

Supporting Information

Mössbauer Properties of the Diferric Cluster and the Differential Iron(II)- Binding Affinity of the Iron Sites in Protein R2 of Class Ia *Escherichia coli* Ribonucleotide Reductase: A DFT/Electrostatics Study

Wen-Ge Han,[†] Gregory M. Sandala,[†] Debra Ann Giammona,[‡]
Donald Bashford,[‡] and Louis Noodleman^{*,†}

[†] Department of Molecular Biology, TPC15, The Scripps Research Institute, 10550
North Torrey Pines Road, La Jolla, CA 92037

[‡] Structural Biology, St. Jude Children's Research Hospital, 262 Danny Thomas
Place, Memphis, TN 38105

*To whom correspondence should be addressed.

E-mail: lou@scripps.edu.

Tel: (858) 784-2840.

Cartesian coordinates of the OPBE/COSMO optimized met-diferric cluster 'Cys-71':

162

Fe	5.321077	9.939453	48.262022
Fe	4.006520	9.624968	45.249955
C	11.598304	13.667180	41.478804
C	10.527534	13.978209	42.492599
O	9.447109	13.366253	42.514508
N	10.806287	14.985203	43.339684
H	11.531061	14.427072	40.691653
C	13.747888	18.618548	50.167965
C	12.520465	17.767296	50.100990
C	11.832421	17.431319	48.956963
C	11.859961	17.073145	51.171488
N	10.787335	16.594757	49.246582
C	10.772652	16.354491	50.594066
C	12.068084	16.974569	52.561847
C	9.899883	15.578830	51.362957
C	11.211016	16.191255	53.323036
C	10.134224	15.502278	52.729424
H	14.632685	18.029476	49.907425
C	5.248099	6.763965	50.694911
C	4.486797	7.549682	49.660170
O	3.787766	6.992219	48.801168
O	4.651146	8.843431	49.739594
H	4.930928	5.726455	50.723063
C	9.090209	8.017669	40.133266
C	7.680169	7.608764	40.434069
C	6.967199	7.927450	41.566961
C	6.778995	6.834706	39.617141
N	5.703420	7.399095	41.514885
C	5.550290	6.728749	40.331170
C	6.867594	6.215050	38.354292
C	4.445879	6.028214	39.837207
C	5.769854	5.522576	37.858069
C	4.571947	5.426477	38.593368
H	9.584657	8.475607	41.006200
C	8.567174	6.748702	47.026149
C	7.554267	7.043790	45.935075
C	6.382926	7.920697	46.335415
O	6.430049	8.445326	47.499551
O	5.465997	8.073787	45.478470
H	8.899493	7.672761	47.513045
C	7.940099	10.125837	50.791247
C	7.843074	11.170834	49.742240
N	6.835172	11.220257	48.799952
C	8.662346	12.253336	49.532792
C	7.048790	12.309484	48.065432
N	8.139794	12.953971	48.477220
H	8.580664	10.498104	51.586204
C	6.513518	8.813930	57.333113
C	5.715865	9.305131	56.164463
C	5.131049	10.578054	56.199290
C	5.551828	8.545626	55.005493
C	4.404832	11.086610	55.128770

C	4.822440	9.037864	53.929343
C	4.248360	10.305840	53.983498
O	3.533494	10.818722	52.931628
H	7.046225	9.667139	57.743464
C	-0.109439	9.370145	43.588733
C	0.807884	8.216286	43.985661
C	2.102318	8.183445	43.191889
O	2.081844	7.849663	41.990026
O	3.216880	8.484103	43.782445
H	-1.005990	9.358163	44.211812
C	2.120869	14.067363	45.712767
C	1.157853	12.883727	45.807326
C	1.832904	11.553711	46.112430
O	1.700908	11.046284	47.263936
O	2.481035	11.016283	45.152285
H	2.825016	13.965307	44.877012
C	3.765708	11.106962	41.781544
C	5.016312	11.246040	42.566259
N	5.247393	10.722715	43.826791
C	6.150806	11.904717	42.163184
C	6.487832	11.066674	44.155886
N	7.059779	11.772397	43.174518
H	3.974147	11.464150	40.770355
C	7.160786	15.018115	45.789287
C	8.451307	15.675165	46.249305
O	8.977785	16.554542	45.504644
O	8.942522	15.298720	47.362577
H	6.690327	15.545148	44.958416
O	2.651436	8.500921	46.730616
O	3.733360	11.502116	49.121826
O	4.713775	10.487188	46.701571
O	-0.037001	8.387997	40.236003
H	12.603985	13.714738	41.910369
H	11.421784	12.681480	41.044277
H	11.672939	15.494904	43.265795
H	10.102961	15.342971	43.973661
H	13.697960	19.460165	49.466679
H	13.908470	19.030309	51.169642
H	12.020113	17.727593	47.930944
H	10.161721	16.184586	48.550260
H	9.059309	15.058495	50.908671
H	9.471286	14.899605	53.349185
H	11.370021	16.106298	54.397516
H	12.893283	17.501448	53.040900
H	6.315799	6.812982	50.451819
H	5.127164	7.202648	51.684439
H	9.702121	7.161163	39.820862
H	9.131931	8.747823	39.311800
H	7.280770	8.504662	42.427791
H	4.963486	7.581871	42.180633
H	3.523093	5.962288	40.409079
H	3.725874	4.876956	38.181193
H	5.830249	5.046928	36.879493
H	7.782052	6.278512	37.764315
H	8.143148	6.101978	47.803026
H	9.441591	6.239454	46.603538
H	7.135520	6.124478	45.505422

H	8.032862	7.560942	45.090604
H	6.962479	9.911640	51.229297
H	8.355017	9.185260	50.409741
H	6.415691	12.635027	47.255055
H	8.478788	13.856613	48.059876
H	9.561050	12.569246	50.047111
H	5.875025	8.402958	58.127173
H	7.236264	8.042001	57.049679
H	5.256469	11.198372	57.087772
H	3.963656	12.081032	55.171151
H	3.490402	10.124054	52.258750
H	4.702317	8.439811	53.032758
H	6.011092	7.559008	54.930018
H	0.385092	10.335052	43.731318
H	-0.428675	9.299871	42.545901
H	0.299011	7.261779	43.794125
H	1.034440	8.261005	45.050673
H	1.551011	14.992046	45.556446
H	2.701180	14.189108	46.636446
H	0.621380	12.778243	44.855619
H	0.415343	13.068977	46.591280
H	3.436416	10.067514	41.720610
H	2.944795	11.693420	42.209769
H	6.994821	10.820519	45.075519
H	7.989269	12.178764	43.178063
H	6.379182	12.434787	41.247660
H	7.376734	13.997710	45.456178
H	6.452039	14.961272	46.620759
H	0.662896	8.155299	40.886389
H	-0.663707	7.655527	40.317931
H	2.253969	9.324786	47.104133
H	3.075258	8.031552	47.486861
H	3.020113	11.405003	48.448781
H	3.319363	11.147546	49.921576
C	7.544078	21.950378	45.129163
N	8.701138	21.359865	45.765739
C	9.821063	21.984864	46.110108
N	9.967286	23.305157	46.011248
N	10.864573	21.247052	46.557255
H	6.808277	21.161638	44.962340
H	7.800505	22.387615	44.159508
H	7.077612	22.715454	45.760377
H	8.673512	20.367074	46.028932
H	9.280501	23.892292	45.532834
H	10.898965	23.682563	46.093102
H	10.629547	20.294217	46.822342
H	11.510539	21.717911	47.174366
O	9.218018	18.842256	46.817134
H	8.831977	18.665498	47.683665
H	9.190232	17.963944	46.343209
O	8.297001	25.088000	44.647000
H	8.768150	25.862341	44.307121
H	7.486531	25.467797	45.013969

Cartesian coordinates of the met-diferric cluster 'Cys-17' obtained from the trajectory of the geometry optimization starting from the X-ray crystal structure:

