Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Hydrogen-bonding effect between active site and protein environment on Catalysis Performance in H_2-Producing [NiFe] Hydrogenases

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H-BONDING ENERGY PROFILES FOR CN^- AND S^- LIGANDS

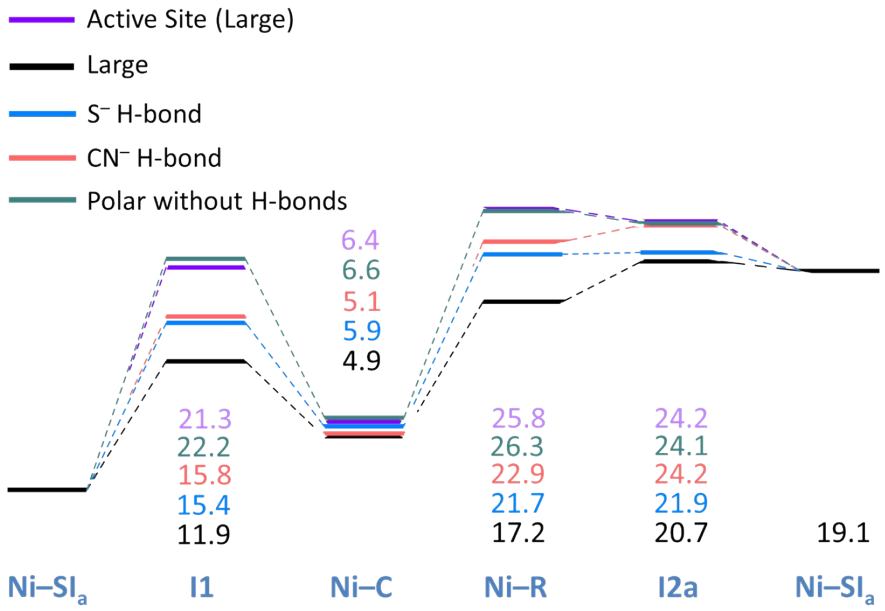

Fig. S1. Gibbs free energy profile, in units of kcal/mol, for the HER referring to different protein environment models. Relative energies referred to the **Ni-SI$_a$** state, in which $\Delta G = 0$ kcal/mol. The pH corrections (pH = 7) are also included in the energy profile for the natural environment of hydrogenases.

ELECTRONIC DENSITY ANALYSIS

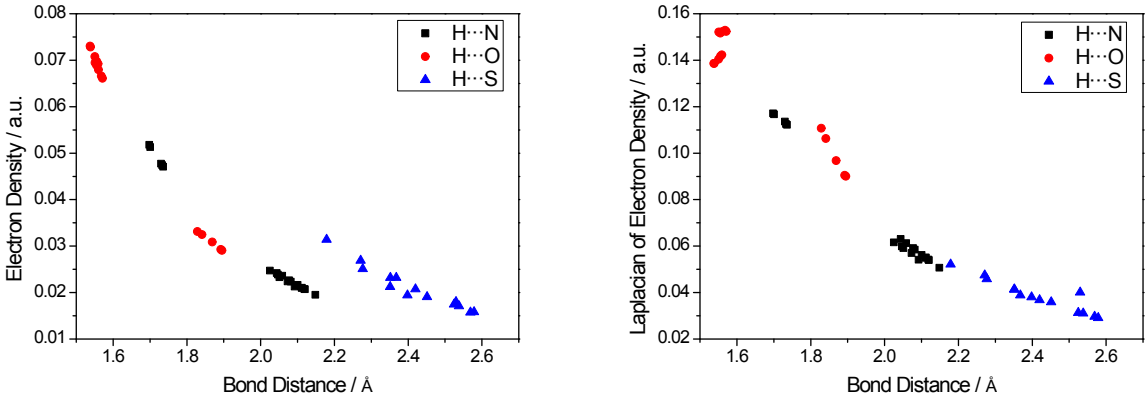

Fig. S2. Electron densities and Laplacian, in a.u., of electron density of the H–N, H–O, and H–S hydrogen bonds *vs*. bond distances, in Å, in the different reaction states of [NiFe] hydrogenases.

PCM CALCULATIONS

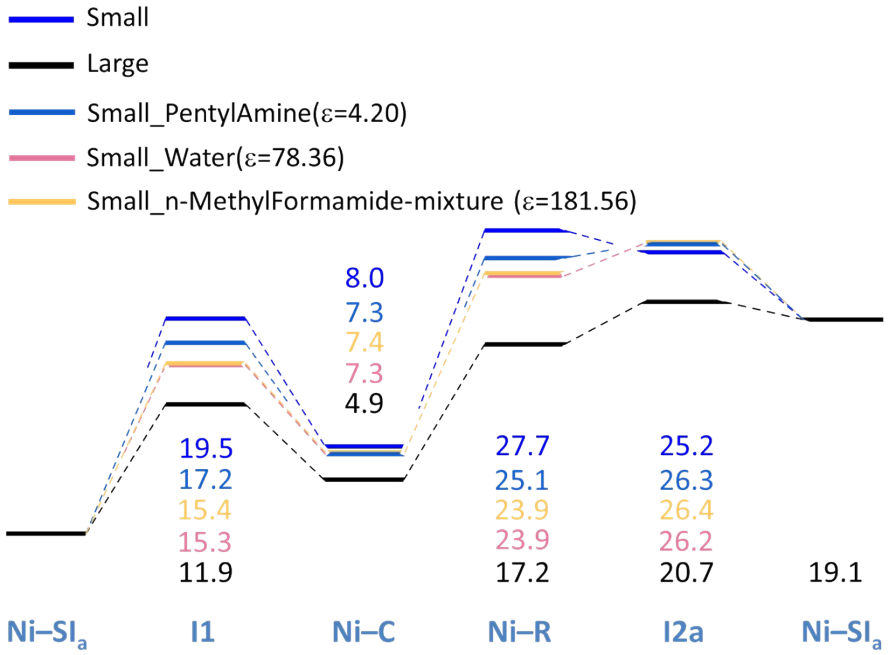

Fig. S3. Gibbs free energy profile, in units of kcal/mol, for the HER attending to different solvent effects through the Polarizable Continuum Model (PCM) in the so-called 'Small' model. Relative energies referred to the **Ni-SI$_a$** state, which $\Delta G = 0$ kcal/mol. The pH corrections (pH = 7) are also included in the energy profile for the natural environment of hydrogenases.

FRACTIONAL CHARGE CALCULATIONS

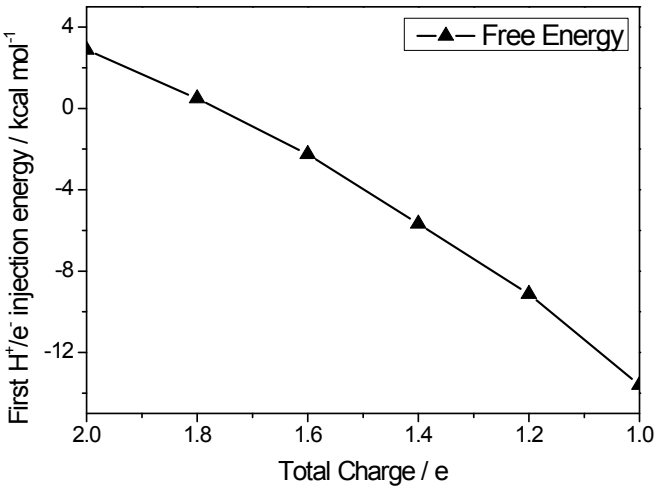

Fig. S4. First H^+/e^- injection free energy change, in units of kcal/mol, *vs*. the fractional charge changes, in e, on the active site conducted by VASP calculations.

HOMO-LUMO DIAGRAMS

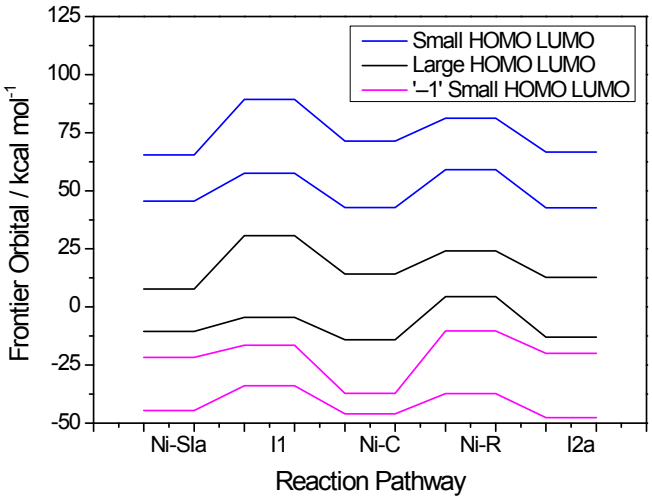

Fig. S5. HOMO and LUMO diagrams, in units of kcal/mol, for the so-called 'Small', 'Large', and '–1 Small' models along the HER path.

PROTON INJECTION

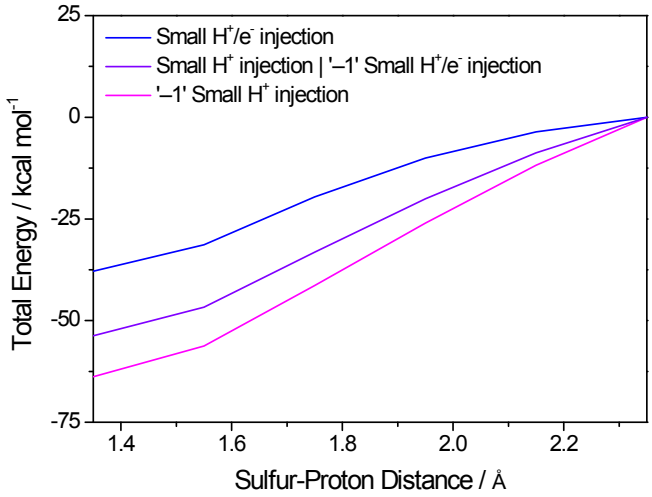

Fig. S6. Binding energy change, in units of kcal/mol, related to the distance, in Å, between the binding sulfur and proton in the H^+/e^- injection for the 'Small', H^+ injection in the 'Small', and H^+/e^- injection in the '–1 Small' models.

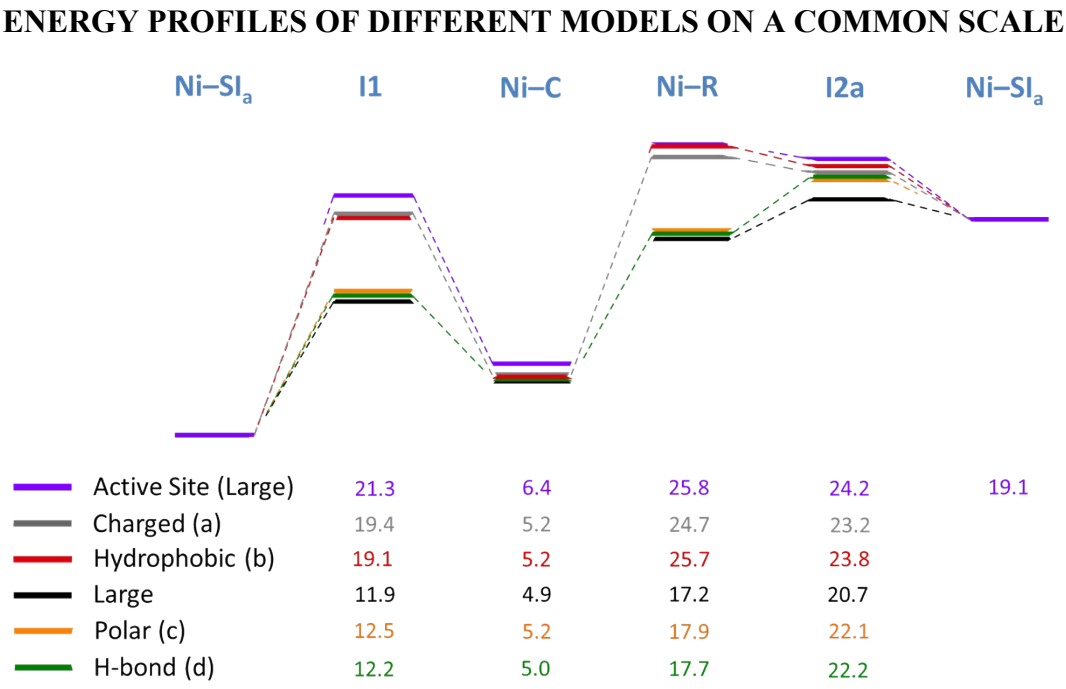

Fig. S7. Gibbs free energy profile, in units of kcal/mol, for the HER reaction on different models. Relative energies referred to the **Ni-SI$_a$** state, in which $\Delta G = 0$ kcal/mol.

ENERGY DIFFERENCE BETWEEN DIFFERENT CHARGED ACTIVE SITE

Tabel S1: Energy difference between '-1', '-3' and '-2' charged active site.[a]

*Free energy / kcal*mol^{-1}*	*Small*	*'-1' Small*	*Δ ('-1'-'-2')*	*'-3' Small*	*Δ ('-3'-'-2')*
Ni-SIa	-3125938.9	-3125943.4	-112.1	-3125839.8	206.8
I1	-3126299.1	-3126317.9	-126.5	-3126188.6	218.2
Ni-C	-3126310.6	-3126312.7	-109.9	-3126214.5	203.7
Ni-R	-3126670.5	-3126687.2	-124.4	-3126556.8	221.3
I2a	-3126673.0	-3126674.0	-108.6	-3126572.1	208.6

[a]Free energy of the electron has been approximated by $G(e^-) = G(1/2H_2) - G(H^+)$, the free energy of the proton is 262.4 kcal/mol (J. Phys. Chem. A, *2001*, **105**, *11534*).

CARTESIAN COORDINATES

Note: * refers to frozen atoms. Frozen atoms in Model 3 are the same with those in Model 1. Also, frozen atoms in Models 4-7 are the same with those in Model 2.

