SUPPORTING INFORMATION

Unraveling the Role of Ligands in the Hydrogen Evolution Mechanism Catalyzed by [NiFe] Hydrogenases

Siyao Qiu,[a] Luis Miguel Azofra,[a, b] Douglas R. MacFarlane,[a, b, *] and Chenghua Sun[a, b, *]

[a]School of Chemistry, Faculty of Science, Monash University, Clayton, VIC 3800, Australia

[b]ARC Centre of Excellence for Electromaterials Science (ACES), School of Chemistry, Faculty of Science, Monash University, Clayton, VIC 3800, Australia

*Authors to whom correspondence should be addressed:
DRM: Tel: (+61) 3 9905 4540. Fax: (+61) 3 9905 4597
E-mail: Douglas.MacFarlane@monash.edu
CS: Tel: (+61) 3 9902 9916. Fax: (+61) 3 9905 4597
E-mail: Chenghua.Sun@monash.edu

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CARTESIAN COORDINATES

Note: * refers to frozen atoms. Frozen atoms in Model 5, 6, and 7 are the same with those in Model 4. Also, frozen atoms in Model 8 are the same.

MODEL 1: PARTIAL FROZEN MODEL (DISTAL CARBONS FROM CYS RESIDUES)

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: **Ni-SI$_a$** (triplet)

Charge, Multiplicity: –2, 3

Gibbs free energy: –4981.487016 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.94710484
C	1.77302265	0.00000000	3.61273328
C	-0.59488852	0.77673458	4.32612683
C	-0.31939178	-1.72464219	3.66349868
N	2.88519193	0.03218885	4.00503839
O	-1.02580442	1.32505013	5.27506933
N	-0.56281590	-2.79712718	4.09002093
*C	-2.24349483	2.88059442	-2.36827060
C	-1.44086769	2.09807237	-1.35562549
S	-1.04635592	0.42422396	-1.98199981
*C	-4.09559921	-1.68589905	0.87106531
C	-2.71049585	-1.75507614	1.55691282
S	-1.74654390	-0.18246171	1.49846278
*C	4.36902243	-1.27416394	-0.15860313
C	2.91932445	-1.28194713	0.32464571
S	1.79448085	-0.71881146	-1.00899072
*C	2.43797702	3.67758669	0.80252267
C	2.19541334	2.31094095	1.49379471
S	0.42829002	1.78231652	1.52511115
H	1.54513200	4.33273743	0.90510120
*H	3.26218366	4.18287386	1.30468373
H	2.65286749	3.56844747	-0.27986297
H	-2.53881453	3.88661933	-1.98398665
H	-1.66893202	3.03288383	-3.30927084
*H	-3.15140718	2.33960521	-2.63569335
*H	4.81503645	-0.28503072	-0.25895930
H	5.01995881	-1.83203549	0.55647112
H	4.45842611	-1.78030774	-1.14598261
H	-4.00573262	-1.61694944	-0.23240027
*H	-4.65491751	-2.59516788	1.15462025
H	-4.67170287	-0.80377463	1.22455731
H	2.51072671	2.33432199	2.55587708
H	2.78062443	1.50468470	1.01031392
H	2.78799856	-0.64961461	1.22742635
H	2.62572649	-2.30883960	0.63083470
H	-0.49513282	2.62321027	-1.11061862
H	-2.00041508	2.00548121	-0.40048553
H	-2.07910836	-2.54654609	1.10588124
H	-2.80200007	-2.00933883	2.63255599

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: **Ni-R** (triplet)
Charge, Multiplicity: –2, 3
Gibbs free energy: –4982.64979 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.57715598
C	0.98219891	0.00000000	4.02662990
C	-1.17068721	1.31586250	3.29416940
C	-1.11781847	-1.40172620	3.18548392
O	1.61298358	0.00506208	5.01865110
N	-1.87656450	2.15346276	3.73204642
N	-1.78813267	-2.31874293	3.51199658
*C	3.51860144	-0.11803604	-2.80987040
C	2.54169975	-0.23321803	-1.65414552
S	0.84569218	0.25706525	-2.13723984
*C	0.74991211	4.16307017	0.15180863
C	0.17508563	3.10910342	1.11837911
S	1.19931338	1.58551834	1.26943096
*C	-3.58340301	-3.17542063	-0.34056156
C	-2.77900390	-1.98084321	0.14867244
S	-1.57579762	-1.36144832	-1.08406355
*C	1.61779524	-4.22942722	0.66781494
C	0.68431442	-3.19818212	1.35468728
S	1.27874344	-1.45670747	1.26280283
H	2.66955413	-3.86904008	0.68147831
*H	1.58727825	-5.15781285	1.23628401
H	1.34517912	-4.41933883	-0.39147023
H	4.54942638	-0.43669661	-2.52030431
H	3.19943564	-0.74044958	-3.67555137
*H	3.56643606	0.91602911	-3.15116564
H	-4.43256892	-3.37626518	0.35279753

H	-4.00993994	-2.99911525	-1.35249331
*H	-3.00450174	-4.09847279	-0.37995944
*H	0.58138339	3.88508965	-0.90923429
H	0.30134912	5.14946659	0.36961609
H	1.84847769	4.26694795	0.29575709
H	-1.06188292	0.09064755	1.32634184
H	-0.78260848	-2.45800941	-1.11050572
H	-0.35129768	-3.25644901	0.96087307
H	0.58095280	-3.41525349	2.43667773
H	-3.42605284	-1.09753749	0.32879361
H	-2.25954669	-2.16229099	1.11351044
H	2.51140784	-1.26970427	-1.25978929
H	2.85612987	0.40379991	-0.79991555
H	0.07594722	3.51621790	2.14534195
H	-0.84954792	2.80183396	0.82476939

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

System: **I2a** (triplet)
Charge, Multiplicity: –2, 3
Gibbs free energy: –4982.64663 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.81901143
C	0.86618754	0.00000000	4.27718375
C	-1.37215555	1.12887963	3.51120253
C	-1.02811422	-1.52312713	3.29214075
O	1.48032721	-0.00747823	5.28186144
N	-2.20780896	1.84582481	3.93327019
N	-1.65581383	-2.48705282	3.55308806
*C	3.92358124	0.61366142	-2.11747456
C	2.81631431	0.30890888	-1.13053792
S	1.17011565	0.65394214	-1.83744946
*C	0.30403401	4.34855530	0.65813047
C	-0.19134735	3.19639729	1.55531410
S	0.92903081	1.73671697	1.56767278
*C	-3.04769693	-3.35238771	-0.86996828
C	-2.40301932	-2.11031200	-0.26929444
S	-0.99258391	-1.56244964	-1.29741427
*C	2.05447708	-3.91902891	0.80988563
C	1.00935738	-3.02405240	1.52392423
S	1.34989722	-1.21209123	1.44686210
H	3.07724858	-3.49267607	0.90470580
*H	2.05411587	-4.88480384	1.31423483
H	1.82919204	-4.03636460	-0.26923280
H	4.93306539	0.38861348	-1.69656808
H	3.80510314	0.02620785	-3.05466439
*H	3.89824090	1.66886696	-2.38806227
*H	-2.36642826	-4.20309449	-0.87931931
H	-3.95232466	-3.66231897	-0.29367519
H	-3.36273696	-3.16980262	-1.92155937
H	0.22965263	4.08578108	-0.41755470
*H	-0.28113130	5.26366857	0.86590790
H	1.37096584	4.58152164	0.86881781
H	-1.51892774	0.29021911	1.08436380
H	-1.59875055	0.63252893	0.35159800
H	0.95827031	-3.25719473	2.60618103
H	-0.00779031	-3.19428327	1.12394388
H	-2.05215529	-2.30146313	0.76808068
H	2.83825388	-0.75788514	-0.82800628
H	2.93618154	0.89511109	-0.19450254
H	-0.30444167	3.52377416	2.60875582
H	-1.19908319	2.85147477	1.24180062
H	-3.14607990	-1.28624846	-0.19350675

System: **I2b** (singlet)
Charge, Multiplicity: –2, 1
Gibbs free energy: –4982.65589 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.76453351
C	1.36604287	0.00000000	3.81844472
C	-0.87993558	1.23244706	3.90412099
C	-0.66819333	-1.57394747	3.61068844
O	2.26599157	0.00055583	4.56265319
N	-1.39998808	2.03622508	4.59183130
N	-1.04494604	-2.57607363	4.10177260
*C	3.06878524	0.71825024	-2.97961741
C	2.19085656	0.41464266	-1.76483955
S	0.45682749	1.03688004	-1.95123965
*C	0.27847518	4.37890821	0.70384644
C	-0.34129124	3.07384815	1.25074344
S	0.83569488	1.63494634	1.28761735
*C	-3.25577774	-3.36400747	0.05615755
C	-2.44297335	-2.11734088	0.44946207
S	-1.43678933	-1.43884233	-0.94886155
*C	2.11714010	-3.86015754	0.29631124
C	0.97987684	-3.11422051	1.05545687
S	1.35372564	-1.32049385	1.20690808
*H	2.26573441	-4.82919155	0.77300443
H	1.88180227	-3.98423261	-0.77992477
H	3.07780966	-3.30550365	0.37461945
H	4.14244513	0.49429760	-2.78525689
H	2.74562173	0.13933704	-3.87266148
*H	2.95716606	1.77485931	-3.22288403
*H	-2.59069827	-4.20391106	-0.14451482
H	-3.94411924	-3.66043892	0.88010052
H	-3.86462187	-3.18185323	-0.85713120
*H	-0.24115339	5.28367740	1.07113311
H	1.33275723	4.46859471	1.04857735
H	0.30051208	4.37788230	-0.40576010
H	-1.24248930	0.04242965	1.45743829
H	-1.60878330	0.06082640	2.22169436
H	2.15520101	-0.67692825	-1.56632341
H	2.62544573	0.87787501	-0.85432570
H	-0.66950416	3.18871342	2.30378333
H	-1.22206037	2.75384398	0.65743908
H	0.02139713	-3.21686658	0.50795649
H	0.83626329	-3.50905629	2.08211564
H	-3.13042328	-1.31884667	0.80773985
H	-1.78472962	-2.35403730	1.31132534

System: **I2b** (triplet)
Charge, Multiplicity: –2, 3
Gibbs free energy: –4982.65308 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.97018141
C	1.37280999	0.00000000	4.01417454

C	-0.78725397	1.36293811	4.04502867
C	-0.73607641	-1.47399659	3.92768146
O	2.27788417	0.00132196	4.75010640
N	-1.24855728	2.23771907	4.68462260
N	-1.16608267	-2.41808497	4.48580534
*C	3.76268887	0.09675423	-2.31660667
C	2.64095582	-0.07593908	-1.31843748
S	1.07330122	0.59946120	-1.96859897
*C	0.88394520	4.27891696	0.67960855
C	0.09354901	3.17788548	1.42445124
S	1.00013220	1.57620456	1.47914497
*C	-3.58672579	-2.88161419	-0.58590455
C	-2.83499497	-1.71995929	0.06706036
S	-1.61435395	-1.00997557	-1.10508499
*C	1.49075120	-4.15064695	0.74863786
C	0.48245400	-3.13791679	1.35210097
S	1.14691259	-1.41994940	1.42398963
*H	1.39187733	-5.10982306	1.25719846
H	1.35193686	-4.27841566	-0.34417804
H	2.53421723	-3.80461592	0.91628332
H	4.74396947	-0.25852443	-1.91822502
H	3.55538800	-0.46244690	-3.25643037
*H	3.86407196	1.14714091	-2.58955039
*H	-3.03085630	-3.81780075	-0.63719831
H	-4.52328176	-3.11665527	-0.02237389
H	-3.88925306	-2.61481998	-1.62235439
*H	0.44559764	5.26489926	0.92284059
H	1.94217584	4.29241663	1.01978205
H	0.88425633	4.11069012	-0.41687328
H	-1.27951667	0.08082416	1.73275707
H	-1.62483935	-0.04493997	2.47079677
H	2.49800776	-1.14837367	-1.07248431
H	2.88472825	0.43133179	-0.36043349
H	-0.09959710	3.46456084	2.47903803
H	-0.89429833	3.00719027	0.94743991
H	-0.45823541	-3.11716325	0.76759439
H	0.22088495	-3.39920965	2.39772360
H	-3.55795567	-0.93055410	0.37204626
H	-2.32529257	-2.04751222	0.99883351

MODEL 2: FREE MODEL

System: **Ni-SI$_a$** (singlet)
Charge, Multiplicity: –2, 1
Gibbs free energy: –4981.470304 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.84564148
C	1.69220441	0.00000000	3.71097296
C	-0.76055693	0.71526226	4.18582672
C	-0.27714635	-1.77022708	3.48477199
N	2.74524605	0.03960444	4.24085093
O	-1.29285033	1.23259316	5.10049904
N	-0.45850194	-2.86868035	3.87320260
C	-3.42866257	0.04162652	-3.13432475

C	-2.47186408	0.50270551	-2.02996013
S	-0.98321400	-0.58051180	-1.92226140
C	-3.48252041	-2.01580959	0.26294984
C	-2.37032833	-1.80801495	1.28745844
S	-1.76073232	-0.06938926	1.36346793
C	4.38578817	-0.96623635	0.41682890
C	2.88038979	-1.23502241	0.49750670
S	1.95001833	-0.53054490	-0.92547276
C	2.82899094	2.86500893	0.32219891
C	2.35939139	2.06833686	1.53788486
S	0.59187628	1.58432230	1.39517286
H	2.20606494	3.77138142	0.15734365
H	3.88663543	3.19179361	0.45018100
H	2.76543393	2.22569606	-0.58377949
H	-4.30720460	0.72283374	-3.23230089
H	-2.91520753	0.00353806	-4.12060145
H	-3.80896322	-0.98180148	-2.92486733
H	4.59112726	0.12571110	0.40304229
H	4.91735166	-1.40371915	1.29197461
H	4.82633319	-1.39591463	-0.51093841
H	-3.08030961	-1.87708001	-0.76328713
H	-3.88997263	-3.04997647	0.33837235
H	-4.32427375	-1.30486100	0.41593211
H	2.42235304	2.64532939	2.48411444
H	2.96459942	1.15811321	1.69764658
H	2.45802452	-0.82201601	1.43877938
H	2.68373832	-2.32751431	0.54411321
H	-2.14216502	1.54820246	-2.21974066
H	-2.98684838	0.51424874	-1.04684401
H	-1.49600111	-2.45267113	1.07580688
H	-2.69114009	-2.04592165	2.32148610

System: **I1** (doublet)
Charge, Multiplicity: –2, 2
Gibbs free energy: –4982.045437 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.63277903
C	0.82098174	0.00000000	4.13433387
C	-1.24906596	1.33120552	3.14072393
C	-1.27787556	-1.29308567	3.17474890
O	1.40864274	-0.00075038	5.15876210
N	-2.05812659	2.14764411	3.41663149
N	-2.08899706	-2.09482261	3.48248937
C	2.03040075	-2.31588941	-3.42782536
C	1.95520953	-1.24341626	-2.33636659
S	0.28177627	-0.49783856	-2.16720502
C	0.57314648	3.66044657	-0.25155392
C	0.40899491	3.10861649	1.16564488
S	1.19118008	1.44884456	1.30224039
C	-4.71018362	0.00811935	0.35175920
C	-3.26344876	-0.13499040	0.81303818
S	-2.07556614	0.86219249	-0.17486221
C	0.44439983	-3.75656635	-0.20638771
C	0.18953963	-3.09884687	1.14965277

S	1.09450104	-1.49823418	1.29649011
H	-0.09979218	-4.72584391	-0.29197356
H	0.09851911	-3.08053305	-1.01956661
H	1.52591675	-3.95606849	-0.37389497
H	3.06212379	-2.73124579	-3.53301249
H	1.34465293	-3.15870674	-3.19500413
H	1.72322993	-1.90634567	-4.41597844
H	-4.85561567	-0.36910468	-0.68548347
H	-5.38356325	-0.57295683	1.02006527
H	-5.03579379	1.07016018	0.37412527
H	0.12824084	2.95212154	-0.98353152
H	0.07255760	4.65046320	-0.36347644
H	1.64449246	3.78054206	-0.52599729
H	-2.45326725	0.36052312	-1.38603990
H	-0.88698818	-2.89768685	1.30853528
H	0.51901668	-3.74243371	1.99410450
H	-3.10986023	0.24764892	1.84074988
H	-2.90899817	-1.18257326	0.81928334
H	2.23472745	-1.66807994	-1.34860513
H	2.68538484	-0.43001187	-2.54869349
H	-0.65862314	3.00933756	1.44312879
H	0.88049827	3.77333781	1.92272917

System: **Ni-C** (doublet)
Charge, Multiplicity: –2, 2
Gibbs free energy: –4982.058004 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.57150145
C	0.86709652	0.00000000	4.06851131
C	-1.17990775	1.37015773	3.17327465
C	-1.20717903	-1.32962913	3.20228561
O	1.45209440	0.01063952	5.08676931
N	-1.89199826	2.24125133	3.52353445
N	-1.94380212	-2.17291479	3.57063785
C	3.70888914	0.16122852	-2.79392907
C	2.82875956	0.19031676	-1.54097487
S	1.04479290	0.17439796	-1.96972890
C	0.84164341	3.69372442	-0.27415076
C	0.31339730	3.00272503	0.98391761
S	1.21974503	1.43190013	1.27710325
C	-4.47556679	-1.31724025	-0.34407603
C	-3.17589952	-0.78677294	0.26452385
S	-1.85588630	-0.63837648	-1.01449138
C	0.54699626	-3.62477083	-0.37747578
C	0.22479414	-3.05286245	1.00295949
S	1.19938422	-1.52806755	1.31093908
H	-0.05003419	-4.54430740	-0.57602442
H	0.30279398	-2.86996921	-1.15536996
H	1.62442361	-3.88387920	-0.47612182
H	4.79290366	0.17317267	-2.53226647
H	3.51228620	-0.74986643	-3.40082376
H	3.50704909	1.03872272	-3.44759081
H	-4.32353271	-2.32065863	-0.79930999
H	-5.26927835	-1.41004037	0.43164491

H	-4.85527715	-0.64624041	-1.14675322
H	1.91482419	3.96696002	-0.16988015
H	0.75322341	3.00794257	-1.14588322
H	0.26982487	4.62508028	-0.49075085
H	-1.01545635	0.05589152	1.22293000
H	-2.81861060	-1.45400760	1.07495697
H	-3.33169315	0.20473260	0.73677920
H	-0.84491466	-2.78599468	1.08755248
H	0.44791760	-3.76800524	1.82388956
H	3.03530445	-0.68535100	-0.88997317
H	3.04154370	1.09067978	-0.92632502
H	0.41524293	3.62614590	1.89710322
H	-0.76026787	2.74726301	0.89517017

System: **Ni-R** (singlet)
Charge, Multiplicity: –2, 1
Gibbs free energy: –4982.627527 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.57075249
C	0.79669098	0.00000000	4.10472648
C	-1.19733292	1.37552286	3.12405227
C	-1.24025771	-1.33234342	3.11423653
O	1.33024794	0.00714188	5.15238537
N	-1.93677904	2.23821682	3.44152639
N	-2.02513350	-2.17148871	3.38661164
C	3.66100552	-0.34774767	-2.81187851
C	2.79429666	-0.11738253	-1.57083260
S	1.02373427	0.11061900	-1.99768961
C	0.88521144	3.66160748	-0.28278928
C	0.49930300	3.04201580	1.06150377
S	1.24240009	1.36761842	1.23139271
C	-4.23756067	-1.96223108	-0.33456809
C	-3.09474493	-1.10849241	0.20839615
S	-1.68264176	-0.95344477	-0.96561839
C	0.93030110	-3.74219750	-0.19122002
C	0.41498766	-3.14246081	1.12126916
S	1.36183178	-1.62590884	1.51697653
H	2.00445759	-4.02076781	-0.11087708
H	0.36152937	-4.65693610	-0.48419598
H	0.85414223	-2.99078293	-1.00920506
H	4.73524816	-0.47981827	-2.54157763
H	3.33257548	-1.25604034	-3.36379344
H	3.59127947	0.50780691	-3.52055798
H	-5.07196653	-1.99909799	0.39960532
H	-4.63574466	-1.57200736	-1.29693294
H	-3.90480013	-3.00888038	-0.50727216
H	0.58857643	2.97968797	-1.10980859
H	0.39337439	4.65111976	-0.43108707
H	1.98483913	3.80866394	-0.36430137
H	-0.99303951	0.10826333	1.22090420
H	-1.36488258	-2.28755438	-0.92186894
H	-0.66088657	-2.88269652	1.04349415
H	0.48558677	-3.86818676	1.96033481
H	-3.39764519	-0.05818894	0.39257380

H	-2.70073092	-1.49088364	1.17292303
H	2.86166613	-0.97170114	-0.86403915
H	3.13822446	0.77527254	-1.00556749
H	0.85037021	3.65228933	1.92241249
H	-0.59619967	2.93205294	1.17367142

