020	-3.93476477	-1.07333887
H	0.54814859	-2.94377196	0.41474727

H	2.65955414	3.82333792	0.53179482
H	2.65695748	3.51740859	-1.23312728
C	4.35017017	0.94325096	-1.17261468
C	4.39736613	-0.61967605	-1.24788237
H	4.19577767	-0.96456381	-2.27416247
H	5.37639555	-1.01857144	-0.93443743
H	4.11405110	1.37185452	-2.15899965
H	5.30874479	1.36784420	-0.83061690
C	3.72848183	1.30325032	1.66102245
C	3.78779281	-1.32249023	1.52508030
H	2.97580691	-1.53046528	2.24054209
H	4.50080370	-2.16453352	1.56944097
H	4.40318803	2.16798104	1.78874432
H	2.90956869	1.39800398	2.39161336
C	4.52313624	-0.00561397	1.85754578
P	-2.93877494	1.33593911	-0.11712997
P	-2.79221935	-1.42067068	-0.01806807
C	-1.97588317	0.03591402	-2.41566925
N	-2.37279132	0.05796260	-3.54807301
H	2.86106779	-3.23154813	-1.63642062
H	2.88815405	-3.76655778	0.07297207
C	-3.15929735	-1.22737421	1.82901266
C	-3.30171850	1.28841111	1.73626291
N	-2.62454965	0.08694255	2.32495459
H	-2.62980131	-2.01958495	2.37944619
H	-4.23716060	-1.27757608	2.04779693
H	-2.85977788	2.17665007	2.21249523
H	-4.37882210	1.23839342	1.95786328
C	-2.54212071	0.14283254	3.81680666
H	-2.07020359	1.09197401	4.10540585
H	-1.93667041	-0.70529337	4.16620679
H	-3.55872660	0.07973465	4.22897216
C	-4.44005034	-0.93464088	-0.75086505
C	-4.52918491	0.61083509	-0.79010537
C	-2.71676608	-3.24877360	-0.17614353
H	-2.60833376	-3.50064399	-1.24276488
H	-3.63505697	-3.71148623	0.22186587
H	-1.84023466	-3.62568422	0.37300686
C	-3.05815326	3.13229084	-0.47422804
H	-2.24902313	3.66489709	0.04811632
H	-4.03534371	3.52596499	-0.14903825
H	-2.94415962	3.27657879	-1.56013358
H	4.84413667	-0.05329453	2.91266503
H	5.44987414	0.04498262	1.25982216
H	-4.63556568	0.97831593	-1.82267223
H	-5.37653674	0.99591693	-0.19962404
H	-5.25298136	-1.38850330	-0.16043255
H	-4.47149294	-1.36219445	-1.76558046
O	0.64391381	0.81307781	2.67897687
C	0.46616079	-0.30918748	2.28505211
H	-0.50640973	-0.01221695	0.78266607
Fe	-1.30806180	0.01698923	-0.67492106

O	0.47047164	-1.50806461	2.36367763
H	-1.65779050	0.13064842	1.88808827
P	3.03519275	-1.31092029	-0.16866292
P	2.96368438	1.43459177	-0.02041896

Name-TSPy:G=-2963.607796//H=-2963.485236//SPE=-2964.15051026

Angstroms

Atom	X	Y	Z
S	0.49685704	1.99306614	-0.41280674
Ni	1.94242281	0.36004445	-0.48395378
S	0.64811735	-0.69377265	-1.89643772
C	1.16799591	2.60799176	1.20938654
C	2.68563916	2.62567725	1.04727698
H	0.83611980	1.95682184	2.03312283
H	0.78571223	3.62613281	1.39180603
C	1.53232281	-2.30977083	-1.62424241
C	3.02273546	-1.98361262	-1.64123252
H	1.27950303	-2.98997520	-2.45457712
H	1.21180886	-2.77725596	-0.68214232
N	3.17706373	1.23592503	0.75703658
N	3.34258718	-1.01061770	-0.54275144
H	3.19071294	3.02114422	1.94949446
H	2.95759931	3.26494067	0.19214557
C	4.45846503	1.18157457	-0.02012727
C	4.55629653	-0.16582985	-0.80255795
H	4.57500761	0.04461332	-1.88093366
H	5.47380449	-0.72710273	-0.54609214
H	4.43496068	2.01384724	-0.73756120
H	5.32231317	1.33244061	0.65326755
C	3.28787006	0.47290556	2.04485127
C	3.47245492	-1.74881434	0.75678930
H	2.48945676	-2.17579264	0.99607696
H	4.17471450	-2.59061291	0.60244939
H	3.85756166	1.09500201	2.76178321
H	2.27026743	0.34280976	2.43675022
C	3.99487976	-0.87063951	1.89040205
P	-2.80711865	1.34456185	0.29222908
P	-2.67608363	-1.23111396	-0.69908556
H	3.28739762	-1.50561523	-2.59796179
H	3.64119687	-2.89479101	-1.52516307
C	-3.29495524	-1.74678164	1.01654347
C	-3.41394875	0.60403963	1.91995882
N	-2.82931571	-0.76946026	2.06088849
H	-2.85479748	-2.72245460	1.27238525
H	-4.39311645	-1.81225839	1.05861269
H	-3.03363309	1.20750669	2.75807763
H	-4.51125506	0.53455217	1.97153382
C	-2.96239187	-1.31155938	3.44782162
H	-2.52742533	-0.58642488	4.14910557
H	-2.42355516	-2.26782710	3.50513858

