

Supplementary Information

Table S1. Experimental and calculated g-tensor for large Ni-A models with varying bridging ligands.

	g_z	g_y	g_x
Experimental			
Ni-A	2.01	2.24	2.32
Ni-B	2.01	2.16	2.33
Calculated			
OH α	2.04	2.14	2.20
OH β	2.04	2.14	2.19
OOH $^-$	2.05	2.13	2.15
S=O, OH α	2.04	2.18	2.19
H $_2$ O	2.07	2.08	2.18
O $^{2-}$	2.08	2.16	2.20
OH α rotated Cys549	2.04	2.15	2.19

Table S2. Mulliken spin populations of selected atoms in the large OH α model. The numbering of the atoms according to the geometry as specified for the OH α model.

Ni	0.81	S26 Cys-549	0.24
Fe	-0.01	S34 Cys-84	-0.02
S10 Cys-81	-0.02	O3 OH $^-$ bridge	0.01
S18 Cys-546	-0.01		

Cartesian Coordinates for Geometry Optimized Small Models (Angstroems)

OOH Model

Ni	58.181945	47.547701	85.300216
Fe	57.511263	50.068614	86.613667
O	57.391089	48.040960	87.045782
C	55.735211	50.534470	87.066094
N	54.618261	50.867931	87.282594
C	58.134115	50.398770	88.371942
N	58.596845	50.598131	89.445524
C	57.816259	51.683507	86.139952
O	58.024236	52.794120	85.803847
S	59.470473	46.671528	83.759636
C	60.661482	47.958701	83.178382
H	61.336985	48.254589	84.003023
H	60.089742	48.865504	82.901493
C	61.452790	47.423572	81.981015
H	62.173215	48.178456	81.595520
H	62.023424	46.514172	82.261799
H	60.769928	47.139729	81.154498
S	56.880298	45.689976	85.106736
C	57.633885	44.695034	86.476941
H	57.875040	45.390171	87.304384
H	56.841154	44.011475	86.849535
C	58.867056	43.901998	86.039082
H	59.317352	43.343975	86.891000
H	58.603487	43.177034	85.242345
H	59.627231	44.587854	85.615448
S	59.558892	49.224562	85.944424
C	60.328287	48.410400	87.413664
H	60.603188	49.224073	88.111064
H	59.525359	47.834056	87.907696
C	61.511796	47.536966	86.997994
H	62.326732	48.146254	86.555340
H	61.194657	46.797439	86.234359
H	61.929849	46.987873	87.869644
S	56.909800	49.356428	84.453358
C	55.150866	48.823190	84.542870
H	54.549373	49.742444	84.675253
H	55.037754	48.244973	85.476489
C	54.749165	48.019982	83.306468
H	54.903872	48.606359	82.376864
H	53.678018	47.724315	83.356161
H	55.354916	47.096116	83.227832
O	56.069458	47.504166	87.357117
H	56.025081	46.784104	86.649442

H₂O Model

Ni	59.216145	47.743041	85.279003
Fe	57.952497	50.319783	86.864937
O	56.831352	48.669037	87.708885
C	56.220597	51.057012	86.699173
N	55.057248	51.277198	86.632641
C	58.091639	50.805694	88.684478
N	58.141081	50.902091	89.865221
C	58.759878	51.727633	86.319034
O	59.302894	52.699381	85.958989
S	59.704933	47.003067	83.323993
C	59.217887	48.135059	81.947429
H	60.121574	48.714719	81.673374
H	58.474755	48.859563	82.330165
C	58.686269	47.354994	80.743468
H	58.455917	48.039041	79.899634
H	59.426363	46.611031	80.387223
H	57.760057	46.806338	81.002057
S	59.397171	45.895237	86.399511
C	58.607857	44.586476	85.363690
H	57.551159	44.864642	85.187776
H	59.105762	44.586813	84.373794
C	58.716084	43.223751	86.051143
H	58.243394	42.428828	85.437180
H	59.776574	42.949479	86.215600
H	58.217553	43.235235	87.040587
S	59.898607	49.074868	86.944614
C	59.992244	48.202696	88.568758
H	59.745429	48.967937	89.329045
H	59.205200	47.423577	88.573453
C	61.374059	47.585552	88.781893
H	62.166544	48.357695	88.738044
H	61.587775	46.821615	88.010347
H	61.426090	47.093235	89.775083
S	57.850278	49.440633	84.723319
C	56.281136	48.450305	84.727896
H	55.488832	49.191606	84.950165
H	56.345375	47.749494	85.580320
C	56.036601	47.710862	83.416690
H	55.959087	48.411805	82.563003
H	55.088730	47.136982	83.473058
H	55.969627	49.145415	87.612581
H	56.860595	46.999699	83.211001
H	57.110706	48.858058	88.636817

O²⁻ Model

Ni	58.327267	47.502589	85.094526
Fe	57.744251	49.718315	86.777250
O	57.425014	47.830600	86.650128
C	55.939416	50.118233	87.153637
N	54.798345	50.396026	87.347456
C	58.216897	49.611135	88.602497
N	58.551765	49.561516	89.743256
C	58.178953	51.387955	86.698897
O	58.500843	52.531572	86.617337
S	59.172953	46.923268	83.014841
C	59.925560	48.493381	82.436631
H	60.696027	48.811992	83.170299
H	59.143508	49.282414	82.447470
C	60.531399	48.344446	81.036023
H	60.995511	49.290617	80.663710
H	61.308102	47.548843	81.031825
H	59.748162	48.031312	80.311804
S	58.498666	45.264403	85.539805
C	57.603470	45.058092	87.127716
H	57.268223	46.099550	87.374878
H	56.707103	44.412100	86.977958
C	58.489792	44.482352	88.238438
H	57.922266	44.331233	89.189363
H	58.938523	43.505732	87.945265
H	59.324497	45.178264	88.450680
S	59.965912	48.944229	86.017734
C	60.547556	47.860732	87.384256
H	60.946817	48.508843	88.190518
H	59.637262	47.373799	87.779434
C	61.566172	46.830418	86.892420
H	62.437744	47.323257	86.407453
H	61.072097	46.166250	86.154332
H	61.945027	46.199427	87.732495
S	57.301573	49.476157	84.413721
C	55.601531	48.773892	84.320672
H	54.875398	49.587485	84.519431
H	55.546048	48.068568	85.172468
C	55.374728	48.083286	82.972629
H	55.396412	48.817638	82.137056
H	54.393029	47.552172	82.938438
H	56.192176	47.355619	82.782960