System: **I2a** (singlet)
Charge, Multiplicity: –2, 1
Gibbs free energy: –4982.627159 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.67263345
C	0.88308886	0.00000000	4.12665406
C	-1.12144779	1.41985221	3.25213609
C	-1.25483070	-1.27306737	3.30838368
O	1.50823437	-0.00914096	5.12428504
N	-1.77986523	2.33257137	3.60558493
N	-2.01236211	-2.09240366	3.69181487
C	3.53609999	0.40048863	-2.90928283
C	2.64258819	0.12800494	-1.69462082
S	0.94444523	0.77600028	-1.93759892
C	-0.55854763	3.39987864	0.48913049
C	0.70421626	3.10233319	1.29273386
S	1.26042111	1.34125524	1.32480646
C	-3.01565601	-3.39132733	-0.43429646
C	-2.45574617	-2.00783645	-0.09395074
S	-1.12308630	-1.49510754	-1.25527710
C	1.44136036	-4.22281662	1.77830320
C	0.41677150	-3.17592975	1.33889360
S	1.13241328	-1.48800702	1.37159002
H	1.76013512	-4.05683892	2.82967005
H	1.01004849	-5.24870407	1.71325586
H	2.35423687	-4.19597202	1.14349864
H	4.56615681	-0.00083990	-2.75990729
H	3.11571056	-0.06522315	-3.82773136
H	3.62067283	1.49235785	-3.10563273
H	-2.22420106	-4.16651496	-0.34803702
H	-3.84348265	-3.66885296	0.25716332
H	-3.40723628	-3.43154399	-1.47582466
H	-0.45906335	3.01843943	-0.54770051
H	-1.43265144	2.92497955	0.97352814
H	-0.74190731	4.49874223	0.45744492
H	-1.37093569	0.41625038	0.91163876
H	-1.42495737	0.78332049	0.13514367
H	-0.47546701	-3.18998986	1.99611924
H	0.08395468	-3.33138232	0.28796320
H	-2.05983581	-2.00106994	0.94052595
H	2.57195998	-0.96268196	-1.49490376
H	3.07522703	0.58218292	-0.77685047
H	0.56108052	3.38811301	2.35554016
H	1.57324608	3.66110542	0.88190250
H	-3.26560387	-1.24483394	-0.11468906

MODEL 3: TOTALLY FROZEN MODEL (BOTH CARBONS FROM CYS RESIDUES)

System: **Ni-SI$_a$** (singlet)
Charge, Multiplicity: –2, 1
Gibbs free energy: –4981.49866 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.78254741
C	1.76727594	0.00000000	3.47513975
C	-0.71416424	0.56570762	4.22945331
C	-0.19450318	-1.83423528	3.26173039
N	2.87435655	0.05229857	3.88071966
O	-1.21317344	0.97937713	5.21402916
N	-0.34387388	-2.97086405	3.53958831
*C	-2.25170033	3.03615253	-2.40875947
*C	-1.50636406	2.21013513	-1.35505782
S	-1.12849355	0.49894185	-1.94914483
*C	-3.80545874	-1.95653616	0.31794034
*C	-2.76532880	-1.70355279	1.42683499
S	-1.85399776	-0.06960919	1.33012900
*C	4.61002603	-0.94973132	-0.70532008
*C	3.30162968	-1.05806286	0.05929387
S	1.89237940	-0.46268715	-1.03345162
*C	2.41383064	3.74801695	0.80543404
*C	2.17293605	2.34469770	1.40401538
S	0.45419645	1.67203914	1.36429710
H	1.50809872	4.38676785	0.91114439
*H	3.21411484	4.24150183	1.35580783
H	2.66222695	3.70580276	-0.27496892
H	-2.57205688	4.02709032	-2.01082755
H	-1.62194917	3.20835286	-3.30923084
*H	-3.13064644	2.47663947	-2.72928235
*H	4.99818635	0.06849799	-0.69858643
H	5.39658538	-1.59417269	-0.24426838
H	4.49236263	-1.27206842	-1.76297316
H	-3.31775807	-1.97504839	-0.67891098
*H	-4.30919756	-2.92204237	0.50246307
H	-4.57732726	-1.15707182	0.29072133
H	2.44447011	2.32245160	2.47936635
H	2.81930335	1.58780160	0.92197950
H	3.30994558	-0.48673457	1.01318086
H	3.08166926	-2.10975298	0.33683199
H	-0.55672826	2.70646928	-1.06762589
H	-2.10888970	2.12987987	-0.42599467
H	-2.00129319	-2.50480398	1.46321351
H	-3.22983501	-1.67623749	2.43426405

System: **I1** (doublet)
Charge, Multiplicity: –2, 2
Gibbs free energy: –4982.080299 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.54793265
C	0.75701240	0.00000000	4.08921356
C	-0.78802336	1.71736676	2.68634983

C	-1.60559901	-0.73224603	3.22473207
O	1.31181078	0.00834776	5.13254508
N	-1.29145072	2.78571764	2.72112836
N	-2.59685545	-1.22833676	3.63689123
*C	2.88812857	-1.76849230	-2.86980652
*C	2.00163843	-1.35844093	-1.68952934
S	0.76181396	-0.09280349	-2.17087766
*C	2.68123334	3.28486419	0.15945679
*C	1.95141983	2.59273424	1.32486734
S	1.74453362	0.75727540	1.21905257
*C	-4.74909661	-0.89561874	-0.26270634
*C	-3.50790568	-0.32219873	0.39861768
S	-2.08978076	-0.11025845	-0.76345724
*C	-0.75629001	-4.42150607	0.63364024
*C	-1.01349344	-3.07275565	1.33718796
S	0.38173252	-1.86887886	1.28704771
*H	-1.23809558	-5.21773878	1.20201349
H	-1.11395966	-4.43589340	-0.41732575
H	0.33223921	-4.65122457	0.61222621
H	3.62050336	-2.56307415	-2.58794117
H	2.28079891	-2.14149315	-3.72388087
*H	3.44143554	-0.89288337	-3.20898413
*H	-4.70981093	-1.98391980	-0.31650858
H	-5.65588754	-0.65218624	0.33674144
H	-4.90680405	-0.49267468	-1.28715496
H	2.11422999	3.16491902	-0.78759945
*H	2.79042335	4.36104331	0.38981008
H	3.69526001	2.85820284	-0.00622886
H	-2.08748595	-1.38369197	-1.23327308
H	-1.91346124	-2.56996619	0.93087625
H	-1.23731495	-3.22311744	2.41198910
H	-3.66655606	0.71172346	0.76833013
H	-3.17738481	-0.89667650	1.28819256
H	1.47575430	-2.24082426	-1.27070897
H	2.61970127	-0.95338018	-0.86083806
H	0.94034090	3.02449600	1.46955286
H	2.50054739	2.75826420	2.27769589

System: **Ni-C** (doublet)
Charge, Multiplicity: –2, 2
Gibbs free energy: –4982.097114 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.55438936
C	0.85904302	0.00000000	4.05607502
C	-1.15909851	1.38265384	3.16927002
C	-1.20912546	-1.32072635	3.18914299
O	1.43723603	0.00562993	5.07757963
N	-1.84799727	2.26115280	3.54674456
N	-1.92693106	-2.17178731	3.57708087
*C	3.83857407	-0.32453921	-2.50955932
*C	2.73465169	-0.34309409	-1.44698147
S	1.10987437	0.31570629	-1.97209516
*C	1.15413554	4.12951183	0.26806882
*C	0.66291541	3.18161091	1.37730070

S	1.26832181	1.43099432	1.25849475
*C	-3.68168376	-2.82878218	-0.76192237
*C	-2.88799754	-1.78331193	0.00222699
S	-1.50098753	-1.19414543	-1.08205072
*C	1.30296612	-4.31038882	0.69775483
*C	0.41803936	-3.20666776	1.31228311
S	1.23044757	-1.54834651	1.34811033
*H	1.14646568	-5.24053862	1.24381464
H	1.09762514	-4.46069329	-0.38200048
H	2.38157153	-4.05703228	0.80013830
H	4.79329221	-0.73074059	-2.10519466
H	3.55747980	-0.91640196	-3.40856228
*H	4.00016098	0.70625668	-2.82440620
*H	-3.17654350	-3.79475751	-0.76610259
H	-4.67943280	-2.99610994	-0.29052696
H	-3.85879510	-2.52269868	-1.81653321
H	2.26424558	4.17791433	0.22881100
H	0.80304263	3.78613109	-0.72736059
*H	0.76722931	5.14659078	0.46352175
H	-1.04925316	-0.00412140	1.20322674
H	-2.48590234	-2.17279191	0.96048878
H	-3.52154995	-0.91122062	0.26904501
H	-0.53537625	-3.09010607	0.76436085
H	0.15439899	-3.42941437	2.36510843
H	2.57596184	-1.38090089	-1.08877907
H	3.06468796	0.22905641	-0.55316984
H	0.99159838	3.52127526	2.38189017
H	-0.44329648	3.14428071	1.41801258

System: **Ni-R** (singlet)
Charge, Multiplicity: –2, 1
Gibbs free energy: –4982.671913 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.55168401
C	0.81865884	0.00000000	4.07140668
C	-1.19662474	1.36116884	3.14194677
C	-1.21213504	-1.34276332	3.12384964
O	1.37100667	0.00016863	5.10911914
N	-1.92264123	2.21839036	3.50225779
N	-1.95660825	-2.20312263	3.44009745
*C	3.86760601	-0.35911919	-2.49094310
*C	2.76889415	-0.38543689	-1.42414167
S	1.10962311	0.17270063	-1.98001321
*C	1.03537891	4.07308008	0.17355082
*C	0.58348917	3.14127314	1.31024851
S	1.21838654	1.40897434	1.20677659
*C	-3.55000385	-3.08230298	-0.63372400
*C	-2.79096203	-1.98878568	0.09671057
S	-1.45455892	-1.27648303	-0.98734760
*C	1.49188159	-4.34098825	0.84193584
*C	0.56826952	-3.25529602	1.42870415
S	1.38893609	-1.61738661	1.50929974
H	2.55801037	-4.03911932	0.93641074
*H	1.37098776	-5.25994423	1.41418999

H	1.29805966	-4.53939556	-0.23372739
H	4.83872392	-0.71560252	-2.07772182
H	3.60967892	-0.98926243	-3.37127813
*H	3.98999380	0.66747553	-2.83614696
H	-4.52800746	-3.27450333	-0.13624411
H	-3.75740479	-2.81478696	-1.69252346
*H	-3.00996748	-4.02927606	-0.61308761
H	0.68886925	3.68843235	-0.80888139
*H	0.61214645	5.08016007	0.34146415
H	2.14293803	4.15897790	0.12357517
H	-1.03300266	0.05338183	1.19810522
H	-0.75074800	-2.44467692	-1.07974814
H	-0.36934198	-3.17768244	0.83417708
H	0.23416750	-3.51641483	2.45259192
H	-3.42537759	-1.10525812	0.31368627
H	-2.35883309	-2.29769357	1.07106254
H	2.65734891	-1.40186970	-0.99262634
H	3.06089251	0.25745472	-0.56672673
H	0.92415605	3.51389523	2.29997082
H	-0.52030355	3.08308060	1.37245532

System: **I2a** (singlet)
Charge, Multiplicity: –2, 1
Gibbs free energy: –4982.673812 au

Ni	0.00000000	0.00000000	0.00000000
Fe	0.00000000	0.00000000	2.61875574
C	0.81695549	0.00000000	4.11437020
C	-1.13133535	1.44579354	3.11687028
C	-1.32835014	-1.21974159	3.19472168
O	1.39929492	-0.01079546	5.13814647
N	-1.81774835	2.36137250	3.40328551
N	-2.13375871	-2.00832526	3.54210480
*C	3.98352002	-0.61848491	-2.31906065
*C	2.82867098	-0.56083770	-1.31401301
S	1.29483244	0.23171329	-1.94391615
*C	1.37638766	4.02172880	0.21569380
*C	0.78600165	3.12533467	1.32039454
S	1.33855295	1.34789814	1.28132836
*C	-3.72209805	-2.73460222	-0.89384006
*C	-2.91957061	-1.70683047	-0.11563429
S	-1.34894789	-1.44758123	-1.09607290
*C	1.11104583	-4.40245395	0.84809359
*C	0.24898772	-3.24320741	1.39162825
S	1.04757385	-1.57756205	1.36970817
H	2.19616861	-4.19916960	0.99005596
*H	0.88410441	-5.30994736	1.40780451
H	0.94253351	-4.56818187	-0.23597517
H	4.89872830	-1.06205609	-1.86393842
H	3.71500746	-1.21449411	-3.21925110
*H	4.20788247	0.39529172	-2.64958421
*H	-3.26275511	-3.72206682	-0.85031443
H	-4.75478634	-2.83722612	-0.48213895
H	-3.81503249	-2.44880034	-1.96485214
H	1.06437473	3.66490965	-0.78782571

*H	1.02717822	5.06006826	0.36735387
H	2.48768318	4.01931560	0.23611586
H	-1.28379050	0.68231823	0.72925223
H	-1.19720252	1.06548042	-0.06095152
H	-0.04804089	-3.40889207	2.44604278
H	-0.68459729	-3.14039133	0.80135279
H	-2.69002757	-2.03524581	0.91933525
H	2.56887650	-1.58388309	-0.96952041
H	3.15109798	-0.01386407	-0.40139983
H	1.07194959	3.47837992	2.33322775
H	-0.32115887	3.12947196	1.30165735
H	-3.46268641	-0.74027344	-0.03975001

MODEL 4: INORGANIC LIGAND REPLACEMENT: ORIGINAL MODEL

System: **Ni-SI$_a$** (singlet)
Charge, Multiplicity: –2, 1
Gibbs free energy: –6207.814167 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.34633523
S	3.20054391	0.00000000	0.31238393
S	1.88837432	2.11433698	2.68282369
Ni	1.51884186	0.20985322	1.69385554
Fe	1.95384619	0.71570067	4.42310513
C	1.46030640	1.68787061	5.74069969
C	3.76582934	1.03413623	4.73059588
O	1.16246798	2.39682089	6.63142184
N	4.90747895	1.26361401	4.92765815
C	2.03141115	-0.84486496	5.50769348
N	2.02615508	-1.76832891	6.24293072
O	8.65799769	3.32091069	7.83576678
*C	7.52229077	2.99384624	7.45725206
N	7.22221619	2.68110352	6.16736795
C	8.24072172	2.68779924	5.12778959
C	7.65879979	2.38241660	3.73713321
O	7.25478890	1.04561299	3.56851669
H	8.75219694	3.68028712	5.12401594
H	6.26787326	2.36259465	5.90847462
H	9.03122805	1.93494547	5.35702517
H	6.82557386	3.10453965	3.53101654
H	8.45741061	2.59510360	2.98769764
H	6.38532081	0.95695287	4.06140107
C	4.09696065	1.83454369	8.36916130
C	3.99533445	3.33965556	8.65403134
H	3.77648144	1.63451868	7.32883995
H	3.46117282	1.22297678	9.03958463
H	3.10846261	3.80347608	8.17369526
H	3.91507006	3.52335928	9.76354110
C	6.32107247	2.92845315	8.43967786
C	5.61100087	1.53365802	8.51795503
H	5.84643429	1.04930541	9.48781779
H	5.95727955	0.85153190	7.71635648
H	6.77412039	3.17466176	9.43449786

*N	5.22983163	3.84659922	8.06359625
H	5.43993468	4.82252146	8.29796217
N	3.51489597	-3.47514814	8.01660849
*C	3.30817650	-4.49100285	8.89170782
H	2.75256807	-2.91317187	7.57525452
*O	4.21622199	-5.21504972	9.32358061
C	4.85203526	-3.15766444	7.55112398
H	5.33946673	-4.03939209	7.07864091
H	5.50527059	-2.83534050	8.39143268
*H	1.47668184	4.46476332	10.82001440
*C	0.74830732	3.95429927	10.19024174
C	-0.14216000	4.86684941	9.33771212
C	0.69340410	5.74832027	8.39491630
C	-1.17223599	4.03981869	8.54583390
H	0.12612477	3.32495910	10.86461566
H	1.30869795	3.25204717	9.53740058
H	0.05460153	6.45584590	7.82331597
H	1.23138899	5.11431044	7.65797969
H	1.45108061	6.34165315	8.95086349
H	-1.84349675	4.69662552	7.95125707
H	-1.80755089	3.42993534	9.22397727
H	-0.66388631	3.34920826	7.84178902
*H	-0.71373051	5.51767199	10.03517179
*C	-1.68818690	2.14974331	-0.66461018
*H	-2.46847674	1.38951605	-0.69908054
C	-0.61409357	1.70932528	0.32902537
*C	-1.75698421	-2.27509727	3.23048537
H	-2.52596077	-1.54271214	3.56034628
C	-0.35005828	-1.80362591	3.66399454
H	6.89946365	-0.42018788	1.08619677
*C	6.02551163	-0.10385312	0.47722553
*H	6.19019255	0.94005770	0.21021271
C	4.73663587	-0.24223562	1.31567219
H	3.23406947	4.09009173	0.34809669
*C	3.14420634	4.36678661	1.41662090
C	3.38864372	3.14867316	2.35765655
H	-2.14065138	3.12577800	-0.37696753
*H	3.89606088	5.10364610	1.70017384
H	-0.20181668	-1.92258666	4.75621039
H	0.45176648	-2.38936744	3.17164069
H	4.68573245	-1.25001909	1.77729537
H	4.75232014	0.47368209	2.16585807
H	0.24832872	2.40705175	0.30480376
H	-1.01127901	1.74118650	1.36533573
H	5.98129653	-0.71303218	-0.45092691
H	-1.27612724	2.24617638	-1.69275907
H	2.14069537	4.81068967	1.58729220
H	4.18969167	2.48618681	1.97673464
H	3.71000294	3.48325696	3.36547965
*H	-2.01725913	-3.24524439	3.69352824
C	1.01686798	-2.55378271	10.00549423
O	1.79473301	-2.49710137	10.95538522
N	0.94593308	-3.59314352	9.12280363
C	1.82832752	-4.76164853	9.24490452
C	1.19870870	-5.79069993	8.26057016

*C	-0.24106163	-5.28484971	8.04103649
C	-0.05735635	-3.75692457	8.06405675
H	0.33362371	-3.36634786	7.09549318
H	-0.98133360	-3.19399709	8.31050080
H	-0.69124540	-5.64919992	7.09461984
H	-0.89812963	-5.60051624	8.88192279
H	1.75287394	-5.75804008	7.29870590
H	1.26138031	-6.82683178	8.64795133
H	1.83151618	-5.12066134	10.29652877
H	0.26325309	-1.74776434	9.76710080
H	4.77522182	-2.33686322	6.81210547
H	-1.83073152	-2.35128046	2.12614199

System: **I1** (doublet)
Charge, Multiplicity: –2, 2
Gibbs free energy: –6208.39418 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.58281652
S	3.10687471	0.00000000	0.51115146
S	1.33798145	2.48338569	2.56757571
Ni	1.34037464	0.33560852	1.83386741
Fe	1.90994537	1.06180518	4.28504370
C	1.51922400	2.03094449	5.64844153
C	3.69060464	1.61918068	4.25202782
O	1.26685635	2.73183227	6.56239804
N	4.80854087	2.00876947	4.27953236
C	2.41203431	-0.41440398	5.36466772
N	2.68537203	-1.29576198	6.10324927
H	2.97536983	1.07977353	-0.29663635
O	8.53011773	4.83468441	6.73833526
*C	7.41642840	4.33072284	6.52395287
N	7.02508524	3.87944971	5.29948622
C	7.91757644	3.96037700	4.15249684
C	7.25119170	3.48501963	2.85149965
O	7.04097630	2.09583768	2.79432586
H	8.27352396	5.01303162	4.04294371
H	6.09847248	3.43100118	5.17012591
H	8.83049526	3.34477035	4.33083330
H	6.29937803	4.06090804	2.70631067
H	7.92752563	3.76809645	2.00963198
H	6.23819778	1.91926445	3.38421406
C	4.39687140	2.67200759	7.80913265
C	4.01143296	4.13904556	8.03125775
H	4.09865360	2.36585896	6.78749199
H	3.90813650	1.97885591	8.52182158
H	3.02299074	4.38625293	7.59242859
H	3.96427865	4.36974909	9.13350781
C	6.36030564	4.17307922	7.64873134
C	5.94018031	2.68803222	7.93145025
H	6.27277151	2.39797035	8.94985717
H	6.41056554	1.98216159	7.21824889
H	6.86777096	4.59845147	8.55192761
*N	5.08461486	4.84075346	7.33134514
H	5.11358884	5.85092312	7.50212439