H	-4.02875969	-1.46316360	3.66617447
C	-4.21245277	-0.41215462	-1.37479061
C	-4.29764328	1.02410724	-0.79851817
C	-2.55431729	-2.85857590	-1.53930799
H	-2.33528909	-2.68047771	-2.60397578
H	-3.49349124	-3.42856007	-1.44404460
H	-1.72329650	-3.42750181	-1.09285084
C	-2.85376679	3.14447455	0.64530736
H	-2.08838156	3.38702106	1.39890003
H	-3.84969917	3.44462972	1.01053323
H	-2.62398690	3.68269378	-0.28783952
H	3.87454627	-1.42593472	2.83532971
H	5.07868422	-0.70959599	1.76564300
H	-4.27125845	1.77686757	-1.60145431
H	-5.21438453	1.18291734	-0.20728543
H	-5.09641574	-1.01980134	-1.12036891
H	-4.10975323	-0.39510433	-2.47140424
O	0.44200410	-0.95809212	2.92314951
C	0.16144987	-1.66489323	1.99348985
H	-0.55713124	-0.45718082	0.87092936
Fe	-1.11702450	0.26934513	-0.53844057
O	0.03800648	-2.69704310	1.39514850
H	-1.80887086	-0.61473674	1.81063145
N	-1.59321951	1.07135967	-2.23950230
C	-1.85595510	0.37738685	-3.41698816
C	-1.74301177	2.43415685	-2.47921985
C	-2.17611550	1.30646408	-4.41659602
H	-1.79803435	-0.70941493	-3.46182148
C	-2.10446528	2.61043995	-3.82214740
H	-1.57499085	3.17134954	-1.69516522
H	-2.43053524	1.08230161	-5.44705908
H	-2.29468186	3.55554748	-4.31954593

Name-TSSCH3:G=-3192.176459//H=-3192.073601//SPE=-3192.6826118

Angstroms

Atom	X	Y	Z
S	0.52630250	-1.80598804	-0.74480298
Ni	1.99253426	-0.55362928	0.27607803
S	0.61092801	-0.36136495	1.96285945
C	1.34055162	-1.51823489	-2.39611399
C	2.83671737	-1.71794628	-2.16457720
H	1.10402946	-0.51309391	-2.77865067
H	0.95840978	-2.26193443	-3.11585859
C	1.50820722	1.14206169	2.60353171
C	2.99389475	0.79388956	2.55864240
H	1.18968384	1.32735239	3.64343392
H	1.26643188	2.03225973	2.00351558

N	3.32606409	-0.71972628	-1.15381144
N	3.40154469	0.50714046	1.14172770
H	3.41739549	-1.61612548	-3.10179216
H	3.01507813	-2.72663217	-1.75831072
C	4.52173099	-1.16482239	-0.36557323
C	4.57247511	-0.42058917	1.00787453
H	4.49277485	-1.15761374	1.81909557
H	5.51924711	0.13520308	1.14105424
H	4.40437595	-2.24246287	-0.18465118
H	5.44743347	-1.01146659	-0.95122805
C	3.58826342	0.58742406	-1.84237211
C	3.65908137	1.80010565	0.42705454
H	2.70438538	2.33830038	0.36127799
H	4.34516553	2.40568409	1.05065204
H	4.22724679	0.38612981	-2.72387073
H	2.62382174	0.96961639	-2.20188868
C	4.28851134	1.60794218	-0.94987220
P	-2.75433970	-0.60358889	-1.12002882
P	-2.62562359	0.73399271	1.27338734
H	3.17710137	-0.11706940	3.15087826
H	3.62148257	1.60785559	2.97127584
C	-3.09915258	2.29830099	0.31646567
C	-3.26149660	1.05997844	-1.88091962
N	-2.62275759	2.17213776	-1.10316506
H	-2.57200568	3.16016231	0.75381836
H	-4.18407722	2.48651946	0.31315917
H	-2.86706344	1.11878996	-2.90665582
H	-4.35212812	1.20939768	-1.89076420
C	-2.64485030	3.47255916	-1.83712638
H	-2.19555189	3.32332125	-2.82877097
H	-2.06648200	4.21168766	-1.26501431
H	-3.68788153	3.80368914	-1.93869477
C	-4.25423930	-0.18944209	1.19121196
C	-4.32062161	-0.96067042	-0.14833964
C	-2.55201747	1.39062969	2.99158362
H	-2.42987399	0.53999049	3.68088793
H	-3.47334437	1.94074995	3.24610921
H	-1.67954116	2.05583898	3.08901806
C	-2.85990136	-1.67983234	-2.61207411
H	-2.04446405	-1.41082268	-3.30226246
H	-3.83221244	-1.55877984	-3.11843435
H	-2.73319110	-2.72909140	-2.30568124
H	4.27352321	2.58047033	-1.46941454
H	5.35195169	1.33766823	-0.83816190
H	-4.37049291	-2.04675971	0.02009128
H	-5.19393110	-0.66993919	-0.75660449
H	-5.08345972	0.52885907	1.30590549
H	-4.26961019	-0.88321555	2.04524574
O	0.65813844	2.15284581	-2.19990665
C	0.46822185	2.42821392	-1.04847725
H	-0.45475613	0.92601811	-0.48903280
Fe	-1.08856030	-0.38145212	0.23631970