OH-a model

Ni	58.174677	47.392177	85.098313
Fe	57.730524	49.763481	86.747995
O	57.314198	47.761524	86.800059
C	55.907380	50.111576	87.099941
N	54.736479	50.242794	87.247913
C	58.206188	49.777721	88.577226
N	58.547616	49.781209	89.713060
C	58.130671	51.419056	86.585849
O	58.401041	52.561622	86.467109
S	58.904197	46.857685	83.074735
C	59.779442	48.361852	82.471722
H	60.548605	48.637409	83.219586
H	59.059982	49.203195	82.429116
C	60.407441	48.098080	81.100324
H	60.946726	48.992856	80.718458
H	61.126371	47.254518	81.150747
H	59.628856	47.822154	80.359077
S	58.580760	45.246037	85.556675
C	57.837382	44.902449	87.210239
H	57.503425	45.882758	87.606767
H	56.940968	44.258030	87.079888
C	58.840522	44.234785	88.156856
H	58.376797	43.997698	89.141086
H	59.238755	43.291322	87.727409
H	59.702317	44.905206	88.337219
S	59.801711	48.898440	86.082613
C	60.395597	47.865073	87.483600
H	60.690525	48.559586	88.293145
H	59.523284	47.299994	87.856366
C	61.527706	46.940408	87.038979
H	62.368686	47.516722	86.599730
H	61.147447	46.230252	86.277626
H	61.922424	46.353364	87.897909
S	57.315096	49.403992	84.465989
C	55.548971	48.956271	84.174063
H	54.937124	49.838082	84.443041
H	55.263038	48.159484	84.886006
C	55.359122	48.498433	82.726577
H	55.576253	49.326201	82.021049
H	54.318488	48.150391	82.543685
H	56.339514	47.749571	86.714281
H	56.065519	47.675086	82.495176

OH-b model

Ni	58.325502	47.478474	85.202096
Fe	57.680376	49.879495	86.680446
O	57.248954	47.879542	86.754153
C	55.870253	50.318968	87.008472
N	54.727964	50.601438	87.158622
C	58.116843	49.825923	88.515416
N	58.424372	49.683905	89.653287
C	58.095255	51.530923	86.509451
O	58.388370	52.668350	86.394864
S	59.106163	46.856177	83.225440
C	59.787780	48.396295	82.477429
H	60.454144	48.871808	83.223857
H	58.959644	49.108298	82.291385
C	60.546425	48.073542	81.187131
H	60.966897	48.991015	80.719036
H	61.381295	47.371142	81.387723
H	59.877829	47.585843	80.447315
S	58.972485	45.444739	85.865447
C	58.030293	45.066843	87.409683
H	58.558962	45.489496	88.290989
H	57.043468	45.564127	87.353631
C	57.870567	43.552345	87.578758
H	57.324121	43.296640	88.513912
H	57.316663	43.125674	86.718647
H	58.860801	43.052686	87.611107
S	59.828717	49.115432	86.040073
C	60.646199	48.281592	87.463731
H	60.912256	49.069033	88.194447
H	59.905009	47.634654	87.965820
C	61.848857	47.463083	86.995309
H	62.575659	48.096307	86.445930
H	61.499610	46.656176	86.321156
H	62.374757	46.996831	87.858133
S	57.271341	49.373578	84.440980
C	55.561206	48.687732	84.373747
H	54.869432	49.533529	84.547918
H	55.461984	48.015589	85.245511
C	55.322090	47.971349	83.043672
H	55.371599	48.681570	82.192250
H	54.324057	47.480605	83.025489
H	56.104627	47.203478	82.875273
H	57.694896	47.602124	87.577837

Volbeda S model

C	6.258210	0.804389	6.505860
C	7.205992	1.178513	7.649768
S	6.374339	1.246517	9.291079
C	11.044679	-2.033731	9.524973
C	9.913698	-3.000654	9.867099
S	8.473099	-2.722472	8.737698
O	8.154665	-1.146814	9.093378
C	3.009432	-1.618208	12.838425
C	4.522945	-1.534437	12.621780
S	4.963403	-0.114914	11.529195
C	2.975407	-0.992755	8.563301
C	3.683393	-2.288064	8.958042
S	5.453269	-2.223113	8.465980
Fe	6.678143	-3.893405	9.552277
C	5.126564	-4.654747	10.334796
N	4.145236	-5.099859	10.828236
C	7.777391	-5.028010	10.595040
N	8.513376	-5.685640	11.254063
C	6.588498	-5.006102	8.249165
O	6.517688	-5.766989	7.350970
Ni	6.525407	-0.819560	10.107722
O	6.696281	-2.508015	11.015968
H	6.778574	0.821615	5.519626
H	5.393573	1.498656	6.459311
H	5.862872	-0.215983	6.676701
H	7.658281	2.181222	7.483656
H	8.018990	0.432461	7.741778
H	11.429820	-2.215470	8.500575
H	11.890206	-2.132451	10.238744
H	10.182537	-4.068473	9.766698
H	9.553553	-2.862676	10.903425
H	2.751010	-2.477403	13.494859
H	2.488950	-1.763600	11.872375
H	2.606482	-0.690928	13.299379
H	5.046953	-1.425407	13.595798
H	4.917698	-2.451990	12.146449
H	1.911177	-1.013214	8.886033
H	3.003540	-0.833473	7.465560
H	3.474376	-0.133701	9.052780
H	3.242228	-3.180808	8.472929
H	3.637122	-2.465983	10.044038
H	10.664355	-0.994712	9.566045
H	7.530663	-2.584759	11.517263

Cartesian Coordinates for Geometry Optimized Large Models (Angstroems)

OOH Model

Ni	57.942657	47.213736	85.018751
Fe	57.475330	49.490793	86.662039
O	56.578415	47.730400	86.279899
C	55.737264	50.005536	87.096982
N	54.625405	50.218273	87.415075
C	57.830756	49.065047	88.420212
N	58.030701	48.683739	89.518880
C	58.029121	51.104543	86.827683
O	58.342876	52.215446	86.987774
S	58.688517	46.576851	83.029553
C	59.464733	48.049346	82.256243
H	59.856504	48.676234	83.077953
H	58.692613	48.646889	81.733410
C	60.594032	47.640669	81.310369
H	61.035246	48.533047	80.819866
H	61.397336	47.116828	81.863421
H	60.237146	46.961454	80.514294
S	58.643554	45.285825	85.795881
C	58.089229	45.202880	87.544364
H	58.372307	46.144067	88.054328
H	56.991175	45.150444	87.561387
C	58.671699	44.019532	88.315733
H	58.348358	44.095830	89.372678
H	58.327716	43.049965	87.904055
H	59.780582	44.019594	88.299540
S	59.576071	48.613557	85.952726
C	60.722999	47.941882	87.244172
H	60.627354	48.614647	88.116313
H	60.325215	46.957085	87.544183
C	62.197482	47.815237	86.787498
H	62.619739	48.799235	86.505894
H	62.282905	47.137851	85.916693
H	62.802237	47.398210	87.616699
S	57.198636	49.354891	84.332902
C	55.383249	49.281415	84.010352
H	54.968994	50.229405	84.400517
H	54.966103	48.463529	84.624864
C	55.016466	49.114833	82.524202
H	55.416736	49.964643	81.932333
H	53.914599	49.108475	82.423837
N	55.486442	47.849739	81.983358
H	56.462068	47.572295	82.165646
C	54.629806	46.909464	81.485954
O	53.412815	47.071628	81.365562
C	55.310749	45.576321	81.109317
H	54.618611	45.050831	80.429385
H	55.435690	44.967797	82.025935
N	56.609286	45.724205	80.477460