162

Fe	5.203431	9.927497	48.272202
Fe	4.062224	9.662733	45.243479
C	11.637773	13.716375	41.515203
C	10.578512	14.059071	42.531059
O	9.477415	13.488108	42.550305
N	10.891577	15.057145	43.378992
H	11.531061	14.427072	40.691653
C	13.707678	18.536223	50.194517
C	12.517801	17.637034	50.060737
C	11.889253	17.300154	48.881738
C	11.796930	16.946543	51.095589
N	10.827445	16.469815	49.117815
C	10.735564	16.236980	50.462449
C	11.927518	16.839780	52.495065
C	9.803644	15.482690	51.180398
C	11.017524	16.067393	53.205827
C	9.959698	15.401249	52.556997
H	14.632685	18.029476	49.907425
C	5.227951	6.753305	50.834207
C	4.530905	7.616636	49.821814
O	3.755000	7.139571	48.974737
O	4.827012	8.878798	49.917925
H	4.930928	5.726455	50.723063
C	9.017217	8.077183	40.148689
C	7.635276	7.670097	40.557336
C	7.022052	8.009908	41.740588
C	6.661868	6.900487	39.824013
N	5.753598	7.497998	41.797766
C	5.492662	6.825595	40.634400
C	6.636234	6.264357	38.567092
C	4.334579	6.153170	40.236283
C	5.485150	5.596079	38.166707
C	4.344667	5.541282	38.991742
H	9.584657	8.475607	41.006200
C	8.501690	6.758621	47.058985
C	7.537937	7.096839	45.940044
C	6.353672	7.958161	46.329525
O	6.342307	8.440007	47.508792
O	5.472760	8.137928	45.437058
H	8.899493	7.672761	47.513045
C	7.764479	10.220475	50.920743
C	7.698477	11.191009	49.800324
N	6.683215	11.228332	48.860393
C	8.558600	12.222700	49.517393
C	6.939811	12.261471	48.058989
N	8.059902	12.881797	48.423945
H	8.580664	10.498104	51.586204
C	6.449063	8.830841	57.389178
C	5.709793	9.288682	56.170753
C	5.095386	10.549106	56.134915
C	5.639095	8.499043	55.023594

C	4.426063	11.010346	55.006508
C	4.974534	8.948432	53.890642
C	4.366049	10.199611	53.872784
O	3.711750	10.667655	52.764007
H	7.046225	9.667139	57.743464
C	-0.155505	9.370662	43.529214
C	0.822623	8.264105	43.911376
C	2.127507	8.324911	43.137847
O	2.112145	8.186574	41.899273
O	3.239201	8.485935	43.785608
H	-1.005990	9.358163	44.211812
C	2.053906	14.019065	45.657436
C	1.097882	12.825501	45.609031
C	1.761404	11.500855	45.953366
O	1.522507	10.959629	47.072669
O	2.520345	11.004361	45.057495
H	2.825016	13.965307	44.877012
C	3.822204	11.052082	41.765571
C	5.081971	11.215172	42.526964
N	5.308587	10.744349	43.809422
C	6.223916	11.842175	42.094758
C	6.552710	11.088503	44.123371
N	7.132582	11.743597	43.111128
H	3.974147	11.464150	40.770355
C	7.185829	14.933847	45.709222
C	8.477298	15.566997	46.189460
O	8.972582	16.512032	45.505989
O	9.004980	15.108982	47.252795
H	6.690327	15.545148	44.958416
O	2.688798	8.457545	46.717582
O	3.388900	11.069686	49.069270
O	4.718133	10.554144	46.690622
O	-0.037001	8.387997	40.236003
H	12.652546	13.812072	41.914365
H	11.473822	12.706338	41.134921
H	11.780934	15.528176	43.317366
H	10.202760	15.426432	44.022102
H	13.616261	19.420158	49.551057
H	13.831679	18.891379	51.222238
H	12.129417	17.595528	47.865786
H	10.226099	16.065498	48.398933
H	8.976366	14.985027	50.680638
H	9.249060	14.815758	53.139359
H	11.119073	15.975410	54.286542
H	12.735194	17.347916	53.021718
H	6.312643	6.854919	50.730949
H	4.962302	7.058609	51.845113
H	9.587595	7.235889	39.735321
H	8.997550	8.856235	39.372877
H	7.413735	8.593346	42.563135
H	5.063590	7.723016	42.503279
H	3.455995	6.128396	40.876563
H	3.451375	5.019389	38.649135
H	5.454987	5.111560	37.190677
H	7.502144	6.299917	37.905777
H	8.010541	6.182735	47.851274
H	9.338212	6.164362	46.673402

H	7.134975	6.198881	45.454771
H	8.052898	7.648062	45.139776
H	6.842609	10.237004	51.507490
H	7.920418	9.192937	50.574852
H	6.318436	12.548790	47.225667
H	8.442398	13.748103	47.957207
H	9.474127	12.530118	50.004704
H	5.771698	8.540556	58.203271
H	7.108914	7.983957	57.176742
H	5.149249	11.197727	57.010183
H	3.960034	11.994248	54.988795
H	3.832863	10.007391	52.067188
H	4.937570	8.328577	53.004632
H	6.117267	7.518748	55.005035
H	0.310940	10.356926	43.598993
H	-0.539445	9.253665	42.513600
H	0.375993	7.284557	43.687404
H	1.030218	8.284444	44.979946
H	1.490233	14.948011	45.504567
H	2.554988	14.092361	46.631471
H	0.675705	12.742563	44.599243
H	0.268691	12.978806	46.308791
H	3.537280	10.001908	41.661744
H	2.986522	11.574969	42.242001
H	7.055278	10.882032	45.055470
H	8.060809	12.151139	43.105709
H	6.461161	12.326082	41.156195
H	7.404290	13.960847	45.257923
H	6.498519	14.777511	46.544540
H	0.707189	8.279972	40.878517
H	-0.653853	7.689952	40.495998
H	2.176739	9.249739	47.003614
H	3.061776	8.060011	47.536829
H	2.741390	11.110673	48.322788
H	2.944844	10.490364	49.704065
C	7.549522	21.928961	45.208527
N	8.685643	21.290936	45.835244
C	9.833341	21.881137	46.163186
N	10.055431	23.171461	45.916717
N	10.796414	21.145508	46.736423
H	6.808277	21.161638	44.962340
H	7.834820	22.422852	44.275075
H	7.076629	22.661778	45.874403
H	8.620707	20.303546	46.114740
H	9.348896	23.768229	45.499819
H	10.938127	23.584347	46.170710
H	10.592209	20.185099	46.982520
H	11.640017	21.581700	47.070068
O	9.096784	18.778309	46.889610
H	8.548071	18.591134	47.666098
H	9.112939	17.913421	46.393012
O	8.297001	25.088000	44.647000
H	8.786510	25.826057	44.261909
H	7.379713	25.392312	44.613768

Cartesian coordinates of the met-diferric cluster 'Rotate-Tyr122-Fix-Asp84':

162

Fe	5.203431	9.927497	48.272202
Fe	3.981389	9.636887	45.236768
C	11.613289	13.678352	41.492225
C	10.540833	13.990184	42.504293
O	9.452782	13.391978	42.513613
N	10.826688	14.986346	43.362426
H	11.531061	14.427072	40.691653
C	13.734068	18.591302	50.192371
C	12.507610	17.737829	50.098816
C	11.840756	17.405755	48.939819
C	11.813389	17.052615	51.155130
N	10.783575	16.577698	49.206673
C	10.736143	16.340754	50.553628
C	11.981461	16.958448	52.551630
C	9.835126	15.575393	51.301005
C	11.096796	16.185857	53.292169
C	10.030833	15.501928	52.673276
H	14.632685	18.029476	49.907425
C	5.162919	6.766678	50.887412
C	4.530905	7.616636	49.821814
O	3.755000	7.139571	48.974737
O	4.827012	8.878798	49.917925
H	4.930928	5.726455	50.723063
C	9.066906	8.008270	40.147904
C	7.660607	7.603424	40.476923
C	6.971921	7.933957	41.621193
C	6.736677	6.829706	39.683004
N	5.703351	7.416680	41.598536
C	5.520348	6.741464	40.422116
C	6.789148	6.198771	38.423384
C	4.396689	6.053153	39.956051
C	5.671723	5.517312	37.954216
C	4.487763	5.442069	38.713529
H	9.584657	8.475607	41.006200
C	8.514167	6.757961	47.045089
C	7.506043	7.068434	45.954116
C	6.322229	7.931445	46.348262
O	6.332030	8.434460	47.520668
O	5.424204	8.091971	45.471596
H	8.899493	7.672761	47.513045
C	7.879714	10.152003	50.824762
C	7.772255	11.167827	49.747657
N	6.750257	11.206604	48.814215
C	8.597815	12.237789	49.506537
C	6.969966	12.280033	48.055929
N	8.072008	12.921404	48.441730
H	8.580664	10.498104	51.586204
C	6.452526	8.811835	57.418449
C	5.670477	9.235208	56.212982
C	4.695117	10.238211	56.302690
C	5.952002	8.714621	54.949833
C	4.013535	10.700882	55.182799

