# Supplementary Information for

# Sulfur K-edge XAS and DFT calculations on superoxide reductase: Role of the axial thiolate in reactivity

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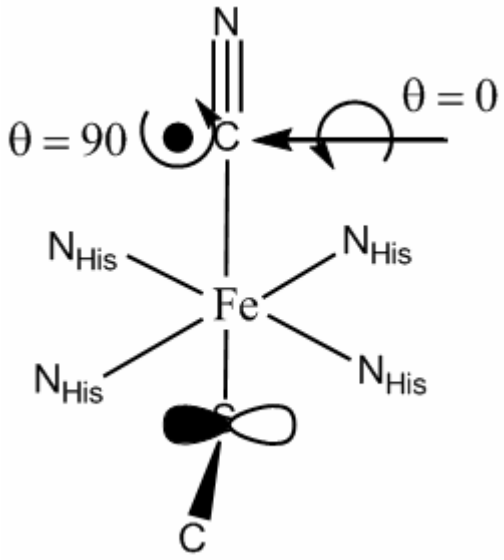
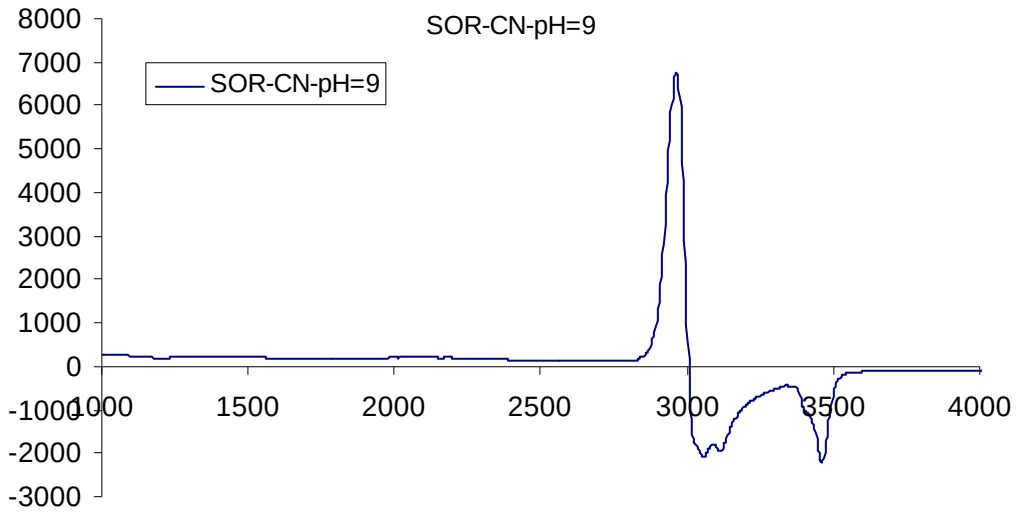



The orientation of the H-bonding or the direction of bending has a significant effect on the localization of the $t_2$ hole in the low-spin $CN^-$ bound form. Both of the above mentioned perturbations can be caused either along (θ=90) or perpendicular to (θ=0) the Fe-C-S plane (Figure on the left). Bending the Fe-CN along θ=90 axis selectively weakens the Fe-CN

backbonding to the Fe-S dπ orbital which now ends up as the LUMO. Likewise H-bonding from the θ=0 orientation only will weaken the backbonding to the Fe-S dπ orbital.

Fig. S1: EPR spectrum of the CN bound form @8K, 10mW, ModAmp 20




Full reference 41:

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

Scheme S1: Reaction scheme without H-bonding:

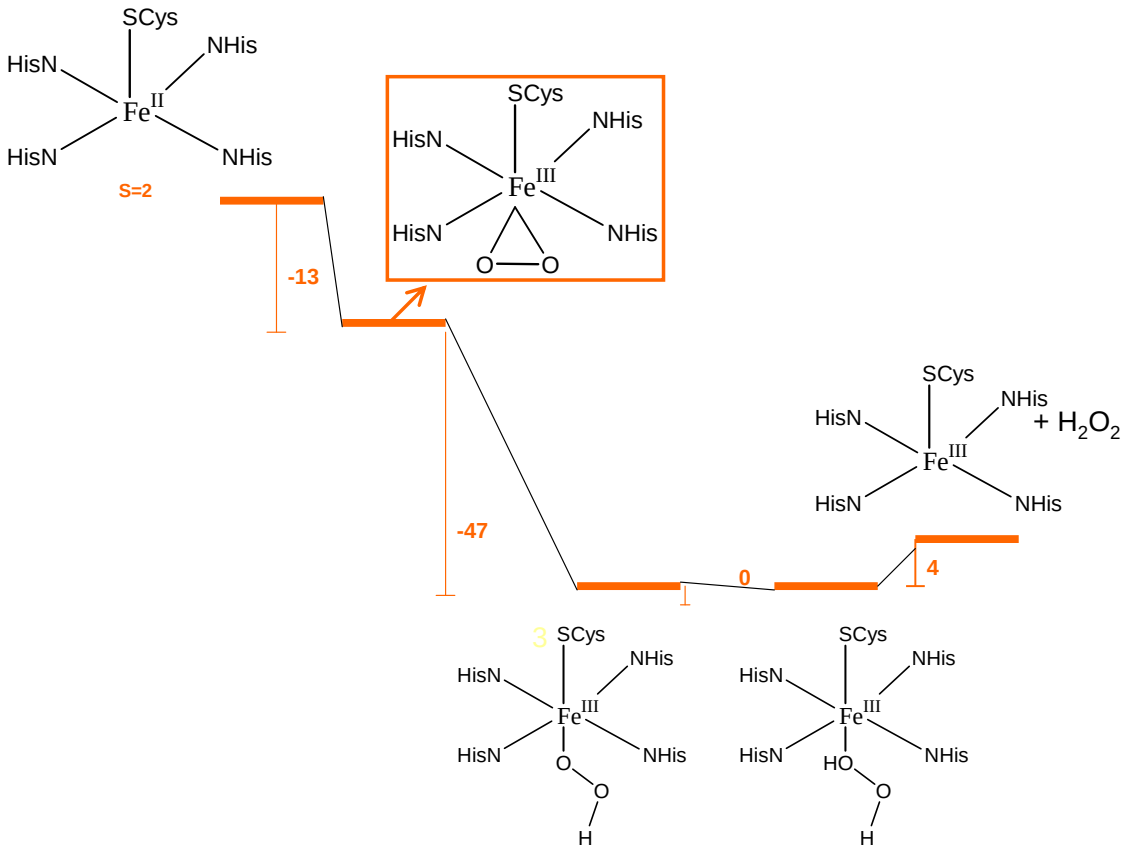
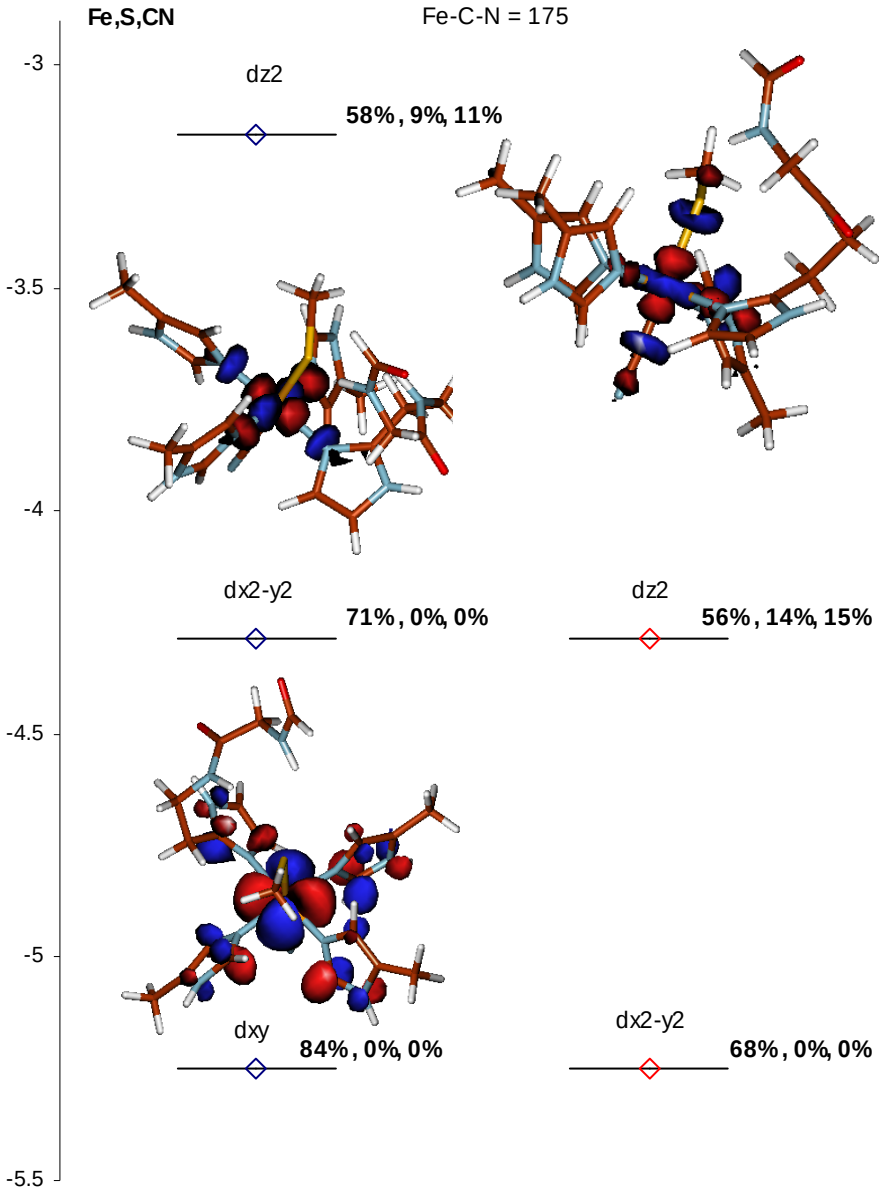