H	57.433328	45.751242	81.096733
C	56.698662	46.157936	79.182172
O	55.701769	46.318286	78.467715
C	58.111648	46.439855	78.681637
H	58.379247	47.492616	78.899752
H	58.136349	46.302991	77.586541
H	58.867791	45.785992	79.153398
O	51.290404	47.484983	84.802228
O	49.597533	46.164067	85.516411
C	50.088539	47.078793	84.779401
C	49.122932	47.780945	83.803824
H	49.646297	48.039977	82.865023
H	48.770464	48.726731	84.262370
H	48.241414	47.148899	83.592082
H	52.304745	47.149186	86.092766
N	52.846937	46.922172	86.981564
H	53.774548	47.328196	87.145637
C	52.339607	46.003894	87.813535
N	51.229919	45.325643	87.463238
H	50.630749	45.642254	86.620253
H	50.733201	44.829401	88.202441
N	52.946833	45.709643	89.002237
H	52.451840	45.035067	89.584284
C	53.823692	46.648853	89.706055
H	54.321511	46.090404	90.520089
H	54.624769	46.961716	89.014392
C	53.085738	47.890049	90.224196
H	52.404136	47.615752	91.055977
H	52.442707	48.260883	89.402271
C	54.025889	49.028002	90.638248
H	54.534279	48.801781	91.597858
H	54.823126	49.144657	89.875253
C	53.275722	50.366429	90.767665
H	53.993922	51.172894	91.022401
H	52.517014	50.322941	91.571308
N	52.565179	50.714904	89.548807
H	53.125374	50.759308	88.681067
C	51.206930	50.798319	89.492411
O	50.453327	50.597383	90.455016
C	50.633133	51.106191	88.094454
H	49.639634	51.563171	88.270913
C	50.544788	49.854114	87.188186
H	51.366902	49.153366	87.431281
H	49.592871	49.309088	87.316161
C	50.759898	50.410109	85.770318
H	51.071052	49.615802	85.067910
H	49.828178	50.883707	85.397998
C	51.836569	51.478662	85.990387
H	52.849883	51.025955	86.005473
H	51.813657	52.274586	85.224005
N	51.492601	52.017821	87.319405
C	51.831600	53.234815	87.842208

O	51.353073	53.627024	88.918634
C	52.904062	54.031948	87.104230
H	52.809676	55.077757	87.451341
H	52.740160	54.024534	86.008859
C	54.303759	53.473892	87.432890
H	54.469580	53.468743	88.527776
H	54.433758	52.436265	87.080925
H	55.096579	54.098432	86.976315
H	58.046901	47.249377	90.520711
O	58.266628	46.455725	91.084261
C	59.551610	46.678722	91.631506
H	59.934816	45.704792	91.996059
H	60.268569	47.035093	90.853192
C	59.556609	47.665756	92.808503
H	60.559076	47.662995	93.290304
H	58.827092	47.341213	93.576751
N	59.214152	49.011057	92.367012
H	59.127864	49.180424	91.357791
C	58.764699	49.960963	93.232721
O	58.645259	49.773580	94.448697
C	58.336398	51.285034	92.575574
H	58.272820	52.016673	93.404117
C	56.998037	51.171712	91.799004
H	56.131864	51.364673	92.456336
H	56.888569	50.153993	91.378212
C	57.136559	52.184983	90.646820
H	56.915607	53.211877	91.000376
H	56.470039	51.960225	89.793107
C	58.618067	52.065611	90.264652
H	58.763850	51.229007	89.555154
H	59.021858	52.981632	89.799423
N	59.282655	51.782054	91.548271
C	60.571226	52.092561	91.903707
O	60.970036	51.897265	93.061993
C	61.511307	52.649357	90.821691
H	61.089576	53.573248	90.375808
H	62.441409	52.927097	91.352243
C	61.830930	51.633265	89.693786
H	60.903249	51.457498	89.109903
C	62.288210	50.282613	90.268700
H	62.538529	49.571950	89.457026
H	63.189258	50.407823	90.903082
H	61.501838	49.819049	90.894360
C	62.877653	52.216490	88.731110
H	63.836914	52.404433	89.255994
H	63.083492	51.516285	87.897505
H	62.537697	53.175769	88.294704
C	58.643450	56.266527	90.155414
H	59.068931	57.290797	90.140489
H	57.831875	56.250466	90.909024
H	59.437371	55.583604	90.517817
C	58.119935	55.859793	88.768664

H	57.251145	56.501707	88.509681
H	57.722107	54.822344	88.807429
C	59.151708	55.947869	87.620814
H	59.527456	56.996123	87.589822
C	60.361640	55.023528	87.846433
H	60.030220	53.971742	87.957389
H	61.051424	55.053945	86.980344
H	60.936611	55.301646	88.751405
C	58.484136	55.643188	86.267270
H	59.218625	55.683879	85.439268
H	57.667005	56.360688	86.050562
H	58.053695	54.622786	86.265768
C	60.868915	54.214538	82.008458
H	61.922583	54.495698	81.807186
H	60.321803	55.152717	82.232838
H	60.444641	53.784803	81.082045
C	60.773618	53.240810	83.150912
N	61.263133	53.543725	84.414408
C	61.020186	52.470430	85.162363
H	61.253311	52.360641	86.224882
N	60.400439	51.484883	84.446905
H	60.106281	50.564160	84.816357
C	60.228101	51.957088	83.158848
H	59.733357	51.352367	82.381975
O	55.971632	47.026016	87.432026
H	56.487422	47.415184	88.177071

H₂O Model

Ni	57.950388	47.179535	85.011958
Fe	57.497361	49.434463	86.707041
O	56.817593	47.506903	86.547335
C	55.738102	49.920345	87.059730
N	54.599671	50.133045	87.268579
C	57.888253	49.074337	88.479405
N	58.170046	48.775552	89.580901
C	57.983797	51.070171	86.869920
O	58.267574	52.183761	87.049806
S	58.791465	46.546009	83.076375
C	59.954946	47.893404	82.668763
H	60.716228	47.930928	83.468680
H	59.410816	48.855871	82.688428
C	60.594032	47.640669	81.310369
H	61.362395	48.410895	81.100189
H	61.087821	46.650115	81.269661
H	59.847243	47.683303	80.497348
S	58.533939	45.213293	85.782507
C	58.027614	45.184296	87.565883
H	58.321303	46.141019	88.037654
H	56.922509	45.122778	87.639782
C	58.671699	44.019532	88.315733
H	58.422869	44.106660	89.391315