C	5.285456	9.172603	53.819886
C	4.309756	10.160512	53.930186
O	3.629754	10.632330	52.836900
H	7.046225	9.667139	57.743464
C	-0.134884	9.366044	43.557661
C	0.790674	8.222512	43.958992
C	2.089230	8.207118	43.176611
O	2.076245	7.921309	41.963143
O	3.200638	8.468562	43.793170
H	-1.005990	9.358163	44.211812
C	2.078369	14.070224	45.673259
C	1.116200	12.883479	45.717776
C	1.786276	11.555905	46.039510
O	1.623271	11.044520	47.185111
O	2.462299	11.021780	45.098130
H	2.825016	13.965307	44.877012
C	3.755397	11.115933	41.779103
C	5.006278	11.250058	42.563170
N	5.238035	10.730278	43.824140
C	6.142571	11.901663	42.153072
C	6.481947	11.067813	44.147646
N	7.054478	11.767840	43.161636
H	3.974147	11.464150	40.770355
C	7.159006	15.007104	45.780569
C	8.445190	15.662245	46.252640
O	8.965774	16.561036	45.527495
O	8.936798	15.263140	47.357444
H	6.690327	15.545148	44.958416
O	2.613071	8.489508	46.757320
O	3.566395	11.325633	49.112402
O	4.658404	10.504352	46.697173
O	-0.037001	8.387997	40.236003
H	12.619186	13.740911	41.922237
H	11.448348	12.682223	41.076586
H	11.705263	15.477373	43.306049
H	10.124194	15.348548	43.994545
H	13.672322	19.460826	49.526367
H	13.889909	18.967906	51.208462
H	12.053431	17.698605	47.917299
H	10.166175	16.169397	48.500892
H	9.002160	15.061922	50.825648
H	9.345026	14.909426	53.277720
H	11.223330	16.107960	54.371505
H	12.795332	17.482999	53.051783
H	6.246912	6.915451	50.903088
H	4.765143	7.051728	51.865129
H	9.670728	7.148448	39.828464
H	9.092445	8.731074	39.319090
H	7.308335	8.513261	42.471427
H	4.977374	7.611236	42.276260
H	3.485003	6.007143	40.546938
H	3.624565	4.904813	38.320730
H	5.703674	5.037792	36.975916
H	7.689513	6.248274	37.810833
H	8.071183	6.143594	47.837226
H	9.361025	6.203954	46.622385
H	7.094680	6.151495	45.511864

H	7.987957	7.594805	45.117384
H	6.916808	10.007838	51.313910
H	8.213164	9.177349	50.449241
H	6.335080	12.592766	47.242024
H	8.420735	13.816782	48.016207
H	9.505965	12.554059	50.002229
H	5.808586	8.519071	58.255871
H	7.134755	7.986035	57.195018
H	4.468045	10.681313	57.273213
H	3.262547	11.484914	55.266762
H	3.927176	10.113149	52.076516
H	5.538317	8.769186	52.846171
H	6.719091	7.947825	54.835507
H	0.357812	10.336174	43.666738
H	-0.484593	9.273577	42.526700
H	0.293258	7.263266	43.759960
H	1.006829	8.264327	45.026069
H	1.516547	14.993600	45.484399
H	2.609516	14.194074	46.625787
H	0.621797	12.783279	44.743076
H	0.341029	13.058765	46.471989
H	3.417729	10.080286	41.716341
H	2.938109	11.713525	42.197864
H	6.991562	10.820114	45.065176
H	7.987247	12.164363	43.159261
H	6.371593	12.425239	41.234140
H	7.378551	13.992120	45.434383
H	6.448059	14.937985	46.608912
H	0.670500	8.177248	40.887569
H	-0.659413	7.654848	40.338718
H	2.179692	9.315895	47.079882
H	3.022403	8.071610	47.547503
H	2.890984	11.310864	48.391601
H	3.098173	10.904451	49.846192
C	7.539193	21.950688	45.143428
N	8.685944	21.353153	45.790440
C	9.811265	21.969311	46.131249
N	9.972066	23.286009	46.009768
N	10.842836	21.226933	46.598612
H	6.808277	21.161638	44.962340
H	7.808262	22.393350	44.179618
H	7.065303	22.712156	45.773984
H	8.640304	20.366169	46.074606
H	9.287687	23.870929	45.528484
H	10.906080	23.657650	46.086990
H	10.593114	20.282666	46.880371
H	11.487778	21.702239	47.213223
O	9.148967	18.846111	46.867079
H	8.748590	18.655603	47.724566
H	9.137814	17.972242	46.385243
O	8.297001	25.088000	44.647000
H	8.729101	25.889428	44.321883
H	7.428298	25.408524	44.935770

Cartesian coordinates of Mono-Fe1(II)-S1:

153

Fe	5.253468	9.366459	47.748880
C	5.034534	6.590584	50.955930
C	4.692505	7.765164	50.060133
O	5.309905	7.754898	48.929221
O	3.911193	8.667497	50.432878
H	5.173067	5.680679	50.367543
C	8.317193	6.489885	46.739588
C	7.506872	6.660880	45.459629
C	6.247877	7.529032	45.570353
O	6.396785	8.586582	46.293777
O	5.216944	7.203937	44.946928
H	8.679154	7.444420	47.147180
C	7.831131	9.910238	50.511765
C	7.747583	10.836708	49.355149
N	6.765455	10.789982	48.385340
C	8.576063	11.901909	49.088379
C	7.007657	11.815391	47.580451
N	8.089616	12.507508	47.962201
H	8.477626	10.363691	51.265000
C	6.391465	8.889401	57.271288
C	5.613700	9.336047	56.070942
C	5.303084	10.690994	55.895803
C	5.205669	8.443298	55.078481
C	4.636763	11.151302	54.765688
C	4.528976	8.883794	53.947963
C	4.260775	10.243094	53.772076
O	3.640554	10.721903	52.655050
H	7.068570	9.698540	57.537608
C	-0.425492	8.619909	42.000777
C	0.376598	7.335429	41.876081
C	1.476855	7.077364	42.877149
O	1.818139	8.152263	43.607492
O	2.025508	5.992536	43.001667
H	-0.845305	8.715486	43.001082
C	2.028876	12.907696	45.042055
C	2.568903	12.417171	46.372810
C	3.374671	11.125164	46.333743
O	3.577471	10.518281	45.263249
O	3.808781	10.737110	47.487332
H	2.831130	13.047393	44.304230
C	3.706313	10.754528	41.235181
C	5.015006	10.992085	41.879855
N	5.300422	10.770278	43.206578
C	6.184821	11.415304	41.310738
C	6.583393	11.038709	43.435134
N	7.135126	11.434327	42.293550
H	3.858927	10.924995	40.169709
C	11.661904	13.177686	40.733289
C	10.474096	13.133834	41.653224
O	9.610082	12.242624	41.538845
N	10.395221	14.125344	42.552524
H	11.464496	13.953922	39.987328

C	13.705735	18.456339	49.625733
C	12.506394	17.562298	49.567169
C	11.830844	17.201431	48.423478
C	11.859890	16.856947	50.639753
N	10.808416	16.337755	48.717005
C	10.796825	16.102084	50.065073
C	12.065731	16.770969	52.030999
C	9.949260	15.296750	50.831537
C	11.233159	15.961075	52.791248
C	10.182305	15.232499	52.198448
H	14.589106	17.942519	49.233390
C	8.847092	7.635087	39.655381
C	7.525203	7.104270	40.126868
C	7.072862	7.169401	41.422318
C	6.471915	6.449588	39.385611
N	5.829376	6.611470	41.539390
C	5.425252	6.159522	40.312673
C	6.279243	6.067534	38.041473
C	4.234191	5.526074	39.944468
C	5.096400	5.435813	37.671534
C	4.082328	5.167723	38.611975
H	9.447039	8.058236	40.488698
C	7.010054	14.538853	45.299564
C	8.279048	15.279694	45.693302
O	8.673688	16.214682	44.930077
O	8.868287	14.913934	46.755970
H	6.495139	14.991929	44.451835
H	5.994653	6.802201	51.445759
H	4.278337	6.426595	51.726965
H	7.715960	6.014250	47.524160
H	9.188728	5.848979	46.550276
H	7.206722	5.685273	45.059607
H	8.140081	7.125207	44.688631
H	6.848116	9.761772	50.965658
H	8.228672	8.925307	50.238139
H	6.406374	12.083725	46.727089
H	8.420566	13.385643	47.517461
H	9.456609	12.263712	49.602386
H	5.747302	8.685859	58.137905
H	6.976786	7.985618	57.071026
H	5.612371	11.412241	56.653961
H	4.427795	12.211874	54.631435
H	3.630809	10.010223	51.988762
H	4.223396	8.176696	53.185745
H	5.433257	7.380396	55.176458
H	0.178892	9.511336	41.799873
H	-1.256745	8.608668	41.285155
H	0.855763	7.269057	40.888018
H	-0.278855	6.457805	41.934028
H	1.314755	12.195929	44.612644
H	1.514788	13.868511	45.171262
H	1.755427	12.265769	47.096035
H	3.215674	13.175952	46.837448
H	3.371998	9.721854	41.374379
H	2.922477	11.423692	41.608414
H	4.617330	10.550957	43.966088
H	7.095814	10.924472	44.376973