MODEL 1: SMALL MODEL

System: **Ni-SI$_a$** (singlet)

Charge, Multiplicity: –2, 1

Gibbs free energy: –4981.496567 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.79268735
C	1.70583828	0.00000000	3.62761379
C	-0.77910889	0.57587997	4.19604476
C	-0.26490295	-1.82824639	3.24410891
N	2.76684348	0.06139506	4.14059109
O	-1.32352013	0.99912838	5.15147357
N	-0.45985208	-2.96347136	3.49916226
*C	-1.96547216	2.82672368	-2.64545167
C	-1.29175409	2.03190327	-1.53384493
S	-1.10245859	0.24877619	-1.96810467
*C	-4.18168275	-1.49042708	0.70513395
C	-2.72454384	-1.60208615	1.21514245
S	-1.82941125	0.02738735	1.31094543
*C	4.33333023	-1.49708692	0.09334978
C	2.84473276	-1.31043707	0.43267603
S	1.89744165	-0.54836365	-0.95691358
*C	2.58585735	3.57509730	0.72082642
C	2.33424782	2.22836773	1.45544185
S	0.58800275	1.62218206	1.37222965
H	1.69612448	4.23841877	0.78667686
*H	3.40674581	4.06814763	1.24015947
H	2.82699478	3.42578402	-0.35064687
H	-2.21144430	3.86666915	-2.32828520
H	-1.32431691	2.88284722	-3.55291572
*H	-2.88290272	2.31318624	-2.93343122
*H	4.82846042	-0.53425236	-0.03036129
H	4.85495588	-2.04820157	0.90827565
H	4.46444862	-2.07152431	-0.85061329
H	-4.21194621	-1.36800941	-0.39765531
*H	-4.79526556	-2.35960004	1.00190636
H	-4.67177532	-0.59367339	1.14578219
H	2.55287713	2.30577237	2.53966235
H	2.98163890	1.42265067	1.05963294
H	2.72055371	-0.69100670	1.34750559
H	2.37989632	-2.28733012	0.67749415
H	-0.29290197	2.45643813	-1.30130609
H	-1.88353956	2.10126227	-0.59711585
H	-2.11435660	-2.27556830	0.58124211

H	-2.67541956	-2.01176978	2.24379461

System: **I1** (doublet)
Charge, Multiplicity: –2, 2
Gibbs free energy: –4982.07052 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.54295090
C	0.80666830	0.00000000	4.05981267
C	-0.46420213	1.83244512	2.51108924
C	-1.66698241	-0.38321397	3.35413553
O	1.40219310	0.01363790	5.08054854
N	-0.78941831	2.96484929	2.41728089
N	-2.69785611	-0.66144738	3.86245157
*C	2.22494587	-2.33773318	-2.99633997
C	1.48253595	-1.77264775	-1.80073853
S	0.69373809	-0.16181734	-2.18578592
*C	3.64259643	2.33738811	0.30313083
C	2.41775627	2.05912504	1.19955073
S	1.86997756	0.29423052	1.21280487
*C	-4.70037077	0.54196420	0.10721408
C	-3.27813772	0.74121435	0.61875545
S	-2.01734995	0.55207801	-0.69860741
*C	-1.88932606	-4.04654620	0.57486140
C	-1.77779776	-2.71980051	1.36870447
S	-0.12828518	-1.90039294	1.27222955
*H	-2.55997256	-4.70497677	1.12710635
H	-2.25530498	-3.90052994	-0.46251522
H	-0.90079984	-4.55214616	0.51397277
H	2.71244301	-3.31658110	-2.76563012
H	1.54067014	-2.49519240	-3.86035749
*H	2.99711259	-1.64056989	-3.32113279
*H	-4.98560127	-0.50399500	-0.00671377
H	-5.42900212	0.97449054	0.83066455
H	-4.86262608	1.05250707	-0.86801715
H	3.37047721	2.32927538	-0.77251064
*H	4.07326227	3.31678523	0.58359649
H	4.43145375	1.56833416	0.45707230
H	-2.44377508	-0.65782938	-1.14774216
H	-2.55037689	-1.99254853	1.04653084
H	-1.97143712	-2.88420800	2.44721046
H	-3.09359500	1.76951148	0.99137829
H	-3.01924135	0.07934596	1.46896052
H	0.70975107	-2.48508637	-1.44378558
H	2.17401209	-1.62770222	-0.94354171
H	1.54829371	2.68615701	0.92179270
H	2.64461670	2.29849829	2.25981366

System: **Ni-C** (doublet)
Charge, Multiplicity: –2, 2
Gibbs free energy: –4982.08882 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.55387681

C	0.88657662	0.00000000	4.04102859
C	-1.14842401	1.38491336	3.18044109
C	-1.20565244	-1.31781308	3.20623851
O	1.48317264	0.00570766	5.05223851
N	-1.82149112	2.27234816	3.56578605
N	-1.92734696	-2.16146701	3.60300224
*C	3.69497783	-0.28911451	-2.62585333
C	2.69952536	-0.36960775	-1.47880389
S	1.07937353	0.34412386	-1.94082970
*C	1.34892880	4.15668894	0.45480980
C	0.49499460	3.11356432	1.20063847
S	1.24492967	1.42485831	1.24473006
*C	-3.84420603	-2.53106911	-0.62361136
C	-2.92331334	-1.48228448	0.00276931
S	-1.52850547	-1.08630603	-1.12914087
*C	1.12838657	-4.29220618	0.53480849
C	0.38734352	-3.18395714	1.32369077
S	1.22374204	-1.54655255	1.32727379
*H	0.95443404	-5.23673318	1.05009235
H	0.79100533	-4.34908333	-0.51978216
H	2.22678352	-4.11608516	0.53330715
H	4.67031912	-0.75840971	-2.35484857
H	3.30928978	-0.81086921	-3.52985838
*H	3.88914184	0.74605505	-2.90620687
*H	-3.38530542	-3.51755454	-0.69084622
H	-4.77424200	-2.64854924	-0.01926797
H	-4.15234001	-2.23526191	-1.65192337
H	2.41653484	4.07478151	0.75675433
H	1.30613913	4.00826507	-0.64427299
*H	1.01878376	5.18068708	0.70955625
H	-1.04401540	0.02353064	1.21501298
H	-2.52409348	-1.82758314	0.97875559
H	-3.48672214	-0.54975529	0.21776840
H	-0.63994093	-3.03398114	0.94302464
H	0.27996085	-3.45701531	2.39259973
H	2.54134012	-1.42337546	-1.17193470
H	3.08129735	0.15892903	-0.57922906
H	0.34231380	3.39188057	2.26313381
H	-0.52030166	3.01558946	0.76798078

System: **Ni-R** (singlet)
Charge, Multiplicity: –2, 1
Gibbs free energy: –4982.66238 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.55765023
C	0.84227295	0.00000000	4.06451032
C	-1.17643762	1.37726134	3.15089738
C	-1.22222144	-1.32469473	3.15561663
O	1.41224502	0.00181830	5.09287042
N	-1.88334581	2.24969638	3.51242450
N	-1.97627267	-2.16988738	3.48977335
*C	3.75088360	-0.40007426	-2.57809439
C	2.72773038	-0.46216553	-1.44885972
S	1.08898848	0.18723180	-1.95898071

*C	1.21290597	4.08168489	0.29218517
C	0.50700673	3.09351947	1.23366378
S	1.21535715	1.39221461	1.20927659
*C	-3.67665996	-2.87770629	-0.43840994
C	-2.80901810	-1.75099297	0.11611354
S	-1.46409918	-1.21952248	-1.02693142
*C	1.37318032	-4.35551802	0.78497241
C	0.51293341	-3.24393434	1.43706839
S	1.37258790	-1.63173547	1.50536596
H	2.45258948	-4.09312166	0.83714035
*H	1.24260428	-5.28009662	1.34555076
H	1.12308390	-4.52225432	-0.28428298
H	4.73958622	-0.80470915	-2.25651104
H	3.41582900	-0.98868385	-3.46168814
*H	3.89723478	0.62791300	-2.90967875
H	-4.57597264	-3.00905240	0.20437322
H	-4.03116821	-2.65749633	-1.47002996
*H	-3.17331769	-3.84465348	-0.45937246
H	1.03849126	3.82164145	-0.77286083
*H	0.83683577	5.10055424	0.49731861
H	2.31233175	4.08296507	0.45982951
H	-1.02856108	0.06764444	1.20421312
H	-0.82598066	-2.43056852	-1.02448119
H	-0.45113056	-3.13273476	0.89106511
H	0.22035741	-3.51836199	2.47008284
H	-3.39178766	-0.81920002	0.26523941
H	-2.36737391	-1.99037513	1.10552768
H	2.59686212	-1.49726949	-1.07183691
H	3.06921543	0.13000641	-0.57377689
H	0.57239565	3.42507857	2.29081977
H	-0.57396310	3.00833517	1.01355786

System: **I2a** (singlet)
Charge, Multiplicity: –2, 1
Gibbs free energy: –4982.66643 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.65044395
C	0.86021657	0.00000000	4.12062142
C	-1.07156338	1.49282017	3.14552409
C	-1.34068290	-1.16696687	3.31090210
O	1.47363901	-0.01142492	5.12607662
N	-1.71523566	2.43820189	3.43373303
N	-2.14457437	-1.92501017	3.72379990
*C	3.79429704	-0.73035868	-2.41198457
C	2.68810806	-0.66996347	-1.36201419
S	1.22950503	0.28459054	-1.92978038
*C	1.71741068	3.98577888	0.45133536
C	0.84103846	3.04102754	1.29620166
S	1.38307061	1.27148813	1.29723641
*C	-3.91205433	-2.36691496	-0.45760049
C	-2.83674316	-1.37692930	0.00644681
S	-1.39289526	-1.35706770	-1.13548326
*C	0.90879699	-4.41788589	0.85673352
C	0.09062695	-3.24449629	1.45537193

S	0.93817066	-1.60975627	1.37878330
H	2.00097066	-4.24655227	0.98045150
*H	0.66180810	-5.32688510	1.40427001
H	0.70686622	-4.54847418	-0.22598105
H	4.70754393	-1.23818735	-2.02238124
H	3.45856966	-1.27830473	-3.32056108
*H	4.06390094	0.27667176	-2.72905568
*H	-3.52126649	-3.38415638	-0.47869571
H	-4.78836911	-2.34955473	0.22898258
H	-4.27120707	-2.12487968	-1.48302070
H	1.60276596	3.77665895	-0.63266504
*H	1.45444436	5.03955145	0.65983387
H	2.79373309	3.85594716	0.69930610
H	-1.25578623	0.78697879	0.76204977
H	-1.18179070	1.12638188	-0.02724935
H	-0.13432638	-3.40501896	2.52827989
H	-0.88081401	-3.13452677	0.93281342
H	-2.49607754	-1.62305305	1.03374693
H	2.35464339	-1.69116708	-1.08280061
H	3.06897815	-0.20785924	-0.42576645
H	0.84095444	3.33638773	2.36513615
H	-0.21957806	3.07248915	0.98012236
H	-3.26139696	-0.35063720	0.06373440

MODEL 2: LARGE MODEL

System: **Ni-SI$_a$** (singlet)

Charge, Multiplicity: –2, 1

Gibbs free energy: –7996.462622 au

*C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.37201953
C	2.06162039	0.00000000	0.60601112
*N	1.23039819	-0.00407841	-0.50137980
C	1.31795881	-0.00113927	1.78214872
*H	-0.92687097	-0.06855984	-0.57929303
H	3.15574194	-0.00254305	0.50548782
H	1.58090037	-0.01541174	2.84612603
H	-0.81874563	-0.01662657	2.00017874
O	-9.22446019	-3.60485712	-0.01898321
*C	-8.11689988	-3.43397062	0.50723659
N	-7.85660309	-2.43997488	1.40618020
C	-8.88345279	-1.50440790	1.84319014
C	-8.32219103	-0.42896624	2.78803010
O	-7.97555403	-0.91669704	4.06790981
H	-9.34451219	-1.02644912	0.94741916
H	-6.93030831	-2.38602582	1.86561065
H	-9.70544803	-2.04825727	2.36458856
H	-7.45588520	0.07363724	2.28511690
H	-9.10896834	0.34768484	2.92342545
H	-7.11008667	-1.40274403	3.94579090
C	-4.72203046	-4.81885600	1.24115027

C	-4.58332806	-4.39326874	-0.22618221
H	-4.38377139	-3.99415128	1.89849958
H	-4.11926027	-5.71560500	1.48788101
H	-3.65890801	-3.81149083	-0.41480593
H	-4.55198070	-5.29889744	-0.89273166
C	-6.89955823	-4.32833153	0.17488905
C	-6.24725670	-5.03658539	1.41182468
H	-6.51891383	-6.11154879	1.41391566
H	-6.60306023	-4.60786939	2.36983070
H	-7.30903579	-5.10211414	-0.52194535
*N	-5.77796646	-3.56842942	-0.42111377
H	-5.95531270	-3.33371728	-1.40429779
*H	-5.77206671	3.87587871	10.00555382
*C	-4.97878413	3.29041816	9.54068664
H	-4.60746385	2.57384951	10.30254947
H	-5.42498247	2.68974018	8.72456456
C	-3.80641896	4.09444050	8.99035991
C	-4.15005653	4.95140955	7.80066512
O	-3.09370160	5.70612966	7.40072151
O	-5.22924569	4.97722258	7.22111494
H	-3.01639928	3.40630653	8.60368884
H	-3.30469837	4.73090957	9.75142098
N	-4.91474121	-2.35425842	8.19020081
C	-3.84400960	-2.84769374	8.88624031
N	-3.69440719	-2.54605918	10.19294443
N	-4.29968387	-6.79094904	6.04768675
C	-5.30961050	-2.84455422	6.86482414
N	-2.91838573	-3.59862839	8.28574752
*C	-4.10105886	-7.91253880	6.80461007
H	-3.49680202	-6.22266383	5.72985957
H	-2.95725183	-3.81829536	7.27857639
H	-2.13445738	-4.03923768	8.89747553
H	-4.49251547	-2.12450320	10.66787409
H	-3.01120909	-3.14554563	10.80793649
H	-5.61782084	-1.85814177	8.73709548
*O	-5.01662878	-8.63227939	7.22763053
C	-5.61155068	-6.45584808	5.50378697
C	-5.85970613	-4.93986592	5.47285201
C	-5.75054998	-4.31583187	6.87273158
H	-5.12025736	-4.46462631	4.79544316
H	-6.85258065	-4.73849855	5.01654760
H	-6.70587230	-4.42407460	7.43467917
H	-4.99426502	-4.89822332	7.44023650
H	-6.35855192	-6.98213014	6.13497276
H	-5.70937088	-6.87093618	4.47289590
H	-6.10738695	-2.17972302	6.48111974
H	-4.45950371	-2.69714200	6.16682167
*H	-1.91256699	-5.71473257	-2.00787482
*C	-1.22381602	-5.35758204	-1.24259015
C	-0.33537300	-4.17376733	-1.65608514
C	-1.16823811	-2.95771869	-2.08996342
C	0.63543815	-3.78131201	-0.52575147
H	-0.59821509	-6.22660012	-0.94008959
H	-1.82912175	-5.08636848	-0.35140501
H	-0.51956594	-2.13088371	-2.44852915