Figure S1: MO diagram with H-bonding from backbone and no solvent



Optimized Geometries:

1. Resting 6C

Fe -0.8223 -0.0864  0.1140
N  3.8952 -1.4255 -0.7693
C  3.2859 -2.7455 -0.8032
C  1.7935 -2.7398 -0.3718
C  1.5932 -2.0638  0.9541
N  0.5819 -1.2637  1.3067
N  2.4127 -2.2492  2.0192
C  0.7602 -0.9610  2.6482
C  1.9051 -1.5513  3.0955
H  3.5741 -0.7364 -1.4382
H  3.3604 -3.1560 -1.8158
H  3.8856 -3.3896 -0.1545
H  1.1899 -2.2198 -1.1140
H  1.4370 -3.7777 -0.3200
H  3.3599 -2.6272  1.9685
H  0.0537 -0.3467  3.1824
N  4.6826  1.2526 -0.9579
C  5.1743  0.4637  0.1540
C  4.7676 -1.0101  0.1878
O  5.2045 -1.7189  1.0879
H  3.7053  1.5207 -0.9956
H  6.2659  0.5060  0.1227
H  4.8612  0.8909  1.1147
H  5.0519  2.5147 -2.5500
C  5.5649  1.8841 -1.7991
O  6.7673  1.7642 -1.7419
C  0.3085  0.2582 -3.2193
S  0.8898  0.5173 -1.4980
H  1.0123  0.7435 -3.8992
H -0.6805  0.7006 -3.3690
H  0.2747 -0.8079 -3.4634
C  0.1630  3.8258  1.7273
N -0.8335  3.3693  2.5749
C  0.4059  2.7769  0.8859
C -1.1627  2.1076  2.2358
N -0.4264  1.7157  1.2022
C  0.7440  5.1921  1.7926
H  1.1032  2.7203  0.0651
H -1.9381  1.5261  2.7289
N -4.2188  1.8454 -1.7680
C -3.2770  2.8385 -1.9792
C -3.5967  0.7786 -1.2132
C -2.0977  2.3039 -1.5421

N -2.3074  1.0268 -1.0623
H -5.2074  1.9167 -1.9799
H -4.1034 -0.1296 -0.9277
H -1.1183  2.7558 -1.5271
N -2.6639 -3.3383 -2.0115
C -2.5215 -3.8696 -0.7386
C -2.0009 -2.1587 -2.0608
C -1.7525 -2.9654 -0.0677
N -1.4455 -1.9021 -0.8910
H -3.1811 -3.7490 -2.7750
H -1.9631 -1.5280 -2.9358
H -1.4414 -2.9831  0.9637
C -4.5696 -1.1979  1.5494
C -3.3772 -0.3762  2.0412
O -3.5006  0.3532  3.0164
O -2.2672 -0.4996  1.3623
H -4.2972 -1.8975  0.7558
H -5.3523 -0.5162  1.1975
H -4.9953 -1.7515  2.3920
C -3.5955  4.1748 -2.5360
H  2.3981 -1.5416  4.0550
C -3.1642 -5.1149 -0.2576
H -1.2757  3.8882  3.3200
H  1.5033  5.3114  1.0154
H  1.2248  5.3898  2.7586
H -0.0167  5.9674  1.6372
H -2.6813  4.7673 -2.6229
H -4.2917  4.7297 -1.8948
H -4.0445  4.1118 -3.5351
H -2.8874 -5.2895  0.7850
H -2.8571 -5.9961 -0.8345
H -4.2588 -5.0556 -0.3047

2.  Resting 5C Ferric
Fe  0.8194  0.0550 -0.1649
N -3.6195 -1.5259  0.5554
C -3.0965 -2.7870  0.0669
C -1.6358 -2.6876 -0.4318
C -1.4701 -1.7290 -1.5844
N -0.5981 -0.6303 -1.6098
C -2.1725 -1.7350 -2.7616
C -0.7949 -0.0130 -2.7773
N -1.7318 -0.6571 -3.4898
H -0.9926 -2.3771  0.3960
H -1.3055 -3.6928 -0.7272
H -3.1478 -3.5301  0.8691