H	8.113890	11.752137	42.155861
H	6.407891	11.689110	40.288525
H	12.584846	13.434930	41.264395
H	11.773087	12.212713	40.235230
H	11.117331	14.827245	42.610444
H	9.595132	14.229290	43.158684
H	13.566249	19.364908	49.026170
H	13.930630	18.771649	50.649128
H	12.014163	17.495024	47.396174
H	10.202016	15.901601	48.029214
H	9.130611	14.744964	50.374480
H	9.540924	14.608656	52.819723
H	11.390742	15.888930	53.866870
H	12.868604	17.328580	52.513380
H	9.453383	6.850231	39.181932
H	8.720656	8.426299	38.902688
H	7.565063	7.588731	42.289131
H	5.314686	6.544723	42.405380
H	3.457187	5.319316	40.678467
H	3.165002	4.671733	38.294280
H	4.945026	5.141029	36.633100
H	7.044289	6.261820	37.289399
H	7.266260	13.510199	45.031051
H	6.325887	14.500325	46.152814
H	2.551682	7.877748	44.190625
C	7.384571	21.284734	44.312945
N	8.536346	20.837128	45.066365
C	9.636703	21.528108	45.333777
N	9.861715	22.750171	44.833965
N	10.567991	20.974050	46.136398
H	6.720405	20.422489	44.174073
H	6.827299	22.063869	44.847295
H	7.670545	21.657415	43.322739
H	8.540277	19.881398	45.450141
H	10.593307	23.287582	45.277114
H	9.081802	23.310621	44.509971
H	11.504721	21.345053	46.087121
H	10.484747	19.972445	46.282286
O	9.200601	18.411350	46.228816
H	9.067740	17.536107	45.746099
H	8.865869	18.242456	47.118672
O	8.049000	24.956000	44.152000
H	8.426561	25.844223	44.229130
H	7.164705	25.125333	43.802624

Cartesian coordinates of Mono-Fe1(II)-S2:

153

Fe	5.089052	9.535556	48.025480
C	5.407975	6.633522	50.844684
C	4.973449	7.766908	49.954853
O	5.381341	7.692429	48.732009
O	4.306330	8.748718	50.362024

H	5.173067	5.680679	50.367543
C	8.255595	6.511006	46.750203
C	7.440573	6.715580	45.480228
C	6.279749	7.662046	45.613237
O	6.324607	8.716029	46.239975
O	5.208436	7.253305	44.928535
H	8.679154	7.444420	47.147180
C	7.720965	9.994917	50.577877
C	7.676990	10.891617	49.398952
N	6.693944	10.841886	48.430473
C	8.539346	11.914357	49.086969
C	6.969344	11.822079	47.579665
N	8.072052	12.490126	47.936589
H	8.477626	10.363691	51.265000
C	6.401412	8.888266	57.266507
C	5.638960	9.324468	56.053305
C	5.275736	10.668573	55.890281
C	5.294197	8.430432	55.038696
C	4.613555	11.116443	54.752818
C	4.619150	8.858906	53.902567
C	4.293782	10.206671	53.742036
O	3.670592	10.669285	52.619798
H	7.068570	9.698540	57.537608
C	-0.196552	8.795963	42.128504
C	0.699567	7.577327	41.955289
C	1.888439	7.374626	42.927862
O	2.183863	8.292320	43.740308
O	2.500891	6.271513	42.789114
H	-0.845306	8.715486	43.001082
C	2.018229	12.843917	45.016250
C	2.530406	12.482255	46.399234
C	3.413267	11.250704	46.507524
O	3.894603	10.675544	45.513679
O	3.649616	10.865808	47.725428
H	2.831129	13.047393	44.304231
C	3.734155	10.614328	41.203726
C	5.038517	10.865513	41.843740
N	5.292815	10.777902	43.190850
C	6.231138	11.193496	41.257904
C	6.578186	11.036957	43.419399
N	7.162883	11.283759	42.253730
H	3.858926	10.924995	40.169709
C	11.589741	13.220616	40.790393
C	10.475072	13.445710	41.775720
O	9.457480	12.731453	41.780228
N	10.629280	14.485513	42.608999
H	11.464495	13.953923	39.987328
C	13.667219	18.451050	49.528098
C	12.487368	17.535559	49.427024
C	11.853574	17.160636	48.262736
C	11.808527	16.834473	50.482817
N	10.829372	16.291761	48.528551
C	10.769624	16.071199	49.877398
C	11.960717	16.761350	51.881802
C	9.885610	15.283112	50.619444
C	11.094778	15.963448	52.618364
C	10.063817	15.234134	51.994714

H	14.589104	17.942522	49.233390
C	8.795514	7.639895	39.684183
C	7.453541	7.129820	40.138681
C	6.886477	7.289332	41.383550
C	6.467303	6.408869	39.363319
N	5.638426	6.726214	41.433584
C	5.346619	6.179746	40.214202
C	6.390145	5.918316	38.042187
C	4.190521	5.507533	39.804170
C	5.245897	5.243600	37.628854
C	4.155391	5.040395	38.498315
H	9.447038	8.058237	40.488698
C	7.041843	14.479249	45.241186
C	8.343442	15.171020	45.611091
O	8.779481	16.077137	44.836935
O	8.926069	14.793425	46.673045
H	6.495139	14.991927	44.451834
H	6.499282	6.672459	50.947481
H	4.952532	6.670477	51.832701
H	7.643091	6.063830	47.538995
H	9.083288	5.826040	46.532641
H	7.066349	5.762536	45.092917
H	8.077590	7.139802	44.689737
H	6.763163	9.992381	51.106508
H	7.966166	8.961478	50.308372
H	6.379417	12.069545	46.712245
H	8.433194	13.341618	47.455251
H	9.434266	12.263684	49.583273
H	5.746379	8.691903	58.126068
H	6.992498	7.985712	57.080919
H	5.537133	11.392387	56.663782
H	4.360308	12.168609	54.628316
H	3.718522	9.967828	51.946927
H	4.351101	8.153485	53.124652
H	5.567862	7.377903	55.126991
H	0.389035	9.716024	42.235015
H	-0.856583	8.914611	41.255858
H	1.143943	7.589226	40.948689
H	0.100252	6.656771	41.983210
H	1.403577	12.040713	44.593538
H	1.398254	13.747352	45.075407
H	1.696926	12.341630	47.100491
H	3.117190	13.311120	46.826123
H	3.470772	9.553124	41.230716
H	2.921466	11.180451	41.668572
H	4.604299	10.661168	43.960628
H	7.068766	11.026228	44.378193
H	8.116441	11.644208	42.140130
H	6.479250	11.356182	40.218462
H	12.576725	13.378113	41.237798
H	11.519402	12.211631	40.379688
H	11.452550	15.065152	42.559972
H	9.888682	14.774866	43.234498
H	13.557167	19.326636	48.876139
H	13.807763	18.817919	50.549730
H	12.069106	17.445321	47.238440
H	10.237735	15.853740	47.828251