H	-1.74483243	-2.56908078	-1.22642828
H	-1.89221253	-3.21134142	-2.89438903
H	1.26581545	-2.91570603	-0.81966198
H	1.30237595	-4.62675486	-0.25032820
H	0.07545787	-3.47860169	0.38285184
*H	0.28211895	-4.51169608	-2.51634340
*C	0.77122478	3.66734308	5.20647733
*H	1.52467310	3.38072081	5.94006496
C	-0.28185410	2.56847696	5.10322533
N	0.64768396	-0.55248632	8.25471829
*C	0.83224872	-1.76448549	7.49715652
H	1.70790200	-1.65079116	6.81368073
C	-0.41498591	-2.10591982	6.64920613
H	-7.84024480	0.83778234	6.38789164
*C	-6.96709080	1.52420580	6.39377203
*H	-7.10685783	2.21646981	5.56345357
C	-5.67980081	0.69389486	6.21935303
H	-3.97480345	3.58869282	2.71617682
*C	-3.91056402	2.67632706	2.09238164
C	-4.22625993	1.39714376	2.91713689
H	1.26960916	3.83552504	4.22697530
C	0.61499591	-0.53860985	9.61872219
O	0.82363351	-1.51267513	10.34104354
*H	-4.62768547	2.72917049	1.27289129
H	-0.30740564	-3.09875574	6.16936877
H	-1.31415527	-2.14762183	7.29113533
H	0.33614034	0.28456902	7.73006589
H	-5.65495805	-0.12516139	6.96375572
H	-5.66901343	0.20354233	5.22215302
H	-1.09507113	2.85565715	4.40616246
H	0.16384671	1.63824112	4.69482701
H	-6.96264091	2.11009443	7.33586218
H	0.32623552	4.62831518	5.54285864
H	-2.89642319	2.62547598	1.64160687
H	-4.90490155	1.61408301	3.76116587
H	-4.70205276	0.61321404	2.30352487
*H	1.07685390	-2.59934171	8.18014846
*H	2.40499065	3.14179095	8.83330041
*C	2.06421193	2.32864507	9.47429896
O	2.87913872	1.80170611	10.23815449
N	0.73336625	1.99702983	9.43830705
H	0.17181756	2.30538656	8.61838146
*C	0.25047016	0.83629920	10.20744169
*H	-0.83217719	0.87853888	10.32658263
H	0.71184415	0.86143903	11.21372780
*H	-7.54459197	4.95612458	4.28636675
*C	-6.71945774	5.40678447	3.73494966
O	-6.91826087	5.76003918	2.56713117
*N	-5.56655622	5.54874939	4.37944429
*H	-4.68326999	5.94826446	3.88113461
H	-5.45161683	5.22952939	5.35901932
S	-1.06383639	2.14419347	6.71910702
S	-0.76903383	-0.93142445	5.23525753
S	-4.13221035	1.67163398	6.46865131
S	-2.71295242	0.60211066	3.63876468

Ni	-2.40122076	0.54325338	5.78758443
Fe	-2.64351360	-1.60878256	3.98724690
C	-2.20508055	-2.27652382	2.46883492
C	-4.44799315	-1.84012417	3.60603260
O	-1.98184003	-2.70676762	1.40181060
N	-5.58973216	-2.00101444	3.35921823
C	-2.58498242	-3.31322194	4.80591097
N	-2.53782076	-4.38150362	5.30755924
*H	-0.56318454	-5.82934907	12.91345682
*C	-0.59650686	-5.92957645	11.82855512
C	-1.36722649	-4.83887777	11.06632611
O	-2.19323235	-4.12012181	11.70364159
O	-1.13772036	-4.79742818	9.81279300
H	0.43936486	-5.97888720	11.43502873
H	-1.07040827	-6.90598851	11.58479854
H	-3.38198848	6.17262751	6.58715158
*C	-0.94249195	-8.04263729	3.68241799
C	-1.91689827	-8.47223905	4.78494650
O	-2.85733071	-9.24357565	4.55704879
C	-1.46491822	-8.39388401	2.28849316
N	-1.71158185	-7.94792257	6.03790415
C	-2.65396719	-8.27803924	7.11748183
C	-2.10751376	-7.51147488	8.33549003
*C	-0.61149933	-7.43117524	8.04641666
C	-0.57585548	-7.14991057	6.53204509
*C	-4.10469895	-0.94795313	-1.13382440
C	-4.77810706	-0.66715679	-2.48376920
*C	-4.94842589	-0.57248019	0.05502928
H	-5.92435699	-1.09494086	0.03907037
H	-4.46272442	-0.87446046	1.00471348
H	-5.13572770	0.52398310	0.09039726
H	-3.12969341	-0.40917716	-1.09817113
H	-3.84058132	-2.02013855	-1.07386033
H	-5.74166062	-1.21685988	-2.56867941
H	-5.01506616	0.41330022	-2.60242996
H	-4.13757272	-0.96927364	-3.34005501
H	-1.68745929	-9.47714120	2.21356812
H	-2.41248180	-7.85544558	2.08278136
H	-0.73169362	-8.11513260	1.50388015
H	0.04224965	-8.53061656	3.87328095
H	-0.75744795	-6.94935903	3.77080432
H	-0.73895493	-6.06813098	6.31715785
H	0.37499118	-7.46236897	6.05256378
H	-0.13305958	-6.62985211	8.64459309
H	-0.11465654	-8.40411716	8.26018817
H	-2.52417536	-6.48365360	8.37416658
H	-2.36239311	-8.00800326	9.29167017
H	-2.67513316	-9.37637247	7.28817992

System: **I1** (doublet)

Charge, Multiplicity: –2, 2

Gibbs free energy: –7997.048695 au

C	0.00000000	0.00000000	0.00000000

N	0.00000000	0.00000000	1.36939101
C	2.06145122	0.00000000	0.60308808
N	1.22949920	-0.00175460	-0.50344951
C	1.31667894	0.00064041	1.77930311
H	-0.92804568	-0.05615783	-0.57872897
H	3.15572850	-0.00608249	0.50195715
H	1.57816905	-0.01546874	2.84373700
H	-0.82749917	0.03314198	1.99456578
O	-9.24824045	-3.55277284	-0.04284342
C	-8.13025853	-3.40768284	0.46929301
N	-7.85323308	-2.44298787	1.39713256
C	-8.87570755	-1.51182482	1.85425835
C	-8.30993849	-0.43323649	2.79128838
O	-7.95495144	-0.91613550	4.07011281
H	-9.35333569	-1.03789320	0.96521854
H	-6.91758133	-2.39057419	1.83532950
H	-9.68717632	-2.05977280	2.38805014
H	-7.44678480	0.06808635	2.28130599
H	-9.09828362	0.34287464	2.92584759
H	-7.08106659	-1.39747285	3.94125466
C	-4.79271819	-4.74866214	1.25388472
C	-4.58603803	-4.32762179	-0.20392390
H	-4.56408213	-3.89198899	1.91831463
H	-4.14580047	-5.59496103	1.55969325
H	-3.67020499	-3.71967614	-0.34207647
H	-4.49214109	-5.23391049	-0.86325625
C	-6.92989240	-4.30551403	0.09438699
C	-6.30296254	-5.07815653	1.30876747
H	-6.48814269	-6.16548302	1.19074342
H	-6.75180943	-4.77365716	2.27556269
H	-7.35576426	-5.03855327	-0.63456494
N	-5.79374240	-3.53783179	-0.46510051
H	-5.93143851	-3.31434781	-1.45657670
H	-5.74030169	3.74886330	10.07218185
C	-4.94931591	3.16877413	9.59706793
H	-4.63518179	2.40017476	10.33312323
H	-5.38780082	2.62019190	8.74218826
C	-3.72366521	3.94827801	9.12970858
C	-3.92915542	4.70567664	7.84564457
O	-2.96518401	5.62622097	7.62669714
O	-4.83914462	4.49344736	7.04928227
H	-2.89634186	3.24417129	8.86622002
H	-3.30022368	4.63133890	9.89524621
N	-5.00331852	-2.50471865	8.20402261
C	-3.91470388	-3.00328557	8.88389162
N	-3.79979214	-2.78293034	10.20869455
N	-4.31626643	-6.87897768	5.92976273
C	-5.37381707	-2.98543306	6.86482649
N	-2.94834831	-3.66543110	8.24926656
C	-4.12350374	-7.99642460	6.69209647
H	-3.51749806	-6.28619308	5.64371041
H	-2.98947264	-3.87860296	7.23695292
H	-2.16631398	-4.11889789	8.84793113
H	-4.60302439	-2.37820280	10.68907049
H	-3.09624232	-3.38435271	10.80816713

H	-5.77704379	-2.21324267	8.80353153
O	-5.04090196	-8.71884104	7.10604246
C	-5.62489772	-6.54343382	5.38161349
C	-5.89230688	-5.03155149	5.40922760
C	-5.77027999	-4.46531793	6.83142387
H	-5.16517121	-4.51984692	4.74466014
H	-6.89395243	-4.82371157	4.97501710
H	-6.71147647	-4.62333782	7.40667994
H	-4.98657501	-5.04813132	7.35994078
H	-6.37115370	-7.10432211	5.98315142
H	-5.70239831	-6.91845937	4.33393990
H	-6.19544877	-2.34704145	6.48641627
H	-4.52461646	-2.78720536	6.17869929
H	-1.93955885	-5.67606158	-2.09004321
C	-1.24772967	-5.33370389	-1.32042806
C	-0.35646657	-4.14665464	-1.71815885
C	-1.18792323	-2.92303101	-2.13296598
C	0.61361642	-3.77046214	-0.58170552
H	-0.62496189	-6.20951185	-1.03190652
H	-1.85056494	-5.07226497	-0.42472949
H	-0.53835087	-2.09169234	-2.47916283
H	-1.76151352	-2.54706520	-1.26177087
H	-1.91378893	-3.16302147	-2.94007484
H	1.24598553	-2.90228919	-0.86350734
H	1.27808053	-4.62090388	-0.31543349
H	0.05170669	-3.47708135	0.32899476
H	0.25916081	-4.47464374	-2.58412071
C	0.79480936	3.58550400	5.25947238
H	1.54809758	3.28507585	5.98742367
C	-0.26544441	2.50211070	5.12703100
N	0.51171969	-0.71450878	8.24874612
C	0.83708556	-1.88012765	7.46824619
H	1.75198272	-1.68635925	6.85673304
C	-0.30680724	-2.31219057	6.53149568
H	-7.91578875	0.90800198	6.49277958
C	-6.95191865	1.45612530	6.42646413
H	-7.08796322	2.16279202	5.60802197
C	-5.83849417	0.43606018	6.19479455
H	-3.97691561	3.57052457	2.76689435
C	-3.89606251	2.66088146	2.13841855
C	-4.12290187	1.36892182	2.96720210
H	1.30209385	3.76564468	4.28556055
C	0.62812587	-0.68572009	9.60812808
O	0.95959059	-1.64135029	10.30911260
H	-4.61437130	2.72883324	1.32121880
H	-0.06414455	-3.27697016	6.04303207
H	-1.23470472	-2.45985007	7.11205578
H	0.17207046	0.11781294	7.73684775
H	-5.99415036	-0.45321658	6.83145628
H	-5.80796872	0.07310528	5.15069536
H	-1.02212794	2.77403518	4.36414095
H	0.19113052	1.55470087	4.77269974
H	-6.81262451	2.03156462	7.36446176
H	0.35867628	4.54790432	5.60609307
H	-2.88568302	2.65653016	1.67648509

H	-4.70603192	1.57556615	3.88540439
H	-4.68705064	0.60410052	2.40350414
H	1.07886750	-2.72583619	8.13873611
H	2.43202574	2.99922294	8.87529636
C	2.08888645	2.17797115	9.50454280
O	2.89341494	1.65336620	10.28041777
N	0.75821030	1.83993564	9.44311251
H	0.19840308	2.15155855	8.61960260
C	0.27009577	0.68235726	10.21840581
H	-0.81213841	0.72724912	10.33993388
H	0.74318556	0.70065551	11.21863653
H	-7.51718594	4.92254104	4.37243125
C	-6.69099666	5.37771891	3.82651155
O	-6.89912714	5.77002903	2.67415229
N	-5.53653355	5.50566523	4.47100206
H	-4.65233506	5.90872456	3.97741868
H	-5.37206953	5.09822511	5.40819778
S	-1.17164279	2.11942164	6.68887114
S	-0.66678203	-1.11653237	5.15280712
S	-4.16826026	0.99514107	6.72067249
S	-2.54171193	0.57723112	3.50924093
Ni	-2.29450714	0.29340770	5.74718936
Fe	-2.57953664	-1.66063529	4.00607176
C	-2.21110075	-2.33630337	2.46533024
C	-4.40597356	-1.80140507	3.68135092
O	-2.01396075	-2.76284649	1.39048274
N	-5.55337661	-1.93622500	3.43176153
C	-2.59759528	-3.35382089	4.82450952
N	-2.59879600	-4.42510930	5.32615645
H	-0.56706910	-6.01953449	12.82569282
C	-0.60214872	-6.10363280	11.73953371
C	-1.40154285	-5.01392673	11.00546546
O	-2.24634724	-4.33610602	11.66659037
O	-1.17545550	-4.92745450	9.75540246
H	0.43203907	-6.12245570	11.33956531
H	-1.05752451	-7.08503926	11.48118101
H	-3.09299801	5.96151381	6.71285536
H	-4.25432483	2.25335970	6.22564970
C	-0.97011505	-8.09295848	3.56321877
C	-1.93958391	-8.54178687	4.66393785
O	-2.87689574	-9.31472603	4.42862060
C	-1.49681505	-8.42633611	2.16659735
N	-1.73441497	-8.03177220	5.92310735
C	-2.67725325	-8.37046053	7.00027242
C	-2.12521696	-7.62284442	8.22710715
C	-0.62965985	-7.54824308	7.93532679
C	-0.59823457	-7.24004768	6.42603630
C	-4.11053283	-0.91402101	-1.14109282
C	-4.78969954	-0.61928325	-2.48538228
C	-4.95076993	-0.55290863	0.05452730
H	-5.92541904	-1.07767193	0.03544462
H	-4.45833063	-0.85938936	1.00005549
H	-5.13948156	0.54309812	0.10272753
H	-3.13680243	-0.37364222	-1.10240931
H	-3.84268422	-1.98576753	-1.09602116

H	-5.75313533	-1.16914987	-2.57222172
H	-5.02843463	0.46224153	-2.59128611
H	-4.15233490	-0.91100352	-3.34775680
H	-1.71710420	-9.50905136	2.07772267
H	-2.44612374	-7.88711664	1.97154964
H	-0.76710274	-8.13484690	1.38337692
H	0.01695148	-8.58031662	3.74343468
H	-0.78835738	-7.00049628	3.66646797
H	-0.76428323	-6.15467494	6.23148378
H	0.35128791	-7.54312155	5.93818152
H	-0.14315741	-6.76044405	8.54502680
H	-0.13850723	-8.52796926	8.13049735
H	-2.53421222	-6.59245183	8.27954982
H	-2.38162187	-8.13018860	9.17726232
H	-2.70330963	-9.47074447	7.15743203

System: **Ni-C** (doublet)