N	4.60112042	-2.65203051	7.77074494
*C	4.65271729	-3.63296591	8.70672311
H	3.71772325	-2.24120905	7.38629845
*O	5.70462107	-4.17761497	9.07072220
C	5.81495693	-2.15138446	7.15394979
H	6.39034923	-2.96741278	6.66187840
H	6.48839824	-1.68719366	7.90757781
*H	1.56538886	5.01207338	10.43824372
*C	0.87345658	4.35553977	9.91070812
C	-0.23626760	5.05917998	9.11962592
C	0.34548962	5.99844418	8.05035108
C	-1.19280572	4.03151788	8.48592872
H	0.43393978	3.67494682	10.67353409
H	1.47466573	3.71568689	9.23084246
H	-0.45442567	6.55587523	7.51655627
H	0.90569212	5.40966529	7.29296200
H	1.04505168	6.74049036	8.49263051
H	-2.01884715	4.53620563	7.93946589
H	-1.64834219	3.37473792	9.25854005
H	-0.65218093	3.38606693	7.76356528
*H	-0.83398124	5.65395840	9.84417613
*C	-2.27125932	1.55225618	-0.54253702
*H	-2.91512555	0.67661013	-0.46317991
C	-1.08320641	1.42906656	0.39953397
*C	-1.23272559	-2.59056010	3.52097066
H	-2.19223110	-2.05752449	3.69557349
C	-0.04172700	-1.78602616	4.08577164
H	6.83006273	0.47247165	0.21656577
*C	5.78362985	0.63080424	-0.12269578
*H	5.74514742	1.66935830	-0.45074357
C	4.83335988	0.35605562	1.04568086
H	2.39806810	4.27562871	-0.12233383
*C	2.30838017	4.63061427	0.92402383
C	2.72377713	3.54704809	1.96387343
H	-2.88578562	2.45382992	-0.30872473
*H	2.95202655	5.49356633	1.09621437
H	-0.06174761	-1.77334660	5.19547617
H	0.92651918	-2.24265184	3.80285432
H	5.12306027	-0.55871840	1.60178703
H	4.83887761	1.17738089	1.78655080
H	-0.46869768	2.35261536	0.37732562
H	-1.42572395	1.32126810	1.45051827
H	5.58815461	-0.03621756	-0.98937231
H	-1.94230083	1.63100446	-1.60241750
H	1.25811717	4.95339834	1.08871488
H	3.52098616	2.88788232	1.56568713
H	3.15334877	4.01979146	2.87027522
*H	-1.28316968	-3.56127017	4.04864767
C	2.19216389	-2.01868333	9.96151936
O	3.03567065	-1.78251851	10.82410002
N	2.20780120	-3.11121193	9.14270634
C	3.27819183	-4.11351731	9.22673855
C	2.73465192	-5.29115655	8.36446935
*C	1.21732458	-5.03269159	8.26768284
C	1.15294967	-3.49595051	8.19723938

H	1.38616053	-3.10917254	7.17723208
H	0.17638633	-3.06966127	8.50689977
H	0.74704784	-5.52305233	7.39038962
H	0.70056096	-5.39266503	9.18527334
H	3.18428241	-5.23511324	7.35052378
H	3.00041651	-6.27717511	8.79456585
H	3.44206275	-4.39929081	10.28806656
H	5.52962674	-1.39185348	6.40041386
H	-1.13280120	-2.75295793	2.42818873
H	1.30085293	-1.35589718	9.76175723

System: **Ni-C** (doublet)
Charge, Multiplicity: –2, 2
Gibbs free energy: –6208.409578 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.34080202
S	3.06128112	0.00000000	0.12500663
S	1.49233934	2.42081531	2.41869709
Ni	1.50533212	0.19091392	1.65774301
Fe	2.01578268	0.85894228	4.07624116
C	1.59245683	1.87295142	5.41708858
C	3.80591660	1.37689364	4.18842003
O	1.35995387	2.58052560	6.32217467
N	4.93444786	1.71102901	4.27319757
H	2.61947564	-0.09321655	2.79629797
C	2.33148934	-0.59213790	5.25562667
N	2.46497690	-1.44914279	6.05500958
C	1.82810119	-2.01967047	9.92623580
O	8.84809732	4.10478131	6.69475708
*C	7.69217632	3.73073519	6.44142850
N	7.28408454	3.34083527	5.20348975
C	8.20850647	3.30609850	4.07996245
C	7.54749094	2.77081300	2.79918591
O	7.23300207	1.40108084	2.85474997
H	8.61660490	4.33089083	3.90064533
H	6.32024600	2.98362197	5.05455171
H	9.08562045	2.66576839	4.33153965
H	6.64736270	3.39860999	2.56963595
H	8.26732220	2.92693636	1.96102014
H	6.39403033	1.34031601	3.40292172
C	4.46840134	2.41909584	7.74756494
C	4.26578899	3.93087133	7.92054655
H	4.08966227	2.10979706	6.75479533
H	3.93666430	1.81990648	8.51302039
H	3.30847301	4.28346769	7.48288207
H	4.25877094	4.20253877	9.01479713
C	6.59298391	3.67875465	7.53526016
C	6.00852969	2.24751863	7.79514356
H	6.35665875	1.87528557	8.78054756
H	6.34877444	1.52300365	7.02893418
H	7.11255957	4.04445760	8.45816072
*N	5.40380530	4.47648583	7.18802204
H	5.55041456	5.48244263	7.32111390
N	4.21206830	-2.92384536	7.79306179

*C	4.15133072	-3.88266970	8.75050444
H	3.37864941	-2.44334642	7.38314507
*O	5.14110766	-4.51346915	9.14879928
C	5.48036192	-2.55801363	7.19043770
H	5.98819813	-3.44069023	6.74180372
H	6.17652272	-2.12980070	7.94459195
*H	1.85907430	5.05414630	10.21603677
*C	1.11863232	4.45235676	9.68929771
C	0.09880173	5.24083692	8.85802864
C	0.78996732	6.10338894	7.78929375
C	-0.93339772	4.29469952	8.21663997
H	0.60027785	3.83625568	10.45720483
H	1.67073930	3.74103606	9.03932674
H	0.05827243	6.72342611	7.22763701
H	1.31107718	5.45420646	7.05345352
H	1.54585782	6.78434893	8.23665202
H	-1.69566714	4.86261595	7.64058184
H	-1.46611959	3.69653810	8.98729685
H	-0.43887100	3.58782199	7.51919047
*H	-0.45790283	5.90252882	9.55712528
*C	-2.08058391	1.69418263	-0.75952564
*H	-2.80546708	0.88479676	-0.67297568
C	-0.95634653	1.54265969	0.25974171
*C	-1.51172593	-2.42472149	3.41982496
H	-2.35979769	-1.76676323	3.70997460
C	-0.16834813	-1.77992130	3.82072469
H	6.82404056	-0.20502325	0.31150710
*C	5.84120481	0.03363056	-0.15122987
*H	5.90883343	1.06337881	-0.50238354
C	4.72875311	-0.14703465	0.89268797
H	2.84529600	3.93551257	-0.28404546
*C	2.73987550	4.36665989	0.73088713
C	2.99606382	3.30905888	1.83928196
H	-2.62375849	2.65676853	-0.61707357
*H	3.45856669	5.16943315	0.89609697
H	-0.02529854	-1.79830671	4.92068333
H	0.69701850	-2.32004129	3.38768582
H	4.81052265	-1.14058702	1.38185804
H	4.83889263	0.60278540	1.70204166
H	-0.25425691	2.39813002	0.19191717
H	-1.35436624	1.54859046	1.29685708
H	5.69070906	-0.62882673	-1.03152700
H	-1.68498013	1.67911296	-1.79874601
H	1.72259898	4.80515160	0.82071371
H	3.73142888	2.55021842	1.51220999
H	3.41761268	3.78594509	2.74768551
*H	-1.64097582	-3.35923535	3.92473549
O	2.67454137	-1.84247680	10.79959816
N	1.75872490	-3.12466423	9.12711406
C	2.72900678	-4.22086664	9.25177709
C	2.09372621	-5.36033777	8.40155744
*C	0.60887833	-4.96521796	8.27238526
C	0.68715378	-3.43121878	8.17234194
H	0.97072504	-3.09042148	7.14898312
H	-0.25073973	-2.91092673	8.45708938

H	0.10967001	-5.42809253	7.39616165
H	0.04607863	-5.25748089	9.18690151
H	2.56361599	-5.36658078	7.39532886
H	2.25982612	-6.35766280	8.85473711
H	2.84575611	-4.49802846	10.32151742
H	-1.57277694	-2.57313482	2.32207852
H	5.28446924	-1.80406452	6.40374136
H	1.00306966	-1.28367015	9.69828881

System: **Ni-R** (singlet)
Charge, Multiplicity: –2, 1
Gibbs free energy: –6208.989386 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.34122005
S	3.03838957	0.00000000	0.19313364
S	1.42612458	2.57910885	2.49886656
Ni	1.46104310	0.13730733	1.70187858
Fe	1.98407897	0.89251788	4.08823740
C	1.56967631	1.93206851	5.40775042
C	3.76953521	1.42544704	4.16292417
O	1.33791173	2.66085093	6.29766512
N	4.89883728	1.76858957	4.22971656
H	2.56063812	-0.11872613	2.83669170
C	2.32805697	-0.54121085	5.28113776
N	2.49684396	-1.39053089	6.08391143
H	3.05172223	1.28349266	-0.26876765
O	8.72117298	4.37730055	6.71626822
*C	7.58561599	3.93256453	6.48539427
N	7.19432165	3.48237713	5.26061389
C	8.11164366	3.49070744	4.12997080
C	7.43691398	3.06684987	2.81457363
O	7.13466998	1.69427177	2.74307548
H	8.54948212	4.51254327	4.02828374
H	6.24611105	3.08532139	5.11648836
H	8.97119167	2.80650955	4.32434829
H	6.52918816	3.70613289	2.65625234
H	8.14611917	3.30656242	1.98662659
H	6.31750471	1.56920697	3.32350356
C	4.44428801	2.47739351	7.72186015
C	4.14330411	3.96775765	7.91919511
H	4.15428301	2.17846686	6.69582876
H	3.89775683	1.82295828	8.42930243
H	3.18386076	4.27006325	7.45028032
H	4.07929769	4.21315447	9.01751242
C	6.49986876	3.85360547	7.59143869
C	5.98227926	2.40145475	7.88267232
H	6.27085941	2.10656196	8.91306766
H	6.42572703	1.65759821	7.19118796
H	7.01655837	4.25756357	8.49927897
*N	5.27492190	4.59532158	7.24270958
H	5.36134829	5.60388019	7.40210255
N	4.31575525	-2.84419937	7.74978834
*C	4.29084168	-3.82087296	8.69043657
H	3.46449798	-2.38047875	7.35081799

*O	5.30040744	-4.42475250	9.07977336
C	5.56891606	-2.41972211	7.15510262
H	6.10589748	-3.27173781	6.68105782
H	6.25296148	-1.98892287	7.91906283
*H	1.71604189	5.01766236	10.27934237
*C	0.99486075	4.39990073	9.74445387
C	-0.04553129	5.17176586	8.92299859
C	0.62441276	6.07845174	7.87736063
C	-1.03937063	4.20455856	8.25322226
H	0.49447571	3.75713521	10.50226411
H	1.56910037	3.71660819	9.08368717
H	-0.12381368	6.68391429	7.32164795
H	1.17260856	5.46202396	7.13320262
H	1.35246326	6.77629196	8.34485914
H	-1.81777058	4.75770929	7.68447334
H	-1.55491868	3.56998805	9.00632936
H	-0.51444753	3.53301770	7.54272187
*H	-0.62722017	5.80083004	9.63278290
*C	-2.12238447	1.68502450	-0.74038730
*H	-2.82109273	0.85190677	-0.66472687
C	-0.97816324	1.53504721	0.26281710
*C	-1.41976363	-2.47063616	3.38188504
H	-2.34840390	-1.87767909	3.52693269
C	-0.19489980	-1.73296120	3.95166065
H	6.83442012	0.07680784	0.31773752
*C	5.84887966	0.26958370	-0.15695675
*H	5.88316781	1.30556184	-0.49409886
C	4.75009844	0.04547180	0.88866818
H	2.69012553	4.13434466	-0.26290053
*C	2.61151652	4.48917462	0.78530993
C	2.93109416	3.37520200	1.82247068
H	-2.68767340	2.62883778	-0.56353042
*H	3.30447382	5.31188973	0.96138618
H	-0.25525164	-1.64901629	5.05733928
H	0.74844338	-2.26926958	3.73385763
H	4.84290282	-0.94551277	1.37841459
H	4.79523957	0.79567361	1.70172818
H	-0.28781805	2.40230546	0.21895175
H	-1.36733950	1.51436261	1.30251354
H	5.73180897	-0.39587392	-1.03873623
H	-1.74318732	1.70789017	-1.78613320
H	1.58349222	4.88319758	0.93526341
H	3.58890965	2.60085581	1.37103990
H	3.50846086	3.78788577	2.67479249
*H	-1.54084705	-3.43032095	3.91808611
C	1.91930943	-2.05550004	9.90316248
O	2.76673988	-1.86715510	10.77369373
N	1.87539330	-3.15050969	9.08927960
C	2.88141621	-4.21643824	9.18669077
C	2.28160048	-5.35609126	8.31188717
*C	0.78396640	-5.00872930	8.19835982
C	0.80978688	-3.47109629	8.13198139
H	1.07671059	-3.09591176	7.11597332
H	-0.14374155	-2.98991158	8.43313977
H	0.29595206	-5.46833887	7.31410114

H	0.23629452	-5.34081817	9.10858697
H	2.74627050	-5.32116526	7.30380493
H	2.48416797	-6.35793259	8.73980727
H	3.01085488	-4.51470742	10.24935938
H	1.07261248	-1.33984565	9.69118190
H	5.34444127	-1.65108667	6.39023942
H	-1.30799501	-2.65699843	2.29389271

System: **I2a** (singlet)
Charge, Multiplicity: –2, 1
Gibbs free energy: –6208.985172 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.34947094
S	3.15841034	0.00000000	0.07743646
S	1.90612617	2.07105555	2.50946054
Ni	1.57405457	-0.04921034	1.68617376
Fe	2.07813325	0.57265870	4.20495589
C	1.77047380	1.58875591	5.54167453
C	3.92601954	0.78007476	4.36001946
O	1.59826097	2.31665926	6.44864392
N	5.08898923	0.93352442	4.49152746
C	2.16483529	-0.96835548	5.31200023
N	2.18183840	-1.88066075	6.06059354
H	2.38783358	-1.16066621	2.59774436
H	1.97968868	-1.59227750	1.95513667
O	9.17299875	2.83197341	7.15349396
*C	7.99309482	2.58410792	6.86042975
N	7.58397489	2.27258920	5.59973339
C	8.53077579	2.18668747	4.49710885
C	7.85458125	1.79559949	3.17230067
O	7.39718172	0.46580216	3.13938298
H	9.05728708	3.16557908	4.38392151
H	6.59316795	2.03087047	5.41132370
H	9.32167464	1.43784743	4.73466119
H	7.03227866	2.52680822	2.95796156
H	8.61180182	1.92133318	2.36249257
H	6.53446835	0.46620390	3.65266954
C	4.60012154	1.60515478	7.98196052
C	4.56410503	3.11663961	8.24306098
H	4.24820924	1.40282952	6.95205395
H	3.95819714	1.02770458	8.67633948
H	3.67406571	3.60359016	7.79262263
H	4.53988815	3.32248287	9.35118347
C	6.86372011	2.61325179	7.92481984
C	6.10437758	1.25267592	8.10221214
H	6.34891582	0.81725026	9.09303661
H	6.40337306	0.51212661	7.33404029
H	7.39760453	2.87157946	8.87506711
*N	5.78950758	3.56564727	7.58938359
H	6.04612202	4.53746435	7.79093925
N	3.69558023	-3.65633938	7.76952493
*C	3.49115672	-4.64550061	8.67598197
H	2.93793453	-3.05837295	7.37045332
*O	4.38428337	-5.41091452	9.06504443

C	5.01569332	-3.41665106	7.21675020
H	5.42589733	-4.32958246	6.73044712
H	5.73624508	-3.11771051	8.00930931
*H	2.24957809	4.42096159	10.55601412
*C	1.45801256	3.94075971	9.98083850
C	0.56751989	4.88830258	9.16735754
C	1.39115462	5.71219999	8.16393254
C	-0.54920195	4.10717557	8.44986569
H	0.84575406	3.35565445	10.70245356
H	1.93988542	3.20050379	9.30764637
H	0.75748963	6.44427514	7.61820355
H	1.85236546	5.04141547	7.40781308
H	2.20906340	6.27274361	8.66600478
H	-1.21959041	4.79105963	7.88569109
H	-1.17379352	3.53960580	9.17324536
H	-0.11975503	3.38256307	7.72765429
*H	0.07310665	5.57736864	9.88677875
*C	-1.72710172	2.11459621	-0.67663763
*H	-2.54860914	1.39749462	-0.64763948
C	-0.62093772	1.70264082	0.29810734
*C	-1.78933644	-2.24429562	3.29432221
H	-2.60924494	-1.51618542	3.47512400
C	-0.45539055	-1.72151220	3.86717190
H	6.80225930	-0.89212774	0.59429752
*C	5.91218797	-0.52773626	0.03802722
*H	6.11508959	0.50171543	-0.25607477
C	4.67463622	-0.57851658	0.95354330
H	3.37302866	3.76914121	0.01644704
*C	3.33041808	4.10216037	1.07222649
C	3.48671320	2.90605440	2.05385167
H	-2.12829904	3.12386710	-0.42915729
*H	4.13623481	4.80162090	1.29718691
H	-0.48224139	-1.68343313	4.97564350
H	0.38983622	-2.38777977	3.60544836
H	4.50343475	-1.61672931	1.31347868
H	4.85600993	0.03810919	1.85792334
H	0.23715663	2.40338766	0.22886964
H	-0.98631201	1.76728559	1.34569329
H	5.77172946	-1.13669515	-0.88102783
H	-1.35170028	2.14141056	-1.72319227
H	2.36784151	4.63335278	1.23452477
H	4.16425670	2.13623439	1.63404838
H	3.92139901	3.23536884	3.01934509
*H	-2.07093645	-3.19299463	3.78786304
C	1.37663036	-2.56628113	9.88049162
O	2.21203510	-2.53424845	10.78133851
N	1.19774245	-3.61720370	9.02698435
C	2.02293487	-4.82909419	9.12329234
C	1.28086513	-5.84179127	8.20204317
*C	-0.14052620	-5.26214962	8.05525817
C	0.12595193	-3.74635067	8.03250525
H	0.47832013	-3.39595123	7.03408678
H	-0.75023025	-3.12902861	8.31996903
H	-0.66501740	-5.62007181	7.14533621
H	-0.76232486	-5.52464710	8.94005473

H	1.77751189	-5.85934493	7.20884741
H	1.31081385	-6.87173345	8.60932581
H	2.07091347	-5.16686077	10.18084547
H	4.93583746	-2.60309948	6.47010799
H	-1.72027268	-2.39681229	2.19771061
H	0.65432939	-1.72503327	9.66876890

MODEL 5: INORGANIC LIGAND REPLACEMENT: $[CN]^-$ REPLACES CO

System: **Ni-SI$_a$** (singlet)
Charge, Multiplicity: –3, 1
Gibbs free energy: –6187.202559 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.40617294
S	3.25485483	0.00000000	0.38287661
S	1.94405809	2.06472110	2.82886860
Ni	1.52063316	0.21804314	1.73993352
Fe	1.97076793	0.61273088	4.52580209
C	1.41565310	1.64873782	5.95698553
C	3.74045902	0.91384632	4.91982901
N	1.08523201	2.36000479	6.84568869
N	4.89148688	1.10867171	5.15038843
C	1.95802283	-0.93635335	5.60422318
N	1.91016221	-1.88622411	6.31605767
O	8.58521624	3.10836795	8.10140620
C	7.44791762	2.78845338	7.70721223
N	7.16343631	2.46978550	6.41786164
C	8.19907901	2.46237619	5.39735342
C	7.64183038	2.11008480	4.00530978
O	7.23172160	0.77496952	3.88464013
H	8.70241354	3.46087672	5.37378525
H	6.20837797	2.14301370	6.13526641
H	8.99486243	1.72481998	5.66099244
H	6.81603148	2.82867355	3.76086877
H	8.45876854	2.29818106	3.26492893
H	6.32119561	0.73456531	4.33519800
C	4.00527124	1.65939270	8.54322955
C	3.89209357	3.16461666	8.81025401
H	3.70774254	1.45887127	7.49607544
H	3.33944443	1.05707648	9.19194973
H	3.02372854	3.60187329	8.27522971
H	3.76464585	3.36533617	9.91430508
C	6.23139102	2.74547792	8.67266134
C	5.51056666	1.35468391	8.74912707
H	5.71540400	0.88711419	9.73582472
H	5.88060351	0.65923321	7.96938057
H	6.67714822	2.99282025	9.67345481
N	5.15533891	3.66772015	8.27418704
H	5.36048129	4.64366040	8.51090869
N	3.30669254	-3.60722003	8.06939540
C	3.08065846	-4.65075206	8.90144653
H	2.56488744	-3.02066374	7.59157873
O	3.96632846	-5.39722385	9.34150517