H -3.7512 -3.1283 -0.7394
H -3.5047 -1.2798  1.5300
H -2.0953 -0.3666 -4.3896
H -2.9786 -2.3629 -3.1053
H -0.2930  0.8799 -3.1145
N -4.2149  0.9349  1.6870
C -4.9316  0.5392  0.5081
C -4.3858 -0.6971 -0.2114
O -4.6409 -0.9056 -1.3866
H -3.3128  1.3827  1.5905
H -5.9608  0.3226  0.8162
H -4.9835  1.3419 -0.2366
C -4.8840  1.1414  2.8674
O -6.0211  0.8139  3.0963
H -4.2176  1.6393  3.5721
C  0.1367 -0.7799  3.0592
S -0.4575  0.2831  1.6849
H -0.5038 -0.5848  3.9213
H  1.1698 -0.5336  3.3170
H  0.0645 -1.8364  2.7897
C -0.7146  5.5053 -1.2152
C -0.0123  4.1839 -1.2265
N  1.2757  4.0219 -1.7145
C -0.3682  2.9325 -0.7898
C  1.6561  2.7398 -1.5562
N  0.6793  2.0390 -0.9895
H -1.7167  5.3938 -0.7948
H -0.8185  5.9156 -2.2261
H -0.1738  6.2382 -0.6057
H  1.8408  4.7531 -2.1309
H -1.2995  2.6224 -0.3408
H  2.6315  2.3671 -1.8332
C  6.3285  1.4442  0.7975
C  4.8500  1.2907  0.9040
N  4.0827  1.9417  1.8566
C  3.9476  0.5497  0.1860
C  2.7899  1.5947  1.6981
N  2.6677  0.7439  0.6858
H  6.7082  0.8494 -0.0365
H  6.8360  1.1051  1.7082
H  6.6161  2.4878  0.6242
H  4.4380  2.5645  2.5731
H  4.1426 -0.1235 -0.6354
H  1.9823  1.9760  2.3063
C  3.7950 -4.7231  0.9058
C  2.9713 -3.6640  0.2510

N  2.4554 -3.7843 -1.0309
C  2.5456 -2.4330  0.6748
C  1.7555 -2.6766 -1.3365
N  1.7858 -1.8228 -0.3170
H  2.7437 -1.9468  1.6169
H  1.2379 -2.5304 -2.2721
H  2.5840 -4.5817 -1.6436
H  4.0882 -4.4025  1.9081
H  4.7095 -4.9311  0.3382
H  3.2385 -5.6623  1.0037

3. $Fe^{II}$-$O_2^-$

Fe -0.8935  0.0439  0.4376
N  3.5565 -1.5937 -0.7082
C  3.0356 -2.8691 -0.2439
C  1.6658 -2.7332  0.4465
C  1.6599 -1.8039  1.6280
N  0.7156 -0.7952  1.7778
C  2.5053 -1.7861  2.7100
C  0.9793 -0.1999  2.9277
N  2.0572 -0.7651  3.5241
H  0.9307 -2.3640 -0.2712
H  1.3350 -3.7380  0.7479
H  2.9363 -3.5542 -1.0958
H  3.7845 -3.2872  0.4324
H  2.9223 -1.0248 -1.2662
H  2.4749 -0.4742  4.3956
H  3.3954 -2.3521  2.9337
H  0.4142  0.6163  3.3497
N  4.3386  0.9293 -1.7501
C  4.9140  0.4621 -0.5028
C  4.5744 -0.9698 -0.0569
O  5.2135 -1.4747  0.8570
H  3.3257  1.0171 -1.8334
H  5.9996  0.5198 -0.6032
H  4.6271  1.1219  0.3272
C  5.1114  1.2848 -2.8157
O  6.3283  1.2680 -2.8602
H  4.4914  1.6094 -3.6748
C  0.2982 -0.7547 -3.0224
S  0.7516  0.3264 -1.5999
H  0.9980 -0.5926 -3.8475
H -0.7100 -0.5264 -3.3899
H  0.3287 -1.8170 -2.7544
C  0.8614  5.5477  0.7864