H	58.323087	43.039265	87.939251
H	59.774199	44.051215	88.220781
S	59.590998	48.631473	85.990752
C	60.724504	47.899762	87.258805
H	60.618641	48.523555	88.165601
H	60.330335	46.898029	87.501256
C	62.197482	47.815237	86.787498
H	62.602139	48.816910	86.547662
H	62.292325	47.176586	85.889083
H	62.812984	47.374370	87.595056
S	57.192028	49.304126	84.353853
C	55.376369	49.241657	84.018172
H	54.959292	50.176305	84.436190
H	54.931792	48.404555	84.586259
C	55.016466	49.114833	82.524202
H	55.407031	49.981947	81.954589
H	53.914070	49.097456	82.433394
N	55.500526	47.868065	81.948434
H	56.497284	47.641705	82.061398
C	54.649820	46.876541	81.538301
O	53.424350	46.989818	81.508860
C	55.343215	45.553150	81.140508
H	54.638837	45.020244	80.479763
H	55.490118	44.947072	82.055933
N	56.628232	45.701574	80.480581
H	57.461540	45.736767	81.081180
C	56.703021	46.141252	79.185199
O	55.701518	46.295424	78.478661
C	58.111648	46.439855	78.681637
H	58.324332	47.518509	78.819490
H	58.156251	46.226338	77.599272
H	58.892737	45.858547	79.204054
O	51.417487	47.981894	84.503478
O	50.344493	46.042815	84.945597
C	50.403259	47.216085	84.461455
C	49.122932	47.780945	83.803824
H	49.373397	48.275832	82.846787
H	48.685887	48.551064	84.470234
H	48.375685	46.985233	83.636590
H	52.607238	47.696116	85.612277
N	53.284245	47.499857	86.415342
H	53.701534	48.309809	86.893995
C	53.256152	46.273996	86.962504
N	52.517526	45.323308	86.367678
H	51.705163	45.616617	85.720445
H	52.431137	44.418300	86.829462
N	54.010771	45.960620	88.058950
H	53.864376	45.027660	88.441958
C	54.610819	46.941392	88.968450
H	55.283970	46.387674	89.647761
H	55.277127	47.615976	88.386382
C	53.583946	47.778982	89.735851

H	53.014347	47.123276	90.423594
H	52.850389	48.180984	89.009294
C	54.203098	48.961180	90.495792
H	54.663405	48.629867	91.447485
H	55.022805	49.397430	89.891515
C	53.162509	50.053376	90.791324
H	53.651300	50.902585	91.313662
H	52.361387	49.677809	91.455153
N	52.507695	50.523305	89.578772
H	53.101541	50.719231	88.763274
C	51.154593	50.624675	89.464320
O	50.358465	50.302730	90.354771
C	50.633133	51.106191	88.094454
H	49.666786	51.598607	88.319504
C	50.454454	49.973011	87.059310
H	51.247984	49.209559	87.180779
H	49.480696	49.463969	87.167027
C	50.643313	50.689768	85.711793
H	50.878387	49.969332	84.907756
H	49.732520	51.264599	85.447880
C	51.800373	51.650019	86.016707
H	52.776295	51.126116	85.945561
H	51.824297	52.529959	85.349427
N	51.531488	52.049598	87.411177
C	51.873247	53.218800	88.035460
O	51.422267	53.500258	89.156184
C	52.902451	54.102595	87.336904
H	52.874146	55.078206	87.855165
H	52.635616	54.279080	86.276110
C	54.303759	53.473892	87.432890
H	54.564024	53.262822	88.488528
H	54.370346	52.516718	86.887489
H	55.076494	54.155718	87.028179
H	58.124968	47.247081	90.463650
O	58.326633	46.456192	91.032492
C	59.595418	46.684335	91.625963
H	59.969213	45.710022	91.997126
H	60.334222	47.047618	90.872827
C	59.556609	47.665756	92.808503
H	60.541891	47.669143	93.322452
H	58.807205	47.325117	93.551215
N	59.218753	49.011769	92.362322
H	59.075253	49.160786	91.354686
C	58.782769	49.963400	93.231619
O	58.684961	49.783020	94.450118
C	58.336398	51.285034	92.575574
H	58.263885	52.008308	93.411126
C	56.997513	51.166966	91.806105
H	56.130024	51.322167	92.471555
H	56.909209	50.159590	91.358532
C	57.112062	52.214993	90.682892
H	56.870264	53.226902	91.063032

H	56.445575	52.001263	89.826273
C	58.594837	52.135682	90.289579
H	58.751883	51.330734	89.548417
H	58.977586	53.077796	89.859706
N	59.272395	51.807808	91.553756
C	60.573825	52.075257	91.896565
O	60.985561	51.831994	93.040439
C	61.511307	52.649357	90.821691
H	61.112661	53.606984	90.427925
H	62.457724	52.873322	91.348047
C	61.786402	51.679470	89.641867
H	60.850953	51.567270	89.054627
C	62.195517	50.285084	90.147209
H	62.430542	49.611937	89.299935
H	63.095294	50.347049	90.791995
H	61.389933	49.814336	90.742277
C	62.852283	52.268356	88.702917
H	63.822261	52.380414	89.228987
H	63.018828	51.608984	87.827830
H	62.555592	53.265387	88.323767
C	58.643450	56.266527	90.155414
H	59.101378	57.275085	90.103640
H	57.845367	56.296504	90.922650
H	59.421129	55.566638	90.521948
C	58.084048	55.837998	88.788339
H	57.216037	56.483111	88.535317
H	57.678055	54.805110	88.857921
C	59.090647	55.891514	87.614799
H	59.467514	56.937006	87.545923
C	60.304592	54.971809	87.838872
H	59.973549	53.924686	87.987066
H	60.973897	54.978224	86.956191
H	60.898788	55.273420	88.723487
C	58.392635	55.548371	86.285368
H	59.111218	55.542593	85.442639
H	57.582265	56.269917	86.057535
H	57.947305	54.535923	86.332511
C	60.868915	54.214538	82.008458
H	61.919024	54.547631	81.885053
H	60.257882	55.125247	82.170380
H	60.542465	53.746744	81.061259
C	60.734218	53.258981	83.159946
N	61.096012	53.610899	84.453636
C	60.846318	52.541492	85.202662
H	60.986448	52.464322	86.283847
N	60.342203	51.511510	84.458316
H	60.072989	50.585663	84.822008
C	60.259793	51.949334	83.147787
H	59.873913	51.316177	82.351336
H	56.625989	46.576584	86.305736
H	56.248139	47.682163	87.329213

O²⁻ Model

Ni	57.888928	47.271637	85.048054
Fe	57.486699	49.450931	86.719488
O	56.971679	47.615964	86.549367
C	55.729890	49.880916	87.059022
N	54.584773	50.114550	87.243473
C	57.914916	49.074944	88.469519
N	58.225907	48.790625	89.573931
C	57.967808	51.108131	86.863821
O	58.247516	52.241818	87.014570
S	58.633857	46.595148	82.993303
C	59.460629	48.051069	82.250142
H	59.855735	48.657170	83.088191
H	58.712429	48.680039	81.726888
C	60.594032	47.640669	81.310369
H	61.074120	48.530494	80.848203
H	61.372088	47.077503	81.862399
H	60.231811	46.991199	80.491614
S	58.428503	45.219750	85.774544
C	57.915419	45.109308	87.533382
H	58.068171	46.106133	87.987167
H	56.823664	44.931533	87.578392
C	58.671699	44.019532	88.315733
H	58.374038	44.056191	89.383564
H	58.469545	43.003223	87.919568
H	59.765967	44.190153	88.265526
S	59.664271	48.681680	85.878977
C	60.689651	47.775736	87.109508
H	60.474772	48.204737	88.106052
H	60.317598	46.733455	87.100743
C	62.197482	47.815237	86.787498
H	62.582083	48.854864	86.783772
H	62.401141	47.373907	85.792126
H	62.765588	47.239006	87.546992
S	57.144400	49.362948	84.354238
C	55.340602	49.269474	84.019777
H	54.878357	50.193310	84.415507
H	54.928434	48.420772	84.590953
C	55.016466	49.114833	82.524202
H	55.440656	49.964959	81.948317
H	53.918469	49.104528	82.385737
N	55.513867	47.848923	82.004724
H	56.466307	47.555483	82.294007
C	54.679804	46.907819	81.477462
O	53.474808	47.078255	81.262322
C	55.374604	45.564378	81.161681
H	54.689002	44.994162	80.512635
H	55.527730	45.007040	82.106753
N	56.661698	45.716687	80.505728
H	57.467998	45.903455	81.140234
C	56.725753	46.043291	79.181952