C	4.65551477	-3.27372910	7.64877507
H	5.15509331	-4.13594630	7.15184970
H	5.28881505	-2.98438633	8.51627621
H	1.34698868	4.29762485	10.95102002
C	0.62609499	3.81082036	10.29456455
C	-0.23826287	4.74251426	9.43721040
C	0.63096624	5.59888368	8.50070977
C	-1.25705798	3.92603861	8.61889674
H	-0.01894305	3.17651494	10.94459631
H	1.18128966	3.11514557	9.62947197
H	0.01644568	6.32876077	7.92843681
H	1.13699204	4.93320814	7.76761654
H	1.40768496	6.16585083	9.06061111
H	-1.91255140	4.59385423	8.01651893
H	-1.91022648	3.31514355	9.28149930
H	-0.71428667	3.24532956	7.92214983
H	-0.80655307	5.40059852	10.13357519
C	-1.57541046	2.24374261	-0.64699101
H	-2.36674545	1.49724826	-0.71422085
C	-0.53412000	1.73204682	0.35006555
C	-1.80960935	-2.24924800	3.16272563
H	-2.57749473	-1.50977105	3.48212285
C	-0.40836025	-1.80355042	3.65193389
H	6.92478855	-0.49661804	1.26530714
C	6.07121623	-0.15710011	0.63719201
H	6.25898513	0.88863428	0.39353047
C	4.75276010	-0.29796666	1.42637108
H	3.33143970	4.10412004	0.51160456
C	3.24009504	4.34270150	1.59001003
C	3.46139103	3.08132610	2.48942566
H	-2.01198159	3.22352257	-0.34014180
H	3.99658906	5.06179870	1.90502462
H	-0.29537208	-1.96465918	4.74386137
H	0.39430843	-2.39303547	3.16442207
H	4.67936268	-1.32002910	1.85497416
H	4.75409548	0.38683706	2.30210435
H	0.35963528	2.39077489	0.35633495
H	-0.94416208	1.76271498	1.38197670
H	6.04892191	-0.74508080	-0.30720415
H	-1.14391559	2.35587460	-1.66701079
H	2.23827281	4.78832234	1.77146618
H	4.22598350	2.40927899	2.05375064
H	3.82623223	3.37430955	3.49575076
H	-2.09655346	-3.22319860	3.60133166
C	0.72156315	-2.82451743	10.15319344
O	1.43344490	-2.87247309	11.15666910
N	0.71227906	-3.76454655	9.16506481
C	1.59322778	-4.93668113	9.21967694
C	0.96948807	-5.90631323	8.17198983
C	-0.45920439	-5.37028536	7.95155638
C	-0.24753738	-3.84645295	8.05702322
H	0.19622377	-3.41073333	7.12935966
H	-1.16762189	-3.27423174	8.29511732
H	-0.89383241	-5.67608579	6.97710750
H	-1.13876429	-5.71783844	8.76265960

H	1.54063352	-5.82959976	7.22286215
H	1.01241160	-6.96262465	8.50654619
H	1.58848251	-5.35561266	10.24903786
H	-0.01498827	-1.99441798	9.95107808
H	4.59012626	-2.42371860	6.94143254
H	-1.84829043	-2.29905737	2.05436501

System: **I1** (doublet)
Charge, Multiplicity: –3, 2
Gibbs free energy: –6187.770695 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.69620105
S	3.13226185	0.00000000	0.67398228
S	1.43868267	2.43410734	2.78522198
Ni	1.34250833	0.32561239	1.90481584
Fe	1.94878496	0.99261327	4.54035919
C	1.43502252	2.04475271	5.97974436
C	3.68922069	1.56249495	4.64015669
N	1.10249040	2.75284862	6.87174903
N	4.82033908	1.94127928	4.70148252
C	2.31541427	-0.46912826	5.66268547
N	2.51378313	-1.38201139	6.40032090
H	3.07476854	1.08544195	-0.14614939
O	8.40402104	4.70288824	7.27114897
C	7.30103882	4.18120656	7.01993886
N	6.95688800	3.72265852	5.78664833
C	7.88546176	3.81736813	4.67139135
C	7.25337126	3.37857156	3.33748512
O	7.02744117	1.99888670	3.24431578
H	8.26016541	4.86805393	4.60009527
H	6.04208016	3.24304988	5.61404715
H	8.78617781	3.18392922	4.85967500
H	6.31410942	3.97251378	3.18059053
H	7.96201497	3.67945071	2.52479902
H	6.18327285	1.82947969	3.80569328
C	4.23127984	2.52987343	8.18692757
C	3.84144802	3.99390102	8.40612674
H	3.95247804	2.23839062	7.15550053
H	3.70853596	1.83460262	8.87222143
H	2.87147833	4.22261799	7.91843073
H	3.74980416	4.22132410	9.50829238
C	6.20822093	4.01998184	8.10929580
C	5.76888203	2.53409185	8.36175984
H	6.07039244	2.23352215	9.38843946
H	6.25836925	1.83373775	7.65531631
H	6.69593013	4.43002775	9.03376249
N	4.94960052	4.70003821	7.76230429
H	4.97770968	5.70804806	7.94405364
N	4.34166613	-2.77808420	8.01178057
C	4.36998349	-3.80108683	8.89714950
H	3.47129522	-2.33470231	7.58816879
O	5.40261315	-4.36742865	9.28193752
C	5.57290571	-2.24110334	7.46271525
H	6.16545613	-3.02429253	6.93683522

H	6.22342099	-1.82255823	8.26236223
H	1.33008639	4.83550730	10.75359493
C	0.64851340	4.20198079	10.18603301
C	-0.43058897	4.93187339	9.37762502
C	0.19961368	5.86743690	8.33181413
C	-1.36590145	3.91769149	8.69145140
H	0.17752925	3.50564934	10.91725704
H	1.25208588	3.57394698	9.49597094
H	-0.57561322	6.45346650	7.78971370
H	0.74768981	5.25238831	7.58443745
H	0.91245762	6.58510457	8.79621270
H	-2.17320590	4.43679956	8.12789606
H	-1.84796889	3.24521379	9.43622155
H	-0.77574197	3.29981110	7.97482002
H	-1.04005713	5.52352768	10.09705648
C	-2.17582314	1.71315512	-0.43694828
H	-2.83246477	0.84410810	-0.40228840
C	-0.97751564	1.48209821	0.47344990
C	-1.32454265	-2.54734411	3.54771716
H	-2.27458448	-1.99462150	3.71786389
C	-0.12734447	-1.78623918	4.16363989
H	6.87371726	0.50989750	0.62599502
C	5.84879706	0.67736621	0.22678381
H	5.83370631	1.72453369	-0.07478265
C	4.82299741	0.36922808	1.32219769
H	2.45638883	4.40720762	0.19271501
C	2.38822478	4.69317125	1.26279088
C	2.81329658	3.53784774	2.22525369
H	-2.76586021	2.61396973	-0.13560026
H	3.03640429	5.54264839	1.47888761
H	-0.18354800	-1.80022003	5.27304383
H	0.83090990	-2.27812988	3.90282487
H	5.08998271	-0.55179780	1.87952830
H	4.76822956	1.17260005	2.08265101
H	-0.31206373	2.37110524	0.48339103
H	-1.31272696	1.35285869	1.52514085
H	5.70625681	0.03584166	-0.67048426
H	-1.86177170	1.84762026	-1.49740842
H	1.34049452	5.00180941	1.46947119
H	3.60301387	2.91021812	1.76201171
H	3.26387912	3.95031122	3.15183274
H	-1.40436050	-3.53075028	4.04746622
C	1.86417408	-2.31545833	10.28110425
O	2.66161410	-2.18985845	11.21129128
N	1.91722712	-3.30717972	9.34663544
C	2.98480733	-4.31295081	9.36229726
C	2.44685080	-5.42460199	8.41299119
C	0.93465678	-5.14379034	8.30706025
C	0.89421399	-3.60226522	8.33568820
H	1.17718548	-3.14463993	7.35634944
H	-0.08567267	-3.17853014	8.63733180
H	0.47588489	-5.56708205	7.38914432
H	0.39574121	-5.55664933	9.19018026
H	2.91325416	-5.30242248	7.41271396
H	2.69653045	-6.44105562	8.77960378

H	3.13954549	-4.67430167	10.40196063
H	5.30266036	-1.43746275	6.74934558
H	-1.20337102	-2.67536730	2.45167244
H	0.99006958	-1.62338764	10.11172677

System: **Ni-C** (doublet)
Charge, Multiplicity: –3, 2
Gibbs free energy: –6187.797298 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.38521194
S	3.09965515	0.00000000	0.16125600
S	1.53994372	2.39706543	2.51793986
Ni	1.50569015	0.16236140	1.70170462
Fe	2.03723915	0.79543733	4.12693012
C	1.57923117	1.87970229	5.61922674
C	3.80781053	1.30209186	4.28554453
N	1.31487207	2.58629518	6.52942809
N	4.94743657	1.61862226	4.39805972
H	2.62599192	-0.14860004	2.86141124
C	2.30644902	-0.66224230	5.30679210
N	2.42588048	-1.54791600	6.08683225
C	1.68208511	-2.30723749	10.06904413
O	8.79986921	4.03385902	6.88688899
C	7.64800000	3.63220849	6.63497014
N	7.25627183	3.21142251	5.40407209
C	8.19374720	3.18653680	4.29233030
C	7.55313815	2.64634140	3.00119995
O	7.24096959	1.28156972	3.06155913
H	8.59853710	4.21588323	4.12313982
H	6.29752264	2.82612043	5.23830886
H	9.07409009	2.55147045	4.55187272
H	6.65450212	3.27193419	2.75986136
H	8.28838532	2.80975747	2.17392910
H	6.35960134	1.23762299	3.56870766
C	4.44761677	2.27490427	7.84775591
C	4.18837616	3.77331256	8.02969096
H	4.13412347	1.98129525	6.82735993
H	3.87510066	1.64740026	8.55828541
H	3.24099325	4.07744168	7.53896762
H	4.11935797	4.03590220	9.12571401
C	6.54617273	3.58626541	7.72633873
C	5.98229612	2.14818848	8.00469345
H	6.27162843	1.83306467	9.03033467
H	6.39818955	1.40114178	7.29907168
H	7.06704306	3.96946969	8.64410907
N	5.35014808	4.36379342	7.36622258
H	5.46610109	5.37017323	7.51990323
N	4.12358865	-3.03357736	7.80028124
C	4.06671607	-4.02802818	8.71717392
H	3.29333083	-2.54082588	7.36411459
O	5.05023431	-4.66833153	9.11499151
C	5.39358836	-2.62629046	7.22674701
H	5.91788053	-3.48149736	6.74347579
H	6.07693587	-2.22141134	8.00551392

H	1.76355080	4.87628426	10.35650717
C	1.02998787	4.28783746	9.80562427
C	0.01186880	5.08263411	8.98014241
C	0.71299450	5.93341394	7.90766346
C	-1.00668961	4.13046099	8.32432676
H	0.50542597	3.65202428	10.55515235
H	1.57806118	3.59285757	9.13384667
H	-0.01260730	6.56513956	7.34891843
H	1.20842089	5.25797302	7.17652766
H	1.48418008	6.60261452	8.35009780
H	-1.76661263	4.69757488	7.74177080
H	-1.54454956	3.52661329	9.08925735
H	-0.47427215	3.43835731	7.63118904
H	-0.54295660	5.74291281	9.68471914
C	-2.02416056	1.77624716	-0.74831901
H	-2.75106764	0.96608991	-0.69068665
C	-0.90899262	1.56712211	0.27376636
C	-1.51893189	-2.43890444	3.34236942
H	-2.39324694	-1.79824853	3.59390493
C	-0.21024510	-1.78231676	3.83681181
H	6.86698448	-0.15677610	0.40087996
C	5.88656339	0.09096338	-0.06676781
H	5.96005503	1.12845071	-0.39315071
C	4.75719470	-0.12398288	0.95228430
H	2.87246897	4.02555844	-0.16541380
C	2.77757136	4.40697514	0.87137339
C	3.03847681	3.29169449	1.92804017
H	-2.56336812	2.73974101	-0.58119434
H	3.49481455	5.20452763	1.06512956
H	-0.14203308	-1.81517087	4.94465118
H	0.68228043	-2.32094746	3.46017003
H	4.85930396	-1.12322917	1.42847381
H	4.84271768	0.61060516	1.77846784
H	-0.18101989	2.40379000	0.23541706
H	-1.31565679	1.56632036	1.30848438
H	5.75015374	-0.54783747	-0.96864797
H	-1.62072523	1.78612852	-1.78595725
H	1.75838375	4.83592411	0.99181602
H	3.74521730	2.53335237	1.53894487
H	3.50235489	3.71892328	2.84103464
H	-1.65625159	-3.38463650	3.82364787
O	2.48176066	-2.22623271	11.00176816
N	1.66504201	-3.31522769	9.15017395
C	2.64465446	-4.40645815	9.19797875
C	2.01302585	-5.49896101	8.28407097
C	0.52999498	-5.09370710	8.16432886
C	0.62104117	-3.55422988	8.14598500
H	0.94185874	-3.15553220	7.15315321
H	-0.31910823	-3.03889465	8.43099670
H	0.03782820	-5.50489712	7.25837690
H	-0.04296070	-5.43108289	9.05785062
H	2.48844450	-5.45148431	7.28173397
H	2.17431108	-6.52008760	8.68521952
H	2.77015237	-4.74533396	10.24892926
H	-1.51151332	-2.56194523	2.23914616

H	5.18903942	-1.84115325	6.47260909
H	0.86336860	-1.55410777	9.88301511

System: **Ni-R** (singlet)
Charge, Multiplicity: –3, 1
Gibbs free energy: –6188.365674 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.41566938
S	3.04517514	0.00000000	0.26023727
S	1.44294531	2.55993023	2.56994720
Ni	1.46042441	0.12698622	1.75699071
Fe	2.00158329	0.83106069	4.15872101
C	1.57245857	1.92318143	5.64291949
C	3.76089414	1.37903425	4.25007510
N	1.31143069	2.62547792	6.55920707
N	4.89992443	1.72251331	4.31280920
H	2.58269995	-0.13571948	2.91222230
C	2.31741344	-0.59920368	5.33702750
N	2.48374120	-1.48330672	6.11503145
H	3.08575271	1.29661663	-0.18081341
O	8.71559752	4.31115829	6.79425315
C	7.57307671	3.86491699	6.57620637
N	7.17697855	3.39535831	5.36256094
C	8.09499071	3.39227238	4.23381717
C	7.42440613	2.94001010	2.92360039
O	7.11974453	1.57258257	2.88739228
H	8.52907207	4.41585151	4.11710219
H	6.22620173	2.98613581	5.21472429
H	8.95968532	2.71604641	4.43999888
H	6.51799571	3.57833040	2.75167662
H	8.14050764	3.16906107	2.09412141
H	6.26190411	1.48112368	3.44593857
C	4.47091745	2.39191515	7.79786240
C	4.12069843	3.87135209	7.97170638
H	4.21515990	2.08464807	6.76477515
H	3.90679302	1.72877538	8.48188648
H	3.16558736	4.11464746	7.46219140
H	4.01667819	4.12991248	9.06547496
C	6.49504506	3.81182862	7.69003398
C	6.00050522	2.35941380	8.02274827
H	6.25428739	2.12107638	9.07854458
H	6.49373628	1.59854067	7.38473757
H	7.02068109	4.24481979	8.58224248
N	5.26105865	4.52714760	7.32995669
H	5.32085578	5.53770181	7.48530701
N	4.25803791	-2.90263369	7.77205480
C	4.24440599	-3.90050428	8.68621844
H	3.40644936	-2.43132096	7.33944012
O	5.25042724	-4.51139874	9.07396030
C	5.50821185	-2.45130579	7.18950908
H	6.05591732	-3.28538086	6.69426074
H	6.18700363	-2.03029575	7.96404951
H	1.68994827	4.92926548	10.35494166
C	0.96931891	4.31944056	9.81044356

C	-0.07711502	5.08641239	8.99442662
C	0.59332600	5.96218867	7.92232678
C	-1.06631072	4.10462026	8.33733707
H	0.46947605	3.66813776	10.56365301
H	1.53051366	3.64155312	9.13175954
H	-0.15350776	6.57288706	7.36813038
H	1.10622838	5.30416313	7.18710920
H	1.34504991	6.65374805	8.36436944
H	-1.84530445	4.64879347	7.75808133
H	-1.58247636	3.48078880	9.10132316
H	-0.51170375	3.43229919	7.64114085
H	-0.64799889	5.72639407	9.70604862
C	-2.10927989	1.72254498	-0.71562765
H	-2.81089534	0.89088608	-0.65169093
C	-0.96498667	1.53741058	0.28436450
C	-1.43800938	-2.47759469	3.36662839
H	-2.37889835	-1.89479523	3.47647024
C	-0.24460133	-1.73442477	3.99914200
H	6.84702809	0.07216991	0.34793588
C	5.85490554	0.27614206	-0.11130417
H	5.89384339	1.31541923	-0.43762033
C	4.76342550	0.03599073	0.93977478
H	2.69849482	4.16565983	-0.19828661
C	2.62632460	4.49596951	0.86006059
C	2.93815816	3.35060765	1.87040514
H	-2.67157899	2.66812628	-0.52461411
H	3.32111834	5.31458114	1.04764262
H	-0.36149165	-1.66417473	5.10240420
H	0.70642756	-2.27510869	3.82807254
H	4.86712812	-0.96098089	1.41534836
H	4.81304707	0.77167865	1.76651672
H	-0.26695860	2.40037536	0.26764490
H	-1.35661831	1.49912163	1.32357144
H	5.72576377	-0.37487861	-1.00390851
H	-1.73051177	1.75710768	-1.76268658
H	1.59832827	4.88630635	1.02490061
H	3.57802651	2.58032611	1.38051650
H	3.54648649	3.73256501	2.71709183
H	-1.56450513	-3.44237497	3.89230637
C	1.83205424	-2.25567392	10.06691709
O	2.64295404	-2.15260924	10.98832668
N	1.82637717	-3.26649023	9.15177995
C	2.84001713	-4.32630140	9.18051963
C	2.23241965	-5.43117283	8.26542126
C	0.73624714	-5.07209528	8.16640467
C	0.77918086	-3.53025868	8.15672042
H	1.07758977	-3.11239993	7.16391756
H	-0.17334026	-3.04672574	8.45616312
H	0.24613234	-5.49242157	7.26342434
H	0.18517542	-5.43365649	9.06446112
H	2.69365796	-5.35949240	7.25790575
H	2.43119082	-6.45001978	8.65584847
H	2.98864390	-4.66931430	10.22722220
H	0.99273522	-1.52339107	9.89072285
H	5.26969153	-1.66736258	6.44373650

H	-1.27562509	-2.64886737	2.28186228

System: **I2a** (singlet)
Charge, Multiplicity: –3, 1
Gibbs free energy: –6188.37415 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.40960956
S	3.22914328	0.00000000	0.17106986
S	1.97252611	2.00616452	2.67170678
Ni	1.56861409	-0.07493423	1.71955556
Fe	2.06843569	0.51002567	4.41041684
C	1.67093822	1.62915356	5.82852838
C	3.87740462	0.71727813	4.67851842
N	1.44048116	2.37789582	6.71812275
N	5.04881081	0.84737033	4.84032009
C	2.04116987	-1.00670007	5.52593344
N	1.99197886	-1.95004694	6.24757060
H	2.34376565	-1.24656647	2.63417719
H	1.93036297	-1.65766788	1.99892184
O	8.99817792	2.70209912	7.60087900
C	7.82626158	2.44365282	7.26865273
N	7.46009484	2.12599702	5.99915798
C	8.44266769	2.04233235	4.93037657
C	7.80528165	1.66206583	3.58079816
O	7.33180624	0.34307158	3.53527881
H	8.98096219	3.01907244	4.84285660
H	6.47532349	1.85581484	5.76995759
H	9.22229554	1.28541940	5.18612045
H	7.00002055	2.40571066	3.34487466
H	8.59357676	1.78484913	2.79687751
H	6.43450849	0.36919891	4.01360862
C	4.38732029	1.48223209	8.28142279
C	4.34746556	2.99423564	8.52875782
H	4.04153933	1.28055878	7.24922584
H	3.72311167	0.91685316	8.96419253
H	3.47432914	3.45845772	8.02525885
H	4.27931201	3.21587634	9.63403453
C	6.65979172	2.47588827	8.29384963
C	5.88566309	1.11854331	8.43531112
H	6.11009498	0.66807024	9.42577018
H	6.19628007	0.38851383	7.66117973
H	7.16619025	2.72230061	9.26564425
N	5.60525851	3.43477553	7.92849280
H	5.86012582	4.40593216	8.13408307
N	3.41511854	-3.74583393	7.90883239
C	3.18284342	-4.77044950	8.76247322
H	2.67737169	-3.12312108	7.47144567
O	4.05216404	-5.55232409	9.17194487
C	4.75582748	-3.47218799	7.42431039
H	5.19411417	-4.35633408	6.90841064
H	5.44115381	-3.20806270	8.25975298
H	1.95840930	4.27166698	10.76809987
C	1.18564448	3.81112548	10.15266109
C	0.32574978	4.77230493	9.32338124