C  0.1861  4.2451  1.0199
N -1.0016  4.1154  1.7259
C  0.4959  2.9728  0.6227
C -1.3633  2.8063  1.7216
N -0.4710  2.0893  1.0593
H  1.7706  5.3920  0.1993
H  1.1539  6.0425  1.7225
H  0.2262  6.2493  0.2291
H -1.5180  4.8653  2.1625
H  1.3312  2.6418  0.0238
H -2.2615  2.3955  2.1713
C -6.1174  1.6385 -1.6963
C -4.6536  1.4070 -1.5004
N -3.6974  1.7963 -2.4298
C -3.9342  0.8236 -0.4880
C -2.4718  1.4459 -1.9563
N -2.5826  0.8519 -0.7822
H -6.6681  1.2651 -0.8287
H -6.5034  1.1190 -2.5835
H -6.3567  2.7044 -1.8067
H -3.8772  2.2645 -3.3063
H -4.2800  0.4234  0.4538
H -1.5349  1.6333 -2.4640
C -3.7460 -4.5919 -1.5408
C -2.9339 -3.6610 -0.7158
N -2.7801 -3.7890  0.6555
C -2.2260 -2.5352 -1.0407
C -2.0137 -2.7570  1.0967
N -1.6624 -1.9792  0.0887
H -2.0943 -2.0878 -2.0144
H -1.7898 -2.5637  2.1341
H -3.1922 -4.5052  1.2358
H -3.7115 -4.2827 -2.5892
H -4.8007 -4.6030 -1.2349
H -3.3783 -5.6256 -1.4906
O -2.0357 -0.1771  2.2538
O -3.1108  0.5465  2.5435

4.  a) High-spin $Fe^{III}$-OOH
Fe -0.9758  0.0841  0.4569
N  3.5917 -1.5976 -0.8452
C  2.9672 -2.8620 -0.4998
C  1.5512 -2.6911  0.0990
C  1.5460 -1.8618  1.3555
N  0.5940 -0.8821  1.6434

C  2.4201 -1.9330  2.4108
C  0.8886 -0.4014  2.8426
N  1.9865 -1.0061  3.3345
H  0.8982 -2.2240 -0.6380
H  1.1442 -3.6922  0.3012
H  2.9008 -3.4934 -1.3938
H  3.6381 -3.3619  0.2028
H  3.1578 -1.0348 -1.5650
H  2.4291 -0.8029  4.2204
H  3.3278 -2.4984  2.5499
H  0.3295  0.3560  3.3675
N  4.3948  0.9545 -1.6936
C  5.0168  0.3840 -0.5141
C  4.6032 -1.0403 -0.1266
O  5.1673 -1.5842  0.8104
H  3.4137  1.2115 -1.6746
H  6.0947  0.3776 -0.6906
H  4.8362  1.0108  0.3681
C  5.1527  1.3435 -2.7675
O  6.3519  1.1986 -2.8551
H  4.5398  1.8090 -3.5638
C -0.1274 -0.4957 -2.9654
S  0.5286  0.3361 -1.4638
H  0.5546 -0.3025 -3.7968
H -1.1164 -0.1097 -3.2348
H -0.2009 -1.5772 -2.8194
C  0.9763  5.5356  0.8588
C  0.3288  4.2264  1.1253
N -0.5977  4.0169  2.1341
C  0.4403  3.0166  0.4976
C -1.0083  2.7300  2.0835
N -0.3950  2.0944  1.0976
H  1.6631  5.4443  0.0136
H  1.5564  5.8930  1.7188
H  0.2427  6.3123  0.6087
H -0.9217  4.7114  2.7942
H  1.0487  2.7533 -0.3535
H -1.7500  2.2882  2.7311
C -6.0845  1.8316 -1.7051
C -4.6324  1.6263 -1.4382
N -3.6396  2.2468 -2.1809
C -3.9525  0.8631 -0.5246
C -2.4347  1.8487 -1.7170
N -2.5894  1.0042 -0.7109
H -6.6800  1.2515 -0.9955
H -6.3627  1.5080 -2.7157

H -6.3754  2.8841 -1.5999
H -3.7897  2.8869 -2.9496
H -4.3427  0.2308  0.2576
H -1.4854  2.1768 -2.1146
C -3.8558 -4.4530 -1.6577
C -2.9946 -3.5572 -0.8450
N -2.5158 -3.8972  0.4095
C -2.5104 -2.2980 -1.0714
C -1.7875 -2.8658  0.8904
N -1.7639 -1.8773  0.0128
H -2.6613 -1.6683 -1.9338
H -1.3279 -2.8502  1.8648
H -2.6853 -4.7706  0.8904
H -4.1090 -3.9692 -2.6046
H -4.7960 -4.6922 -1.1452
H -3.3567 -5.4009 -1.8944
O -2.1350 -0.8517  2.9982
O -2.1844  0.1619  1.9820
H -2.9754 -0.6939  3.4574