Charge, Multiplicity: –2, 2

Gibbs free energy: –7997.059728 au

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.36887221
C	2.06199313	0.00000000	0.60253858
N	1.22972421	0.00368574	-0.50310063
C	1.31727360	0.00036049	1.77858383
H	-0.92842651	-0.02566775	-0.58047979
H	3.15617143	-0.00840042	0.50103119
H	1.58232797	-0.01668184	2.84205928
H	-0.83092054	0.06626925	1.99083946
O	-9.27996647	-3.47013058	-0.17544336
C	-8.16526977	-3.33784204	0.34719386
N	-7.88894652	-2.39516621	1.29571939
C	-8.91131463	-1.48332053	1.79093932
C	-8.35646623	-0.49925469	2.83347112
O	-8.02406371	-1.10243904	4.06680308
H	-9.34966320	-0.92307183	0.93174165
H	-6.95723458	-2.36504177	1.74528392
H	-9.74934598	-2.06006670	2.24662932
H	-7.48309106	0.04295664	2.38760321
H	-9.14265348	0.26555444	3.02845597
H	-7.14462565	-1.55385892	3.91248914
C	-4.80783574	-4.76733886	1.04516687
C	-4.63745679	-4.28939588	-0.40138861
H	-4.50933100	-3.95599480	1.73743139
H	-4.19335190	-5.65862443	1.28268993
H	-3.71006387	-3.70000340	-0.54831685
H	-4.58857129	-5.16977562	-1.09993444
C	-6.96489015	-4.23199430	-0.03944137
C	-6.33106336	-5.02234262	1.15821982
H	-6.57836394	-6.09942541	1.06619984
H	-6.72277341	-4.67959883	2.13672913
H	-7.39008921	-4.95568920	-0.77877666
N	-5.82956957	-3.45899601	-0.59090507
H	-5.98848936	-3.18758215	-1.56747219

H	-5.70549678	3.44845070	10.19835794
C	-4.92137029	2.87581944	9.70307010
H	-4.56953500	2.11417414	10.42997282
H	-5.37947736	2.32262699	8.86039226
C	-3.72491297	3.66671875	9.18909679
C	-4.03032845	4.54672005	8.00558875
O	-2.94376190	5.26136493	7.61573113
O	-5.10816090	4.61998216	7.42856301
H	-2.94311286	2.96799954	8.80766627
H	-3.22513104	4.28271202	9.96834117
N	-5.04344768	-2.75239570	8.14348425
C	-3.95083228	-3.25760104	8.79415162
N	-3.79652195	-3.03857411	10.11800189
N	-4.39456658	-7.03132897	5.69594244
C	-5.43951154	-3.15822703	6.79048932
N	-3.00862678	-3.93714748	8.13769497
C	-4.20826934	-8.18615729	6.40337527
H	-3.59006799	-6.44081151	5.42353700
H	-3.06055773	-4.10668688	7.12107841
H	-2.22701918	-4.42389295	8.71353995
H	-4.61049863	-2.69280047	10.62662640
H	-3.09997231	-3.66940676	10.68328281
H	-5.74833099	-2.30329894	8.72712207
O	-5.13382939	-8.91301777	6.79122446
C	-5.70412665	-6.66149066	5.16978943
C	-5.96489205	-5.14982997	5.25508114
C	-5.85558153	-4.63291573	6.69755467
H	-5.23187666	-4.61763606	4.61361348
H	-6.96154373	-4.92301378	4.81888530
H	-6.80412470	-4.80099287	7.25629641
H	-5.08415241	-5.24228834	7.21459203
H	-6.45128453	-7.23989901	5.75313612
H	-5.79106178	-6.99530088	4.10888765
H	-6.24957063	-2.48108259	6.45649383
H	-4.59597847	-2.95037205	6.10166991
H	-1.99691833	-5.57782684	-2.29061642
C	-1.30220496	-5.26987826	-1.50933170
C	-0.39800293	-4.07926382	-1.86360090
C	-1.21545641	-2.83157824	-2.23141835
C	0.57471694	-3.75641655	-0.71318777
H	-0.68900164	-6.16197452	-1.25200043
H	-1.90361552	-5.03608122	-0.60492740
H	-0.55722458	-1.99552467	-2.54851670
H	-1.78341634	-2.48027352	-1.34589184
H	-1.94663018	-3.03282793	-3.04406848
H	1.21523704	-2.88367515	-0.96018556
H	1.23064893	-4.62255704	-0.47866907
H	0.01463639	-3.49374156	0.20833266
H	0.21432641	-4.38222934	-2.74144915
C	0.82923524	3.38837570	5.38362902
H	1.57926672	3.05421418	6.10046612
C	-0.19289461	2.28545211	5.12757685
N	0.58801069	-0.98941775	8.21536988
C	0.81401459	-2.15257940	7.39707482
H	1.70733598	-1.99118952	6.74647192

C	-0.39733393	-2.48429016	6.50667990
H	-7.85076570	0.66529833	6.45572785
C	-6.93806924	1.29965181	6.47456102
H	-7.06847066	2.03490971	5.68039767
C	-5.71193281	0.39046776	6.30131022
H	-3.95972664	3.49479506	2.91005383
C	-3.86949704	2.62348285	2.23124951
C	-4.09605974	1.29355241	2.98714497
H	1.34836025	3.66892496	4.44134192
C	0.62025292	-1.03174465	9.57906158
O	0.87195241	-2.03127525	10.25014210
H	-4.58644910	2.72781609	1.41689968
H	-0.25207612	-3.45376578	5.98941394
H	-1.31500461	-2.57258101	7.11797702
H	0.27350472	-0.13019069	7.73160958
H	-5.75485226	-0.43718850	7.03661558
H	-5.71620563	-0.08407506	5.29888435
H	-0.95249932	2.61307973	4.39069191
H	0.29174583	1.38549111	4.69480678
H	-6.90971445	1.85252408	7.43714613
H	0.34729615	4.29947949	5.79888851
H	-2.85947564	2.65353966	1.76856861
H	-4.66395785	1.44592564	3.92297525
H	-4.64686333	0.55497444	2.37888870
H	1.04730085	-3.02418891	8.03664279
H	2.45886407	2.65689111	8.97648740
C	2.10702696	1.81734145	9.57613171
O	2.90572784	1.24696006	10.32326713
N	0.77057739	1.50057514	9.51097916
H	0.21099046	1.85804865	8.71499576
C	0.27260450	0.31618550	10.23613021
H	-0.80920723	0.36789976	10.35915075
H	0.74125355	0.29369218	11.23847213
H	-7.46788615	4.84150917	4.54395990
C	-6.63688631	5.30756243	4.01460745
O	-6.83371496	5.72620888	2.86839412
N	-5.48138700	5.40014303	4.66341506
H	-4.59293154	5.81160113	4.18443462
H	-5.36579562	5.02109118	5.62155491
S	-1.09674374	1.76441191	6.64327682
S	-0.71672458	-1.24527552	5.16577713
S	-4.11508775	1.26432163	6.56924855
S	-2.51234879	0.48401210	3.46844374
Ni	-2.40762593	0.12938769	5.78841425
Fe	-2.67328278	-1.74873575	4.06085287
C	-2.22668480	-2.36423787	2.49591894
C	-4.47158493	-1.90516909	3.59578699
O	-2.00552610	-2.76307503	1.42217697
N	-5.60154084	-2.04104418	3.29155040
H	-3.34485513	-1.16048591	5.53269689
C	-2.67446123	-3.50352666	4.74900303
N	-2.64398957	-4.61161393	5.15390026
H	-0.63486821	-6.46527460	12.60362839
C	-0.67034467	-6.50998668	11.51510444
C	-1.44577388	-5.37712293	10.82092458

O	-2.26266954	-4.69391824	11.50796518
O	-1.22856727	-5.26341869	9.56999747
H	0.36398798	-6.53639834	11.11544979
H	-1.14526064	-7.47179694	11.22088703
H	-3.20252726	5.73846898	6.79870727
C	-1.05507963	-8.20382934	3.27328731
C	-2.03268920	-8.67734500	4.35561369
O	-2.98127608	-9.42656970	4.09108169
C	-1.58912355	-8.46940573	1.86485971
N	-1.82007084	-8.21797002	5.63253711
C	-2.76652817	-8.58640529	6.69631344
C	-2.20775570	-7.88907120	7.94954275
C	-0.71102797	-7.81836861	7.66199780
C	-0.67342476	-7.46088103	6.16381178
C	-4.11893931	-0.83016422	-1.17327668
C	-4.78810133	-0.46665808	-2.50567939
C	-4.95615042	-0.50320910	0.03448255
H	-5.94146955	-1.00605646	-0.00886624
H	-4.47495294	-0.86075197	0.96698136
H	-5.12250123	0.59308303	0.12856211
H	-3.13525564	-0.31016546	-1.11008215
H	-3.87342086	-1.90834130	-1.17290191
H	-5.76038004	-0.99568606	-2.61842616
H	-5.00775815	0.62226738	-2.56567960
H	-4.15291622	-0.73234229	-3.37799419
H	-1.83244145	-9.54272761	1.73324015
H	-2.52710632	-7.90309413	1.69278390
H	-0.85368921	-8.16265595	1.09284097
H	-0.07842489	-8.71883488	3.43222806
H	-0.85017593	-7.12059114	3.42042020
H	-0.82340826	-6.36739514	6.00583398
H	0.27258054	-7.76088417	5.66710331
H	-0.21936617	-7.05565650	8.29882900
H	-0.22901760	-8.80839149	7.82531713
H	-2.60739254	-6.85769776	8.03970902
H	-2.46955672	-8.42803042	8.88054910
H	-2.80354531	-9.69137296	6.81310927

System: **Ni-R** (singlet)

Charge, Multiplicity: –2, 1

Gibbs free energy: –7997.645182 au

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N	0.00000000	0.00000000	1.36563044
C	2.06126541	0.00000000	0.59363591
N	1.22642402	0.00575617	-0.51089061
C	1.31761801	0.00022973	1.77170966
H	-0.93238644	-0.01352702	-0.57473772
H	3.15554784	-0.00961644	0.49011698
H	1.58598763	-0.01770009	2.83446683
H	-0.84891743	0.08165474	1.97631612
O	-9.29988577	-3.40769076	-0.16053820
C	-8.17684368	-3.30904477	0.35228847
N	-7.88195440	-2.40593173	1.33496249

C	-8.89173253	-1.49180349	1.85269806
C	-8.30917940	-0.45130937	2.82288643
O	-7.95070110	-0.97868950	4.08421542
H	-9.38492284	-0.98203850	0.99272778
H	-6.94394146	-2.38864767	1.77149052
H	-9.69506408	-2.05881277	2.37931666
H	-7.44535672	0.05993130	2.32478573
H	-9.09047700	0.32553962	2.98968032
H	-7.08719955	-1.46878327	3.92955624
C	-4.87195355	-4.72361349	1.06887639
C	-4.64318334	-4.22710987	-0.36144679
H	-4.65750679	-3.90232915	1.78109572
H	-4.22771440	-5.58354523	1.34066903
H	-3.72606209	-3.61104980	-0.45117406
H	-4.53421381	-5.09748600	-1.06510586
C	-6.99499816	-4.20434056	-0.08396873
C	-6.38065104	-5.06038966	1.07959767
H	-6.55678275	-6.13712632	0.87869525
H	-6.84504683	-4.83070424	2.05964864
H	-7.44033035	-4.88286408	-0.85264409
N	-5.84751717	-3.42596142	-0.60304691
H	-5.97390563	-3.15707417	-1.58435300
H	-5.62561494	3.32506176	10.28340676
C	-4.84690927	2.75659353	9.77502270
H	-4.51645110	1.96119591	10.47457669
H	-5.30520498	2.24946050	8.90515957
C	-3.63637577	3.56064675	9.31361466
C	-3.91671419	4.45599317	8.13693455
O	-2.90365692	5.32112850	7.89413741
O	-4.92306211	4.40271653	7.43802531
H	-2.83915677	2.87608093	8.93413831
H	-3.15832395	4.15825253	10.11840779
N	-5.05022535	-2.85379900	8.14136311
C	-3.95881579	-3.39839401	8.78135539
N	-3.83741575	-3.26565010	10.11747986
N	-4.38511053	-7.09728655	5.61774081
C	-5.43098286	-3.24421811	6.77554640
N	-2.99602105	-4.01908215	8.10161121
C	-4.20172178	-8.25985230	6.31247411
H	-3.58058450	-6.49842311	5.35912607
H	-3.04437384	-4.16994243	7.07962194
H	-2.21503948	-4.51690628	8.66509953
H	-4.63985669	-2.89770915	10.62790198
H	-3.12942126	-3.90381377	10.67201460
H	-5.82230094	-2.60918131	8.76376330
O	-5.12770269	-8.98841457	6.69599816
C	-5.69282495	-6.71875154	5.09458777
C	-5.95099009	-5.20813280	5.20264684
C	-5.84102530	-4.71733263	6.65392907
H	-5.21559189	-4.66617505	4.57229496
H	-6.94718173	-4.97241706	4.77005086
H	-6.78860627	-4.90105389	7.21068807
H	-5.06573350	-5.33343375	7.15720939
H	-6.44244764	-7.30498747	5.66709668
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H	-6.24146443	-2.56736943	6.43969566
H	-4.57842080	-3.01898036	6.10369987
H	-2.03507069	-5.53620555	-2.35725419
C	-1.33425688	-5.24217672	-1.57613434
C	-0.43096533	-4.04825183	-1.92187591
C	-1.25045320	-2.79779737	-2.27555955
C	0.54203359	-3.73453871	-0.76925987
H	-0.72163581	-6.13903447	-1.33462151
H	-1.92955263	-5.01774921	-0.66534383
H	-0.59357505	-1.95806239	-2.58549795
H	-1.81541473	-2.45549980	-1.38465639
H	-1.98363713	-2.99139124	-3.08845264
H	1.18114658	-2.85838457	-1.00759445
H	1.19866444	-4.60222955	-0.54216501
H	-0.01921257	-3.47994645	0.15412767
H	0.17825398	-4.34335918	-2.80521760
C	0.87789913	3.30725589	5.42623191
H	1.63111872	2.95977449	6.13328183
C	-0.16720268	2.21833968	5.18897887
N	0.58137737	-1.12577032	8.20232868
C	0.85225357	-2.26194867	7.36003634
H	1.75710018	-2.06460332	6.73526797
C	-0.32466236	-2.61137729	6.44058557
H	-7.80745894	0.60867223	6.50375877
C	-6.89109785	1.23505432	6.53713348
H	-7.02334185	1.98222706	5.75460942
C	-5.68619882	0.31597349	6.31656015
H	-3.93895205	3.46710962	2.98779233
C	-3.84407756	2.60715627	2.29358857
C	-4.05750435	1.25484256	3.01328190
H	1.38750484	3.57250012	4.47442474
C	0.67922479	-1.17350284	9.56144637
O	0.98337521	-2.16980390	10.21650563
H	-4.56580878	2.72598971	1.48549885
H	-0.11576168	-3.54050128	5.87302456
H	-1.24224857	-2.77930523	7.03192011
H	0.23728389	-0.26891492	7.73579989
H	-5.69553675	-0.53572114	7.02504750
H	-5.67161364	-0.11935485	5.29861680
H	-0.93103082	2.53360940	4.45063043
H	0.30299594	1.30803482	4.76336182
H	-6.84593035	1.76125855	7.51265736
H	0.42123446	4.23069620	5.84412772
H	-2.83526643	2.65255217	1.83144845
H	-4.61534840	1.39978898	3.96289407
H	-4.66856473	0.55775539	2.41275759
H	1.08597036	-3.14352721	7.98562929
H	2.52743000	2.51758314	8.99758056
C	2.17588454	1.67099799	9.58741507
O	2.97474745	1.09749206	10.33257334
N	0.83879480	1.35689730	9.51928855
H	0.28445151	1.70761185	8.71304679
C	0.33944468	0.16807696	10.23773943
H	-0.74133468	0.22246464	10.36840149
H	0.81685132	0.13346483	11.23546901