C	1.18794055	5.57622340	8.33524942
C	-0.76969145	3.99671937	8.56665697
H	0.54351941	3.21500292	10.84075289
H	1.67648153	3.08366326	9.47120249
H	0.58100080	6.32831019	7.78394910
H	1.62545844	4.87864393	7.58772656
H	2.01589420	6.11209329	8.85074875
H	-1.42314921	4.68914655	7.99038029
H	-1.41598831	3.42276597	9.26806400
H	-0.29323616	3.28712948	7.85091787
H	-0.17787164	5.46411503	10.03556691
C	-1.58928202	2.22315108	-0.65657141
H	-2.41844163	1.51453556	-0.67422798
C	-0.52378662	1.72886132	0.32501328
C	-1.85394369	-2.20977183	3.22305151
H	-2.66755958	-1.47078622	3.39277881
C	-0.53016497	-1.71925983	3.85619532
H	6.84181840	-0.88875974	0.91752680
C	5.98845348	-0.51485570	0.30960260
H	6.21322254	0.51778022	0.04390285
C	4.68944073	-0.57997477	1.13101788
H	3.45982515	3.85843855	0.25422016
C	3.41399851	4.12221368	1.33042269
C	3.55529042	2.85815083	2.23695808
H	-1.97991986	3.23124755	-0.37953200
H	4.21726991	4.80839546	1.60074111
H	-0.59636184	-1.71275103	4.96439172
H	0.30766868	-2.40185498	3.60894268
H	4.50280232	-1.62443154	1.46768154
H	4.80206219	0.01984636	2.05922669
H	0.37428237	2.38089996	0.29565565
H	-0.90407720	1.78675619	1.36815487
H	5.91136026	-1.10753713	-0.62935654
H	-1.18831122	2.28012721	-1.69379443
H	2.44861782	4.63990552	1.52195479
H	4.21269434	2.10902052	1.75059456
H	4.01410478	3.11803310	3.21298997
H	-2.16453088	-3.16461288	3.68645151
C	0.98045651	-2.81911441	10.09238806
O	1.74116490	-2.88755063	11.05810268
N	0.87197011	-3.77366966	9.12421129
C	1.69989474	-4.98465837	9.15160117
C	0.98508551	-5.93326264	8.14399812
C	-0.42711022	-5.33551533	7.98606343
C	-0.14373238	-3.82185813	8.06514081
H	0.27267992	-3.41222421	7.11303143
H	-1.02528663	-3.20797211	8.34232887
H	-0.92127936	-5.62989109	7.03672993
H	-1.08169243	-5.64590853	8.83205898
H	1.51348575	-5.88897374	7.16838187
H	0.99710450	-6.98797104	8.48609290
H	1.72368817	-5.39447769	10.18440267
H	4.69446635	-2.62175843	6.71703781
H	-1.74732886	-2.33254358	2.12502616
H	0.27699437	-1.95584491	9.91314345

MODEL 6: INORGANIC LIGAND REPLACEMENT: CO REPLACES $[CN]^-$

System: **Ni-SI$_a$** (singlet)
Charge, Multiplicity: –1, 1
Gibbs free energy: –6228.30423 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.33830463
S	3.12046559	0.00000000	0.23467455
S	1.84576934	2.13407474	2.59403457
Ni	1.49881486	0.18929853	1.64873372
Fe	2.03615019	0.71062281	4.32954121
C	1.43824105	1.42321418	5.81867062
C	3.81994789	1.22704600	4.58330813
O	1.05571451	1.85087916	6.83329239
N	4.93863909	1.55906663	4.72767122
C	2.38443056	-0.86968604	5.01274465
O	2.59795728	-1.90323862	5.51478892
O	8.83483160	3.39075029	7.45092994
C	7.66556804	3.19708703	7.09410496
N	7.29904128	2.99684073	5.79765394
C	8.28200364	2.95466652	4.72382924
C	7.63871468	2.72297919	3.34794361
O	7.16826811	1.40826073	3.14094034
H	8.85824075	3.90986957	4.71891921
H	6.31623406	2.76393771	5.57935894
H	9.02674952	2.14745085	4.91325867
H	6.83313562	3.48932635	3.19463103
H	8.41485567	2.92057957	2.57449887
H	6.37962121	1.29653391	3.73873703
C	4.26967720	2.08702446	8.23623328
C	4.20779545	3.60711686	8.46176914
H	3.83974603	1.84700857	7.24449095
H	3.70344978	1.51954018	9.00192137
H	3.29012632	4.06942997	8.04183085
H	4.22161664	3.83550120	9.56395207
C	6.49750009	3.16315378	8.11137249
C	5.79040094	1.77139159	8.23471460
H	6.11750405	1.26146787	9.16305646
H	6.05358190	1.11322684	7.38247368
H	6.97591974	3.42420950	9.08917386
N	5.39387592	4.06854903	7.74996199
H	5.62531804	5.05409068	7.91609743
N	3.70867605	-3.22920612	8.07148665
C	3.53445685	-4.23334533	8.98216564
H	2.89769937	-2.67271032	7.79332584
O	4.46044201	-4.93703479	9.40936189
C	5.00594738	-2.85068977	7.54206172
H	5.75897778	-3.53849795	7.97231025
H	5.26577291	-1.80663112	7.82013284
H	1.74225489	4.78901115	10.61629188
C	0.99358509	4.25224544	10.03392836
C	0.10401411	5.16292034	9.17525475

C	0.94159753	6.06948653	8.25814235
C	-0.90917636	4.34068449	8.35978505
H	0.37975197	3.66033644	10.74708891
H	1.53004137	3.51986353	9.39405860
H	0.30154650	6.76886703	7.67888334
H	1.51393963	5.45968123	7.52562675
H	1.67398564	6.67394736	8.83470659
H	-1.58727546	4.99877343	7.77539190
H	-1.53856867	3.70456544	9.01822387
H	-0.38855699	3.66909547	7.64606352
H	-0.47917898	5.80469192	9.87111663
C	-1.83434383	2.00684727	-0.64183313
H	-2.61259170	1.24415621	-0.61690513
C	-0.72589119	1.65861085	0.34367137
C	-1.74375183	-2.25776677	3.42760718
H	-2.48265656	-1.50724932	3.78112751
C	-0.31132987	-1.79000321	3.74789434
H	6.81957772	-0.47471226	0.89152514
C	5.92429509	-0.18224813	0.30404017
H	6.07525986	0.85042321	-0.01054241
C	4.67186662	-0.28174612	1.19715327
H	3.14939583	3.95950177	0.12494107
C	3.06319529	4.31631084	1.16914013
C	3.31694884	3.17845366	2.19730158
H	-2.29334713	2.98903441	-0.39369998
H	3.82235632	5.06561237	1.39464759
H	-0.10970665	-1.86770413	4.83581756
H	0.45564995	-2.39850920	3.22792575
H	4.60199948	-1.28163781	1.67179670
H	4.73017647	0.45287959	2.03008971
H	0.08802875	2.40983929	0.29428813
H	-1.10857157	1.67077821	1.38508839
H	5.84521420	-0.83109915	-0.59294738
H	-1.45037286	2.06020088	-1.68274821
H	2.06515364	4.77975859	1.31172426
H	4.14979065	2.51381072	1.89699905
H	3.59954828	3.59498742	3.18596845
H	-1.98308354	-3.20909567	3.93851703
C	1.23079537	-2.24427519	10.07361115
O	2.03351161	-2.14200404	10.99287421
N	1.19267887	-3.29806540	9.19385593
C	2.06579806	-4.47119545	9.38433571
C	1.40593129	-5.56152626	8.49272229
C	-0.04079244	-5.06817752	8.29589108
C	0.13562733	-3.54425399	8.20576055
H	0.46360668	-3.24152556	7.18270504
H	-0.77756326	-2.96485329	8.45257193
H	-0.53219793	-5.50095127	7.40087013
H	-0.66095720	-5.31778725	9.18403467
H	1.92658095	-5.59838565	7.51208588
H	1.48198870	-6.56785904	8.94734732
H	2.08545700	-4.74743895	10.45966140
H	0.43382615	-1.47609685	9.84896550
H	5.02254108	-2.92643497	6.43467362
H	-1.89025935	-2.37679865	2.33504577

System: **I1** (doublet)
Charge, Multiplicity: –1, 2
Gibbs free energy: –6228.899198 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.48206903
S	3.07953097	0.00000000	0.39381841
S	1.28016409	2.51969988	2.44255547
Ni	1.33445958	0.36344193	1.74985044
Fe	1.94706902	1.03569680	4.09885981
C	1.55517475	1.75706150	5.65247750
C	3.67876792	1.74809464	4.01184420
O	1.32274727	2.15283835	6.72688837
N	4.76732585	2.19168482	3.99136994
C	2.64461543	-0.41831409	4.76188914
O	3.12263906	-1.36231596	5.26607647
H	2.94945564	1.08013111	-0.41064114
O	8.64397026	4.18637505	6.29663158
C	7.45837668	4.50004132	6.14258473
N	6.86519256	4.79850529	4.95414335
C	7.56491587	4.88309540	3.68766631
C	6.86728158	4.15684996	2.51843565
O	6.95274391	2.75780240	2.56682807
H	7.70626580	5.95610709	3.40026520
H	5.86912778	5.05226820	5.05311472
H	8.57308096	4.44605815	3.84801914
H	5.80221322	4.51101593	2.46501660
H	7.35998966	4.50553383	1.57888416
H	6.23787742	2.46076337	3.20717343
C	5.12105208	2.65106467	7.31472329
C	4.20691431	3.87697369	7.12816924
H	5.41928947	2.26343505	6.31863660
H	4.61354605	1.82990468	7.85997036
H	3.55868809	3.76521340	6.23386185
H	3.53806086	4.00987967	8.00975611
C	6.50214942	4.60624181	7.36075024
C	6.33845804	3.23255626	8.05257969
H	6.11395629	3.37759907	9.13248999
H	7.26034306	2.62358607	7.96908961
H	6.98446530	5.34743718	8.03530358
N	5.13914462	5.02691678	6.97496069
H	4.82622932	5.84486483	7.50366370
N	4.71529142	-2.41947818	7.73077599
C	4.79240168	-3.38819983	8.69142131
H	3.80134564	-2.02074229	7.50350651
O	5.85529658	-3.91126005	9.05602374
C	5.87758348	-1.86375039	7.06206848
H	6.77204442	-2.39272604	7.44337933
H	5.97982707	-0.77691751	7.26928183
H	1.67976327	5.29952587	10.14018215
C	0.98193448	4.61791751	9.65481014
C	-0.11018170	5.33107041	8.84615524
C	0.50665352	6.31118913	7.83405965
C	-1.03190390	4.31915993	8.14330889

H	0.54105204	3.97016538	10.44283554
H	1.57549277	3.95286587	8.98977694
H	-0.27332762	6.84672561	7.25177720
H	1.14845265	5.76363456	7.10937179
H	1.14056962	7.07376559	8.33584740
H	-1.85279528	4.83143294	7.59744133
H	-1.49394968	3.61865361	8.87141497
H	-0.46255311	3.71034057	7.41079349
H	-0.73537600	5.90264447	9.56788672
C	-2.34416407	1.38417669	-0.61783946
H	-2.98038088	0.50848274	-0.49159640
C	-1.17346665	1.36858059	0.34887214
C	-1.19858980	-2.58810902	3.58463007
H	-2.13171281	-2.03153194	3.81521467
C	0.03986492	-1.78074690	4.00761141
H	6.78243520	0.37584733	-0.02079422
C	5.72351805	0.52996486	-0.31951060
H	5.67145131	1.55432733	-0.68769015
C	4.82030043	0.31574881	0.89633234
H	2.35822922	4.11139647	-0.37572898
C	2.24137656	4.54650176	0.63604121
C	2.65093893	3.55698718	1.76618490
H	-2.97859649	2.28511760	-0.45569506
H	2.88221092	5.41947579	0.76175728
H	0.13313870	-1.75056019	5.11401999
H	0.97039400	-2.23477003	3.61473080
H	5.09371350	-0.59930460	1.46049862
H	4.87555717	1.15875324	1.61298437
H	-0.60658707	2.31955504	0.29658026
H	-1.52017625	1.27451466	1.39886376
H	5.49120646	-0.17295142	-1.14644487
H	-1.99860987	1.40366325	-1.67383367
H	1.18891087	4.88026383	0.75239555
H	3.46843599	2.88290324	1.44472073
H	3.05132369	4.10890567	2.64018997
H	-1.23240604	-3.53733028	4.15130526
C	2.28943930	-1.75011361	9.92835090
O	3.13580224	-1.47702695	10.77073285
N	2.35462374	-2.83623605	9.09095888
C	3.42422990	-3.83981344	9.24063027
C	2.87920658	-5.06870699	8.45763309
C	1.35938925	-4.82522366	8.37526857
C	1.27524987	-3.29932354	8.21051529
H	1.46435434	-3.00125830	7.15182128
H	0.30282445	-2.86131503	8.51551239
H	0.87267640	-5.37772506	7.54592842
H	0.86548553	-5.12392476	9.32535702
H	3.31384392	-5.07456916	7.43531817
H	3.15797892	-6.02382661	8.94279663
H	3.58438618	-4.05189859	10.31877476
H	5.80513642	-1.99657397	5.96233009
H	-1.19255837	-2.79887789	2.49635906
H	1.36153273	-1.13200452	9.74876663

System: **Ni-C** (doublet)
Charge, Multiplicity: –1, 2
Gibbs free energy: –6228.89908 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.30893040
S	3.04285406	0.00000000	0.10956840
S	1.49829374	2.43056411	2.39770188
Ni	1.50017994	0.22579018	1.62688190
Fe	2.04821857	0.81629396	4.02602837
C	1.57629242	1.89437551	5.34159008
C	3.84054729	1.39467710	4.12565827
O	1.32874756	2.62031224	6.21258172
N	4.95609038	1.74471399	4.22113806
H	2.63803852	-0.08930845	2.75287830
C	2.39814150	-0.55918570	5.03765243
O	2.61717560	-1.47004567	5.73232061
C	1.82371690	-1.95053162	9.96994139
O	8.93627331	3.55879218	6.64590200
C	7.74582294	3.71745325	6.36035481
N	7.26077178	3.91999507	5.09995871
C	8.08299876	3.92459093	3.90410784
C	7.44417574	3.16699743	2.72432949
O	7.33808676	1.78090980	2.92012771
H	8.29917745	4.97371406	3.57824356
H	6.23770903	4.00648310	5.03315323
H	9.05401785	3.46010524	4.17590481
H	6.44832025	3.63381023	2.49605579
H	8.08436061	3.34707608	1.82861320
H	6.53661232	1.65015187	3.50105795
C	4.48911873	2.44098003	7.68353052
C	4.33569995	3.96122204	7.87094109
H	3.99417511	2.13179596	6.74304119
H	4.03104730	1.86941924	8.51574901
H	3.37740801	4.35106996	7.46894592
H	4.37190165	4.22276020	8.96300541
C	6.63537674	3.65121481	7.43170210
C	6.02141763	2.21778857	7.55685506
H	6.45562746	1.68887203	8.42814863
H	6.24719137	1.62142038	6.65027065
H	7.13497588	3.92791424	8.39405046
N	5.46959106	4.49134904	7.11517495
H	5.64773514	5.48743831	7.28764889
N	4.22047082	-2.85501823	7.84435140
C	4.16010826	-3.83743526	8.78974842
H	3.36562774	-2.34413246	7.61505083
O	5.14778999	-4.47128942	9.18842461
C	5.45880283	-2.40851039	7.23390491
H	6.26922219	-3.07757937	7.58174100
H	5.70290586	-1.36413820	7.52614161
H	1.95331534	5.13565360	10.16294273
C	1.20387022	4.53377488	9.64915412
C	0.17868778	5.31674984	8.81860631
C	0.85820999	6.15561503	7.72428581
C	-0.87967692	4.37335175	8.21741851

H	0.69062839	3.93127918	10.43083956
H	1.74628955	3.80983186	9.00422671
H	0.12286627	6.77296664	7.16548459
H	1.36355914	5.49345699	6.98837780
H	1.62580235	6.83774529	8.14804216
H	-1.64436194	4.94049228	7.64477007
H	-1.40682729	3.80026575	9.01014090
H	-0.41405275	3.64366888	7.52434907
H	-0.36163386	5.99524518	9.51150445
C	-2.09899386	1.67475050	-0.74001954
H	-2.82985612	0.87258001	-0.63796611
C	-0.96060177	1.54197106	0.26339983
C	-1.53182490	-2.39732952	3.48518062
H	-2.34610134	-1.71561412	3.81172891
C	-0.15696698	-1.78160712	3.80583505
H	6.79532805	-0.29283525	0.28516950
C	5.81328666	-0.04442719	-0.17199717
H	5.88667042	0.98035023	-0.53630404
C	4.70607238	-0.18840660	0.88271827
H	2.86117143	3.86501817	-0.32073997
C	2.75482683	4.32483848	0.68048297
C	3.01107025	3.30150511	1.81731001
H	-2.63315411	2.64028154	-0.59706906
H	3.48135999	5.12356381	0.83030192
H	0.02733978	-1.79949420	4.90021785
H	0.67182597	-2.33713718	3.32243445
H	4.75358343	-1.18205913	1.37554297
H	4.83909398	0.56672197	1.68546748
H	-0.26163034	2.39671279	0.16911651
H	-1.34196009	1.55745997	1.30572471
H	5.64754088	-0.71813038	-1.03921423
H	-1.71959379	1.65239800	-1.78412788
H	1.74332092	4.77685603	0.75687808
H	3.75399017	2.53880351	1.52059586
H	3.41290491	3.80534562	2.71952613
H	-1.66486026	-3.32447656	4.00254453
O	2.68320740	-1.77027538	10.82376584
N	1.78321036	-3.03334983	9.12771156
C	2.73488286	-4.14913539	9.28457500
C	2.08945706	-5.29364863	8.45445476
C	0.60531326	-4.89588642	8.35227390
C	0.67572924	-3.36660686	8.22370645
H	0.90931996	-3.06355780	7.17581210
H	-0.25331500	-2.84232808	8.52831748
H	0.08080700	-5.37763025	7.50207538
H	0.06605310	-5.16588266	9.28616645
H	2.54377951	-5.31266519	7.44086753
H	2.26137719	-6.28539732	8.91493218
H	2.83598048	-4.40208286	10.36110119
H	-1.65191561	-2.55552575	2.39439972
H	5.39242119	-2.44814855	6.12645777
H	0.96784557	-1.23723998	9.78229757

System: **Ni-R** (singlet)
Charge, Multiplicity: –1, 1
Gibbs free energy: –6229.48873 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.28625331
S	3.04511438	0.00000000	0.14647717
S	1.43756495	2.57143989	2.44156351
Ni	1.46259591	0.17284314	1.66707114
Fe	1.99920944	0.88329854	4.02959806
C	1.54635861	2.08470901	5.23549162
C	3.80503324	1.42599617	4.07757511
O	1.31773119	2.89721556	6.03379949
N	4.93174620	1.74987388	4.14383115
H	2.56939377	-0.12204060	2.79973742
C	2.31259411	-0.39750296	5.16844443
O	2.50702641	-1.21948160	5.97735455
H	3.05291021	1.27048217	-0.34023739
O	8.85291240	3.86269147	6.67371120
C	7.65157693	3.92134343	6.39655494
N	7.14317548	4.05096774	5.13503703
C	7.95248951	4.12959437	3.93284124
C	7.30355937	3.44202797	2.71582931
O	7.24726968	2.04104903	2.79617561
H	8.15925714	5.19752648	3.66617886
H	6.11685499	4.09820331	5.07749829
H	8.93212454	3.65896020	4.16033029
H	6.28687537	3.89233112	2.55386301
H	7.91067194	3.71642868	1.82083319
H	6.47183316	1.83075180	3.39506527
C	4.44388116	2.48655591	7.62902447
C	4.22762246	3.98558843	7.89144618
H	4.01007637	2.21927472	6.64602333
H	3.96693325	1.84861671	8.40003628
H	3.26037329	4.35783488	7.49501278
H	4.24301600	4.19498828	8.99537515
C	6.54818189	3.78802395	7.47303566
C	5.98808104	2.32770039	7.57251799
H	6.39880216	1.82205379	8.46897245
H	6.28207908	1.73414933	6.68373339
H	7.04148361	4.06645004	8.43763462
N	5.34932553	4.58976444	7.17430551
H	5.48269136	5.58629364	7.38022380
N	4.38256475	-2.82068541	7.72314456
C	4.36568461	-3.82132235	8.65186533
H	3.51138192	-2.32641171	7.51656470
O	5.37795507	-4.42586383	9.03307446
C	5.60231672	-2.30542845	7.13021581
H	6.43628520	-2.96573109	7.43714731
H	5.81747929	-1.27028068	7.47431145
H	1.82029242	5.02518914	10.24377098
C	1.09319170	4.40745813	9.71710544
C	0.04146633	5.17562131	8.90589476
C	0.69157431	6.07704869	7.84358292
C	-0.97230495	4.20804664	8.26758352