H	9.077632	14.737406	50.138046
H	9.391053	14.624384	52.596544
H	11.210446	15.901652	53.699796
H	12.746924	17.321862	52.387467
H	9.372335	6.842656	39.195711
H	8.676680	8.433124	38.930969
H	7.296885	7.781286	42.255861
H	5.001585	6.730074	42.220837
H	3.357582	5.372071	40.493430
H	3.271317	4.509608	38.144780
H	5.185299	4.862820	36.609198
H	7.214055	6.060600	37.342881
H	7.272157	13.470621	44.886880
H	6.399722	14.393189	46.122011
H	4.484582	7.910097	44.999611
C	7.377721	21.278816	44.340802
N	8.506275	20.792891	45.100207
C	9.616205	21.454007	45.401528
N	9.852403	22.696460	44.954706
N	10.541858	20.838823	46.150589
H	6.720405	20.422489	44.174073
H	6.813848	22.043380	44.889367
H	7.681081	21.678031	43.366330
H	8.486706	19.820496	45.441133
H	10.602967	23.205512	45.399637
H	9.076085	23.277863	44.665187
H	11.441590	21.264985	46.298673
H	10.420678	19.852303	46.344933
O	9.012048	18.326371	46.190923
H	8.982072	17.462630	45.685254
H	8.553481	18.132775	47.017610
O	8.049000	24.956000	44.152000
H	8.413068	25.837218	43.991621
H	7.100881	25.081798	44.009037

Cartesian coordinates of Mono-Fe1(II)-S3:

153

Fe	5.251818	9.446474	47.777195
C	5.185228	6.598494	50.965758
C	4.697604	7.782140	50.149583
O	5.275467	7.880508	48.997149
O	3.841708	8.573089	50.589268
H	5.173067	5.680679	50.367543
C	8.184693	6.513899	46.830941
C	7.434545	6.662861	45.515760
C	6.410613	7.796028	45.410753
O	6.439311	8.682415	46.329782
O	5.663715	7.821143	44.399397
H	8.679154	7.444420	47.147180
C	7.798389	9.943761	50.528963
C	7.770978	10.858729	49.363571
N	6.819898	10.805651	48.369093

C	8.625927	11.903339	49.098554
C	7.103285	11.800738	47.542177
N	8.183939	12.485938	47.941969
H	8.477626	10.363691	51.265000
C	6.402915	8.889752	57.253620
C	5.608955	9.364757	56.076044
C	5.318675	10.726893	55.925419
C	5.160102	8.490688	55.084951
C	4.623130	11.212198	54.823106
C	4.454672	8.955669	53.982428
C	4.197663	10.320513	53.835434
O	3.539988	10.818540	52.746667
H	7.068570	9.698540	57.537608
C	-0.536552	8.643794	41.960771
C	0.679883	7.738689	41.911231
C	1.696225	7.992866	43.002475
O	1.444002	9.120165	43.671157
O	2.639729	7.249155	43.228743
H	-0.845305	8.715486	43.001082
C	1.984341	12.775120	44.954674
C	2.419423	12.298665	46.332336
C	3.171882	10.974671	46.440490
O	3.026393	10.036622	45.634230
O	3.941297	10.903225	47.479283
H	2.831130	13.047393	44.304230
C	3.845554	10.413059	41.133430
C	5.112431	10.749782	41.820379
N	5.596013	10.183270	42.980588
C	6.051181	11.670487	41.440965
C	6.776207	10.721171	43.277883
N	7.061747	11.632724	42.359298
H	3.858927	10.924995	40.169709
C	11.548255	13.150606	40.719625
C	10.427197	13.366888	41.692003
O	9.377985	12.702499	41.605286
N	10.601671	14.338127	42.597358
H	11.464496	13.953922	39.987328
C	13.693579	18.494508	49.528389
C	12.490824	17.607273	49.472570
C	11.812433	17.240625	48.332620
C	11.849503	16.904878	50.550050
N	10.791429	16.378314	48.633893
C	10.785074	16.148711	49.982649
C	12.065606	16.819499	51.939878
C	9.940515	15.345735	50.754776
C	11.239768	16.007615	52.705257
C	10.184039	15.279824	52.119403
H	14.589106	17.942519	49.233390
C	8.887504	7.589298	39.650013
C	7.559386	7.060280	40.101294
C	7.104789	7.121648	41.394526
C	6.501221	6.420807	39.353243
N	5.857728	6.574334	41.507574
C	5.447425	6.142474	40.276980
C	6.309572	6.042101	38.008493
C	4.246062	5.534401	39.900809
C	5.119468	5.427485	37.632526

C	4.094936	5.178977	38.566950
H	9.447039	8.058236	40.488698
C	7.022734	14.509987	45.273956
C	8.282358	15.266192	45.662567
O	8.628915	16.231852	44.912470
O	8.911085	14.892349	46.697498
H	6.495139	14.991929	44.451835
H	6.234699	6.771096	51.237870
H	4.599896	6.457314	51.877010
H	7.510219	6.222689	47.642438
H	8.953676	5.734826	46.736513
H	6.912974	5.732788	45.256798
H	8.144758	6.825678	44.692402
H	6.811527	9.864827	50.991027
H	8.130794	8.933521	50.265622
H	6.538630	12.047189	46.657585
H	8.527781	13.352486	47.488935
H	9.495487	12.264371	49.631633
H	5.770356	8.652043	58.119893
H	6.999455	8.000969	57.021519
H	5.664641	11.433620	56.680760
H	4.427047	12.277330	54.708575
H	3.486707	10.105416	52.087145
H	4.116572	8.267347	53.215651
H	5.376798	7.424015	55.164185
H	-0.307339	9.659858	41.619893
H	-1.357149	8.253991	41.348538
H	1.214630	7.812033	40.954027
H	0.394348	6.683227	42.005915
H	1.390077	12.021713	44.429529
H	1.363022	13.674029	45.061087
H	1.529217	12.168096	46.967971
H	3.022259	13.062286	46.837660
H	3.754440	9.338670	40.951215
H	2.970237	10.747791	41.698582
H	5.267478	9.359846	43.527950
H	7.398904	10.444492	44.114393
H	7.952808	12.152989	42.270763
H	6.075079	12.334465	40.588546
H	12.535021	13.216687	41.187628
H	11.424038	12.187359	40.220975
H	11.450268	14.882783	42.614156
H	9.848891	14.618552	43.207230
H	13.600201	19.350613	48.848972
H	13.865775	18.889200	50.534729
H	11.994085	17.527778	47.303368
H	10.186104	15.934640	47.949546
H	9.119106	14.794293	50.302187
H	9.547171	14.655371	52.744116
H	11.407993	15.930275	53.778737
H	12.873430	17.376939	52.413755
H	9.524777	6.797159	39.230852
H	8.775318	8.348235	38.862968
H	7.597781	7.527899	42.265441
H	5.316462	6.584260	42.360827
H	3.460015	5.345819	40.631362
H	3.170331	4.701434	38.242277

H	4.971561	5.131771	36.593808
H	7.082971	6.222116	37.261125
H	7.287872	13.493365	44.968094
H	6.353701	14.435665	46.136944
H	2.121486	9.311001	44.375177
C	7.397552	21.276948	44.266470
N	8.566454	20.826144	44.986763
C	9.650367	21.535687	45.264084
N	9.853507	22.765014	44.771693
N	10.588486	20.996060	46.071693
H	6.720405	20.422489	44.174073
H	6.869830	22.073155	44.804818
H	7.650234	21.623502	43.257717
H	8.583851	19.865492	45.366181
H	10.559670	23.319312	45.235256
H	9.066912	23.311712	44.432197
H	11.526497	21.356101	45.990117
H	10.510588	19.993594	46.217391
O	9.202058	18.419554	46.163395
H	9.036346	17.538924	45.699929
H	8.825419	18.294443	47.041543
O	8.049000	24.956000	44.152000
H	8.432506	25.707941	43.681431
H	7.110766	25.012161	43.926675

Cartesian coordinates of Mono-Fe1(II)-S4:

153

Fe	5.295908	9.526105	48.049122
C	5.143433	6.598652	50.967576
C	4.794475	7.795339	50.112707
O	5.324369	7.771260	48.932405
O	4.114228	8.756942	50.523354
H	5.173067	5.680679	50.367543
C	8.143912	6.572724	46.737562
C	7.290843	6.907049	45.519799
C	6.231072	7.994809	45.677022
O	6.483770	8.905815	46.548501
O	5.230501	7.996606	44.919401
H	8.679154	7.444420	47.147180
C	7.760373	9.989468	50.542993
C	7.704570	10.958441	49.425497
N	6.654359	11.017961	48.536953
C	8.606591	11.942237	49.095952
C	6.928230	12.015236	47.704851
N	8.093618	12.596528	48.007463
H	8.477626	10.363691	51.265000
C	6.455018	8.857824	57.234488
C	5.645013	9.319708	56.063568
C	5.341697	10.679562	55.914904
C	5.195020	8.438471	55.079290
C	4.638459	11.157681	54.813959
C	4.480472	8.896288	53.979677