H	-7.41823683	4.80643767	4.66107958
C	-6.58870475	5.27670598	4.13312512
O	-6.79209257	5.71587694	2.99720991
N	-5.42865662	5.35505873	4.77571650
H	-4.54160202	5.76976897	4.29690198
H	-5.29652666	4.95983207	5.72369200
S	-1.07111796	1.68911418	6.70887491
S	-0.69130831	-1.30938405	5.18273187
S	-4.05056858	1.07487166	6.68288229
S	-2.46435539	0.44101483	3.39351720
Ni	-2.32470244	0.00194584	5.87949593
Fe	-2.64105075	-1.80318269	4.09277443
C	-2.23220120	-2.37484215	2.50565361
C	-4.44785213	-1.91439370	3.65237505
O	-2.03100951	-2.73965340	1.41469482
N	-5.58500223	-2.02346888	3.35695972
H	-3.23996906	-1.28176655	5.62650178
C	-2.65100122	-3.56669209	4.74811423
N	-2.63731246	-4.68151369	5.14011062
H	-0.58121357	-6.64277452	12.51358494
C	-0.62418642	-6.67196409	11.42482631
C	-1.43272435	-5.54565524	10.75762251
O	-2.26970575	-4.90455704	11.46421534
O	-1.22122586	-5.39141147	9.51166309
H	0.40657074	-6.66646144	11.01577240
H	-1.07987760	-7.63953086	11.11937338
H	-3.12590104	5.79191413	7.06197718
H	-4.16282024	2.10812225	5.80147709
C	-1.06866805	-8.24558653	3.16223513
C	-2.04035521	-8.73287410	4.24437016
O	-2.99361128	-9.47470098	3.97515180
C	-1.60715313	-8.49998643	1.75355325
N	-1.81746411	-8.29385634	5.52671010
C	-2.75971514	-8.67060024	6.59138224
C	-2.19001936	-7.99191916	7.84988058
C	-0.69488507	-7.92458560	7.55368623
C	-0.66595484	-7.54585925	6.06044719
C	-4.12992512	-0.79647377	-1.15809120
C	-4.80962804	-0.41928086	-2.48150560
C	-4.95797854	-0.48324853	0.05936572
H	-5.94127061	-0.99071839	0.02040985
H	-4.46287419	-0.84178943	0.98437765
H	-5.12738490	0.61180472	0.16269208
H	-3.14694074	-0.27584480	-1.09495256
H	-3.88131856	-1.87364641	-1.17324908
H	-5.78283203	-0.94736131	-2.59231944
H	-5.03015494	0.67023633	-2.52823459
H	-4.18121468	-0.67512804	-3.36177372
H	-1.84497914	-9.57330684	1.61166935
H	-2.54890815	-7.93723833	1.59113874
H	-0.87661795	-8.18105870	0.98184145
H	-0.08884916	-8.75710919	3.31252772
H	-0.86857273	-7.16277381	3.31934455
H	-0.81566352	-6.45010284	5.91876110
H	0.27612208	-7.84095651	5.55348408

H	-0.19467712	-7.17324025	8.19735434
H	-0.21647750	-8.91901059	7.70023134
H	-2.58361908	-6.95966547	7.95484400
H	-2.44894244	-8.54116074	8.77574516
H	-2.80189132	-9.77675954	6.69479608

System: **I2a** (singlet)

Charge, Multiplicity: –2, 1

Gibbs free energy: –7997.639588 au

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.37041181
C	2.06191893	0.00000000	0.60385656
N	1.22994811	0.00318440	-0.50240313
C	1.31765670	-0.00090741	1.77989267
H	-0.92806037	-0.02735131	-0.58067134
H	3.15607375	-0.00642481	0.50266212
H	1.58199826	-0.01667537	2.84353131
H	-0.82366837	0.03563960	1.99848319
O	-9.28318577	-3.47125273	-0.15670627
C	-8.16400868	-3.33919687	0.35574352
N	-7.88109869	-2.39963609	1.30635455
C	-8.90218308	-1.49556703	1.81909438
C	-8.34995276	-0.53455141	2.88453166
O	-8.01787080	-1.16494048	4.10478706
H	-9.33727593	-0.91440366	0.97209845
H	-6.94392529	-2.36705064	1.74220742
H	-9.74226987	-2.08172746	2.25818643
H	-7.47639222	0.01895730	2.45360987
H	-9.13756262	0.22462589	3.09482965
H	-7.13050192	-1.59779700	3.94340137
C	-4.81835867	-4.77403131	1.06015619
C	-4.63518031	-4.29085849	-0.38285394
H	-4.53037632	-3.96354815	1.75829939
H	-4.20208404	-5.66319946	1.30110010
H	-3.70792825	-3.69844250	-0.51735420
H	-4.57724053	-5.16861550	-1.08383017
C	-6.96757033	-4.23487814	-0.03912932
C	-6.34116138	-5.03824427	1.15455131
H	-6.58064256	-6.11541584	1.04415872
H	-6.74620797	-4.71204312	2.13339932
H	-7.39595995	-4.95011674	-0.78470207
N	-5.82774118	-3.46295319	-0.58073540
H	-5.97861583	-3.18747532	-1.55730207
H	-5.71197703	3.48477807	10.18251973
C	-4.92713893	2.91046983	9.69018833
H	-4.57211617	2.15162729	10.41865908
H	-5.37796317	2.35664698	8.84323226
C	-3.73521809	3.71117898	9.17852318
C	-4.05343839	4.61954221	8.01996896
O	-2.97092804	5.34432564	7.63694301
O	-5.13464490	4.70532447	7.45007603
H	-2.96030690	3.02137401	8.76664883
H	-3.22453025	4.30778171	9.96580643

N	-4.97884546	-2.66736050	8.12439370
C	-3.89835394	-3.19704871	8.78050567
N	-3.73247558	-2.96180771	10.09902093
N	-4.39749637	-6.99956089	5.73745623
C	-5.40229316	-3.09426250	6.78518835
N	-2.97578361	-3.90792994	8.12957852
C	-4.20868963	-8.16297728	6.43196044
H	-3.59158856	-6.41893694	5.45097756
H	-3.04003988	-4.10205222	7.11706359
H	-2.19943146	-4.39815451	8.71315927
H	-4.52770473	-2.56975226	10.60371135
H	-3.04946400	-3.60222831	10.67618209
H	-5.67626774	-2.20694939	8.70880131
O	-5.13334602	-8.88934005	6.82202200
C	-5.71031404	-6.62303899	5.22280514
C	-5.95441776	-5.10737755	5.28671376
C	-5.83894575	-4.56567857	6.72053291
H	-5.21659218	-4.59359404	4.63585989
H	-6.94876548	-4.87656648	4.84767319
H	-6.78998693	-4.70910101	7.28147030
H	-5.07644556	-5.17641420	7.24901523
H	-6.45633699	-7.18509014	5.82341192
H	-5.81537611	-6.97149920	4.16827926
H	-6.20511870	-2.40882322	6.45062452
H	-4.56689006	-2.91812122	6.07687575
H	-1.99376162	-5.58626250	-2.27061108
C	-1.29906675	-5.27570866	-1.49023498
C	-0.39440206	-4.08639936	-1.84779497
C	-1.21117150	-2.83912378	-2.21873441
C	0.58018252	-3.76208197	-0.69934211
H	-0.68614609	-6.16713492	-1.22981727
H	-1.90055176	-5.03833696	-0.58681370
H	-0.55215948	-2.00466082	-2.53842868
H	-1.77868605	-2.48512519	-1.33419025
H	-1.94205357	-3.04239448	-3.03116565
H	1.22095236	-2.89037896	-0.94936872
H	1.23612449	-4.62824151	-0.46474639
H	0.02178136	-3.49714640	0.22238267
H	0.21730695	-4.39168534	-2.72487570
C	0.82358377	3.41095711	5.37257239
H	1.57567751	3.07759679	6.08893697
C	-0.23643398	2.32774016	5.17755252
N	0.52302359	-0.97360007	8.22148065
C	0.81144821	-2.12449736	7.40502372
H	1.72752435	-1.93517645	6.79348826
C	-0.35170583	-2.47263194	6.45641214
H	-7.81498466	0.63718003	6.42327125
C	-6.94122730	1.32199235	6.46613266
H	-7.07246903	2.05362626	5.66930399
C	-5.65325562	0.49861963	6.28721158
H	-3.95639826	3.50527399	2.89558187
C	-3.87094768	2.63102284	2.21972481
C	-4.11683845	1.30741894	2.98633574
H	1.33009120	3.64475584	4.41083450
C	0.61266752	-0.99645471	9.58280506

O	0.90873586	-1.98429152	10.25426336
H	-4.58843459	2.73181971	1.40472665
H	-0.13255718	-3.40068171	5.89185906
H	-1.27650345	-2.65036930	7.03475374
H	0.20502022	-0.11518007	7.73379819
H	-5.57325263	-0.26479675	7.08912229
H	-5.68800042	-0.05193894	5.32399832
H	-1.02489860	2.66541593	4.47455332
H	0.21291805	1.42022471	4.72238085
H	-6.95105394	1.87217917	7.43009865
H	0.37780994	4.34859919	5.76889356
H	-2.85947856	2.64949349	1.75931057
H	-4.71346761	1.48875170	3.90378253
H	-4.64273763	0.55420702	2.37495869
H	1.04451385	-2.99292993	8.04878866
H	2.45339413	2.69194572	8.96775018
C	2.10164397	1.85451731	9.57045300
O	2.90239354	1.29155437	10.32258594
N	0.76717221	1.53503153	9.50476360
H	0.21215389	1.87850148	8.69521816
C	0.26743817	0.35518696	10.23505604
H	-0.81439557	0.40679649	10.35748368
H	0.73687558	0.33471526	11.23707908
H	-7.47208417	4.85603818	4.52232477
C	-6.64096948	5.32033839	3.99162634
O	-6.83698535	5.73419114	2.84337833
N	-5.48588856	5.41599819	4.64069129
H	-4.59731140	5.82585080	4.16054939
H	-5.37137675	5.04251200	5.60041768
S	-1.07871275	1.81335816	6.73025929
S	-0.71440201	-1.18426625	5.16416507
S	-4.14176749	1.54558930	6.36753155
S	-2.56864114	0.49981040	3.57681279
Ni	-2.43935726	0.16120939	5.85313942
Fe	-2.63366896	-1.72569801	3.99148337
C	-2.21937263	-2.33659122	2.44718099
C	-4.44172345	-1.89082393	3.59172022
O	-2.00502067	-2.72688831	1.36474801
N	-5.57865513	-2.03927602	3.31876004
C	-2.64037891	-3.46311774	4.72003059
N	-2.63340787	-4.55938842	5.15961196
H	-0.63846646	-6.41780143	12.62742284
C	-0.67318438	-6.46676008	11.53909996
C	-1.43352032	-5.33011642	10.83432914
O	-2.24177651	-4.62793225	11.51276802
O	-1.21531996	-5.23149035	9.58213325
H	0.36148686	-6.50710258	11.14157388
H	-1.15805147	-7.42469281	11.24859932
H	-3.24074174	5.83988592	6.83439324
H	-3.22576967	-1.16914032	6.36590756
H	-2.88226420	-0.79653184	7.07315649
C	-1.05335904	-8.19138250	3.30342766
C	-2.03407232	-8.65508752	4.38573957
O	-2.98579746	-9.40140259	4.12419307
C	-1.58328379	-8.46581616	1.89510567

N	-1.82096310	-8.19138701	5.66105944
C	-2.76642225	-8.56168431	6.72418746
C	-2.20857686	-7.86344561	7.97779943
C	-0.71156097	-7.78940654	7.69084977
C	-0.67419695	-7.43379461	6.19191477
C	-4.11811813	-0.83565509	-1.17208057
C	-4.78696312	-0.47804889	-2.50624117
C	-4.95597769	-0.50441891	0.03399734
H	-5.94115814	-1.00761737	-0.00812810
H	-4.47427758	-0.85761477	0.96792197
H	-5.12292833	0.59202486	0.12383314
H	-3.13499724	-0.31446867	-1.11044080
H	-3.87036486	-1.91331189	-1.16698560
H	-5.75886533	-1.00815411	-2.61763180
H	-5.00750893	0.61041384	-2.57071293
H	-4.15108469	-0.74673716	-3.37709923
H	-1.82655695	-9.53985368	1.76946675
H	-2.52039494	-7.90017374	1.71637131
H	-0.84526829	-8.16432881	1.12354858
H	-0.07804115	-8.70680176	3.46903002
H	-0.84661719	-7.10745431	3.44328640
H	-0.82348280	-6.34041666	6.03220380
H	0.27189026	-7.73432681	5.69575401
H	-0.22146574	-7.02500319	8.32666924
H	-0.22766294	-8.77824969	7.85535020
H	-2.61059254	-6.83297856	8.06770097
H	-2.46967292	-8.40304865	8.90864069
H	-2.80163584	-9.66672134	6.84092550

MODEL 3: LARGE_ACTIVE SITE MODEL

System: **Ni-SI$_a$** (singlet)

Charge, Multiplicity: –2, 1

Gibbs free energy: –4981.490387 au

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.08994840
C	1.43825695	0.00000000	-0.50848774
C	5.00592113	0.78890279	3.01232182
H	4.36777658	1.69790666	3.12772433
C	5.76602841	0.88642138	1.66922148
H	6.82187788	-4.18826431	-4.41361375
C	5.80867040	-4.03122448	-3.98657891
H	5.14561185	-3.81412470	-4.82408357
C	5.86332723	-2.85128969	-2.99576094
H	1.96870392	-0.70053634	-4.93619491
C	2.61561172	0.18761045	-5.07170866
C	4.00290741	-0.00818224	-4.39845465
H	-0.54999837	0.89707610	-0.35896048
H	2.78396563	0.37249048	-6.13288554
H	6.48467784	1.72958647	1.68171960
H	6.34704329	-0.03708185	1.49066843
H	6.67683006	-3.01154639	-2.26218299