H	0.60265155	3.76753253	10.48339331
H	1.66173183	3.72109003	9.05383250
H	-0.06652491	6.68260596	7.30254082
H	1.22465601	5.46128159	7.08798337
H	1.42831598	6.77556687	8.29487103
H	-1.75639377	4.75939094	7.70593145
H	-1.47953748	3.58825213	9.03790840
H	-0.46998741	3.52270645	7.55464081
H	-0.52775965	5.81056773	9.61758978
C	-2.12847506	1.67206260	-0.73071700
H	-2.82775907	0.84026772	-0.64636579
C	-0.97625011	1.53797976	0.26155709
C	-1.39314600	-2.47469578	3.39482382
H	-2.31220689	-1.87569652	3.56641716
C	-0.15080475	-1.73664664	3.91742668
H	6.83657607	0.04344435	0.23881996
C	5.84572424	0.24511650	-0.21993915
H	5.87844708	1.28020992	-0.55992467
C	4.75931130	0.03623698	0.84036044
H	2.70767174	4.09398718	-0.29528361
C	2.62425862	4.47223171	0.74288084
C	2.94936007	3.38642385	1.80493816
H	-2.69032234	2.61535200	-0.55115582
H	3.32017956	5.29424299	0.91029644
H	-0.18525515	-1.64647105	5.02441820
H	0.78422743	-2.27019691	3.65701529
H	4.84289215	-0.95679343	1.32801495
H	4.82214773	0.78936798	1.65049328
H	-0.28587949	2.40311006	0.19252084
H	-1.35480559	1.53068048	1.30465155
H	5.71361947	-0.42323526	-1.09595932
H	-1.75964769	1.69353185	-1.77900558
H	1.59874473	4.87498076	0.88090102
H	3.63537500	2.61753121	1.39422783
H	3.47984942	3.82953531	2.67111914
H	-1.51067930	-3.43288829	3.93446962
C	1.98072902	-2.03868545	9.85983662
O	2.84636248	-1.83839293	10.70361290
N	1.96081644	-3.11740874	9.01286117
C	2.95438342	-4.19908006	9.14126824
C	2.35161114	-5.34498092	8.28185858
C	0.85238176	-5.00465241	8.19621548
C	0.85952664	-3.47103362	8.10873384
H	1.06962179	-3.12747540	7.06908545
H	-0.08734831	-2.99445440	8.43607601
H	0.34358286	-5.48383143	7.33505967
H	0.32946127	-5.32295143	9.12425450
H	2.80161052	-5.31626882	7.26653786
H	2.56586265	-6.34169112	8.71311957
H	3.06748804	-4.47678619	10.21058938
H	1.10239842	-1.34979354	9.68738924
H	5.52802074	-2.28842915	6.02258746
H	-1.31590638	-2.66692888	2.30555452

System: **I2a** (singlet)
Charge, Multiplicity: –1, 1
Gibbs free energy: –6229.474072 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.34599052
S	3.13418772	0.00000000	0.05703517
S	1.92829001	2.02088538	2.43583220
Ni	1.56687517	-0.05534983	1.66455904
Fe	2.11296364	0.53945273	4.12474110
C	1.78445715	1.53265753	5.51843264
C	3.97565923	0.78963167	4.23117161
O	1.60429098	2.19155712	6.46164724
N	5.13200121	0.94895631	4.35800243
C	2.29869767	-0.95809748	5.01419860
O	2.42496468	-1.93056915	5.64958691
H	2.27430414	-1.39600774	2.40410551
H	1.82248922	-1.69770863	1.76323519
O	9.26883811	2.28129545	6.97108223
C	8.10724577	2.57905502	6.67797163
N	7.66134133	2.85315373	5.41659015
C	8.49786151	2.80950665	4.23143942
C	7.80284719	2.17104717	3.01319399
O	7.55196259	0.79647559	3.14608937
H	8.83387116	3.83959945	3.94872745
H	6.66084866	3.08188710	5.34626533
H	9.40731868	2.23140521	4.49793115
H	6.86383167	2.74711313	2.79370688
H	8.47274712	2.32324251	2.13399993
H	6.71986763	0.72424460	3.69353679
C	4.70358749	1.65893278	7.82095053
C	4.71123036	3.16809158	8.10876547
H	4.28069220	1.48125252	6.81385663
H	4.09701329	1.09029660	8.55414939
H	3.82263354	3.69007927	7.69639610
H	4.72589155	3.35478431	9.21661885
C	6.98453594	2.62014839	7.73861609
C	6.20415234	1.26385059	7.82553609
H	6.49675947	0.71554704	8.74298371
H	6.43949806	0.61748792	6.95635392
H	7.50497841	2.81271353	8.70944598
N	5.93255085	3.60468201	7.43280593
H	6.21403897	4.56308710	7.66813760
N	3.75718595	-3.55306033	7.84325536
C	3.55776731	-4.55004939	8.75493447
H	2.97757482	-2.93056405	7.62036178
O	4.44992220	-5.31762256	9.14183356
C	5.05224816	-3.24839986	7.26361708
H	5.76247172	-4.03300065	7.58823759
H	5.42806015	-2.25913858	7.60408617
H	2.47080861	4.57149089	10.45644702
C	1.66029954	4.08893005	9.91048566
C	0.76502606	5.03210020	9.09606848
C	1.57638142	5.82968274	8.06232540
C	-0.38245740	4.25809563	8.42149261

H	1.05724505	3.53054808	10.65986900
H	2.11736359	3.32552774	9.24526572
H	0.94002888	6.55740842	7.51491111
H	2.02110314	5.14398312	7.30888994
H	2.40749938	6.39247265	8.53844964
H	-1.05607051	4.94317959	7.86356611
H	-0.99765478	3.71429114	9.17014824
H	0.01175482	3.51236030	7.70140661
H	0.29408176	5.74066538	9.80960553
C	-1.78393362	2.06631023	-0.63065988
H	-2.61341188	1.36068927	-0.56726969
C	-0.65039782	1.68698013	0.32132391
C	-1.81149731	-2.20163527	3.43819839
H	-2.59650944	-1.44799158	3.65886457
C	-0.43448929	-1.71154032	3.91783534
H	6.73268816	-1.03128388	0.51273485
C	5.83620957	-0.65736754	-0.02485656
H	6.04510842	0.36257526	-0.34661894
C	4.62500531	-0.64640349	0.92740677
H	3.37010551	3.64654544	-0.07807529
C	3.33556034	4.02724739	0.96087114
C	3.49555371	2.87989348	1.99114531
H	-2.17183095	3.08128896	-0.39227411
H	4.15467686	4.72119186	1.15241269
H	-0.40057182	-1.66059609	5.02638232
H	0.37336515	-2.40061407	3.59989739
H	4.40570787	-1.67161144	1.29782903
H	4.85640332	-0.02698390	1.81887035
H	0.18877205	2.40671846	0.22444487
H	-0.99406662	1.74528176	1.37594927
H	5.65423308	-1.28507122	-0.92193052
H	-1.43649075	2.07465731	-1.68603417
H	2.38331935	4.57916411	1.10704158
H	4.21365430	2.11383036	1.64185567
H	3.87036086	3.26008623	2.96333556
H	-2.09353699	-3.13541792	3.95925431
C	1.45086873	-2.42161236	9.96689289
O	2.30532508	-2.38060821	10.84346362
N	1.29548794	-3.46162598	9.08472019
C	2.09536794	-4.69326237	9.22036668
C	1.32436604	-5.72259291	8.34660408
C	-0.09417555	-5.13340390	8.22873849
C	0.17653049	-3.62301797	8.14842253
H	0.47255463	-3.32429997	7.11501952
H	-0.68383461	-2.99081975	8.44985775
H	-0.65672223	-5.51937940	7.35435803
H	-0.68478142	-5.35679338	9.14364524
H	1.79391856	-5.77464557	7.34114946
H	1.35661513	-6.73980709	8.78181989
H	2.14447422	-4.98725099	10.29003867
H	4.99575653	-3.23067587	6.15525532
H	-1.81394360	-2.37323262	2.34284090
H	0.69606759	-1.60005614	9.78883936

MODEL 7: INORGANIC LIGAND REPLACEMENT: $(CO)_2$ REPLACES $([CN]^-)_2$

System: **Ni-SI$_a$** (singlet)
Charge, Multiplicity: 0, 1
Gibbs free energy: –6248.690872 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.25530643
S	3.05357924	0.00000000	0.14940499
S	1.68037954	2.25622302	2.40398328
Ni	1.49867362	0.22609329	1.61676717
Fe	2.08680110	0.72088595	4.01122968
C	1.48849672	0.65618680	5.68567161
C	3.54659469	1.59108411	4.45280732
O	1.10690324	0.52460972	6.77332318
O	4.46407756	2.22156866	4.78171320
C	2.86863789	-0.86030606	3.80068257
O	3.40902283	-1.88573978	3.74183335
O	8.97259886	3.01228898	6.64983873
C	7.83187605	3.43448603	6.46141551
N	7.23944093	3.59781643	5.23705557
C	7.93796885	3.46602368	3.97184271
C	7.06084947	2.81509373	2.89523419
O	6.73130347	1.46131239	3.17125768
H	8.28323886	4.46072916	3.59848407
H	6.29338175	4.01180090	5.31527740
H	8.84482867	2.85315430	4.16060952
H	6.13709306	3.43678465	2.75440150
H	7.60464609	2.82345811	1.92665955
H	6.41464136	1.44288913	4.09660119
C	5.25051496	2.13280645	8.03332883
C	4.52555568	3.45632766	7.74630430
H	5.38407388	1.56046500	7.09055350
H	4.70198249	1.48856199	8.74934794
H	3.67766168	3.34249019	7.03697452
H	4.10920458	3.87012332	8.69552005
C	6.90888363	3.83531778	7.64037820
C	6.61370890	2.61988631	8.55472580
H	6.52114614	2.95078161	9.61087078
H	7.42522777	1.86791988	8.50552112
H	7.47587864	4.61640909	8.19287251
N	5.58416410	4.32074878	7.17735685
H	5.43574779	5.30912602	7.40219829
N	3.98580034	-2.98715122	7.90656185
C	3.86397417	-3.92238786	8.90546610
H	3.17152395	-2.39859947	7.71989570
O	4.81539124	-4.59719315	9.32335240
C	5.26185294	-2.62342204	7.32057645
H	6.01576885	-3.34789030	7.68535728
H	5.57904796	-1.60174761	7.62641725
H	2.06100273	5.15671228	10.16968772
C	1.29120836	4.58580877	9.65086656
C	0.37629506	5.46346687	8.78660784
C	1.19813771	6.35483734	7.84038446
C	-0.63027303	4.60352089	8.00298154

H	0.71275224	4.02386937	10.41442004
H	1.80977628	3.83067108	9.02012670
H	0.54738401	7.00100388	7.21406254
H	1.81155123	5.73013805	7.15292222
H	1.89280068	7.01531436	8.40159313
H	-1.32711214	5.23005307	7.40704741
H	-1.23959051	3.96874253	8.68041403
H	-0.10149396	3.92485043	7.29731126
H	-0.20218273	6.11732197	9.47849898
C	-2.00015640	1.78766405	-0.75864713
H	-2.76899496	1.02141595	-0.65995645
C	-0.88858671	1.59080912	0.26264204
C	-1.68181424	-2.26705252	3.50903708
H	-2.38256379	-1.49864790	3.89892226
C	-0.22374394	-1.79983894	3.67660975
H	6.76290868	-0.59646249	0.42680281
C	5.81462643	-0.29358323	-0.06461126
H	5.94087786	0.72312976	-0.43682790
C	4.66488913	-0.35367103	0.95488631
H	3.08119079	3.71165118	-0.26662267
C	2.95241767	4.22131441	0.70700945
C	3.15525005	3.25347872	1.90106651
H	-2.48250875	2.77785315	-0.61205208
H	3.71380242	4.98653723	0.85982478
H	0.11315599	-1.87786516	4.73075363
H	0.48615159	-2.38320995	3.05668762
H	4.60171484	-1.35212169	1.43286311
H	4.82943931	0.37865856	1.78051195
H	-0.14048493	2.40372951	0.18099049
H	-1.28292658	1.61599491	1.29877587
H	5.63492516	-0.96856541	-0.92603550
H	-1.61062804	1.75120295	-1.79733033
H	1.95748515	4.71000150	0.73704819
H	4.00424457	2.56075866	1.74209905
H	3.37885181	3.83256413	2.82215931
H	-1.88839622	-3.19320461	4.07728113
C	1.64927555	-1.81094859	9.85282034
O	2.54442205	-1.59432069	10.65950388
N	1.53035627	-2.97114502	9.12488209
C	2.41348875	-4.12708886	9.38168100
C	1.72901275	-5.28184680	8.59662383
C	0.26933570	-4.81730356	8.42710088
C	0.41354174	-3.30116722	8.23155567
H	0.66445737	-3.06075740	7.16964374
H	-0.49283869	-2.72067282	8.50012367
H	-0.25286565	-5.31556718	7.58559018
H	-0.30994062	-5.01669840	9.35411460
H	2.21136919	-5.38379102	7.60100595
H	1.83489986	-6.25282456	9.11649377
H	2.46755184	-4.32145964	10.47348613
H	0.82993565	-1.07299989	9.61032337
H	5.22144370	-2.66642148	6.21114257
H	-1.92863809	-2.43171609	2.44146225

System: **I1** (doublet)
Charge, Multiplicity: 0, 2
Gibbs free energy: –6249.294782 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.37370102
S	3.03393479	0.00000000	0.18120145
S	1.29510087	2.50450000	2.32761938
Ni	1.37635726	0.31391901	1.66788502
Fe	1.99856032	1.00010344	3.95829051
C	1.55798053	0.90808051	5.67005111
C	3.33861424	2.08308533	4.26344454
O	1.29787777	0.75184145	6.79239553
O	4.19373322	2.83828665	4.49475067
C	2.97541530	-0.44424447	3.67856432
O	3.67031249	-1.37781816	3.60094222
H	2.97540016	1.20421629	-0.43465189
O	8.72249961	4.19718801	6.13598890
C	7.52433385	4.44471139	6.00083959
N	6.85239183	4.48549818	4.80761148
C	7.49659375	4.40427149	3.51091085
C	6.64218083	3.64208469	2.49034346
O	6.46809850	2.26722158	2.80667024
H	7.71345355	5.42200288	3.10342790
H	5.86235310	4.76675139	4.92895568
H	8.47357135	3.89725583	3.66002345
H	5.65320451	4.15984901	2.38118059
H	7.13972668	3.68274388	1.49782154
H	6.14158411	2.24174504	3.72893247
C	5.18844236	2.84145256	7.69371952
C	4.29630034	4.06594209	7.44408806
H	5.33955586	2.28425696	6.74461445
H	4.75955059	2.14058624	8.43755944
H	3.42907059	3.84579968	6.78567899
H	3.89012933	4.43940264	8.41447636
C	6.60768411	4.73269606	7.21747264
C	6.50798429	3.49309912	8.14350317
H	6.43075983	3.81535133	9.20353434
H	7.40084983	2.84421239	8.05244025
H	7.09262128	5.58190858	7.74724221
N	5.21296234	5.03901718	6.80934691
H	4.95287661	6.00780189	7.01759504
N	4.64282655	-2.39854221	7.72459025
C	4.69288484	-3.32119259	8.74070900
H	3.74951100	-1.92774191	7.56697019
O	5.74365354	-3.85454859	9.12332546
C	5.83045840	-1.87765991	7.07510796
H	6.68959455	-2.49406408	7.40412954
H	6.02597348	-0.82032769	7.36119060
H	1.74780351	5.46155348	9.95277839
C	1.03872810	4.78195574	9.48005657
C	-0.02361601	5.51098835	8.64681413
C	0.62810968	6.48262496	7.64851616
C	-0.93959765	4.50743299	7.92517504
H	0.57555077	4.16495156	10.27899278

H	1.62427420	4.08861444	8.83734056
H	-0.13093126	7.02263780	7.04389762
H	1.28713318	5.92976184	6.94219619
H	1.25309029	7.24162411	8.16547416
H	-1.74003629	5.02231121	7.35291645
H	-1.42728887	3.81223523	8.64073893
H	-0.35674707	3.89000854	7.20618589
H	-0.65237867	6.09730738	9.35547439
C	-2.31361086	1.35003160	-0.71814768
H	-2.96751597	0.49061152	-0.57180181
C	-1.18385506	1.37026829	0.29564161
C	-1.26281691	-2.53426067	3.59019003
H	-2.16526190	-1.93780945	3.83907121
C	0.02024653	-1.76558082	3.94661310
H	6.77040713	0.18305982	0.00208529
C	5.73443558	0.34412315	-0.36429111
H	5.70397915	1.35962386	-0.75872939
C	4.75870191	0.13900693	0.79147540
H	2.47354332	3.95797866	-0.50647987
C	2.32908551	4.45250276	0.47354135
C	2.68408038	3.53414632	1.67462251
H	-2.93720701	2.26477222	-0.61603782
H	2.98722091	5.31520211	0.57856484
H	0.15857592	-1.69534764	5.04594352
H	0.92489915	-2.25125690	3.53135011
H	4.92538845	-0.82831915	1.30618582
H	4.83933810	0.93419428	1.56074500
H	-0.60892705	2.31521396	0.23503812
H	-1.56237486	1.29576060	1.33534664
H	5.55255482	-0.36871556	-1.19437910
H	-1.93031997	1.32164968	-1.75961272
H	1.28263060	4.81514934	0.53577253
H	3.53688085	2.86282495	1.44543957
H	3.00495949	4.15736845	2.53384747
H	-1.31726072	-3.46774635	4.18082930
C	2.26275389	-1.50546584	9.76379491
O	3.15673326	-1.15922481	10.52551940
N	2.26534654	-2.68583020	9.05867931
C	3.30598733	-3.70828016	9.28806118
C	2.74753378	-4.95915115	8.55215601
C	1.23250537	-4.69704405	8.44739400
C	1.16305650	-3.17908742	8.22438587
H	1.33040996	-2.92854507	7.14869950
H	0.20036749	-2.71948443	8.52876568
H	0.74350165	-5.27691665	7.63880011
H	0.72876392	-4.95357942	9.40403466
H	3.19253963	-5.01470136	7.53567100
H	3.00692294	-5.89707113	9.07882795
H	3.43579869	-3.87252382	10.37847554
H	5.73991191	-1.93514240	5.96938797
H	-1.30264381	-2.77767113	2.50988930
H	1.34497430	-0.88479456	9.54843455

System: **Ni-C** (doublet)
Charge, Multiplicity: 0, 2
Gibbs free energy: –6249.277667 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.23970142
S	3.05407637	0.00000000	0.11802171
S	1.54341620	2.44302074	2.43072776
Ni	1.50308947	0.27739140	1.60152539
Fe	2.08468897	0.74960451	4.01135478
C	1.36137078	1.56312103	5.44160135
C	3.69121049	1.46154010	4.23504905
O	0.93504657	2.03436173	6.40227436
O	4.71557844	1.95689631	4.43262931
H	2.65711808	-0.08540843	2.70821619
C	2.46833178	-0.77672783	4.82237911
O	2.72300306	-1.77764292	5.34242319
C	1.56196179	-1.73454698	9.85149001
O	8.84527194	3.38135344	6.73759738
C	7.67536951	3.64279476	6.47001525
N	7.17914220	3.86839020	5.20777044
C	7.98539610	3.91988208	4.00070119
C	7.34739662	3.11285652	2.86082855
O	7.27661762	1.72250401	3.12884652
H	8.13745706	4.97300889	3.66293828
H	6.18964970	4.16025443	5.20360185
H	8.98142928	3.50408966	4.26060966
H	6.33173274	3.53792543	2.63794698
H	7.95561831	3.23727102	1.93939642
H	6.89705306	1.63857939	4.02578837
C	4.41050596	2.47171410	7.86156558
C	4.25608032	4.00172401	7.93345816
H	3.90778780	2.08750389	6.95131283
H	3.94775937	1.96371849	8.73068961
H	3.30148102	4.36743432	7.50271522
H	4.28752359	4.33904967	9.00096253
C	6.56227479	3.66348729	7.54129041
C	5.94596039	2.24320268	7.77128041
H	6.36314814	1.78736459	8.68966508
H	6.20046992	1.56572580	6.93110306
H	7.05106046	4.01037519	8.48325109
N	5.39854062	4.48215359	7.14970468
H	5.57523224	5.48502539	7.28866205
N	3.97302568	-2.83749854	7.94086295
C	3.84815636	-3.78439069	8.92519855
H	3.14267647	-2.29665620	7.69592664
O	4.80953322	-4.43371869	9.36072794
C	5.25199796	-2.45062915	7.37968948
H	6.02180110	-3.11971435	7.81092269
H	5.51158845	-1.39989617	7.63692577
H	1.81795869	5.25984477	10.08944378
C	1.06853279	4.66671160	9.56560399
C	0.12770076	5.50313874	8.68484756
C	0.91111857	6.38715673	7.70058029
C	-0.88630366	4.61573421	7.94316344

H	0.49645020	4.10252193	10.33297635
H	1.60601872	3.91088979	8.95308416
H	0.23475856	7.03379645	7.10257864
H	1.48613238	5.75962416	6.98367709
H	1.63522511	7.04573963	8.22548088
H	-1.61059436	5.22710291	7.36448371
H	-1.46538096	3.98231483	8.64802842
H	-0.37272480	3.93896867	7.22941355
H	-0.45765877	6.16162820	9.36098323
C	-2.02075558	1.70777578	-0.86137956
H	-2.77287006	0.92464018	-0.76607872
C	-0.92167506	1.58002216	0.18970284
C	-1.66369438	-2.30344076	3.44440517
H	-2.40778752	-1.56834747	3.81746009
C	-0.23070593	-1.79144673	3.68617800
H	6.78452478	-0.45442167	0.45075983
C	5.83057769	-0.18448322	-0.04970889
H	5.93789109	0.83197166	-0.42865982
C	4.67585782	-0.27806368	0.95507275
H	2.97798877	3.77613196	-0.33535250
C	2.85430760	4.26874143	0.64707975
C	3.07768942	3.27974544	1.82483256
H	-2.53416744	2.68749186	-0.75512267
H	3.59552462	5.05251771	0.80326492
H	0.02223615	-1.84945356	4.76504338
H	0.53013582	-2.37533802	3.13056327
H	4.64556135	-1.27416170	1.44380480
H	4.81206321	0.47183247	1.76472607
H	-0.19141338	2.40729955	0.08889205
H	-1.33698217	1.63592675	1.21691714
H	5.68185794	-0.86891811	-0.91007287
H	-1.60423593	1.65568133	-1.88903649
H	1.85200493	4.74297161	0.68998159
H	3.81451149	2.49947106	1.55611457
H	3.46952486	3.82641502	2.70710477
H	-1.83254689	-3.21835330	3.97286542
O	2.43694223	-1.49381113	10.67261022
N	1.48989601	-2.88974861	9.11090980
C	2.39754651	-4.02467929	9.37762653
C	1.75123434	-5.19482540	8.58483352
C	0.28200837	-4.76727481	8.40820332
C	0.39018495	-3.24935134	8.20768633
H	0.64783646	-3.00788562	7.14759113
H	-0.53339531	-2.69166353	8.46661737
H	-0.22478907	-5.28104154	7.56657248
H	-0.29577022	-4.97731203	9.33377411
H	2.24227930	-5.28056652	7.59190551
H	1.87966284	-6.16397383	9.10292006
H	2.44140073	-4.21836042	10.47006790
H	-1.85671674	-2.45511593	2.36400539
H	5.25732443	-2.55679190	6.27373250
H	0.71889788	-1.02243253	9.60684210