C	4.219714	10.260954	53.828884
O	3.563965	10.752048	52.735264
H	7.068570	9.698540	57.537608
C	-0.352328	8.764904	42.027254
C	0.543773	7.557781	41.808001
C	1.739965	7.385635	42.773415
O	1.964841	8.295212	43.618103
O	2.408544	6.318298	42.616208
H	-0.845306	8.715486	43.001082
C	2.048931	13.016178	45.076842
C	2.586458	12.582733	46.430834
C	3.220139	11.225837	46.516107
O	3.174980	10.521222	45.410216
O	3.743854	10.824632	47.571669
H	2.831129	13.047393	44.304231
C	3.818781	10.387040	41.117101
C	5.092730	10.687200	41.799133
N	5.527371	10.138021	42.984828
C	6.089947	11.537636	41.406186
C	6.730505	10.619745	43.296342
N	7.080455	11.476223	42.346357
H	3.858926	10.924995	40.169709
C	11.554753	13.159716	40.739292
C	10.409676	13.327639	41.698007
O	9.398614	12.604484	41.615248
N	10.528118	14.312293	42.598942
H	11.464495	13.953923	39.987328
C	13.676852	18.484423	49.500405
C	12.491387	17.573680	49.451049
C	11.811197	17.200893	48.314610
C	11.861355	16.866893	50.532922
N	10.796642	16.332597	48.621352
C	10.797111	16.103555	49.970960
C	12.080966	16.787962	51.921978
C	9.953654	15.305824	50.750251
C	11.254769	15.981186	52.695847
C	10.197892	15.249308	52.116031
H	14.589104	17.942522	49.233390
C	8.869980	7.573222	39.669989
C	7.522667	7.047766	40.085430
C	6.990309	7.082367	41.353832
C	6.505858	6.427098	39.262524
N	5.730955	6.542108	41.375890
C	5.395946	6.141700	40.110539
C	6.395290	6.068967	37.901995
C	4.208763	5.560048	39.653848
C	5.223833	5.473253	37.444256
C	4.137220	5.228505	38.307965
H	9.447038	8.058237	40.488698
C	7.015597	14.521405	45.285831
C	8.323951	15.218761	45.625766
O	8.745653	16.109021	44.825733
O	8.918244	14.869422	46.691656
H	6.495139	14.991927	44.451834
H	6.164379	6.752789	51.346885
H	4.467425	6.480000	51.818979
H	7.531705	6.159650	47.545697

H	8.891067	5.816769	46.464815
H	6.786803	6.011588	45.136780
H	7.941936	7.249316	44.700030
H	6.790699	9.910295	51.042632
H	8.066152	8.986520	50.220982
H	6.305224	12.327287	46.883240
H	8.465116	13.440772	47.520312
H	9.553239	12.218177	49.543303
H	5.832617	8.562794	58.090195
H	7.104572	8.011894	56.985087
H	5.686410	11.390311	56.667860
H	4.435099	12.222026	54.697001
H	3.568084	10.052097	52.057473
H	4.138239	8.201928	53.221026
H	5.417559	7.373022	55.160380
H	0.219571	9.700005	42.003606
H	-1.139789	8.824599	41.261206
H	0.959512	7.568977	40.789831
H	-0.049908	6.633946	41.861570
H	1.260349	12.342466	44.725334
H	1.622486	14.022334	45.164164
H	1.788880	12.574690	47.188292
H	3.329834	13.290876	46.823912
H	3.704186	9.318383	40.916339
H	2.951314	10.716839	41.697424
H	5.075438	9.409455	43.545409
H	7.316310	10.353836	44.163517
H	7.985283	11.974458	42.267264
H	6.170743	12.163644	40.527821
H	12.526372	13.264663	41.233496
H	11.484254	12.185756	40.251034
H	11.352997	14.891999	42.617593
H	9.760665	14.572969	43.202885
H	13.576643	19.319192	48.795618
H	13.825566	18.909659	50.498530
H	11.984833	17.490002	47.283882
H	10.194685	15.884456	47.938562
H	9.129866	14.753389	50.304308
H	9.558960	14.632082	52.746086
H	11.422791	15.914503	53.770382
H	12.888714	17.350027	52.390999
H	9.502731	6.773125	39.260773
H	8.766488	8.320162	38.869879
H	7.438851	7.456927	42.264752
H	5.102896	6.512954	42.168686
H	3.376297	5.393441	40.336715
H	3.227737	4.769378	37.918935
H	5.138565	5.188431	36.395496
H	7.215422	6.247421	37.206233
H	7.220241	13.476141	45.019806
H	6.357346	14.527753	46.160982
H	3.568243	9.633989	45.547143
C	7.393695	21.274940	44.285004
N	8.545641	20.813377	45.026375
C	9.646439	21.500621	45.299864
N	9.866972	22.727168	44.813649
N	10.579407	20.937698	46.097083

H	6.720405	20.422489	44.174073
H	6.857311	22.067424	44.820199
H	7.669626	21.629521	43.285573
H	8.548869	19.849150	45.383997
H	10.592948	23.266356	45.259726
H	9.089014	23.281462	44.477471
H	11.523204	21.293815	46.023219
H	10.494438	19.934343	46.232556
O	9.171527	18.359983	46.136980
H	9.074569	17.490170	45.650864
H	8.787707	18.187314	47.010850
O	8.049000	24.956000	44.152000
H	8.417422	25.817112	43.914431
H	7.097437	25.081784	44.026839

Cartesian coordinates of Mono-Fe2(II)-S1:

153

Fe	3.963175	8.974976	44.463616
C	5.418527	6.709823	50.659592
C	4.420590	7.687128	50.097884
O	4.652225	7.946229	48.806837
O	3.509571	8.208268	50.731549
H	5.173067	5.680679	50.367543
C	8.184331	6.487394	46.931896
C	7.301533	6.555654	45.695594
C	6.296776	7.697441	45.655706
O	6.525262	8.767044	46.255417
O	5.261340	7.493113	44.911904
H	8.679154	7.444420	47.147180
C	7.820003	9.948064	50.501498
C	7.784253	10.890841	49.360323
N	7.398600	10.571098	48.080306
C	8.107096	12.220953	49.323455
C	7.488666	11.651466	47.310907
N	7.915390	12.669428	48.044744
H	8.477626	10.363692	51.265001
C	6.555180	8.822580	57.150933
C	5.708258	9.271694	56.000346
C	5.439149	10.632549	55.811520
C	5.165868	8.368944	55.082356
C	4.677001	11.089160	54.741256
C	4.389159	8.803946	54.016245
C	4.155002	10.169618	53.829679
O	3.425247	10.648718	52.778199
H	7.068568	9.698540	57.537609
C	-0.254882	8.664594	42.083833
C	0.657009	7.445646	42.037714
C	1.945649	7.443140	42.868311
O	2.207682	8.507244	43.540042
O	2.673718	6.428272	42.808914
H	-0.845304	8.715486	43.001080

C	2.199794	13.175028	45.200052
C	2.812586	12.608699	46.477270
C	3.117606	11.106531	46.509608
O	3.152566	10.546176	45.356989
O	3.316894	10.548632	47.609451
H	2.831130	13.047393	44.304230
C	3.676418	10.492427	41.152266
C	4.939485	10.658844	41.905818
N	5.219463	10.100240	43.135309
C	6.033340	11.372808	41.487493
C	6.457508	10.473875	43.435976
N	6.976905	11.239381	42.465851
H	3.858928	10.924995	40.169708
C	11.503197	13.139853	40.722710
C	10.391970	13.379751	41.710668
O	9.313483	12.768146	41.649385
N	10.627496	14.332846	42.630396
H	11.464496	13.953923	39.987329
C	13.701920	18.544559	49.440815
C	12.491203	17.671499	49.418907
C	11.789001	17.296997	48.297054
C	11.883570	16.971290	50.516259
N	10.778278	16.432770	48.629368
C	10.803615	16.215610	49.980110
C	12.135660	16.885790	51.899282
C	9.965533	15.434709	50.777285
C	11.319690	16.086108	52.688124
C	10.238266	15.372060	52.135707
H	14.589104	17.942521	49.233391
C	8.881667	7.623106	39.636384
C	7.537678	7.070747	40.021874
C	6.978117	7.110214	41.277435
C	6.550962	6.424225	39.184602
N	5.735378	6.537772	41.281662
C	5.432856	6.115466	40.016585
C	6.467453	6.068904	37.822086
C	4.274558	5.492932	39.540576
C	5.318239	5.446620	37.344353
C	4.230120	5.162477	38.193507
H	9.447040	8.058237	40.488699
C	7.018922	14.433873	45.226317
C	8.179614	15.232406	45.787190
O	8.718672	16.090871	45.031056
O	8.558734	14.995765	46.983289
H	6.495139	14.991929	44.451835
H	6.416075	6.914869	50.263717
H	5.426902	6.767622	51.748096
H	7.600869	6.211990	47.818017
H	8.963560	5.726671	46.798997
H	6.765554	5.612713	45.536595
H	7.925573	6.692033	44.798777
H	6.827509	9.813362	50.947180
H	8.206202	8.967544	50.207791
H	7.089832	9.672700	47.671645
H	7.253116	11.676661	46.261357
H	8.121859	13.643692	47.643339
H	8.456961	12.858796	50.119564