H	6.11259857	-1.90955392	-3.53052010
H	1.47300284	-0.05843333	-1.61531623
H	1.95019477	0.94419056	-0.23063709
H	5.46093500	-4.96745908	-3.50350125
H	-0.55059235	-0.90553068	-0.33391237
H	2.08959466	1.07565926	-4.66068465
H	4.28827619	-1.07439570	-4.35655523
H	4.80486377	0.52781234	-4.93419725
H	5.71556098	0.79706283	3.86063738
S	2.45181431	-1.39339949	0.15009085
S	4.69724673	1.19619202	0.16396806
S	4.31192223	-2.63923719	-2.01528354
S	4.06597023	0.63083604	-2.65759205
Ni	4.32140288	-0.72553051	-0.98036484
Fe	5.98473269	1.39651582	-1.79365019
C	6.09081564	3.02047864	-2.33694389
C	6.99986704	0.81180150	-3.23677220
O	6.17333786	4.09915738	-2.78764246
N	7.65367453	0.45231429	-4.14983062
C	7.55291293	1.59307756	-0.75397497
N	8.52877749	1.73012039	-0.10281555
H	4.34903886	-0.10374607	3.05585880

System: **I1** (doublet)

Charge, Multiplicity: –2, 2

Gibbs free energy: –4982.06146 au

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.08977671
C	1.42906412	0.00000000	-0.52268111
C	5.00892495	0.77183464	3.01140175
H	4.30228106	1.62042917	3.18191005
C	5.79747750	1.03226528	1.71408476
H	6.74722147	-4.37677412	-4.45908442
C	5.79492651	-4.05225424	-3.98823027
H	5.13037278	-3.83328343	-4.82378617
C	6.09139530	-2.85098793	-3.09213693
H	1.96876384	-0.71587798	-4.95923548
C	2.61524961	0.17755481	-5.07238864
C	3.96159277	0.01058249	-4.31940899
H	-0.55052710	0.90167421	-0.34956545
H	2.78429168	0.36150588	-6.13351407
H	6.43341193	1.93355870	1.82150509
H	6.46618130	0.17940912	1.50120290
H	7.02790775	-3.01389027	-2.52929822
H	6.22989798	-1.91743074	-3.66841739
H	1.44990978	0.03594914	-1.63028539
H	1.96579327	0.90986561	-0.18258833
H	5.37476339	-4.90986637	-3.42401647
H	-0.56077252	-0.89984264	-0.33524582
H	2.05476057	1.05345769	-4.68134600
H	4.20854205	-1.05775921	-4.16611175
H	4.80898013	0.45121332	-4.87506175

H	5.71875608	0.77690475	3.85954809
S	2.43783113	-1.45481670	-0.00029378
S	4.73747818	1.32927661	0.21470215
S	4.87400246	-2.58689338	-1.74046793
S	3.95043867	0.79843266	-2.64611596
Ni	4.41267597	-0.57807663	-0.90208673
Fe	5.96647799	1.38204296	-1.72345559
C	6.13300071	2.99213419	-2.31170146
C	6.93146768	0.70778605	-3.16404717
O	6.23996774	4.06416521	-2.77582206
N	7.57062182	0.33743932	-4.08672279
C	7.55376740	1.50681097	-0.72246147
N	8.55059954	1.60298236	-0.09286899
H	3.76029405	-2.81497798	-2.47748882
H	4.42864132	-0.17249045	2.97540041

System: **Ni-C** (doublet)

Charge, Multiplicity: –2, 2

Gibbs free energy: –4982.08520 au

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.08998466
C	1.42899159	0.00000000	-0.53360625
C	5.05160168	0.40390715	3.01240081
H	4.45592952	1.33860645	3.14975374
C	5.84167535	0.50577117	1.69497616
H	6.46294328	-4.74200573	-4.43291194
C	5.48365121	-4.46291329	-3.98696542
H	4.83903110	-4.19555567	-4.82439539
C	5.71598249	-3.32758617	-2.97845340
H	1.93636957	-0.87472332	-4.95473382
C	2.62218836	-0.01215978	-5.07194471
C	3.95493248	-0.24518589	-4.32300174
H	-0.54914418	0.90171782	-0.34849575
H	2.80424926	0.15939639	-6.13283755
H	6.60000059	1.31214720	1.75196224
H	6.38111020	-0.43850430	1.49260814
H	6.51802535	-3.61620268	-2.27066904
H	6.07197133	-2.41306517	-3.49516419
H	1.43783920	0.01192640	-1.64135986
H	1.97576714	0.90975397	-0.20882895
H	5.04455635	-5.36118069	-3.50389894
H	-0.55905212	-0.89896250	-0.33785055
H	2.10190663	0.89275973	-4.69043733
H	4.14230338	-1.31976710	-4.14503673
H	4.82159754	0.15776776	-4.87561168
H	5.75965051	0.35776022	3.86075811
S	2.40568493	-1.46493858	0.00099416
S	4.80089465	0.90222271	0.21349393
S	4.22739539	-2.93370015	-1.97133477
S	3.97852164	0.56553469	-2.66851690
Ni	4.39886227	-0.99333285	-0.96198995
Fe	6.07049754	0.80548238	-1.70515133

C	6.30742320	2.44465633	-2.23833592
C	7.00248102	0.19716813	-3.20048034
O	6.48825724	3.51322476	-2.67003562
N	7.62059924	-0.16300357	-4.13644429
H	5.95465721	-0.88093275	-1.37964075
C	7.67199680	0.89754984	-0.71542061
N	8.66701051	0.99549187	-0.08845749
H	4.35788449	-0.46089920	3.02472505

System: **Ni-R** (singlet)

Charge, Multiplicity: –2, 1

Gibbs free energy: –4982.65931 au

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.08995535
C	1.43333431	0.00000000	-0.52897834
C	5.04124698	0.51837783	3.01221014
H	4.39295530	1.41451709	3.16931008
C	5.83787479	0.69801133	1.71385074
H	6.56500385	-4.58709934	-4.44275897
C	5.58345451	-4.33704441	-3.98754530
H	4.93279713	-4.08440889	-4.82475481
C	5.80228090	-3.18300405	-3.00497230
H	1.96328554	-0.83834655	-4.96147972
C	2.62151052	0.04762500	-5.07208755
C	3.96233872	-0.12900810	-4.32159283
H	-0.54464001	0.90386753	-0.34982866
H	2.79972462	0.22333158	-6.13293309
H	6.51208366	1.57507331	1.78624584
H	6.46392653	-0.19030317	1.51688026
H	6.60629675	-3.41932402	-2.28030917
H	6.10210296	-2.24789200	-3.51644501
H	1.46431294	0.02947046	-1.63629881
H	1.97763642	0.90535904	-0.18993295
H	5.17243834	-5.24001365	-3.49126907
H	-0.56281360	-0.89683700	-0.33888903
H	2.06925873	0.93179260	-4.68920403
H	4.16979993	-1.20462716	-4.13729357
H	4.81927769	0.24245027	-4.91119357
H	5.75012473	0.48817117	3.86059137
S	2.43849531	-1.45463496	0.00103576
S	4.77645162	0.98383883	0.22943332
S	4.38805666	-2.84023582	-1.87896858
S	3.94913636	0.74402909	-2.71453034
Ni	4.45181133	-0.90533817	-0.86540075
Fe	6.05354722	0.92274828	-1.66757345
C	6.24400910	2.55298105	-2.23234808
C	6.97519396	0.31043798	-3.16640437
O	6.38809694	3.61992185	-2.68471126
N	7.58819420	-0.04710180	-4.10909942
H	5.99333462	-0.75272365	-1.25276528
C	7.65392067	1.05333079	-0.68712064
N	8.65449567	1.16365922	-0.06796552

H	3.46962114	-2.60438336	-2.85770868
H	4.40039018	-0.38662134	2.99489669

System: **I2a** (singlet)

Charge, Multiplicity: –2, 1

Gibbs free energy: –4982.66175 au

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.09084935
C	1.43400595	0.00000000	-0.52787902
C	5.02488595	0.64392857	3.01796937
H	4.35124787	1.51890999	3.19011111
C	5.79130695	0.86327516	1.69945701
H	6.71156288	-4.34240963	-4.41826598
C	5.69764245	-4.17288660	-3.99697721
H	5.04212061	-3.93501442	-4.83432806
C	5.76812265	-3.02435580	-2.97485393
H	1.97642135	-0.75718915	-4.95106344
C	2.62221356	0.13583151	-5.06881808
C	3.97135531	-0.05037310	-4.33042370
H	-0.55046657	0.89886407	-0.35380972
H	2.79682085	0.31917487	-6.12950982
H	6.43066231	1.76613543	1.76341586
H	6.45561528	0.00385375	1.49596376
H	6.47663638	-3.28112139	-2.15977997
H	6.16094702	-2.10816739	-3.46310543
H	1.44932849	-0.03122385	-1.63634623
H	1.95536581	0.93690453	-0.23964892
H	5.32685532	-5.11345396	-3.53884787
H	-0.55546600	-0.90283699	-0.33361703
H	2.06652844	1.01617334	-4.67945381
H	4.20060201	-1.12721155	-4.19469810
H	4.81566908	0.41841913	-4.86432270
H	5.73352039	0.62867152	3.86681121
S	2.45345942	-1.41076028	0.06826754
S	4.71257236	1.12858485	0.20704970
S	4.13430155	-2.68179317	-2.19995225
S	3.98320109	0.65737747	-2.62843709
Ni	4.45502130	-0.84022575	-0.94095430
Fe	5.99007424	1.18445207	-1.72084660
C	6.15584869	2.79958347	-2.26266872
C	6.96874067	0.57558397	-3.17948633
O	6.27606763	3.87594249	-2.70644614
N	7.62058158	0.22631048	-4.09723924
C	7.57823195	1.31733783	-0.71608302
N	8.57275594	1.42222913	-0.08758510
H	6.04554446	-1.12483933	-0.73986431
H	5.63021832	-1.61420578	-0.15244725
H	4.40844108	-0.27747339	2.99775832

MODEL 4: HYDROPHOBIC MODEL

System: **Ni-SI$_a$** (singlet)

Charge, Multiplicity: –2, 1

Gibbs free energy: –5683.345281 au, –5683.919837 au (**I1**), –5683.94204 au (**Ni-C**), –5684.514304 au (**Ni-R**), –5684.51738 au (**I2a**)

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.42755649
S	3.10303684	0.00000000	0.26855474
S	1.89126788	2.09196995	2.57543775
Ni	1.49216285	0.13360315	1.72480164
Fe	1.97201643	0.81685824	4.41442666
C	1.65071602	1.89639476	5.70866150
C	3.80352191	1.04773946	4.63184624
O	1.50656103	2.67142280	6.57586265
N	4.96368676	1.19256128	4.78486627
C	2.00550187	-0.66135455	5.59447583
N	2.01654763	-1.57745789	6.33995126
C	4.40111224	1.87946962	8.30495376
C	4.29462130	3.38669094	8.57022922
H	3.97413841	1.64855896	7.30944445
H	3.85684280	1.27112335	9.05465525
H	3.33838555	3.81561987	8.20935523
H	4.35980341	3.59308279	9.67412589
C	6.58002823	3.03876929	8.13911101
C	5.92952234	1.62116860	8.29525493
H	6.28030116	1.14988640	9.23557169
H	6.21057491	0.94277428	7.46521897
H	7.07586238	3.32692180	9.09989518
N	5.43167965	3.91326979	7.81172270
H	5.63336706	4.89947747	8.01149479
H	1.80948561	4.43340234	10.75704327
C	1.06355194	3.90418706	10.16449861
C	0.10795387	4.79725564	9.35766081
C	0.86572472	5.71151676	8.38267419
C	-0.93741044	3.95654278	8.59966015
H	0.49205547	3.25783783	10.86713649
H	1.60782098	3.21581971	9.48326124
H	0.17326986	6.39827487	7.85175932
H	1.37382173	5.09931424	7.61050913
H	1.64071697	6.32078258	8.89623645
H	-1.61732819	4.60183306	8.00439134
H	-1.55067817	3.34509815	9.29642109
H	-0.44140180	3.26648848	7.88651787
H	-0.44481449	5.42883305	10.08642245
C	-1.87647978	2.03649330	-0.55407715
H	-2.63745413	1.25618178	-0.54966426
C	-0.74085196	1.64458646	0.38608311
C	-1.63096130	-2.38860188	3.33358925
H	-2.48227861	-1.71805463	3.60277218
C	-0.32622331	-1.78174620	3.89978396
H	6.86297484	-0.31411998	0.73282315
C	5.94159286	-0.01513145	0.18943491
H	6.06508319	1.03272683	-0.08430985

C	4.72860947	-0.21092704	1.12071851
H	2.96542560	4.21370005	0.18638857
C	2.99649205	4.37887905	1.28065051
C	3.37080959	3.07774700	2.04428445
H	-2.34319870	2.99483362	-0.23808086
H	3.74243678	5.13507367	1.52632549
H	-0.33855628	-1.78091102	5.00765930
H	0.54494638	-2.38371949	3.58196446
H	4.73279311	-1.23733142	1.53554646
H	4.79758213	0.47370250	1.99335531
H	0.07804717	2.39186564	0.36021670
H	-1.09780662	1.61052747	1.43594047
H	5.85269313	-0.60848087	-0.74375984
H	-1.51941341	2.14877172	-1.60027616
H	2.00941997	4.76922190	1.60865436
H	3.99423103	2.40775177	1.42585569
H	3.92987012	3.28612137	2.97244165
H	-1.84188613	-3.36515789	3.80808230
N	1.42796550	-3.78116613	9.29505863
C	2.34478800	-4.90294415	9.04285690
C	1.69048854	-5.66260943	7.87470574
C	0.20655804	-5.35767750	8.05646766
C	0.21554661	-3.87155569	8.46274682
C	3.59990381	5.70583151	5.91277660
C	4.30822596	7.03909388	6.18730751
C	4.36105167	4.79325106	4.98861267
H	5.37302701	4.57399717	5.38039703
H	3.85862719	3.80994656	4.89022582
H	4.46429683	5.23717657	3.97331212
H	2.58678126	5.91444422	5.49774653
H	3.41419453	5.18712996	6.87162808
H	5.31288486	6.87015275	6.63445189
H	4.46879901	7.61442046	5.24878050
H	3.72965665	7.68282325	6.88419652
H	0.30659797	-3.20853202	7.57104378
H	-0.68770199	-3.56958221	9.03248002
H	-0.35577008	-5.54457000	7.11961299
H	-0.22506715	-5.97018134	8.87969651
H	2.02721836	-5.25301396	6.89983964
H	1.94012303	-6.74120731	7.88438176
H	2.44046173	-5.53457847	9.95269554
H	3.36742932	-4.55055807	8.79005276
H	1.89681750	-2.89197608	9.07884783
H	7.34136088	3.07907017	7.33069010
H	-1.59999915	-2.48471790	2.22932058