b) Low-spin $Fe^{III}$-OOH
Fe -1.0216  0.0722  0.3952
N  3.6528 -1.6390 -0.7096
C  3.0502 -2.8793 -0.2614
C  1.6144 -2.6876  0.2748
C  1.5115 -1.6701  1.3864
N  0.5347 -0.6657  1.5157
C  2.3461 -1.5885  2.4717
C  0.7929 -0.0347  2.6533
N  1.8779 -0.5564  3.2523
H  0.9646 -2.3750 -0.5442
H  1.2480 -3.6650  0.6189
H  3.0219 -3.6011 -1.0866
H  3.7129 -3.2868  0.5052
H  3.1923 -1.1199 -1.4458
H  2.2834 -0.2375  4.1213
H  3.2518 -2.1245  2.7084
H  0.2091  0.7715  3.0633
N  4.3963  0.9009 -1.6541
C  5.0291  0.3907 -0.4530
C  4.6509 -1.0274 -0.0170
O  5.2229 -1.5278  0.9389
H  3.4072  1.1255 -1.6509
H  6.1074  0.4085 -0.6262
H  4.8284  1.0428  0.4064
C  5.1530  1.2855 -2.7306

O  6.3577  1.1815 -2.7968
H  4.5352  1.7033 -3.5488
C -0.0801 -0.8534 -2.8508
S  0.4690  0.2440 -1.4866
H  0.6318 -0.7383 -3.6728
H -1.0718 -0.5722 -3.2214
H -0.1016 -1.9069 -2.5569
C  0.9590  5.5482  0.8483
C  0.2533  4.2236  0.9610
N -0.8321  4.0450  1.8040
C  0.4264  2.9916  0.3710
C -1.2661  2.7693  1.7064
N -0.5226  2.0928  0.8440
H  1.7772  5.4768  0.1274
H  1.3854  5.8598  1.8092
H  0.2786  6.3371  0.5067
H -1.2408  4.7550  2.3971
H  1.1556  2.6958 -0.3671
H -2.0969  2.3562  2.2564
C -6.0778  1.7143 -1.5874
C -4.6116  1.4853 -1.3788
N -3.6435  2.0368 -2.2039
C -3.8987  0.7646 -0.4531
C -2.4213  1.6497 -1.7751
N -2.5401  0.8710 -0.7117
H -6.6500  1.1906 -0.8175
H -6.4112  1.3418 -2.5635
H -6.3343  2.7789 -1.5283
H -3.8166  2.6309 -3.0039
H -4.2583  0.1907  0.3853
H -1.4845  1.9290 -2.2346
C -3.7842 -4.5446 -1.4085
C -2.9021 -3.5652 -0.6952
N -2.2854 -3.8633  0.5107
C -2.5145 -2.2769 -0.9633
C -1.5774 -2.7914  0.9239
N -1.6891 -1.8031  0.0498
H -2.7772 -1.6622 -1.8083
H -1.0321 -2.7498  1.8504
H -2.3542 -4.7409  1.0083
H -4.1613 -4.1031 -2.3345
H -4.6485 -4.8287 -0.7963
H -3.2420 -5.4604 -1.6728
O -2.0494 -0.8270  2.8738
O -2.1386  0.2050  1.8581
H -2.9557 -0.8100  3.2205

5. $Fe^{III}$-$O_2H_2$

| | | | |
|---|---|---|---|
| Fe | -0.7816 | 0.0186 | 0.1685 |
| N | 3.8167 | -1.4622 | -0.5616 |
| C | 3.2715 | -2.7311 | -0.1229 |
| C | 1.7918 | -2.6378 | 0.3087 |
| C | 1.5700 | -1.7501 | 1.5051 |
| N | 0.5988 | -0.7414 | 1.6004 |
| C | 2.2728 | -1.7689 | 2.6816 |
| C | 0.7365 | -0.1906 | 2.8081 |
| N | 1.7308 | -0.7904 | 3.4800 |
| H | 1.1963 | -2.2805 | -0.5336 |
| H | 1.4396 | -3.6551 | 0.5328 |
| H | 3.3554 | -3.4558 | -0.9391 |
| H | 3.8932 | -3.0925 | 0.7005 |
| H | 3.7173 | -1.1842 | -1.5293 |
| H | 2.0662 | -0.5296 | 4.3994 |
| H | 3.1375 | -2.3366 | 2.9838 |
| H | 0.1431 | 0.6147 | 3.2098 |
| N | 4.5440 | 0.9591 | -1.6864 |
| C | 5.1343 | 0.5932 | -0.4301 |
| C | 4.5630 | -0.6571 | 0.2446 |
| O | 4.7898 | -0.8923 | 1.4212 |
| H | 3.6844 | 1.4925 | -1.6900 |
| H | 6.1982 | 0.4060 | -0.6125 |
| H | 5.0720 | 1.4066 | 0.3012 |
| C | 5.3179 | 1.0131 | -2.8185 |
| O | 6.4331 | 0.5677 | -2.9261 |
| H | 4.7625 | 1.5119 | -3.6122 |
| C | -0.2228 | -0.3410 | -3.2029 |
| S | 0.5985 | 0.1745 | -1.6471 |
| H | 0.3768 | 0.0353 | -4.0339 |
| H | -1.2340 | 0.0671 | -3.2715 |
| H | -0.2578 | -1.4321 | -3.2572 |
| C | 0.6881 | 5.5672 | 0.5217 |
| C | 0.1276 | 4.2220 | 0.8336 |
| N | -0.7954 | 3.9974 | 1.8396 |
| C | 0.3204 | 2.9902 | 0.2650 |
| C | -1.1323 | 2.6916 | 1.8502 |
| N | -0.4736 | 2.0401 | 0.8977 |
| H | 1.3852 | 5.4984 | -0.3168 |
| H | 1.2344 | 5.9866 | 1.3746 |
| H | -0.0993 | 6.2789 | 0.2468 |
| H | -1.1535 | 4.6982 | 2.4780 |
| H | 0.9697 | 2.7291 | -0.5558 |
| H | -1.8321 | 2.2641 | 2.5518 |
| C | -6.0288 | 1.2739 | -2.0474 |