H	5.956389	8.388225	57.963423
H	7.298449	8.072773	56.854720
H	5.846744	11.361152	56.514095
H	4.490540	12.153067	54.600534
H	3.264656	9.912239	52.167053
H	3.967638	8.086089	53.319360
H	5.355598	7.300187	55.195024
H	0.314179	9.596681	42.003616
H	-0.968651	8.633530	41.249532
H	0.990828	7.272386	41.004306
H	0.102815	6.536311	42.308719
H	1.237961	12.695506	44.981573
H	2.010863	14.250049	45.323905
H	2.171255	12.829462	47.340653
H	3.765980	13.112424	46.696175
H	3.412539	9.440403	41.021702
H	2.828258	10.997344	41.627807
H	6.995949	10.185141	44.325156
H	7.901256	11.657570	42.435411
H	6.212456	11.946734	40.587613
H	12.489774	13.154593	41.199795
H	11.348843	12.184074	40.217953
H	11.504028	14.829287	42.657149
H	9.897701	14.623288	43.263042
H	13.652190	19.333469	48.681096
H	13.846481	19.024562	50.414400
H	11.950033	17.573841	47.261573
H	10.128128	16.005670	47.978759
H	9.119686	14.910730	50.341860
H	9.605176	14.764451	52.781173
H	11.513089	16.013542	53.757481
H	12.960236	17.436788	52.351220
H	9.520186	6.849938	39.186458
H	8.779917	8.415747	38.881262
H	7.390860	7.517260	42.190901
H	5.095659	6.522832	42.064063
H	3.438683	5.282596	40.205610
H	3.339862	4.678009	37.791873
H	5.250839	5.174913	36.290985
H	7.289253	6.279391	37.137202
H	7.404096	13.522608	44.759144
H	6.309830	14.154598	46.006915
H	4.027212	8.640869	48.504887
C	7.389299	21.281498	44.289507
N	8.562658	20.820960	44.999044
C	9.644932	21.524546	45.300972
N	9.843774	22.772488	44.859962
N	10.587319	20.958309	46.083040
H	6.720405	20.422489	44.174073
H	6.853610	22.057352	44.849734
H	7.640042	21.660024	43.291868
H	8.580853	19.851060	45.347272
H	10.548534	23.312331	45.341443
H	9.059644	23.324914	44.532500
H	11.519612	21.341049	46.036265
H	10.517882	19.953012	46.201318
O	9.172361	18.396208	46.159258

H	9.053299	17.485259	45.747728
H	8.796667	18.304258	47.043855
O	8.049000	24.956000	44.152000
H	8.373460	25.848173	43.968679
H	7.089698	25.051747	44.077355

Cartesian coordinates of Mono-Fe2(II)-S2:

153

Fe	3.696259	8.757990	44.116514
C	5.509781	6.613730	50.845245
C	4.679072	7.828462	50.398828
O	5.073626	8.478084	49.400781
O	3.640065	8.096642	51.095603
H	5.173067	5.680679	50.367543
C	8.044824	6.557440	46.983571
C	7.197139	6.590010	45.713893
C	6.054790	7.569843	45.628047
O	6.153528	8.622435	46.374533
O	5.110356	7.364729	44.825060
H	8.679154	7.444420	47.147180
C	7.754754	9.961368	50.578742
C	7.658559	10.939853	49.483193
N	6.567220	11.027769	48.664752
C	8.514453	11.930035	49.073944
C	6.737675	12.021177	47.797110
N	7.916165	12.584482	48.028182
H	8.477626	10.363692	51.265001
C	6.343271	8.914038	57.360283
C	5.609332	9.274879	56.105780
C	5.363355	10.615959	55.783377
C	5.185428	8.302991	55.198674
C	4.734743	10.981550	54.596204
C	4.548083	8.647436	54.014796
C	4.331238	9.991660	53.690173
O	3.749743	10.359153	52.519423
H	7.068568	9.698540	57.537609
C	-0.503276	8.501157	41.987529
C	0.320090	7.223664	41.918930
C	1.645608	7.175916	42.677802
O	2.013252	8.283241	43.235406
O	2.300709	6.117957	42.701824
H	-0.845304	8.715486	43.001080
C	2.273545	13.091933	45.253097
C	2.994982	12.324456	46.351480
C	3.466678	10.936021	45.959402
O	2.791116	10.307752	45.087968
O	4.511035	10.486774	46.516482
H	2.831130	13.047393	44.304230
C	3.669896	10.413990	41.108839
C	4.903607	10.570246	41.907985
N	5.135428	9.945244	43.115613

C	6.001180	11.325075	41.585406
C	6.350896	10.325186	43.503205
N	6.897109	11.150977	42.601828
H	3.858928	10.924995	40.169708
C	11.515561	13.138882	40.728767
C	10.428692	13.336473	41.760949
O	9.377487	12.673588	41.754568
N	10.667511	14.297220	42.672301
H	11.464496	13.953923	39.987329
C	13.705491	18.476329	49.604809
C	12.510874	17.574203	49.591407
C	11.821919	17.173770	48.469565
C	11.900085	16.881388	50.693100
N	10.826118	16.293263	48.803125
C	10.848802	16.083722	50.156249
C	12.124811	16.841786	52.083513
C	10.043293	15.267169	50.953612
C	11.329221	16.025857	52.876237
C	10.299963	15.242520	52.317339
H	14.589104	17.942521	49.233391
C	8.850842	7.616187	39.662439
C	7.530657	7.050198	40.104856
C	7.063116	7.006408	41.395822
C	6.478871	6.470754	39.298322
N	5.811223	6.453759	41.447775
C	5.414331	6.121191	40.180963
C	6.300343	6.205848	37.925796
C	4.212953	5.554381	39.745913
C	5.110668	5.630319	37.487354
C	4.074279	5.311717	38.385964
H	9.447040	8.058237	40.488699
C	6.968093	14.497674	45.303877
C	8.299734	15.119056	45.701382
O	8.800342	16.003750	44.950589
O	8.848186	14.710137	46.779778
H	6.495139	14.991929	44.451835
H	6.560270	6.749603	50.574035
H	5.430341	6.458180	51.925232
H	7.416104	6.430990	47.869389
H	8.715498	5.691551	46.923450
H	6.764230	5.602546	45.510795
H	7.828172	6.807725	44.838474
H	6.801032	9.855708	51.098918
H	8.073580	8.973227	50.232077
H	5.776630	10.382520	48.710778
H	6.033135	12.289822	47.032297
H	8.288937	13.440942	47.494594
H	9.492524	12.206148	49.444762
H	5.687054	8.852750	58.238839
H	6.872024	7.959386	57.268044
H	5.690221	11.400950	56.468536
H	4.570453	12.032064	54.356784
H	3.676789	9.544068	51.941009
H	4.228386	7.885845	53.310088
H	5.372671	7.249220	55.410838
H	0.069962	9.369637	41.644783
H	-1.393141	8.415688	41.351337