O	0.46506764	3.09820943	-0.05441794
H	-1.62834537	1.81052081	-0.97758053
S	-1.66651977	-2.36029309	1.45122010
C	-2.06088318	-3.75149493	0.31563853
H	-2.02789397	-4.68958026	0.89620798
H	-3.06529756	-3.66996814	-0.13439401
H	-1.31481103	-3.81961699	-0.49521449

Name-TSSCN:G=-3245.111734//H=-3244.985362//SPE=-3245.61652469

Angstroms

Atom	X	Y	Z
S	1.48253697	1.10984208	-2.18292886
Ni	2.19268418	-0.92652548	-1.85069358
S	0.11793432	-1.60927574	-1.75003037
C	3.10479882	1.83803079	-1.63696214
C	4.18198895	1.02797421	-2.35341386
H	3.19646793	1.79105610	-0.54056092
H	3.14459863	2.89556694	-1.94690108
C	0.60406061	-3.22547175	-0.96329573
C	1.81525892	-3.72745349	-1.74368710
H	-0.23735584	-3.93075252	-1.06648952
H	0.81586472	-3.09140404	0.10721303
N	4.07961058	-0.41507329	-1.94809742
N	2.93333852	-2.72965172	-1.64381433
H	5.19771011	1.40844015	-2.13195007
H	4.02274264	1.08452341	-3.44213448
C	4.59146917	-1.38397681	-2.97189117
C	3.90115119	-2.77248807	-2.79088016
H	3.31833995	-3.00510715	-3.69296110
H	4.63728043	-3.58343044	-2.63886358
H	4.32941255	-0.97733003	-3.95875814
H	5.69297011	-1.45884680	-2.91235170
C	4.76487996	-0.60601299	-0.62639726
C	3.64580562	-2.90650391	-0.33548716
H	2.93619736	-2.65955182	0.46534068
H	3.90854046	-3.97694852	-0.23188743
H	5.77001006	-0.14701326	-0.69404830
H	4.18549970	-0.05366420	0.12543660
C	4.92002846	-2.07264883	-0.23430175
P	-0.78748570	2.52145839	-0.01769790
P	-1.84909955	0.07706667	0.71162091
H	1.55398931	-3.83036571	-2.80905357
H	2.15946783	-4.71269808	-1.37351683
C	-1.41614445	0.60237823	2.48048943
C	-0.44755536	2.83258349	1.81363184
N	-0.21703084	1.51053943	2.48237459
H	-1.14024007	-0.29320349	3.05750048
H	-2.25218822	1.12009912	2.97547527
H	0.47980028	3.41613227	1.91725608
H	-1.27815310	3.35014874	2.31742069

C	0.38834696	1.65168855	3.84206532
H	1.30309708	2.25387516	3.75593394
H	0.62609633	0.65006787	4.22717498
H	-0.33701587	2.14926219	4.50090625
C	-3.25556953	1.25144088	0.35052635
C	-2.65890716	2.62906930	-0.03460925
C	-2.61752901	-1.56411025	1.00400356
H	-3.04488385	-1.91822423	0.05259358
H	-3.41103209	-1.50335563	1.76732950
H	-1.83633612	-2.26901384	1.33026237
C	-0.21378920	4.08465324	-0.78829524
H	0.87999918	4.16027968	-0.68605577
H	-0.69704765	4.95411372	-0.31304362
H	-0.47452698	4.05508947	-1.85805392
H	5.26839658	-2.10745253	0.81123618
H	5.71680853	-2.53790679	-0.83829554
H	-2.95117101	2.91736120	-1.05613769
H	-2.97748966	3.42904578	0.65367422
H	-3.91982294	1.31210238	1.22827520
H	-3.82737171	0.81811814	-0.48534029
O	2.77810338	0.02283015	1.93785514
C	1.85010648	-0.72510016	1.78964054
H	0.86039899	0.19117619	0.52921283
Fe	-0.21869907	0.52598088	-0.64783485
O	1.16896438	-1.68829753	2.00615906
H	0.45456866	1.02709017	1.81671208
C	-1.91286758	2.82743287	-2.86678869
N	-2.03040464	3.90401866	-3.37429639
S	-2.08845698	0.99191267	-2.29265647