O	55.737426	46.034976	78.433512
C	58.111648	46.439855	78.681637
H	58.282967	47.516252	78.881042
H	58.162043	46.277090	77.590803
H	58.916484	45.870950	79.182321
O	51.456022	48.060808	84.300753
O	50.543977	46.017525	84.630313
C	50.492806	47.233760	84.271986
C	49.122932	47.780945	83.803824
H	49.250082	48.439940	82.924279
H	48.682123	48.393887	84.615711
H	48.423515	46.959125	83.563583
H	52.656671	47.770591	85.456698
N	53.297793	47.566670	86.274211
H	53.864677	48.335650	86.669656
C	53.483236	46.292285	86.629884
N	52.885757	45.314363	85.900963
H	52.053346	45.595394	85.299674
H	52.801252	44.402455	86.349541
N	54.229839	45.952811	87.709117
H	54.465528	44.968544	87.810803
C	54.851971	46.913958	88.626978
H	55.535612	46.342666	89.280211
H	55.506806	47.592739	88.045223
C	53.799744	47.677805	89.445495
H	53.262487	46.976803	90.120061
H	53.040835	48.072556	88.742900
C	54.368343	48.864190	90.236600
H	54.872647	48.522415	91.163208
H	55.145595	49.366468	89.629931
C	53.278041	49.883847	90.609590
H	53.733863	50.725077	91.176713
H	52.507490	49.434786	91.265795
N	52.577077	50.399790	89.436689
H	53.142963	50.537318	88.578960
C	51.230090	50.588520	89.423526
O	50.481627	50.326677	90.378120
C	50.633133	51.106191	88.094454
H	49.683805	51.601976	88.377139
C	50.410861	49.985706	87.048614
H	51.173124	49.191099	87.172660
H	49.416302	49.516341	87.154325
C	50.631400	50.689678	85.698395
H	50.872316	49.960595	84.901799
H	49.733011	51.276422	85.414160
C	51.799720	51.631601	86.012116
H	52.768716	51.090925	85.972326
H	51.851482	52.503411	85.335392
N	51.511457	52.054386	87.395356
C	51.869911	53.215998	88.017255
O	51.431452	53.503779	89.144098
C	52.899103	54.090756	87.308457

H	52.859528	55.079055	87.803273
H	52.639640	54.239558	86.241309
C	54.303759	53.473892	87.432890
H	54.568042	53.324043	88.497589
H	54.378240	52.483083	86.950475
H	55.073207	54.134957	86.988599
H	58.067231	47.318613	90.468566
O	58.209792	46.533792	91.079886
C	59.503250	46.680396	91.627882
H	59.838899	45.686865	91.991329
H	60.234623	47.006474	90.851368
C	59.556609	47.665756	92.808503
H	60.570460	47.648997	93.266695
H	58.839839	47.355204	93.595576
N	59.222796	49.013241	92.362671
H	59.060820	49.148988	91.348314
C	58.790068	49.965061	93.230971
O	58.703788	49.791851	94.454623
C	58.336398	51.285034	92.575574
H	58.253623	52.009112	93.409926
C	57.006203	51.153446	91.788253
H	56.129635	51.318311	92.440235
H	56.925936	50.141156	91.349423
C	57.133269	52.182358	90.649209
H	56.891843	53.202308	91.011297
H	56.477844	51.953080	89.788954
C	58.617411	52.089647	90.272158
H	58.776483	51.256677	89.563778
H	59.008587	53.015312	89.816038
N	59.279564	51.808830	91.559447
C	60.570607	52.099413	91.907692
O	60.978310	51.900012	93.064518
C	61.511307	52.649357	90.821691
H	61.103960	53.589245	90.395177
H	62.452518	52.898989	91.347508
C	61.798683	51.647678	89.672064
H	60.869767	51.512701	89.082032
C	62.206716	50.267166	90.211869
H	62.416687	49.569215	89.378375
H	63.117250	50.340332	90.842140
H	61.403522	49.819563	90.826899
C	62.868085	52.218116	88.726539
H	63.834332	52.351760	89.256477
H	63.043509	51.535330	87.871900
H	62.566331	53.202491	88.318182
C	58.643450	56.266527	90.155414
H	59.085459	57.284248	90.142153
H	57.832902	56.261101	90.910587
H	59.425933	55.569250	90.515076
C	58.112315	55.869262	88.768949
H	57.246601	56.517789	88.514698
H	57.710476	54.834101	88.803675

C	59.141783	55.955016	87.619251
H	59.513406	57.005244	87.579532
C	60.352055	55.033130	87.849286
H	60.015315	53.984079	87.961258
H	61.041002	55.061110	86.982640
H	60.926446	55.312152	88.754605
C	58.473614	55.629779	86.271208
H	59.205266	55.673478	85.440803
H	57.643390	56.332211	86.052118
H	58.064616	54.601254	86.284388
C	60.868915	54.214538	82.008458
H	61.914151	54.541742	81.831731
H	60.269337	55.131631	82.182620
H	60.497919	53.736131	81.082591
C	60.780874	53.272037	83.178819
N	61.220809	53.635608	84.444237
C	60.994286	52.575269	85.219498
H	61.194396	52.506662	86.291533
N	60.436238	51.545780	84.522141
H	60.176347	50.616849	84.920492
C	60.285648	51.967816	83.214750
H	59.838186	51.327568	82.456962

OHa model

Ni	57.947754	47.233571	85.027479
Fe	57.505675	49.497536	86.692409
O	56.785996	47.622614	86.470289
C	55.742277	49.967910	87.053206
N	54.603514	50.170961	87.277963
C	57.890812	49.119964	88.458619
N	58.159841	48.783233	89.555144
C	57.988874	51.136326	86.849546
O	58.271377	52.254783	87.031727
S	58.764551	46.581318	83.083646
C	59.965964	47.892975	82.673813
H	60.733298	47.903575	83.469045
H	59.451482	48.872150	82.710463
C	60.594032	47.640669	81.310369
H	61.373209	48.399694	81.092795
H	61.071618	46.642279	81.265337
H	59.840430	47.691627	80.503536
S	58.612556	45.288664	85.822537
C	58.106619	45.243709	87.593728
H	58.485969	46.142825	88.119707
H	57.001692	45.248944	87.663706
C	58.671699	44.019532	88.315733
H	58.410029	44.076855	89.389780
H	58.273792	43.076134	87.894658
H	59.775651	43.991543	88.236934