H	0.574951	6.998629	40.872783
H	-0.268733	6.361825	42.260044
H	1.274009	12.690049	45.063432
H	2.166273	14.145315	45.539558
H	2.349240	12.207152	47.234370
H	3.865844	12.885268	46.706095
H	3.449298	9.364594	40.894093
H	2.792194	10.855687	41.594207
H	6.860811	10.027784	44.406350
H	7.820371	11.569476	42.635900
H	6.214763	11.947911	40.726997
H	12.510764	13.162429	41.189210
H	11.371035	12.177738	40.229355
H	11.529912	14.818847	42.666700
H	9.959084	14.563827	43.342151
H	13.560666	19.354696	48.963393
H	13.931769	18.839798	50.611829
H	11.977904	17.448313	47.432821
H	10.226508	15.821077	48.137453
H	9.236564	14.677584	50.523090
H	9.690134	14.612802	52.964123
H	11.497899	15.991429	53.951925
H	12.910974	17.443309	52.539357
H	9.477093	6.848638	39.184921
H	8.708149	8.406677	38.912352
H	7.548230	7.345161	42.301564
H	5.260491	6.326683	42.283147
H	3.417230	5.322259	40.451431
H	3.149053	4.870972	38.013474
H	4.971244	5.423363	36.426562
H	7.081123	6.443965	37.203555
H	7.120388	13.444126	45.046466
H	6.280155	14.541728	46.153382
H	5.334817	9.284709	46.321623
C	7.397264	21.269380	44.290757
N	8.529780	20.802720	45.057247
C	9.619490	21.496093	45.354698
N	9.840503	22.723556	44.867749
N	10.537748	20.942832	46.171791
H	6.720405	20.422489	44.174073
H	6.854973	22.069063	44.809026
H	7.693243	21.612036	43.292619
H	8.525273	19.838325	45.413776
H	10.541970	23.276276	45.339476
H	9.064381	23.269203	44.510032
H	11.474763	21.313250	46.135777
H	10.454590	19.942230	46.318934
O	9.134292	18.338559	46.220319
H	9.075084	17.458502	45.756598
H	8.739609	18.171498	47.087876
O	8.049000	24.956000	44.152000
H	8.371586	25.790096	43.784446
H	7.097691	24.996055	43.978985

Cartesian coordinates of Mono-Fe₂(II)-S₃:

153

Fe	3.997619	8.660188	44.338047
C	5.549189	6.721100	50.414285
C	4.520595	7.804319	50.033077
O	4.704525	8.455205	48.959906
O	3.565188	8.000516	50.851336
H	5.173067	5.680679	50.367543
C	8.173493	6.477381	47.011677
C	7.315645	6.401735	45.754812
C	6.289869	7.510936	45.567767
O	6.490585	8.648553	46.015779
O	5.243049	7.189669	44.859689
H	8.679154	7.444420	47.147180
C	7.840587	9.860437	50.554117
C	7.774228	10.728653	49.365734
N	6.944249	10.497681	48.302141
C	8.439304	11.891441	49.067035
C	7.085820	11.467150	47.400445
N	7.990557	12.327589	47.849979
H	8.477626	10.363692	51.265001
C	6.390252	8.881442	57.309077
C	5.680735	9.204308	56.027726
C	5.408284	10.533019	55.676581
C	5.278482	8.207207	55.136212
C	4.767332	10.859295	54.485182
C	4.628938	8.512381	53.945387
C	4.373415	9.845913	53.602211
O	3.758195	10.196919	52.443646
H	7.068568	9.698540	57.537609
C	-0.278173	8.666037	42.070785
C	0.699905	7.502093	42.062175
C	1.949837	7.605918	42.923281
O	2.119311	8.678892	43.627107
O	2.792319	6.683169	42.888346
H	-0.845304	8.715486	43.001080
C	2.090827	13.002353	45.117915
C	2.649671	12.595615	46.474066
C	3.124840	11.170009	46.646300
O	3.333652	10.386229	45.729861
O	3.316380	10.879283	47.937632
H	2.831130	13.047393	44.304230
C	3.680904	10.410148	41.114403
C	4.927077	10.546184	41.902604
N	5.176172	9.956467	43.128137
C	6.031621	11.267380	41.530499
C	6.408721	10.322139	43.468331
N	6.950679	11.107853	42.528229
H	3.858928	10.924995	40.169708
C	11.540136	13.107182	40.686604
C	10.444696	13.238210	41.714741
O	9.416768	12.543618	41.673529
N	10.645209	14.175259	42.660838

H	11.464496	13.953923	39.987329
C	13.685715	18.463743	49.572130
C	12.501192	17.548992	49.545758
C	11.817786	17.147414	48.419934
C	11.880511	16.861898	50.645386
N	10.813615	16.274916	48.750167
C	10.822863	16.074991	50.104211
C	12.099890	16.818974	52.036327
C	9.994425	15.280477	50.899563
C	11.285000	16.019515	52.827119
C	10.240449	15.257763	52.265424
H	14.589104	17.942521	49.233391
C	8.876051	7.609184	39.654155
C	7.567653	7.015445	40.088170
C	7.085853	6.983838	41.375790
C	6.543465	6.394741	39.280602
N	5.853788	6.388822	41.424156
C	5.481387	6.026563	40.159015
C	6.389606	6.102716	37.909864
C	4.309295	5.404729	39.719607
C	5.226366	5.480514	37.468701
C	4.193446	5.135892	38.363205
H	9.447040	8.058237	40.488699
C	6.999210	14.400244	45.219595
C	8.236646	15.097429	45.766694
O	8.687883	16.089403	45.128283
O	8.762043	14.631749	46.833141
H	6.495139	14.991929	44.451835
H	6.426315	6.776712	49.768287
H	5.865423	6.877855	51.451319
H	7.565999	6.301614	47.904267
H	8.942970	5.695523	46.981491
H	6.800144	5.435294	45.696371
H	7.956988	6.446123	44.860523
H	6.854823	9.729132	51.009326
H	8.257364	8.872970	50.329186
H	6.319424	9.694308	48.217644
H	6.559757	11.522924	46.463501
H	8.277625	13.252810	47.376078
H	9.198235	12.417297	49.625648
H	5.697099	8.772957	58.155053
H	6.969478	7.954459	57.235848
H	5.715746	11.339378	56.344919
H	4.574254	11.899753	54.226196
H	3.659517	9.388930	51.870035
H	4.319241	7.721819	53.266814
H	5.480441	7.161031	55.372268
H	0.233762	9.625389	41.939860
H	-1.004325	8.558096	41.254757
H	1.070758	7.326471	41.042444
H	0.196111	6.566415	42.341858
H	1.288908	12.327914	44.798268
H	1.662295	14.007990	45.209100
H	1.903887	12.772015	47.259793
H	3.499941	13.234083	46.759231
H	3.446120	9.365086	40.893757
H	2.814374	10.856720	41.613916

H	6.919281	10.006544	44.366115
H	7.881811	11.508460	42.526509
H	6.233673	11.860187	40.647765
H	12.533886	13.133177	41.147658
H	11.412805	12.171004	40.139694
H	11.476053	14.745641	42.666176
H	9.914843	14.397367	43.320192
H	13.545234	19.329263	48.912835
H	13.881490	18.845835	50.578738
H	11.982707	17.415931	47.382633
H	10.206665	15.806471	48.087534
H	9.172882	14.713642	50.465833
H	9.611415	14.645468	52.910360
H	11.451861	15.980152	53.902785
H	12.898369	17.402916	52.493873
H	9.525161	6.858990	39.181222
H	8.722877	8.400920	38.907364
H	7.548286	7.354317	42.281466
H	5.262040	6.335957	42.240615
H	3.517120	5.142891	40.418597
H	3.291346	4.651359	37.989489
H	5.105446	5.254768	36.409569
H	7.170688	6.357937	37.193269
H	7.290077	13.442211	44.773115
H	6.292294	14.192328	46.028536
H	3.650129	9.957718	48.077912
C	7.387914	21.279311	44.267895
N	8.535708	20.838621	45.025785
C	9.635326	21.538473	45.266661
N	9.837273	22.753610	44.741110
N	10.580748	21.000813	46.061930
H	6.720405	20.422489	44.174073
H	6.843005	22.083020	44.777382
H	7.668203	21.606380	43.260282
H	8.531228	19.893535	45.430616
H	10.576662	23.303132	45.155485
H	9.046656	23.312421	44.425136
H	11.513618	21.379338	46.002601
H	10.505782	20.003893	46.233595
O	9.134791	18.420286	46.299279
H	9.013181	17.513540	45.899383
H	8.796917	18.329692	47.199532
O	8.049000	24.956000	44.152000
H	8.434571	25.637028	43.585283
H	7.124038	24.938529	43.867878