System: **Ni-R** (singlet)
Charge, Multiplicity: 0, 1
Gibbs free energy: –6249.873827 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.11582637
S	3.09941475	0.00000000	0.10738687
S	1.48710353	2.61818647	2.43296896
Ni	1.50093616	0.29103891	1.59776680
Fe	1.97070222	0.85521543	4.01007581
C	1.03815733	1.49120572	5.40121493
C	3.43375620	1.77828319	4.36335798
O	0.45664641	1.80279725	6.34744184
O	4.34040036	2.43631733	4.65578585
H	2.66277150	0.08174637	2.72503339
C	2.46938969	-0.64113308	4.80820443
O	2.80977229	-1.62135319	5.32371626
H	3.23721894	1.26365562	-0.37716551
O	8.82394213	3.39069521	6.66423714
C	7.66095203	3.74116219	6.46604488
N	7.06944534	3.86588058	5.23557315
C	7.78995549	3.78108532	3.97834461
C	6.96297248	3.09619492	2.88282941
O	6.69465926	1.72426356	3.14468980
H	8.08869792	4.79519883	3.61724416
H	6.10573492	4.23935669	5.30381299
H	8.72496201	3.21465317	4.17483859
H	6.01221347	3.67027392	2.72815323
H	7.52473339	3.13699991	1.92527525
H	6.35941595	1.68720061	4.06294882
C	5.10175556	2.29084270	7.94253081
C	4.33076910	3.59482774	7.68837026
H	5.27366503	1.75840764	6.98248605
H	4.56860704	1.60082990	8.62688446
H	3.49666771	3.47492075	6.96351127
H	3.88616371	3.96138473	8.64424316
C	6.69963909	4.06969643	7.63702570
C	6.43593453	2.81236671	8.50487573
H	6.31137832	3.10376974	9.56928386
H	7.27642629	2.09351175	8.44751136
H	7.22344373	4.85333704	8.22700812
N	5.36499971	4.51275926	7.16270977
H	5.17252198	5.49084970	7.39837785
N	4.11096747	-2.85491725	7.79735532
C	4.01001062	-3.82440686	8.76099044
H	3.26807455	-2.33100545	7.55826843
O	4.98635704	-4.45997496	9.18307379
C	5.37901953	-2.42622318	7.24249851
H	6.16608476	-3.08394466	7.65986976
H	5.61168499	-1.37414510	7.51884909
H	1.76806935	5.14279598	10.11744564
C	1.03298774	4.54367240	9.58056899
C	0.09986652	5.40572485	8.71558293
C	0.90534890	6.36463354	7.82288001
C	-0.85781361	4.54594113	7.87540919

H	0.46465003	3.94711722	10.32494118
H	1.59156603	3.82209668	8.94482111
H	0.24266486	7.00014720	7.19829611
H	1.56407045	5.79107630	7.13286971
H	1.55321783	7.03758815	8.42398338
H	-1.59542175	5.17541645	7.33416735
H	-1.42293774	3.82605867	8.50446887
H	-0.29992182	3.95891674	7.11763479
H	-0.52824755	6.00621339	9.40764254
C	-1.98853227	1.73581337	-0.90782122
H	-2.72205966	0.93346911	-0.82937618
C	-0.89860262	1.60059854	0.15290522
C	-1.53647232	-2.35670905	3.31154328
H	-2.35451863	-1.66181599	3.59539782
C	-0.17055552	-1.76328954	3.66929021
H	6.86905244	-0.23952988	0.35585772
C	5.90542506	0.01180542	-0.13430820
H	5.98851754	1.03819717	-0.49167678
C	4.77227798	-0.11820561	0.88232991
H	2.96281267	3.91995736	-0.34225906
C	2.82538669	4.37794586	0.65615314
C	3.05163738	3.37464731	1.82303590
H	-2.51955384	2.70445700	-0.78909431
H	3.54795380	5.17538230	0.82942092
H	-0.02853367	-1.72913799	4.77005296
H	0.67230690	-2.33618260	3.23671633
H	4.74859064	-1.12237937	1.35350087
H	4.87169193	0.62207998	1.70232524
H	-0.15531954	2.41950625	0.07468007
H	-1.32809854	1.66083274	1.17388834
H	5.76801571	-0.66239458	-1.00392863
H	-1.56329664	1.70611090	-1.93300845
H	1.81318951	4.83067456	0.69851800
H	3.76155142	2.57284309	1.53245674
H	3.51349179	3.90945106	2.67687596
H	-1.70706371	-3.29916683	3.86458860
C	1.67889020	-1.85132507	9.73419454
O	2.54814335	-1.61116635	10.56190158
N	1.63129006	-2.99126777	8.96895010
C	2.56583752	-4.10968379	9.20876224
C	1.94655851	-5.27647837	8.38977340
C	0.46771460	-4.87940009	8.22231438
C	0.54100975	-3.35504454	8.05584649
H	0.79407480	-3.08341862	7.00222706
H	-0.39533293	-2.82479499	8.32625378
H	-0.02713971	-5.38549383	7.36897592
H	-0.10486070	-5.12367701	9.14273476
H	2.43899860	-5.32802782	7.39514540
H	2.09785668	-6.25390762	8.88575138
H	2.61601647	-4.32742453	10.29641066
H	0.82182237	-1.15143145	9.50406654
H	5.38395547	-2.50953020	6.13459757
H	-1.62017183	-2.54727381	2.22318279

System: **I2a** (singlet)
Charge, Multiplicity: 0, 1
Gibbs free energy: –6249.855788 au

S	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.32426107
S	3.15612013	0.00000000	0.11708960
S	1.94162302	1.96302160	2.36052093
Ni	1.55908244	-0.08074141	1.65882235
Fe	2.12119271	0.54560273	4.10700854
C	1.48694718	1.25908144	5.60841314
C	3.77863263	1.07096776	4.39366207
O	1.09463154	1.65272629	6.62274174
O	4.83057869	1.48175618	4.65340337
C	2.43155169	-1.09142371	4.72098110
O	2.63530730	-2.13493953	5.18729947
H	2.10080311	-1.64904233	2.21425164
H	1.60940345	-1.82056432	1.59707999
O	9.20514500	1.96464380	6.77344072
C	8.13669916	2.54369852	6.57683576
N	7.61638745	2.85078972	5.34724983
C	8.34668508	2.71692224	4.09951968
C	7.49714729	2.10549174	2.97677163
O	7.16036443	0.74385689	3.19124446
H	8.73008035	3.70874602	3.75802452
H	6.73125176	3.38184331	5.42103286
H	9.22741277	2.07323874	4.30827011
H	6.57919845	2.73466886	2.82906063
H	8.07112271	2.14792419	2.02649628
H	6.78261078	0.69486327	4.09148899
C	5.40753713	1.46112445	7.98434036
C	4.82510366	2.85910522	7.71682836
H	5.54416139	0.91519829	7.02660009
H	4.75859506	0.84526326	8.63890285
H	4.03282005	2.85441319	6.93621952
H	4.36248254	3.26051029	8.64865584
C	7.23733256	3.00079745	7.75408202
C	6.77754271	1.79105196	8.60211673
H	6.65591871	2.09275843	9.66417204
H	7.51371682	0.96459933	8.56429322
H	7.87747671	3.68623518	8.35110211
N	5.99466721	3.66323784	7.28851882
H	5.93085318	4.63366899	7.60932728
N	3.62010038	-3.42771231	7.96127777
C	3.38138291	-4.35697514	8.94297341
H	2.86621588	-2.78168190	7.72138359
O	4.25085983	-5.13433128	9.36063023
C	4.93522998	-3.20688408	7.39216526
H	5.61437637	-3.97299527	7.81394975
H	5.32974447	-2.20006255	7.65305238
H	2.56568517	4.85447046	10.26960516
C	1.74044530	4.37408417	9.74369689
C	0.93060309	5.35321022	8.88187693
C	1.84978746	6.15476317	7.94505315
C	-0.16840927	4.62580238	8.08932348

H	1.10020129	3.87439745	10.50118784
H	2.17378900	3.57015872	9.10861286
H	1.27734087	6.87495104	7.32301902
H	2.39030122	5.47045782	7.25306978
H	2.61306049	6.72865548	8.51244609
H	-0.79740456	5.34108737	7.51828449
H	-0.83816813	4.04551002	8.75865825
H	0.27511120	3.91195006	7.36342802
H	0.42394009	6.05985582	9.57511093
C	-1.77255840	2.02489017	-0.70649468
H	-2.62237285	1.34716480	-0.61453684
C	-0.65638387	1.69020505	0.28159357
C	-1.92166301	-2.07062752	3.53340962
H	-2.63282885	-1.26032658	3.79586302
C	-0.48362401	-1.68803401	3.91888151
H	6.65129772	-1.30004423	0.54072096
C	5.76454803	-0.89553015	0.01145371
H	6.00315989	0.10379801	-0.35166589
C	4.57731903	-0.77160674	0.98996565
H	3.46770354	3.41586769	-0.18960921
C	3.40410956	3.89734858	0.80460278
C	3.50658896	2.85842752	1.94616574
H	-2.13891795	3.05873460	-0.52778276
H	4.24375467	4.57385663	0.96737945
H	-0.36598789	-1.64220570	5.02153218
H	0.25348435	-2.42292253	3.53904236
H	4.26587672	-1.76621550	1.37661894
H	4.87545866	-0.15690432	1.86996040
H	0.17883175	2.41185023	0.17014802
H	-1.01865310	1.77231934	1.32801017
H	5.52147324	-1.54524090	-0.85287784
H	-1.41130317	1.97173483	-1.75490470
H	2.46704112	4.48737387	0.86639351
H	4.29609516	2.10668148	1.75322946
H	3.74628216	3.36815468	2.90351567
H	-2.23080718	-2.97346962	4.09219113
C	1.39470452	-2.03721486	9.91492763
O	2.29884140	-1.92853635	10.73268811
N	1.16254741	-3.16302841	9.16219128
C	1.91462890	-4.41064175	9.40594807
C	1.11388795	-5.47437690	8.60326998
C	-0.28681181	-4.85347090	8.44009609
C	0.02161467	-3.36026115	8.26029565
H	0.30469021	-3.13999574	7.20198135
H	-0.81863280	-2.68848657	8.53196597
H	-0.85972874	-5.28323149	7.59378490
H	-0.88445226	-4.99843885	9.36552380
H	1.58479392	-5.61219349	7.60646022
H	1.11447410	-6.45852588	9.10889912
H	1.94067256	-4.62405101	10.49526995
H	4.91806253	-3.30427492	6.28584441
H	-2.01031566	-2.26152946	2.44559874
H	0.65511292	-1.21426164	9.68471428

MODEL 8: LARGE MODEL

System: **I2a** (singlet)
Charge, Multiplicity: –2, 1
SCF energy: –7998.79079658 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

System: **I2a** (triplet)
Charge, Multiplicity: –2, 3
SCF energy: –7998.75523931 au

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.36987733
C	2.06227973	0.00000000	0.60814198
N	1.23168159	0.00013179	-0.49819934
C	1.31575930	0.00029672	1.78260478
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H	3.15651666	-0.00687479	0.50779653
H	1.57429024	-0.01851191	2.84770961
H	-0.82334232	0.04335230	1.99977300
O	-9.29749716	-3.53118254	-0.02087114
C	-8.14238138	-3.38617893	0.40296256
N	-7.81525973	-2.48588927	1.37766588
C	-8.84532453	-1.69968348	2.04593630
C	-8.29656056	-0.85715670	3.20794781
O	-7.86065956	-1.62267404	4.31354728
H	-9.34437469	-1.03242475	1.30343924
H	-6.84456554	-2.43878796	1.73208848
H	-9.63974725	-2.38006110	2.42962494
H	-7.48063567	-0.19282290	2.82347174
H	-9.11708517	-0.18807287	3.55472226
H	-6.95517597	-1.95530964	4.04434311
C	-4.83704324	-5.02861498	0.84464333
C	-4.65987319	-4.28510678	-0.48987083
H	-4.47430355	-4.37887575	1.66698346
H	-4.27229696	-5.98181740	0.88560693
H	-3.71791189	-3.70316459	-0.52255063
H	-4.63635161	-5.01369535	-1.34806330

C	-6.97568568	-4.23869866	-0.11249491
C	-6.37432296	-5.22056565	0.95353452
H	-6.68664878	-6.26067187	0.72994761
H	-6.73592977	-4.97790264	1.97281295
H	-7.40500689	-4.82875568	-0.96347260
N	-5.83059751	-3.41848928	-0.48456931
H	-5.98263015	-2.79186790	-1.29048050
H	-5.77170705	3.67402865	10.08169461
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H	-4.61600918	2.35837567	10.35150371
H	-5.43217935	2.51736904	8.77361243
C	-3.80211441	3.89969453	9.07023374
C	-4.14093522	4.79667109	7.90822452
O	-3.07453159	5.54425225	7.52340370
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H	-3.02126431	3.21543951	8.65895997
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C	-5.42279999	-3.01906996	6.77357010
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H	-2.22684268	-4.25277030	8.76915129
H	-4.61340004	-2.43235851	10.59171668
H	-3.12769301	-3.46098522	10.71675934
H	-5.73928512	-2.13818433	8.68522207
O	-5.09777282	-8.76820150	7.00305674
C	-5.67608247	-6.57537877	5.30584900
C	-5.94572155	-5.06380795	5.32038330
C	-5.87322873	-4.48593169	6.74301132
H	-5.19521200	-4.55744041	4.67710380
H	-6.92989688	-4.85359374	4.84937205
H	-6.84358167	-4.60413631	7.27549259
H	-5.13186419	-5.08692294	7.31159327
H	-6.42494083	-7.13237094	5.90739839
H	-5.74887923	-6.95922005	4.26110799
H	-6.21442954	-2.33739895	6.40496200
H	-4.57443945	-2.87970939	6.07385104
H	-1.94784681	-5.64973418	-2.15094011
C	-1.25810951	-5.31673703	-1.37533902
C	-0.36009604	-4.12970611	-1.75709485
C	-1.18459959	-2.89773995	-2.16116898
C	0.61108395	-3.77184104	-0.61568881
H	-0.64105182	-6.19758841	-1.09026026
H	-1.86649444	-5.06159077	-0.48083263
H	-0.53028925	-2.06578376	-2.49669814
H	-1.75856515	-2.52874971	-1.28745374
H	-1.90963040	-3.12627420	-2.97218719
H	1.24575114	-2.90160655	-0.88560586
H	1.27321958	-4.62767087	-0.36159947
H	0.05177598	-3.48978881	0.29996031

H	0.25663840	-4.45058465	-2.62448064
C	0.78267286	3.53509740	5.29648282
H	1.53280997	3.22496616	6.02383224
C	-0.25394162	2.42875164	5.13624520
N	0.44745839	-0.79977536	8.24360673
C	0.79926916	-1.95141714	7.45379916
H	1.73257183	-1.74403897	6.87436323
C	-0.30603516	-2.36930117	6.46873036
H	-7.89160596	0.83912281	6.50243184
C	-6.97338393	1.41964669	6.41091740
H	-7.10620364	2.13237933	5.59728470
C	-5.72529181	0.55603193	6.26583847
H	-4.07378196	3.46457468	2.85308409
C	-3.89690684	2.65362425	2.14666594
C	-4.05894336	1.26792288	2.82870909
H	1.15545823	3.81960757	4.31186205
C	0.58460490	-0.77574168	9.60099523
O	0.93019717	-1.73332141	10.29278178
H	-4.61165107	2.73120004	1.32694897
H	-0.05620569	-3.34150077	5.99946279
H	-1.25937223	-2.50451910	7.01423253
H	0.11497470	0.03870736	7.73447679
H	-5.66092940	-0.18731122	7.08774026
H	-5.73287995	-0.02822620	5.32053037
H	-1.03253354	2.72575276	4.40500169
H	0.20648777	1.50314014	4.73135844
H	-6.89810271	2.04143257	7.32996781
H	0.29812189	4.44164931	5.72551764
H	-2.87881783	2.75200957	1.71853463
H	-4.78960048	1.30090326	3.65720042
H	-4.41467377	0.50906459	2.11639273
H	1.03591438	-2.80393542	8.11756198
H	2.40316577	2.90979164	8.91305653
C	2.05489197	2.08377877	9.53326474
O	2.85653234	1.54334507	10.30063716
N	0.72327480	1.75289106	9.46886296
H	0.16391058	2.08687141	8.65856505
C	0.22851526	0.58725111	10.22527643
H	-0.85409904	0.63431771	10.34273896
H	0.69735333	0.59131132	11.22759098
H	-7.52074480	4.90542607	4.38606062
C	-6.69091530	5.36339429	3.84786114
O	-6.88433636	5.74605096	2.68863842
N	-5.53879598	5.48135711	4.49856802
H	-4.65132739	5.88647566	4.01233318
H	-5.43147892	5.14301907	5.47208870
S	-1.13013807	1.98747628	6.68504891
S	-0.57903188	-1.15015533	5.10686593
S	-4.21456514	1.58865269	6.34534093
S	-2.48834128	0.56590982	3.51338214
Ni	-2.47240308	0.31696284	5.79581041
Fe	-2.51615886	-1.66929215	3.95600975
C	-2.16449646	-2.30822401	2.41134709
C	-4.31514359	-1.88601963	3.55087406
O	-2.01367336	-2.73647678	1.33272100

N	-5.43734595	-2.10584072	3.26691951
C	-2.54153890	-3.39460810	4.72136233
N	-2.58416051	-4.47463643	5.19597858
H	-0.64024482	-6.13611259	12.76662616
C	-0.67074298	-6.20976297	11.67962730
C	-1.46240563	-5.11506264	10.94184366
O	-2.30302100	-4.42646846	11.59570737
O	-1.23377888	-5.03532890	9.69079675
H	0.36598581	-6.22767016	11.28598313
H	-1.12495845	-7.18882029	11.41050631
H	-3.35819144	6.04007581	6.72570813
H	-3.25974999	-1.26248855	6.05099668
H	-3.07842286	-0.96161121	6.79566993
C	-1.00986818	-8.12207001	3.48365425
C	-1.98994668	-8.57033298	4.57339992
O	-2.93519596	-9.32958208	4.32565918
C	-1.52294452	-8.45175122	2.08104155
N	-1.78551825	-8.07561846	5.83874201
C	-2.73240933	-8.42684511	6.90760609
C	-2.18362794	-7.69653297	8.14618387
C	-0.68657561	-7.61895978	7.86192314
C	-0.64614573	-7.29743137	6.35562004
C	-4.10824373	-0.88983935	-1.16708079
C	-4.70307999	-0.43012694	-2.50569585
C	-4.95269655	-0.53764384	0.02829748
H	-5.99603892	-0.89798364	-0.06655403
H	-4.56030694	-1.00117207	0.95353612
H	-4.99608064	0.56420830	0.16755212
H	-3.09623316	-0.43925018	-1.05186693
H	-3.91876946	-1.97732076	-1.20411976
H	-5.69906505	-0.89442556	-2.68614922
H	-4.85850439	0.67103723	-2.52319111
H	-4.04914715	-0.69439276	-3.36391400
H	-1.73986529	-9.53461448	1.98613321
H	-2.47176943	-7.91428441	1.87879252
H	-0.78613783	-8.15657284	1.30587835
H	-0.02529510	-8.61111149	3.67250342
H	-0.82674472	-7.03013201	3.59135020
H	-0.80194051	-6.20917244	6.16946786
H	0.30375149	-7.60248962	5.86969259
H	-0.20331298	-6.83740298	8.48179249
H	-0.19687019	-8.60068615	8.05042132
H	-2.59348024	-6.66750631	8.21084483
H	-2.44400422	-8.21604191	9.08857898
H	-2.76156897	-9.52909352	7.04954821

System: **I2b** (singlet)
Charge, Multiplicity: –2, 1
SCF energy: –7998.76937289 au

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N	0.00000000	0.00000000	1.36888901
C	2.06127426	0.00000000	0.59736993
N	1.22755949	0.00859710	-0.50853924
C	1.31896705	-0.00279491	1.77528272