C -4.6015  1.2772 -1.6280
N -3.7232  2.2899 -1.9666
C -3.8424  0.3915 -0.9057
C -2.5054  2.0048 -1.4659
N -2.5352  0.8512 -0.8107
H -6.5316  0.3800 -1.6707
H -6.1269  1.2763 -3.1393
H -6.5671  2.1474 -1.6613
H -3.9551  3.1098 -2.5153
H -4.1426 -0.5627 -0.4993
H -1.6444  2.6456 -1.5828
C -3.4253 -4.8425 -1.5210
C -2.7123 -3.7818 -0.7512
N -2.3390 -3.9327  0.5756
C -2.2909 -2.5203 -1.0819
C -1.7310 -2.8076  0.9964
N -1.6838 -1.9166  0.0132
H -2.3907 -2.0122 -2.0282
H -1.3410 -2.6692  1.9920
H -2.4908 -4.7621  1.1377
H -3.6102 -4.5042 -2.5432
H -4.3928 -5.0878 -1.0676
H -2.8367 -5.7656 -1.5767
O -2.6498  0.5432  3.4436
O -2.6547 -0.1570  2.1781
H -2.9132 -0.1523  4.0729
H -3.5003  0.1279  1.7859

6. $Fe^{III}$-$O_2^-$

Fe -0.8242  0.0247  0.3210
N  3.7155 -1.5410 -0.7850
C  3.1298 -2.8124 -0.4085
C  1.7257 -2.6589  0.2148
C  1.6905 -1.7954  1.4464
N  0.7315 -0.8049  1.6675
C  2.5299 -1.8342  2.5304
C  0.9958 -0.2788  2.8571
N  2.0754 -0.8736  3.4069
H  1.0477 -2.2298 -0.5251
H  1.3420 -3.6636  0.4445
H  3.0588 -3.4602 -1.2897
H  3.8235 -3.2842  0.2910
H  3.2893 -1.0108 -1.5335
H  2.4988 -0.6504  4.3004
H  3.4282 -2.4007  2.7167

H  0.4382  0.5150  3.3299
N  4.3413  1.0601 -1.5755
C  5.0053  0.5197 -0.4055
C  4.6565 -0.9217 -0.0233
O  5.1969 -1.4380  0.9422
H  3.3446  1.2541 -1.5562
H  6.0805  0.5655 -0.5951
H  4.8051  1.1330  0.4816
C  5.0641  1.4334 -2.6774
O  6.2642  1.3113 -2.7841
H  4.4247  1.8618 -3.4730
C  0.2522 -0.7674 -2.9087
S  0.6153  0.4696 -1.5907
H  0.9751 -0.6327 -3.7169
H -0.7500 -0.6108 -3.3216
H  0.3228 -1.7968 -2.5444
C  0.7795  5.5437  0.8909
C  0.1190  4.2202  1.0608
N -1.1023  4.0629  1.6967
C  0.4633  2.9562  0.6622
C -1.4503  2.7602  1.6605
N -0.5208  2.0552  1.0340
H  1.7264  5.4224  0.3589
H  0.9981  6.0210  1.8541
H  0.1578  6.2350  0.3088
H -1.6487  4.7969  2.1260
H  1.3385  2.6417  0.1150
H -2.3694  2.3757  2.0769
C -6.1773  1.5676 -1.5469
C -4.7079  1.3413 -1.4148
N -3.7865  1.8306 -2.3276
C -3.9502  0.6886 -0.4769
C -2.5440  1.4750 -1.9248
N -2.6054  0.7779 -0.7998
H -6.7034  1.0945 -0.7138
H -6.5747  1.1423 -2.4767
H -6.4272  2.6356 -1.5349
H -4.0127  2.3562 -3.1648
H -4.2845  0.1795  0.4137
H -1.6311  1.7344 -2.4426
C -3.7474 -4.6404 -1.3997
C -2.9032 -3.6774 -0.6421
N -2.5164 -3.8731  0.6747
C -2.3563 -2.4707 -0.9856
C -1.7786 -2.8166  1.0736
N -1.6612 -1.9438  0.0869