MODEL 5: CHARGED MODEL

System: **Ni-SI$_a$** (singlet)

Charge, Multiplicity: –2, 1

Gibbs free energy: –5494.139578 au, –5494.713697 au (**I1**), –5494.736227 au (**Ni-C**), –5495.310164 au (**Ni-R**), –5495.312666 au (**I2a**)

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.42755649
S	3.10303684	0.00000000	0.26855474
S	1.89126788	2.09196995	2.57543775
Ni	1.49216285	0.13360315	1.72480164
Fe	1.97201643	0.81685824	4.41442666
C	1.65071602	1.89639476	5.70866150
C	3.80352191	1.04773946	4.63184624
O	1.50656103	2.67142280	6.57586265
N	4.96368676	1.19256128	4.78486627
C	2.00550187	-0.66135455	5.59447583
N	2.01654763	-1.57745789	6.33995126
N	4.10865379	-3.30651817	3.06847778
C	3.04863688	-4.14092878	3.30201297
N	2.82057142	-5.18528923	2.47852203
C	4.59595936	-2.32901060	4.04824678
N	2.20847382	-3.92090853	4.31541867
H	2.30714486	-3.10986898	4.94520967
H	1.43389502	-4.65828817	4.51338407
H	3.56370576	-5.43471208	1.82600073
H	2.15806331	-5.99537757	2.80897439
H	4.74843698	-3.58768496	2.32607009
C	5.14471504	-2.97903581	5.32710663
H	6.08025322	-3.53830562	5.09879125
H	4.41017028	-3.73845538	5.66906347
H	5.35773987	-1.69949053	3.54917587
H	3.76820518	-1.63088150	4.29126555
C	-1.87647978	2.03649330	-0.55407715
H	-2.63745413	1.25618178	-0.54966426
C	-0.74085196	1.64458646	0.38608311
C	-1.63096130	-2.38860188	3.33358925
H	-2.48227861	-1.71805463	3.60277218
C	-0.32622331	-1.78174620	3.89978396
H	6.86297484	-0.31411998	0.73282315
C	5.94159286	-0.01513145	0.18943491
H	6.06508319	1.03272683	-0.08430985
C	4.72860947	-0.21092704	1.12071851
H	2.96542560	4.21370005	0.18638857
C	2.99649205	4.37887905	1.28065051
C	3.37080959	3.07774700	2.04428445
H	-2.34319870	2.99483362	-0.23808086
H	3.74243678	5.13507367	1.52632549
H	-0.33855628	-1.78091102	5.00765930
H	0.54494638	-2.38371949	3.58196446
H	4.73279311	-1.23733142	1.53554646
H	4.79758213	0.47370250	1.99335531
H	0.07804717	2.39186564	0.36021670
H	-1.09780662	1.61052747	1.43594047
H	5.85269313	-0.60848087	-0.74375984
H	-1.51941341	2.14877172	-1.60027616
H	2.00941997	4.76922190	1.60865436
H	3.99423103	2.40775177	1.42585569
H	3.92987012	3.28612137	2.97244165
H	-1.84188613	-3.36515789	3.80808230
H	-0.17160059	-9.04279253	4.51624387

C	-0.08400493	-8.10976965	5.07298699
C	0.63540675	-6.95398945	4.35797341
O	1.37713213	-7.22051598	3.36606924
O	0.45787275	-5.80579120	4.88319608
H	-1.09531762	-7.77016173	5.37669389
H	0.47154144	-8.31813356	6.01390836
H	5.31128358	-2.22567996	6.11941954
H	-1.59725358	-2.48721263	2.22988640

MODEL 6: POLAR MODEL

System: **Ni-SI$_a$** (singlet)

Charge, Multiplicity: –2, 1

Gibbs free energy: –6786.585967 au, –6787.171079 au (**I1**), –6787.182679 au (**Ni-C**), –6787.7674 au (**Ni-R**), –6787.760715 au (**I2a**)

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.42755649
S	3.10303684	0.00000000	0.26855474
S	1.89126788	2.09196995	2.57543775
Ni	1.49216285	0.13360315	1.72480164
Fe	1.97201643	0.81685824	4.41442666
C	1.65071602	1.89639476	5.70866150
C	3.80352191	1.04773946	4.63184624
O	1.50656103	2.67142280	6.57586265
N	4.96368676	1.19256128	4.78486627
C	2.00550187	-0.66135455	5.59447583
N	2.01654763	-1.57745789	6.33995126
C	-0.60927651	5.12399060	4.92434922
N	-0.66861074	3.88863032	4.33037783
C	-2.68942101	4.59173483	4.83931537
N	-1.81310216	5.58165019	5.25089098
C	-1.99930907	3.52741873	4.26720501
H	0.34430881	5.60973660	5.15693579
H	-3.77492790	4.68824757	4.97922049
H	-2.30621820	2.56491771	3.84201299
H	0.12115907	3.31048637	4.00293609
O	8.85065684	3.51295510	7.37388929
C	7.71171415	3.12068442	7.08800022
N	7.33932988	2.74538242	5.82928661
C	8.27363237	2.75222320	4.71227469
C	7.59334167	2.37298255	3.38649449
O	7.22904634	1.01066211	3.29987716
H	8.73604182	3.76369940	4.63153181
H	6.39259258	2.36120036	5.66165166
H	9.11060329	2.04083066	4.90386009
H	6.71450406	3.05007601	3.22772843
H	8.31336997	2.58382328	2.56330389
H	6.40835930	0.91479823	3.86332312
H	4.41932228	-2.23636635	-3.38159064
C	3.69279270	-2.06733745	-2.58676563
H	3.34338636	-3.06262732	-2.24166037

H	4.21745066	-1.59671279	-1.73282846
C	2.48859195	-1.21444029	-2.96915093
C	2.81844263	0.22732493	-3.25264344
O	1.72699575	0.92261646	-3.66587030
O	3.91674654	0.75336734	-3.11772910
H	1.76959396	-1.16050537	-2.11632803
H	1.90832872	-1.61955756	-3.82659187
N	3.91965399	-3.30347780	8.03004563
C	3.77273966	-4.47163593	8.72586974
H	3.09109796	-2.76487391	7.72675993
O	4.72031773	-5.17157418	9.10982723
C	5.22514448	-2.67649894	7.85198327
C	5.36057512	-1.99076925	6.48370941
H	4.61771019	-1.16928877	6.41412885
H	6.35445457	-1.49876572	6.41516380
H	5.98134199	-3.47861412	7.98672647
H	5.39815998	-1.92949790	8.66232789
C	-1.87647978	2.03649330	-0.55407715
H	-2.63745413	1.25618178	-0.54966426
C	-0.74085196	1.64458646	0.38608311
N	-1.57029736	-2.54465782	1.90220097
C	-1.63096129	-2.38860188	3.33358925
H	-2.48227861	-1.71805463	3.60277218
C	-0.32622331	-1.78174620	3.89978396
H	6.86297482	-0.31411998	0.73282315
C	5.94159286	-0.01513145	0.18943491
H	6.06508319	1.03272683	-0.08430985
C	4.72860947	-0.21092704	1.12071851
H	2.96542560	4.21370005	0.18638857
C	2.99649205	4.37887905	1.28065051
C	3.37080959	3.07774700	2.04428445
H	-2.34319870	2.99483362	-0.23808086
C	-1.59775433	-3.76697663	1.29643656
O	-1.76415729	-4.83973760	1.87572485
H	3.74243678	5.13507367	1.52632549
H	-0.33855627	-1.78091102	5.00765930
H	0.54494638	-2.38371948	3.58196446
H	-1.29969521	-1.71014823	1.35142928
H	4.73279311	-1.23733142	1.53554646
H	4.79758213	0.47370250	1.99335531
H	0.07804717	2.39186564	0.36021670
H	-1.09780662	1.61052747	1.43594047
H	5.85269313	-0.60848087	-0.74375984
H	-1.51941341	2.14877172	-1.60027616
H	2.00941997	4.76922190	1.60865436
H	3.99423103	2.40775177	1.42585569
H	3.92987012	3.28612137	2.97244165
H	-1.84188613	-3.36515789	3.80808230
H	-3.62178012	-1.44709546	-1.51208432
C	-3.24930690	-2.38019941	-1.08924132
O	-4.05490472	-3.29190806	-0.87700302
N	-1.89711615	-2.50069920	-0.89055995
H	-1.32521453	-1.63194763	-0.86059320
C	-1.36265633	-3.70130725	-0.22351773
H	-0.29234857	-3.79723971	-0.40611648

H	-1.86770478	-4.59342891	-0.64203261
H	6.35195423	3.37158107	-2.02743517
C	5.52010894	4.06948305	-2.12213411
O	5.74231112	5.27336422	-1.95064672
N	4.33303753	3.55843123	-2.42937473
H	3.44477723	4.18664412	-2.49616987
H	4.19998729	2.53830470	-2.55712135
H	2.01457705	1.85621591	-3.75705524
C	0.77067560	-1.69650340	10.46592857
C	1.72583178	-2.88243265	10.29030698
O	2.73017986	-3.01889409	11.00021816
C	1.37764995	-0.59761444	11.33963052
H	1.68344536	-1.00284065	12.32495550
H	2.29039462	-0.18431510	10.86403524
H	0.66028606	0.23487472	11.49223815
H	-0.18223213	-2.07424044	10.90587179
H	0.50090750	-1.29928188	9.46255874
H	2.69926483	-4.79918836	8.81350189
H	1.43674653	-3.63856832	9.50655663
H	5.21254392	-2.68968330	5.63818442
H	6.86848591	3.03576458	7.83314824

MODEL 5: H-BOND MODEL

System: **Ni-SI$_a$** (singlet)

Charge, Multiplicity: –2, 1

Gibbs free energy: –6155.726788 au, –6156.312337 au (**I1**), –6156.323842 au (**Ni-C**), –6156.908563 au (**Ni-R**), –6156.901419 au (**I2a**)

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.42755649
S	3.10303684	0.00000000	0.26855474
S	1.89126788	2.09196995	2.57543775
Ni	1.49216285	0.13360315	1.72480164
Fe	1.97201643	0.81685824	4.41442666
C	1.65071602	1.89639476	5.70866150
C	3.80352191	1.04773946	4.63184624
O	1.50656103	2.67142280	6.57586265
N	4.96368676	1.19256128	4.78486627
C	2.00550187	-0.66135455	5.59447583
N	2.01654763	-1.57745789	6.33995126
C	-0.60927651	5.12399060	4.92434922
N	-0.66861074	3.88863032	4.33037783
C	-2.68942101	4.59173483	4.83931537
N	-1.81310216	5.58165019	5.25089098
C	-1.99930907	3.52741873	4.26720501
H	0.34430881	5.60973660	5.15693579
H	-3.77492790	4.68824757	4.97922049
H	-2.30621820	2.56491771	3.84201299
H	0.12115907	3.31048637	4.00293609
O	8.85065684	3.51295510	7.37388929
C	7.71171415	3.12068442	7.08800022
N	7.33932988	2.74538242	5.82928661

C	8.27363237	2.75222320	4.71227469
C	7.59334167	2.37298255	3.38649449
O	7.22904634	1.01066211	3.29987716
H	8.73604182	3.76369940	4.63153181
H	6.39259258	2.36120036	5.66165166
H	9.11060329	2.04083066	4.90386009
H	6.71450406	3.05007601	3.22772843
H	8.31336997	2.58382328	2.56330389
H	6.40835930	0.91479823	3.86332312
N	3.91965399	-3.30347780	8.03004563
C	3.77273966	-4.47163593	8.72586974
H	3.09109796	-2.76487391	7.72675993
O	4.72031773	-5.17157418	9.10982723
C	5.22514448	-2.67649894	7.85198327
C	5.36057512	-1.99076925	6.48370941
H	4.61771019	-1.16928877	6.41412885
H	6.35445457	-1.49876572	6.41516380
H	5.98134199	-3.47861412	7.98672647
H	5.39815998	-1.92949790	8.66232789
C	-1.87647978	2.03649330	-0.55407715
H	-2.63745413	1.25618178	-0.54966426
C	-0.74085196	1.64458646	0.38608311
N	-1.57029736	-2.54465782	1.90220097
C	-1.63096129	-2.38860188	3.33358925
H	-2.48227861	-1.71805463	3.60277218
C	-0.32622331	-1.78174620	3.89978396
H	6.86297482	-0.31411998	0.73282315
C	5.94159286	-0.01513145	0.18943491
H	6.06508319	1.03272683	-0.08430985
C	4.72860947	-0.21092704	1.12071851
H	2.96542560	4.21370005	0.18638857
C	2.99649205	4.37887905	1.28065051
C	3.37080959	3.07774700	2.04428445
H	-2.34319870	2.99483362	-0.23808086
C	-1.59775433	-3.76697663	1.29643656
O	-1.76415729	-4.83973760	1.87572485
H	3.74243678	5.13507367	1.52632549
H	-0.33855627	-1.78091102	5.00765930
H	0.54494638	-2.38371948	3.58196446
H	-1.29969521	-1.71014823	1.35142928
H	4.73279311	-1.23733142	1.53554646
H	4.79758213	0.47370250	1.99335531
H	0.07804717	2.39186564	0.36021670
H	-1.09780662	1.61052747	1.43594047
H	5.85269313	-0.60848087	-0.74375984
H	-1.51941341	2.14877172	-1.60027616
H	2.00941997	4.76922190	1.60865436
H	3.99423103	2.40775177	1.42585569
H	3.92987012	3.28612137	2.97244165
H	-1.84188613	-3.36515789	3.80808230
H	-3.62178012	-1.44709546	-1.51208432
C	-3.24930690	-2.38019941	-1.08924132
O	-4.05490472	-3.29190806	-0.87700302
N	-1.89711615	-2.50069920	-0.89055995
H	-1.32521453	-1.63194763	-0.86059320

C	-1.36265633	-3.70130725	-0.22351773
H	-0.29234857	-3.79723971	-0.40611648
H	-1.86770478	-4.59342891	-0.64203261
H	2.68944908	-4.75843745	8.86456251
H	5.21201315	-2.69003861	5.63886245
H	6.86839868	3.03595454	7.83287263

MODEL 7: TRANSITION STATES MODEL

System: **I1** to **Ni-C** (doublet)