S	59.604654	48.683161	85.972338
C	60.725448	47.944366	87.246142
H	60.634331	48.580579	88.145130
H	60.311747	46.952848	87.499784
C	62.197482	47.815237	86.787498
H	62.630481	48.803234	86.539065
H	62.278362	47.167186	85.894409
H	62.799621	47.363399	87.600021
S	57.189342	49.338196	84.346085
C	55.375073	49.236971	84.018109
H	54.931511	50.155808	84.442455
H	54.974109	48.380788	84.586948
C	55.016466	49.114833	82.524202
H	55.389724	49.992952	81.959525
H	53.915867	49.064893	82.428894
N	55.538426	47.882593	81.953762
H	56.538980	47.676233	82.092616
C	54.714647	46.855537	81.589495
O	53.484887	46.929594	81.559711
C	55.448922	45.545204	81.238140
H	54.757744	44.957687	80.610598
H	55.636260	44.984811	82.174690
N	56.711341	45.720569	80.547228
H	57.556848	45.826983	81.128741
C	56.734667	46.085425	79.229113
O	55.710159	46.160568	78.540370
C	58.111648	46.439855	78.681637
H	58.264222	47.534720	78.757565
H	58.153237	46.168897	77.611918
H	58.932216	45.936105	79.222185
O	51.434420	48.022931	84.415077
O	50.412044	46.063128	84.890809
C	50.435354	47.238152	84.410207
C	49.122932	47.780945	83.803824
H	49.328935	48.304461	82.851248
H	48.679935	48.522035	84.498515
H	48.393081	46.968477	83.638449
H	52.619046	47.753961	85.544464
N	53.281844	47.568586	86.358020
H	53.845821	48.343799	86.734879
C	53.356166	46.327848	86.846684
N	52.640707	45.349076	86.255722
H	51.811846	45.623503	85.632454
H	52.570207	44.454755	86.738870
N	54.153107	46.021988	87.909460
H	54.043641	45.081771	88.285348
C	54.728575	47.026831	88.803302
H	55.479882	46.514922	89.432187
H	55.285351	47.759281	88.190700
C	53.691302	47.754863	89.667487
H	53.220297	47.048774	90.382350
H	52.882418	48.113867	89.001198

C	54.282486	48.967521	90.399628
H	54.781095	48.662421	91.341441
H	55.068138	49.426948	89.766425
C	53.215655	50.026436	90.715554
H	53.685835	50.884264	91.242153
H	52.428420	49.625840	91.381393
N	52.537054	50.491429	89.515943
H	53.115323	50.678975	88.683541
C	51.184049	50.607401	89.442463
O	50.409032	50.296792	90.357495
C	50.633133	51.106191	88.094454
H	49.673639	51.601824	88.342074
C	50.434448	49.985447	87.050114
H	51.211288	49.205777	87.170063
H	49.449848	49.496955	87.154388
C	50.640959	50.702193	85.705323
H	50.886974	49.984112	84.901112
H	49.732776	51.276481	85.429922
C	51.795060	51.662205	86.017250
H	52.772989	51.143923	85.941895
H	51.814002	52.548416	85.357838
N	51.529042	52.051562	87.413504
C	51.869520	53.218088	88.039818
O	51.420021	53.496096	89.162936
C	52.901092	54.102312	87.345391
H	52.873276	55.075287	87.868931
H	52.630575	54.283267	86.286227
C	54.303759	53.473892	87.432890
H	54.560832	53.240468	88.483540
H	54.368378	52.525678	86.871938
H	55.076146	54.163832	87.042144
H	58.107562	47.312522	90.481720
O	58.294960	46.501072	91.033677
C	59.566843	46.688073	91.625791
H	59.910038	45.701743	91.995043
H	60.315478	47.029385	90.873113
C	59.556609	47.665756	92.808503
H	60.550593	47.658376	93.306232
H	58.815144	47.335350	93.563378
N	59.223595	49.013478	92.364563
H	59.097631	49.170165	91.354312
C	58.783657	49.965288	93.231394
O	58.680087	49.783941	94.450211
C	58.336398	51.285034	92.575574
H	58.258524	52.009888	93.409488
C	57.003026	51.160319	91.800134
H	56.132090	51.311809	92.461961
H	56.922580	50.153635	91.348425
C	57.117509	52.212024	90.682606
H	56.870524	53.220596	91.069159
H	56.454103	52.000852	89.823963
C	58.600078	52.140704	90.291276

H	58.761025	51.344977	89.541407
H	58.979485	53.090571	89.875624
N	59.275721	51.803602	91.554566
C	60.574523	52.075893	91.897754
O	60.987709	51.834644	93.042447
C	61.511307	52.649357	90.821691
H	61.107772	53.602417	90.421350
H	62.453224	52.885235	91.351605
C	61.804892	51.672266	89.654494
H	60.874382	51.541947	89.063565
C	62.232405	50.292380	90.178431
H	62.474301	49.610724	89.341323
H	63.131501	50.376177	90.822157
H	61.434300	49.819968	90.779694
C	62.873242	52.261835	88.720281
H	63.839389	52.376623	89.253275
H	63.047415	51.599152	87.849589
H	62.579325	53.258507	88.337517
C	58.643450	56.266527	90.155414
H	59.104377	57.275093	90.138408
H	57.823270	56.283786	90.899264
H	59.408364	55.557916	90.532060
C	58.122762	55.868386	88.766237
H	57.266175	56.523650	88.501367
H	57.710439	54.837380	88.802573
C	59.163431	55.939259	87.626930
H	59.552033	56.982575	87.595432
C	60.361133	55.003645	87.867808
H	60.017413	53.956510	87.983744
H	61.058783	55.022417	87.007930
H	60.930462	55.282176	88.776222
C	58.502418	55.639572	86.270750
H	59.248097	55.645107	85.452613
H	57.710489	56.379522	86.037286
H	58.040908	54.633374	86.276444
C	60.868915	54.214538	82.008458
H	61.915697	54.547535	81.857341
H	60.261305	55.126898	82.175058
H	60.521393	53.739081	81.072753
C	60.760035	53.269117	83.167753
N	61.158297	53.631535	84.447002
C	60.919662	52.570515	85.214090
H	61.086818	52.505279	86.291539
N	60.388080	51.538044	84.494153
H	60.118629	50.613419	84.873324
C	60.274911	51.962752	83.182517
H	59.858537	51.321728	82.402462
H	57.045639	47.101062	87.247432