H	-0.93101149	0.00012180	-0.57655773
H	3.15537020	-0.00831774	0.49493287
H	1.58874253	-0.02491422	2.83739367
H	-0.83717785	0.04957443	1.98466437
O	-9.28857188	-3.38594996	-0.27898452
C	-8.19216852	-3.27634616	0.28613431
N	-7.93701952	-2.35275103	1.25705321
C	-8.95308252	-1.41793201	1.72049238
C	-8.39353675	-0.41876026	2.74597958
O	-8.10114067	-0.99435349	4.00330556
H	-9.37309319	-0.87399482	0.84241673
H	-7.02495191	-2.35110440	1.74618877
H	-9.80462542	-1.96998821	2.18234753
H	-7.49945465	0.09019672	2.30238218
H	-9.16363026	0.36930599	2.90717073
H	-7.25040620	-1.49969427	3.87836933
C	-4.79596775	-4.74815022	0.90336356
C	-4.68120906	-4.24684217	-0.54270564
H	-4.42198648	-3.96867371	1.59531096
H	-4.21105070	-5.67145164	1.08738547
H	-3.74933352	-3.67432291	-0.72455794
H	-4.68283757	-5.11624610	-1.25676438
C	-6.98375503	-4.16634754	-0.09034429
C	-6.32202573	-4.93554525	1.10251779
H	-6.62119867	-6.00273488	1.07331159
H	-6.64171361	-4.53382316	2.08444825
H	-7.40498475	-4.90467873	-0.81812252
N	-5.86176918	-3.38943580	-0.66619852
H	-6.05464507	-3.09719997	-1.63094481
H	-5.62951876	3.19137347	10.32335811
C	-4.85234911	2.62695800	9.80796978
H	-4.49674945	1.84398032	10.51012500
H	-5.31415850	2.10044834	8.94972765
C	-3.65819749	3.43178086	9.30902165
C	-3.97905452	4.38256441	8.18540282
O	-2.88333296	5.08495260	7.79418557
O	-5.07178260	4.52417858	7.65046719
H	-2.89533269	2.74545726	8.86993659
H	-3.13384005	3.99837382	10.10974301
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N	-4.43985510	-7.17191086	5.48823816
C	-5.59187193	-3.44803970	6.74347254
N	-3.12123763	-4.27956883	8.01731575
C	-4.25103091	-8.33677919	6.17635474
H	-3.63362184	-6.58529717	5.20741307
H	-3.18013132	-4.41099264	6.99902278
H	-2.31334105	-4.75456286	8.57166495
H	-4.66200592	-3.06278985	10.55695574
H	-3.14831939	-4.04534352	10.57479353
H	-5.80467636	-2.57151743	8.68127721
O	-5.18044489	-9.06750766	6.54652731
C	-5.74767272	-6.82956219	4.94279416
C	-6.08868836	-5.34395563	5.11949862

C	-6.04459218	-4.90676499	6.59495750
H	-5.36321417	-4.73897332	4.53500362
H	-7.08020640	-5.13577114	4.66345453
H	-7.02010053	-5.07402502	7.10291391
H	-5.30510196	-5.55082440	7.11760431
H	-6.48109021	-7.48089533	5.46222412
H	-5.78328042	-7.09294672	3.85953605
H	-6.37523984	-2.72917425	6.43178161
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H	-2.05571570	-5.48904134	-2.44642694
C	-1.35438292	-5.21112545	-1.65971447
C	-0.45207537	-4.01214724	-1.98999243
C	-1.27070787	-2.76125156	-2.34423204
C	0.50762418	-3.70379055	-0.82527185
H	-0.74199400	-6.11207408	-1.43428462
H	-1.94941233	-5.00315574	-0.74470414
H	-0.61280606	-1.91900715	-2.64513666
H	-1.84538410	-2.42219915	-1.45806968
H	-1.99668447	-2.95163335	-3.16410234
H	1.14782504	-2.82455856	-1.04847397
H	1.16298564	-4.57128424	-0.59486516
H	-0.06551180	-3.45767838	0.09384286
H	0.16388874	-4.29972173	-2.87192223
C	0.88135125	3.22068384	5.47936375
H	1.63375077	2.85673314	6.18041725
C	-0.17726602	2.14065500	5.26694792
N	0.73314810	-1.21707123	8.17496591
C	0.82864187	-2.37965223	7.32510267
H	1.67964100	-2.25784161	6.61399320
C	-0.46687342	-2.60426795	6.51739244
H	-7.78100204	0.49594328	6.48865788
C	-6.89665420	1.16576390	6.54291878
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C	-5.61666666	0.33596323	6.28551550
H	-3.86652102	3.46325706	3.00630258
C	-3.83549042	2.58910581	2.32669192
C	-4.16406499	1.27864864	3.08624941
H	1.37971841	3.48215668	4.52107524
C	0.64740847	-1.32146295	9.53401801
O	0.78467638	-2.36428763	10.17285326
H	-4.55632617	2.72379155	1.51960623
H	-0.44298182	-3.59125124	6.01338025
H	-1.34835647	-2.59698485	7.18749545
H	0.44052616	-0.33276880	7.71852948
H	-5.56922175	-0.52507177	6.98663837
H	-5.65577705	-0.09556360	5.26318694
H	-0.99564247	2.49749154	4.60926848
H	0.26433428	1.25783386	4.76099043
H	-6.87278281	1.67421422	7.52876917
H	0.44015795	4.14475022	5.91020536
H	-2.82905798	2.54889037	1.85699532
H	-4.63540514	1.50066299	4.06452833
H	-4.83308618	0.61071390	2.51286728
H	1.05699274	-3.27121352	7.93813404
H	2.52218976	2.36673138	9.03994052

C	2.16581130	1.51269068	9.61604007
O	2.97176752	0.90275000	10.32497634
N	0.82576180	1.21928955	9.56793729
H	0.26416078	1.60961650	8.78651636
C	0.32127553	0.00838075	10.23943971
H	-0.75940698	0.06552039	10.36935895
H	0.78800974	-0.06244810	11.24105407
H	-7.40493273	4.76776291	4.72167187
C	-6.57224168	5.24216944	4.20250677
O	-6.76963445	5.69585160	3.06948718
N	-5.41314642	5.30561089	4.84836173
H	-4.52324452	5.72338906	4.37758565
H	-5.30004946	4.90040920	5.79537136
S	-0.95899174	1.54603301	6.83352034
S	-0.76228103	-1.38924085	5.13642162
S	-4.05941154	1.31564790	6.51261582
S	-2.62295642	0.35545270	3.46331974
Ni	-2.30834138	0.17490303	5.70185260
Fe	-2.82796110	-1.94861586	4.19968770
C	-2.32310128	-2.30647507	2.57634472
C	-4.61336373	-2.06337277	3.64592084
O	-2.05718817	-2.57344426	1.47705349
N	-5.73044851	-2.14931498	3.28700216
C	-2.70752823	-3.76251943	4.64071411
N	-2.62963601	-4.90333831	4.92813037
H	-0.63451388	-6.83271120	12.40801431
C	-0.67517025	-6.84495012	11.31887868
C	-1.48262305	-5.71272184	10.66040234
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O	-1.28266666	-5.56173684	9.41055365
H	0.35723700	-6.83110730	10.91379394
H	-1.12578525	-7.80949025	10.99685934
H	-3.16227449	5.61907399	7.02006675
H	-3.28166199	-1.27618854	5.90858926
H	-3.51471761	-2.09014856	5.74167779
C	-1.11163087	-8.28830112	3.03204747
C	-2.09379673	-8.78076707	4.10191021
O	-3.05938723	-9.49990107	3.81582775
C	-1.64757422	-8.51322765	1.61743395
N	-1.86546066	-8.37141184	5.39307268
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C	-2.24101859	-8.09861075	7.71875151
C	-0.74457377	-8.03704495	7.42863704
C	-0.70306939	-7.64994118	5.93836055
C	-4.13124284	-0.75935249	-1.17803994
C	-4.81266020	-0.37193854	-2.49736781
C	-4.95989543	-0.46102669	0.04294252
H	-5.93675975	-0.98033554	0.00575710
H	-4.45777310	-0.81262395	0.96734956
H	-5.14205237	0.63156388	0.15202414
H	-3.14914392	-0.23686116	-1.11181951
H	-3.88386082	-1.83700954	-1.20136428
H	-5.78605466	-0.89859221	-2.61100146
H	-5.03248816	0.71790046	-2.53514744
H	-4.18548106	-0.62154448	-3.38021753

H	-1.89646561	-9.58126250	1.45628711
H	-2.58294195	-7.93799749	1.46153644
H	-0.91080414	-8.18963078	0.85356596
H	-0.13845990	-8.81345002	3.17788921
H	-0.90054878	-7.21041620	3.20819970
H	-0.83043612	-6.55125228	5.80114586
H	0.23605310	-7.95946812	5.43420607
H	-0.24355974	-7.29432690	8.08121311
H	-0.27340595	-9.03536056	7.57190228
H	-2.63154760	-7.06730928	7.83596080
H	-2.50570106	-8.65747708	8.63708316
H	-2.86025344	-9.86394000	6.53969261

System: **I2b** (triplet)
Charge, Multiplicity: –2, 3
SCF energy: –7998.75715801 au

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.36917878
C	2.06213848	0.00000000	0.60393060
N	1.23020734	0.00898880	-0.50180264
C	1.31690173	-0.00277654	1.77947151
H	-0.92769120	-0.00329939	-0.58159549
H	3.15628176	-0.00896952	0.50252404
H	1.58092299	-0.02569872	2.84313874
H	-0.83169429	0.06496147	1.99297688
O	-9.34738477	-3.46230857	-0.15082553
C	-8.18837606	-3.28868049	0.25183825
N	-7.85864810	-2.38673053	1.22110615
C	-8.88327576	-1.68269737	1.98176083
C	-8.35530216	-1.14843551	3.32398023
O	-7.95249746	-2.16319211	4.22500115
H	-9.29294936	-0.82912703	1.38853461
H	-6.88828431	-2.37776362	1.58597593
H	-9.73625481	-2.37578450	2.15694715
H	-7.52313611	-0.42480927	3.12891970
H	-9.17519397	-0.56854773	3.80510930
H	-7.06744968	-2.46349536	3.87808504
C	-4.87669541	-5.04528753	0.52926860
C	-4.73216131	-4.21058802	-0.75768828
H	-4.40229600	-4.50236211	1.37150033
H	-4.39300358	-6.03948731	0.44714194
H	-3.77109811	-3.66047967	-0.79990835
H	-4.77440508	-4.87719474	-1.66434586
C	-7.01802770	-4.12195580	-0.28758369
C	-6.41389567	-5.12674843	0.75080657
H	-6.82025579	-6.14455024	0.58454357
H	-6.67466034	-4.82665632	1.78533369
H	-7.44730644	-4.69396094	-1.15165010
N	-5.86657987	-3.30456596	-0.64506295
H	-6.02485573	-2.63606243	-1.41528840
H	-5.69164634	3.21645753	10.28156009
C	-4.91067862	2.65176033	9.77225432
H	-4.54380447	1.88291573	10.48370351
H	-5.37175268	2.10861813	8.92479837

C	-3.72986048	3.46527853	9.25725927
C	-4.06964813	4.39761784	8.12635935
O	-3.01418596	5.17942451	7.78213022
O	-5.14754453	4.45808269	7.54564471
H	-2.95993645	2.78715350	8.81523523
H	-3.20277716	4.04305088	10.04717475
N	-5.16268725	-3.07549671	7.95314443
C	-4.09062651	-3.63150454	8.60385710
N	-3.94421878	-3.44991963	9.92954997
N	-4.45434642	-7.16937625	5.47143803
C	-5.58172118	-3.45525258	6.60301641
N	-3.15980571	-4.32508936	7.94139220
C	-4.27129783	-8.32334367	6.18053660
H	-3.64091615	-6.60365871	5.17259049
H	-3.20043087	-4.46721572	6.92452257
H	-2.35814091	-4.77876459	8.51900766
H	-4.72376202	-3.03005752	10.43520402
H	-3.24425059	-4.07712106	10.50713244
H	-5.85932984	-2.62345708	8.54494295
O	-5.20221135	-9.05391570	6.54805168
C	-5.74974632	-6.85312266	4.88032174
C	-6.09864142	-5.36488487	5.00453777
C	-6.09630355	-4.89395996	6.47079905
H	-5.35322359	-4.77704958	4.42650648
H	-7.07557842	-5.16296701	4.51583361
H	-7.10119924	-4.99658693	6.93585214
H	-5.41158701	-5.55723347	7.04251913
H	-6.49325194	-7.49133933	5.40151946
H	-5.75450667	-7.15271470	3.80622260
H	-6.32665171	-2.71602525	6.24531167
H	-4.71652436	-3.34002881	5.92018589
H	-2.03330197	-5.50078306	-2.43946533
C	-1.33734485	-5.21825827	-1.64979848
C	-0.41856039	-4.02878480	-1.96701820
C	-1.21967136	-2.75772381	-2.28803895
C	0.56617435	-3.76207597	-0.81245002
H	-0.73523942	-6.12328725	-1.41234313
H	-1.94113184	-5.00316431	-0.74151297
H	-0.55084906	-1.92074150	-2.57919135
H	-1.77812354	-2.42870927	-1.38810463
H	-1.95729047	-2.92160376	-3.10317596
H	1.21001078	-2.88330189	-1.02717339
H	1.21828434	-4.64171558	-0.62210963
H	0.01815876	-3.53663924	0.12563652
H	0.18658816	-4.30903959	-2.85664527
C	0.84718074	3.23873234	5.47265599
H	1.59455832	2.88041103	6.18048014
C	-0.21195411	2.17073962	5.26504515
N	0.59798209	-1.20169788	8.17996031
C	0.79180635	-2.35360359	7.33770971
H	1.66885144	-2.19487113	6.66626260
C	-0.44614881	-2.67063756	6.47520037
H	-7.86120183	0.60456107	6.56492426
C	-6.93505598	1.17613810	6.50120353
H	-7.06002116	1.93275502	5.72666503

C	-5.74276691	0.23301260	6.28036401
H	-4.01644457	3.36550311	3.04611035
C	-3.85324711	2.59052279	2.29706429
C	-4.07552614	1.20171879	2.96445867
H	1.22108718	3.56994139	4.50345598
C	0.59866809	-1.28769983	9.54248782
O	0.81558740	-2.31434585	10.18583621
H	-4.56889031	2.72143942	1.48522605
H	-0.33211105	-3.66111958	5.99058497
H	-1.35188478	-2.71495356	7.11168522
H	0.28485269	-0.32810020	7.71926139
H	-5.82124545	-0.63577415	6.96638403
H	-5.74160006	-0.19162186	5.25275618
H	-0.98998281	2.52220028	4.55701606
H	0.22775620	1.25697421	4.81240776
H	-6.81926052	1.73021497	7.45683944
H	0.38385480	4.13191559	5.95083374
H	-2.83487541	2.69729313	1.87144026
H	-4.68913937	1.29688791	3.87939447
H	-4.58700596	0.49563394	2.28875939
H	1.01829664	-3.24324571	7.95452197
H	2.46836875	2.40081399	9.04582371
C	2.11013553	1.54813824	9.62275317
O	2.90960104	0.95113138	10.35030794
N	0.77236440	1.24586069	9.55502586
H	0.21832121	1.62575867	8.75938538
C	0.26466527	0.04281611	10.24112323
H	-0.81685291	0.09874729	10.36468460
H	0.73136120	-0.01794758	11.24304204
H	-7.43860707	4.77139248	4.66492454
C	-6.60386504	5.24556681	4.14878894
O	-6.79660266	5.69180980	3.01211817
N	-5.44839468	5.31278111	4.80083224
H	-4.55663938	5.73061342	4.33355027
H	-5.34396093	4.91476816	5.75357095
S	-1.05566056	1.69613282	6.81793216
S	-0.71102899	-1.44500078	5.12080057
S	-4.14650877	1.07574678	6.63388795
S	-2.51846539	0.35194054	3.47105015
Ni	-2.36915633	0.15542970	5.72537224
Fe	-2.73846683	-1.96910520	4.03867478
C	-2.17836739	-2.34985912	2.42852602
C	-4.46605324	-2.19075602	3.38613886
O	-1.94236195	-2.65430218	1.33297968
N	-5.54991004	-2.41037757	2.98934681
C	-2.61666519	-3.78882614	4.50142985
N	-2.58245355	-4.92266782	4.81863294
H	-0.69220533	-6.79262237	12.42702767
C	-0.72669844	-6.80827314	11.33776544
C	-1.54966202	-5.69730127	10.65778960
O	-2.40693520	-5.06498971	11.34581023
O	-1.32786060	-5.54685532	9.41166395
H	0.30824362	-6.77762398	10.94025611
H	-1.15621487	-7.78331610	11.01814307
H	-3.29450394	5.69557872	6.99654465

H	-3.40866545	-1.32779243	5.56742084
H	-3.51041478	-2.18233319	5.47716419
C	-1.11517566	-8.27998977	3.05350391
C	-2.10107318	-8.77342401	4.11949746
O	-3.06398035	-9.49514649	3.83060075
C	-1.62994578	-8.53489680	1.63622270
N	-1.88132135	-8.35919868	5.41107652
C	-2.83321986	-8.74180286	6.46550942
C	-2.27012150	-8.08078654	7.73453749
C	-0.77289764	-8.01346757	7.45106926
C	-0.72384170	-7.63261487	5.95981928
C	-4.12354783	-0.76961652	-1.19817917
C	-4.73456092	-0.26737169	-2.51396003
C	-4.95968153	-0.46919981	0.01703109
H	-6.00207237	-0.82904256	-0.08175014
H	-4.55359146	-0.96256923	0.92090904
H	-5.00290177	0.62672512	0.20179074
H	-3.11432839	-0.31395087	-1.07707023
H	-3.92666011	-1.85401746	-1.27494884
H	-5.72921307	-0.73153428	-2.70166062
H	-4.89760027	0.83254891	-2.49075121
H	-4.08741142	-0.49652877	-3.38729592
H	-1.85388604	-9.61007401	1.48569078
H	-2.57528709	-7.98180770	1.46188727
H	-0.89082538	-8.20571016	0.87698118
H	-0.13373165	-8.78350934	3.21835253
H	-0.92780120	-7.19572832	3.21796571
H	-0.85160461	-6.53497266	5.81536731
H	0.21879492	-7.94234738	5.46243207
H	-0.27793008	-7.26682390	8.10362039
H	-0.29872130	-9.00948191	7.60073684
H	-2.66666049	-7.05185099	7.84911440
H	-2.53638802	-8.63955056	8.65246648
H	-2.88259255	-9.84877755	6.55595820

HOMO-LUMO DIAGRAMS

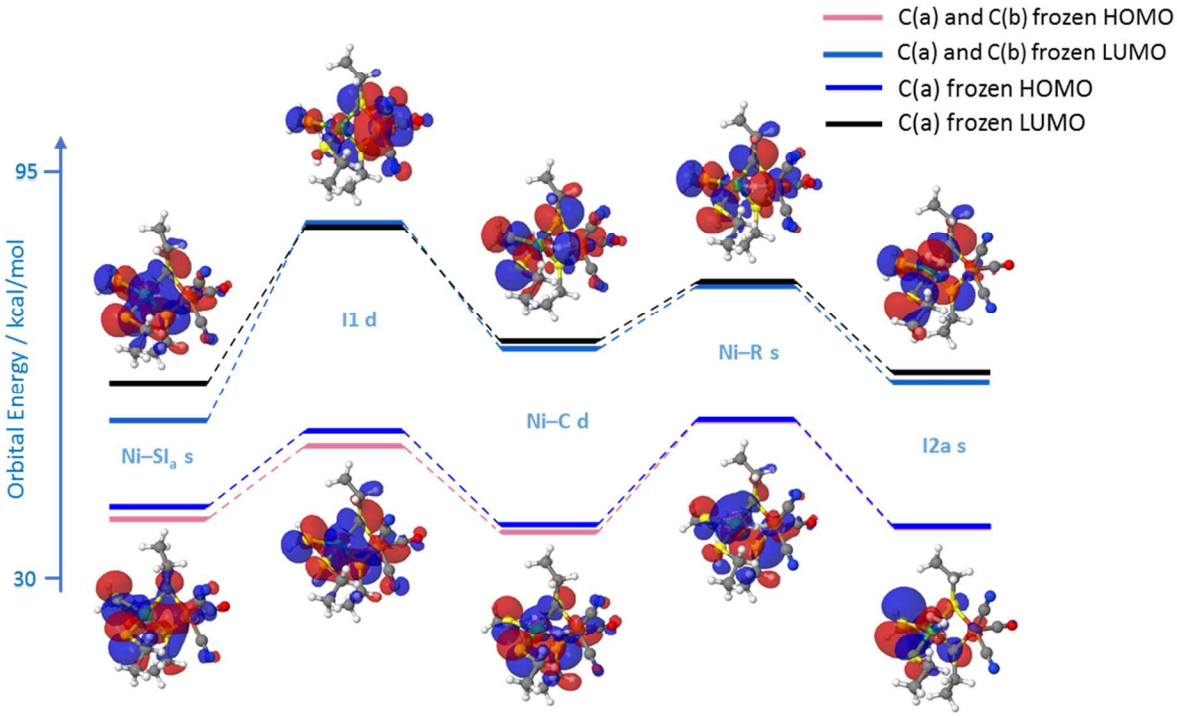

Fig. S1. HOMO and LUMO diagram for the partial and totally frozen models along the HER path. The HOMO and LUMO distributions of the totally frozen models are also shown.