Charge, Multiplicity: –2, 2

Gibbs free energy: –7997.035442 au

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.36771799
C	2.06206053	0.00000000	0.60532158
N	1.23112932	-0.00313391	-0.50077587
C	1.31512085	0.00264574	1.78026117
H	-0.92521616	-0.06024863	-0.58164045
H	3.15647148	-0.00686542	0.50497605
H	1.57436433	-0.01113631	2.84530692
H	-0.83229500	0.05311485	1.98905770
O	-9.26099938	-3.56969975	-0.03585207
C	-8.13304306	-3.40535179	0.44729747
N	-7.84657519	-2.42872178	1.35928348
C	-8.87533368	-1.52357272	1.85246695
C	-8.33918464	-0.56262380	2.92418030
O	-8.00278550	-1.19982979	4.13921049
H	-9.29808791	-0.94122129	0.99938539
H	-6.90006224	-2.36335166	1.76926673
H	-9.72117662	-2.11179892	2.27653912
H	-7.46810002	0.00084354	2.50018956
H	-9.13544782	0.18817029	3.13462628
H	-7.10226614	-1.61597766	3.97100600
C	-4.80353493	-4.76419965	1.22971750
C	-4.59083039	-4.33446486	-0.22483168
H	-4.57031443	-3.91357484	1.90040017
H	-4.16313890	-5.61708674	1.53091702
H	-3.67108868	-3.73153126	-0.35804472
H	-4.50213796	-5.23684626	-0.89019787
C	-6.93435087	-4.30159103	0.06579206
C	-6.31638695	-5.08342361	1.27953217
H	-6.50964913	-6.16892196	1.15810809
H	-6.76570971	-4.77700721	2.24547756
H	-7.36006872	-5.02908350	-0.66890783
N	-5.79298094	-3.53541672	-0.48179319
H	-5.92616695	-3.29962245	-1.47105526
H	-5.76322186	3.74669212	10.05891876
C	-4.97156515	3.16675111	9.58477454
H	-4.65125359	2.40313497	10.32306653
H	-5.43127539	2.61918925	8.73960297
C	-3.75654126	3.96134501	9.11126251
C	-3.98673175	4.70132070	7.81913660

O	-3.01435861	5.60096791	7.55758609
O	-4.92600371	4.48808543	7.06062695
H	-2.90542275	3.27973880	8.86606762
H	-3.35816520	4.66419192	9.87244084
N	-5.10002683	-2.56060098	8.22458769
C	-4.00123130	-3.04015607	8.89925210
N	-3.90288109	-2.84776106	10.23027848
N	-4.33215301	-6.88682682	5.90601984
C	-5.44525146	-3.00698962	6.86718612
N	-3.00769485	-3.65390181	8.25676369
C	-4.14449157	-7.99809286	6.67839797
H	-3.53219795	-6.29099217	5.63051329
H	-3.04234529	-3.86019065	7.24291936
H	-2.22605525	-4.10890500	8.85217998
H	-4.72603228	-2.48849288	10.71327672
H	-3.18561975	-3.44049212	10.82248200
H	-5.88798409	-2.31073166	8.82414493
O	-5.06332106	-8.72018061	7.08974782
C	-5.63376838	-6.55561056	5.33886393
C	-5.90972644	-5.04506894	5.37115821
C	-5.81047235	-4.49360960	6.79964206
H	-5.17512111	-4.52432322	4.72201590
H	-6.90638644	-4.83875000	4.92484061
H	-6.75308973	-4.67952868	7.36427167
H	-5.02022409	-5.06884013	7.32690606
H	-6.38621510	-7.12326317	5.92617622
H	-5.69187001	-6.92584439	4.28829455
H	-6.27725329	-2.37534138	6.50181585
H	-4.59258000	-2.77418650	6.19577514
H	-1.93632906	-5.67685460	-2.09754060
C	-1.24846061	-5.33272376	-1.32571250
C	-0.35230016	-4.14794804	-1.71992778
C	-1.17892996	-2.92023101	-2.13237013
C	0.62059739	-3.77886760	-0.58345116
H	-0.62833523	-6.20889787	-1.03226938
H	-1.85489055	-5.06893691	-0.43329860
H	-0.52600448	-2.09006476	-2.47502295
H	-1.75281204	-2.54499864	-1.26111454
H	-1.90422925	-3.15573278	-2.94134216
H	1.25417078	-2.91088109	-0.86315750
H	1.28382949	-4.63206997	-0.32282571
H	0.06202955	-3.48840029	0.32985001
H	0.26357710	-4.47550176	-2.58551542
C	0.78384977	3.58154288	5.26240415
H	1.53516859	3.28048214	5.99209544
C	-0.26329959	2.49165318	5.10970100
N	0.48870186	-0.71901331	8.24716974
C	0.81744204	-1.88490006	7.46931483
H	1.73520931	-1.69212372	6.86171359
C	-0.31964402	-2.32395209	6.52691475
H	-7.96062311	0.97076670	6.53516918
C	-6.96711538	1.45595044	6.40896379
H	-7.10039985	2.16323544	5.59052231
C	-5.93357795	0.35406393	6.27034240
H	-4.02828815	3.53553926	2.79725993

C	-3.89984497	2.66022005	2.12913429
C	-4.08110386	1.32495795	2.89567365
H	1.29662705	3.77945016	4.29483863
C	0.60294363	-0.69073183	9.60680472
O	0.93285306	-1.64662154	10.30826480
H	-4.61571363	2.72940509	1.31006192
H	-0.08163999	-3.30203659	6.06304787
H	-1.25759419	-2.44827932	7.09749146
H	0.15256734	0.11337446	7.73175915
H	-6.07160317	-0.38800454	7.08014552
H	-6.02229900	-0.18621780	5.30812193
H	-1.02079993	2.76765258	4.34959414
H	0.20496991	1.55519428	4.74221381
H	-6.78902559	2.06558969	7.32089691
H	0.33609859	4.53555412	5.61750802
H	-2.88743337	2.72409983	1.67549372
H	-4.66794230	1.46763694	3.82338072
H	-4.61196899	0.56915567	2.29265264
H	1.05718919	-2.73093916	8.14006083
H	2.41161087	2.99310297	8.88210777
C	2.06642728	2.17181368	9.51019556
O	2.86770757	1.64793189	10.28960638
N	0.73519602	1.83521244	9.44550356
H	0.18233680	2.13982749	8.61533884
C	0.24501237	0.67696215	10.21887612
H	-0.83750858	0.72240894	10.33772702
H	0.71649731	0.69398608	11.21976541
H	-7.52510078	4.92355316	4.35477264
C	-6.69729137	5.37849710	3.81111604
O	-6.90567649	5.77840757	2.66126509
N	-5.54432100	5.50546012	4.45861270
H	-4.65873109	5.90832238	3.96736081
H	-5.38283795	5.07211868	5.38494917
S	-1.16813688	2.07484899	6.66385303
S	-0.64241346	-1.15423730	5.11876485
S	-4.20851026	0.93443873	6.34870064
S	-2.48239120	0.54688859	3.40897722
Ni	-2.23886050	0.29430452	5.65769823
Fe	-2.55075971	-1.68042642	3.96800260
C	-2.19816166	-2.38159519	2.43676559
C	-4.38179917	-1.80799235	3.65756761
O	-2.00958733	-2.82076027	1.36595992
N	-5.53118703	-1.94932153	3.42381952
C	-2.60456676	-3.35712307	4.81848675
N	-2.62735280	-4.41794876	5.34062035
H	-0.60247446	-6.02538835	12.82167199
C	-0.63486821	-6.10908795	11.73538770
C	-1.45587126	-5.03182582	11.00646827
O	-2.31344603	-4.37550668	11.67356959
O	-1.23236099	-4.93200902	9.75735329
H	0.39945616	-6.10644990	11.33540289
H	-1.07157100	-7.09840368	11.47503820
H	-3.16323500	5.92670385	6.64361445
H	-4.33515422	1.94315216	7.23388879
C	-0.98323722	-8.09529198	3.55746334

C	-1.95392687	-8.54680132	4.65667388
O	-2.88872742	-9.32199720	4.41911117
C	-1.51061465	-8.42285130	2.15969399
N	-1.75311793	-8.03576681	5.91626052
C	-2.69924033	-8.37263351	6.99161121
C	-2.14967314	-7.62511204	8.21923687
C	-0.65354601	-7.55232450	7.93061245
C	-0.61845210	-7.24361424	6.42162971
C	-4.10931556	-0.91376152	-1.15230817
C	-4.77556768	-0.59565715	-2.49770631
C	-4.94985950	-0.55016062	0.04172185
H	-5.93878286	-1.04662225	0.00365544
H	-4.47428913	-0.88899199	0.98435686
H	-5.10989305	0.54907309	0.10562092
H	-3.12753983	-0.38930202	-1.10244993
H	-3.85796424	-1.98982209	-1.11606762
H	-5.74462394	-1.13349365	-2.59756744
H	-5.00103471	0.48968662	-2.59290167
H	-4.13560218	-0.88494098	-3.35893643
H	-1.73343589	-9.50474876	2.06747858
H	-2.45864415	-7.88072443	1.96636335
H	-0.78026623	-8.13042133	1.37743590
H	0.00278517	-8.58540218	3.73598410
H	-0.79915376	-7.00360304	3.66432656
H	-0.78445541	-6.15809156	6.22761832
H	0.33226824	-7.54618381	5.93583548
H	-0.16764546	-6.76510120	8.54162770
H	-0.16354473	-8.53245199	8.12666330
H	-2.55727720	-6.59416024	8.27082277
H	-2.40855090	-8.13178829	9.16906503
H	-2.72689075	-9.47281016	7.14914931

System: **Ni-R** to **I2a** (singlet)

Charge, Multiplicity: –2, 1

Gibbs free energy: –7997.625180 au

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.36365127
C	2.06170565	0.00000000	0.59484830
N	1.22749960	0.00343442	-0.50922324
C	1.31620959	0.00216456	1.77202454
H	-0.93042146	-0.02199862	-0.57664113
H	3.15613418	-0.00949811	0.49180296
H	1.58265665	-0.01187625	2.83537566
H	-0.85731156	0.09288883	1.96643148
O	-9.30383003	-3.43372199	-0.13087756
C	-8.17297248	-3.31929282	0.36068560
N	-7.87094132	-2.40420638	1.32987269
C	-8.88380365	-1.50214842	1.86207011
C	-8.31800784	-0.53559712	2.91416579
O	-7.97393049	-1.15905056	4.13544211
H	-9.33710076	-0.92606663	1.02121197
H	-6.92366489	-2.37124078	1.74262199

H	-9.71419674	-2.08903215	2.31880991
H	-7.44677827	0.01150050	2.47047774
H	-9.10242858	0.22680514	3.12693387
H	-7.09120348	-1.60537957	3.95644795
C	-4.88212138	-4.72072680	1.10200828
C	-4.63499409	-4.23075178	-0.32690934
H	-4.68843673	-3.89283073	1.81263379
H	-4.23260173	-5.57048822	1.39022973
H	-3.72033071	-3.60987593	-0.40640994
H	-4.51072158	-5.10406338	-1.02419214
C	-6.99222396	-4.21424845	-0.07867183
C	-6.38641568	-5.07434195	1.08708482
H	-6.54546469	-6.15123052	0.87265371
H	-6.86979838	-4.85967655	2.06134147
H	-7.43788211	-4.88928457	-0.85005470
N	-5.84035888	-3.43800689	-0.58967799
H	-5.95535240	-3.17355378	-1.57343216
H	-5.64688014	3.38578415	10.25108861
C	-4.86675517	2.81476982	9.74773525
H	-4.56364438	2.00137925	10.43833285
H	-5.31823902	2.32560456	8.86380026
C	-3.63204086	3.61620274	9.33688029
C	-3.88441553	4.54751033	8.18172603
O	-2.98204991	5.54820045	8.09311078
O	-4.78796272	4.39842270	7.36406062
H	-2.83905309	2.92898269	8.94738582
H	-3.16414767	4.17703520	10.17185261
N	-5.09036658	-2.83562872	8.16701315
C	-3.99176613	-3.35751884	8.81140313
N	-3.87984760	-3.22396069	10.14883043
N	-4.38038032	-7.07936518	5.63522245
C	-5.45723748	-3.22428238	6.79722123
N	-3.01215371	-3.95593272	8.13560363
C	-4.20093515	-8.22376362	6.36083468
H	-3.57582734	-6.47803695	5.38614526
H	-3.05860360	-4.11639503	7.11476364
H	-2.23325091	-4.45302340	8.70233821
H	-4.69638047	-2.88295009	10.65571422
H	-3.16415665	-3.85112845	10.70450897
H	-5.86763804	-2.59566984	8.78427199
O	-5.12658274	-8.95102379	6.74767854
C	-5.68513268	-6.70044036	5.10549916
C	-5.94394330	-5.18995807	5.21525961
C	-5.83592943	-4.70460875	6.66760692
H	-5.20721553	-4.64621591	4.58782836
H	-6.93955923	-4.95257497	4.78216190
H	-6.77711196	-4.91040741	7.22749413
H	-5.04656302	-5.30788895	7.16437350
H	-6.43729909	-7.28813267	5.67324262
H	-5.76341348	-7.01448943	4.03797496
H	-6.28293829	-2.56472810	6.46548982
H	-4.60804420	-2.97727260	6.12837189
H	-2.02283331	-5.55664339	-2.32377372
C	-1.32627425	-5.25408834	-1.54322165
C	-0.41952798	-4.06404730	-1.89346285

C	-1.23546686	-2.81220726	-2.25023449
C	0.55558536	-3.75080511	-0.74236414
H	-0.71456706	-6.14873413	-1.29093476
H	-1.92492717	-5.02189602	-0.63647211
H	-0.57624061	-1.97455288	-2.56066126
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H	1.61718404	3.00221969	6.11553499
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C	0.84314646	-2.21218622	7.37628352
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C	-0.30798176	-2.58026861	6.43630110
H	-7.85934632	0.70325785	6.55142656
C	-6.90313646	1.26890908	6.51698479
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C	-5.78178876	0.26289256	6.33228695
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C	-3.85130371	2.61605659	2.26926667
C	-4.03896568	1.24918588	2.97051970
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H	-5.85527656	-0.25379644	5.35505195
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C	2.15791606	1.73751515	9.57919004
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C	-4.41180988	-1.89533162	3.65479227
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C	-0.69663964	-7.87543277	7.60552705
C	-0.69269689	-7.45423799	6.12893879
C	-4.12784635	-0.81202380	-1.16009692
C	-4.80488701	-0.44100885	-2.48671908
C	-4.95650750	-0.48948187	0.05429194
H	-5.94413788	-0.98817432	0.01229859
H	-4.46588937	-0.84934720	0.98088761
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H	-3.87995516	-1.88942409	-1.16969882
H	-5.77819498	-0.96919440	-2.59697274
H	-5.02491394	0.64835267	-2.53894399
H	-4.17499359	-0.70116373	-3.36470027
H	-2.70091697	-7.15090686	2.25439395
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H	0.25753920	-7.68930993	5.60882964
H	-0.20373076	-7.13319508	8.26558230
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H	-2.59625467	-6.95518197	8.05451801
H	-2.42818474	-8.55841032	8.82671738
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