OHb model

Ni	57.939894	47.172036	85.021392
Fe	57.488060	49.421605	86.718328
O	56.837999	47.505907	86.552488
C	55.727376	49.893868	87.079864
N	54.587080	50.105503	87.293544
C	57.882650	49.058369	88.488301
N	58.169266	48.763026	89.591285
C	57.972536	51.059753	86.880529
O	58.255657	52.179421	87.057527
S	58.771564	46.541054	83.075432
C	59.941429	47.884367	82.664717
H	60.698275	47.924102	83.469484
H	59.398698	48.849074	82.685277
C	60.594032	47.640669	81.310369
H	61.360024	48.415895	81.101173
H	61.093254	46.652305	81.272888
H	59.851229	47.675803	80.492858
S	58.556538	45.214945	85.787840
C	57.949625	45.122720	87.526286
H	58.109190	46.103567	88.007919
H	56.855706	44.965295	87.520231
C	58.671699	44.019532	88.315733
H	58.347988	44.066381	89.374439
H	58.456530	43.009375	87.914509
H	59.769776	44.167580	88.293666
S	59.584027	48.630707	85.987856
C	60.721088	47.895000	87.250557
H	60.613092	48.512158	88.161631
H	60.328487	46.890558	87.486269
C	62.197482	47.815237	86.787498
H	62.601531	48.819782	86.556091
H	62.296033	47.184418	85.883520
H	62.812828	47.368425	87.593355
S	57.178611	49.298095	84.363766
C	55.362781	49.252206	84.019120
H	54.943138	50.189150	84.429047
H	54.906116	48.418529	84.582448
C	55.016466	49.114833	82.524202
H	55.405612	49.982694	81.953742
H	53.916134	49.077680	82.416104
N	55.537446	47.872226	81.974437
H	56.538448	47.671985	82.118385
C	54.720344	46.839546	81.607107
O	53.490094	46.904893	81.571486
C	55.466317	45.532611	81.258074
H	54.777256	44.935559	80.636797
H	55.663286	44.979435	82.197159
N	56.725195	45.718128	80.560933
H	57.568151	45.846314	81.142237
C	56.738979	46.085241	79.242766
O	55.713504	46.130096	78.552772
C	58.111648	46.439855	78.681637

H	58.258233	47.535925	78.749912
H	58.142861	46.163654	77.612695
H	58.940906	45.942750	79.216183
O	51.425804	47.996797	84.476054
O	50.375060	46.046211	84.920341
C	50.418241	47.223119	84.443273
C	49.122932	47.780945	83.803824
H	49.357571	48.285993	82.847941
H	48.685565	48.541373	84.481239
H	48.381578	46.978920	83.638381
H	52.656240	47.709496	85.576362
N	53.345514	47.513681	86.367207
H	53.765666	48.325768	86.846515
C	53.327211	46.283460	86.910754
N	52.580724	45.332133	86.317697
H	51.760653	45.622060	85.682809
H	52.504422	44.425617	86.776900
N	54.084533	45.969327	87.997226
H	53.935643	45.037836	88.381524
C	54.714270	46.950754	88.889287
H	55.387105	46.390032	89.562794
H	55.383290	47.605374	88.301367
C	53.686220	47.780908	89.672163
H	53.131160	47.130283	90.379897
H	52.935547	48.164772	88.953019
C	54.297147	48.985277	90.401478
H	54.791122	48.675436	91.344493
H	55.089213	49.431660	89.768429
C	53.241864	50.059483	90.718918
H	53.729038	50.920216	91.224845
H	52.464486	49.672705	91.404583
N	52.547214	50.517773	89.523381
H	53.119489	50.703606	88.687100
C	51.191259	50.615973	89.447719
O	50.417532	50.302160	90.362399
C	50.633133	51.106191	88.094454
H	49.669132	51.593697	88.341031
C	50.446780	49.977912	87.054156
H	51.241930	49.215260	87.167254
H	49.474078	49.467347	87.166380
C	50.629905	50.697255	85.706941
H	50.869340	49.980382	84.900248
H	49.715243	51.268095	85.445580
C	51.784207	51.660982	86.009556
H	52.762372	51.141910	85.933614
H	51.800882	52.542930	85.344229
N	51.520433	52.056993	87.405638
C	51.868176	53.223947	88.029976
O	51.417538	53.509870	89.150531
C	52.901633	54.103333	87.330134
H	52.872782	55.081331	87.844625
H	52.637595	54.275788	86.267748

C	54.303759	53.473892	87.432890
H	54.562654	53.271708	88.490215
H	54.368093	52.510091	86.898426
H	55.078006	54.150381	87.021850
H	58.108139	47.251813	90.475638
O	58.306019	46.459860	91.050706
C	59.579507	46.679984	91.629450
H	59.950736	45.704376	92.002211
H	60.313438	47.036152	90.868240
C	59.556609	47.665756	92.808503
H	60.547695	47.668909	93.312655
H	58.813897	47.330065	93.560515
N	59.217523	49.010362	92.360761
H	59.070120	49.153846	91.349967
C	58.784947	49.962938	93.229983
O	58.691340	49.784670	94.450522
C	58.336398	51.285034	92.575574
H	58.260456	52.008039	93.411606
C	57.000365	51.160629	91.801044
H	56.129301	51.311291	92.463388
H	56.919233	50.153876	91.349530
C	57.114041	52.209698	90.679346
H	56.868879	53.221234	91.060322
H	56.450840	51.993286	89.821205
C	58.596892	52.132491	90.288166
H	58.754843	51.326547	89.548770
H	58.978856	53.075422	89.859185
N	59.273405	51.809204	91.555485
C	60.573620	52.077376	91.898264
O	60.985503	51.843247	93.045226
C	61.511307	52.649357	90.821691
H	61.112264	53.606888	90.427150
H	62.458166	52.873950	91.347729
C	61.785670	51.677178	89.643772
H	60.849849	51.562092	89.058780
C	62.196784	50.284854	90.151774
H	62.427309	49.609472	89.305558
H	63.099123	50.348910	90.793772
H	61.392598	49.815937	90.749526
C	62.850670	52.264591	88.702779
H	63.821800	52.376686	89.227715
H	63.015711	51.603872	87.828363
H	62.554047	53.261568	88.322883
C	58.643450	56.266527	90.155414
H	59.101660	57.275317	90.103525
H	57.846401	56.296311	90.923898
H	59.421111	55.566282	90.520932
C	58.081586	55.838744	88.789703
H	57.213468	56.484640	88.538136
H	57.675714	54.806221	88.858335
C	59.086604	55.892666	87.616105
H	59.464129	56.938533	87.547926

C	60.300341	54.971609	87.838777
H	59.968642	53.924808	87.988642
H	60.968728	54.976911	86.955322
H	60.896314	55.273589	88.722479
C	58.385069	55.551641	86.288327
H	59.103178	55.545015	85.445352
H	57.576135	56.275785	86.062044
H	57.936813	54.540450	86.336363
C	60.868915	54.214538	82.008458
H	61.920116	54.546436	81.887413
H	60.258940	55.126474	82.169831
H	60.543776	53.748689	81.059661
C	60.729523	53.256148	83.158845
N	61.091075	53.606780	84.452213
C	60.839086	52.535739	85.200399
H	60.980108	52.457745	86.281351
N	60.333572	51.507136	84.456801
H	60.062251	50.577621	84.822709
C	60.252413	51.946220	83.147522
H	59.864216	51.310449	82.348784
H	55.920850	47.533287	86.217734

Volbeda Model

C	5.770760	1.240605	6.994453
C	7.142542	1.074841	7.648224
S	7.080053	1.132365	9.482004
C	10.538000	3.337000	8.302000
C	10.904095	3.132288	9.761514
O	11.822115	3.731894	10.321787
N	10.193631	2.103504	10.369641
C	10.681071	1.422752	11.477061
C	11.019370	-0.007353	11.365654
O	11.809159	-0.538859	12.169512
N	10.548796	-0.632118	10.234243
C	11.017000	-1.936000	9.829000
C	9.964997	-3.053606	10.026783
S	8.669028	-2.932470	8.743108
O	8.266232	-1.399793	8.835325
C	8.574000	-3.088000	2.447000
C	7.349149	-3.316763	3.285431
N	6.295502	-4.124147	2.869405
C	6.941542	-2.841635	4.532587
C	5.330731	-4.099385	3.849938
N	5.692533	-3.331379	4.864803
C	11.030898	-8.624023	9.168137
C	11.096336	-9.025584	10.637721
O	10.946633	-10.206921	10.991923
C	9.578000	-8.262000	8.803000
N	11.225390	-8.024324	11.558562
C	11.093000	-8.350000	12.983000
C	9.718953	-8.946369	13.366644
O	9.631760	-9.763786	14.295397
C	11.298481	-6.980713	13.689320
C	12.059606	-6.110652	12.673045
C	11.521443	-6.598808	11.319052
N	8.655035	-8.429765	12.697188
C	7.274636	-8.706631	13.081107
C	6.411181	-7.431472	13.084797
C	6.971879	-6.329468	13.994630
C	6.452216	-4.921467	13.660460
N	7.139989	-3.879293	14.415175
C	8.441303	-3.473543	14.129070
N	9.265842	-3.988114	13.266020
N	8.839227	-2.389137	14.915923
C	5.589000	-10.614000	5.464000
C	6.708580	-9.561790	5.509133
C	6.702422	-8.550504	4.340353
C	5.414699	-7.710040	4.295717
C	7.934517	-7.630591	4.411876
C	2.053000	-7.534000	6.431000
C	1.889252	-8.235852	7.763970
O	0.783623	-8.686889	8.108591
C	1.370677	-6.145964	6.416003

C	2.084829	-5.163216	7.354844
C	1.313402	-5.596201	4.982139
N	2.976476	-8.336070	8.579226
C	2.814000	-9.018000	9.866000
C	1.708146	-8.426107	10.755073
O	0.922846	-9.153450	11.375188
C	4.217137	-8.896618	10.517857
C	5.178464	-8.748987	9.325195
C	4.366912	-7.913240	8.324279
N	1.722039	-7.065542	10.836233
C	0.832000	-6.358000	11.729000
C	1.599847	-5.523578	12.768075
S	2.689178	-6.499287	13.870923
C	6.489000	-5.295000	18.099000
C	6.455668	-3.892842	17.519772
O	5.341033	-3.565738	16.806869
O	7.343540	-3.070416	17.645111
C	3.222000	-0.903000	13.249000
C	4.419588	-1.499386	12.471928
S	5.128167	-0.221594	11.354759
C	2.947000	-1.547000	7.924000
C	3.833619	-2.425594	8.798319
S	5.600502	-2.221873	8.391162
Fe	6.733144	-3.942337	9.513366
C	5.144432	-4.750870	10.155395
N	4.166154	-5.305897	10.502189
C	7.724184	-5.215239	10.450365
N	8.356019	-6.054968	10.980156
C	6.688475	-5.013160	8.110731
O	6.659003	-5.718150	7.186926
Ni	6.713030	-1.017827	10.079814
O	6.889655	-2.653415	10.841380
H	5.853856	1.210284	5.887103
H	5.298035	2.200516	7.282660
H	5.103184	0.416577	7.305819
H	7.831754	1.879741	7.320696
H	7.601708	0.106450	7.377588
H	10.931507	4.306585	7.951165
H	9.444535	3.298032	8.134841
H	10.996388	2.527116	7.700271
H	9.368604	1.702143	9.869819
H	11.240843	2.006991	12.215836
H	9.704887	-0.306779	9.746769
H	11.352710	-1.905043	8.770462
H	11.891605	-2.170254	10.464209
H	10.416355	-4.054899	9.889749
H	9.516637	-3.009515	11.037811
H	9.116475	-4.032145	2.234278
H	9.271448	-2.416221	2.979319
H	8.330250	-2.617015	1.472365
H	6.254914	-4.645809	1.994365
H	7.485987	-2.176409	5.211586

H	4.394860	-4.660075	3.765004
H	11.705557	-7.778137	8.935146
H	11.371552	-9.500313	8.584943
H	9.217395	-7.385543	9.372189
H	8.904043	-9.108313	9.038701
H	9.478925	-8.038559	7.722716
H	11.848171	-9.102302	13.280871
H	10.318575	-6.504196	13.886390
H	11.820186	-7.093526	14.656598
H	11.842994	-5.037205	12.828303
H	13.152860	-6.282559	12.741452
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H	12.255677	-6.480584	10.501310
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H	7.311272	-9.179541	14.082084
H	6.826825	-9.452790	12.389102
H	5.377482	-7.700451	13.380431
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H	5.373630	-4.845348	13.899516
H	6.532559	-4.735775	12.571240
H	6.545725	-3.165836	14.836255
H	8.799156	-4.652653	12.635517
H	9.829395	-2.173296	14.792337
H	8.525444	-2.406734	15.891660
H	5.701681	-11.351305	6.282709
H	5.599141	-11.170990	4.504794
H	4.585525	-10.157394	5.574157
H	6.659347	-8.999400	6.466101
H	7.690948	-10.079668	5.518293
H	6.761598	-9.136326	3.394373
H	5.317195	-7.093163	5.211815
H	4.506702	-8.336517	4.200006
H	5.431517	-7.010229	3.437603
H	7.915067	-7.027379	5.340554
H	7.956795	-6.920553	3.560904
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H	3.111275	-7.419244	6.131938
H	1.565035	-8.183163	5.676274
H	0.332029	-6.296023	6.780028
H	3.128432	-4.987035	7.024888
H	2.124609	-5.532627	8.396639
H	1.571594	-4.182388	7.365609
H	2.337241	-5.461562	4.576423
H	0.812132	-4.608396	4.952095
H	0.766767	-6.280473	4.302751
H	2.523059	-10.074153	9.699979
H	4.261446	-7.983715	11.140535
H	4.443514	-9.760912	11.167332
H	6.128335	-8.255053	9.600321
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H	4.485804	-6.832642	8.527570
H	4.659088	-8.109720	7.278795
H	2.539896	-6.537009	10.483951
H	0.186715	-7.113471	12.213954
H	0.174183	-5.667455	11.156299
H	0.899967	-4.917665	13.373019
H	2.301126	-4.836820	12.256612
H	1.698738	-7.197154	14.492018
H	7.292966	-5.362795	18.849835
H	6.711056	-6.013268	17.283850
H	5.522725	-5.580932	18.555751
H	4.725875	-4.326202	16.735666
H	2.792031	-1.661424	13.934865
H	2.425239	-0.571360	12.554587
H	3.531638	-0.028768	13.854996
H	5.209846	-1.863441	13.156073
H	4.103374	-2.374465	11.871853
H	1.875597	-1.737258	8.142269
H	3.122579	-1.754115	6.850206
H	3.141732	-0.472116	8.105542
H	3.598437	-3.492151	8.661744
H	3.704374	-2.201299	9.865310