H -2.4275 -1.9460 -1.9254
H -1.3700 -2.7039  2.0658
H -2.7656 -4.6616  1.2562
H -3.9241 -4.2643 -2.4105
H -4.7244 -4.7879 -0.9234
H -3.2685 -5.6231 -1.4901
O -2.0755 -0.0950  2.1705
O -3.1491  0.3922  2.6161

7. $Fe^{III}$-OH

Fe  1.1046  0.2186  0.4263
N -3.6596  1.1512 -0.9705
C -3.1778  2.5236 -0.9430
C -1.7382  2.6553 -0.3762
C -1.6054  2.0066  0.9706
N -0.5493  1.3363  1.4366
N -2.5576  2.0856  1.9353
C -0.8406  1.0053  2.7507
C -2.0928  1.4460  3.0648
H -3.2035  0.5091 -1.6075
H -3.1980  2.9340 -1.9581
H -3.8924  3.1034 -0.3526
H -1.0231  2.1853 -1.0503
H -1.4852  3.7224 -0.3067
H -3.5361  2.3306  1.7700
H -0.1303  0.4711  3.3600
N -4.1815 -1.5775 -1.2906
C -4.8252 -0.8730 -0.2006
C -4.5616  0.6306 -0.0978
O -5.1354  1.2672  0.7816
H -3.1809 -1.7432 -1.2662
H -5.9027 -1.0128 -0.3170
H -4.5454 -1.3014  0.7698
H -4.3040 -2.7922 -2.9541
C -4.9322 -2.2448 -2.2258
O -6.1419 -2.2374 -2.2659
C  0.2405  0.1633 -3.0429
S -0.3969 -0.4314 -1.4253
H -0.4107 -0.2147 -3.8345
H  1.2553 -0.2015 -3.2331
H  0.2431  1.2570 -3.0906
C  0.2735 -3.7958  1.7529
N  1.0203 -3.2752  2.7978
C  0.0502 -2.7416  0.9167
C  1.2311 -1.9611  2.5612
N  0.6528 -1.6111  1.4235

C -0.0993 -5.2202  1.6217
H -0.4736 -2.7245 -0.0260
H  1.8229 -1.2976  3.1735
N  4.7688 -1.7900 -0.6167
C  3.9644 -2.4889 -1.5057
C  4.0198 -0.8331 -0.0165
C  2.7359 -1.8953 -1.4025
N  2.7817 -0.8707 -0.4770
H  5.7497 -1.9727 -0.4415
H  4.3684 -0.1672  0.7585
H  1.8149 -2.1501 -1.9044
N  3.0544  3.5571 -1.4676
C  2.5750  4.1344 -0.3037
C  2.5484  2.3024 -1.5605
C  1.7765  3.1825  0.2570
N  1.7735  2.0464 -0.5240
H  3.6636  4.0008 -2.1432
H  2.7776  1.6205 -2.3650
H  1.2076  3.2396  1.1716
O  2.2283  0.6163  1.8948
C  4.4343 -3.6414 -2.3226
H -2.6877  1.3649  3.9612
C  2.9470  5.4756  0.1962
H  1.3478 -3.7904  3.6049
H -0.6811 -5.3666  0.7081
H -0.7113 -5.5732  2.4616
H  0.7820 -5.8716  1.5610
H  3.6094 -4.0227 -2.9298
H  4.7961 -4.4664 -1.6964
H  5.2470 -3.3619 -3.0046
H  2.4193  5.6794  1.1313
H  2.6873  6.2741 -0.5103
H  4.0227  5.5535  0.3987
H  2.3091  1.4861  2.3036

8. $Fe^{III}$-$OH_2$

Fe  0.9871  0.1703  0.2991
N -3.6073  1.2186 -0.9606
C -3.1071  2.5849 -0.9557
C -1.6755  2.7182 -0.3458
C -1.5775  1.9751  0.9583
N -0.6064  1.1431  1.3759
N -2.5318  2.0577  1.9132
C -0.9803  0.7095  2.6468
C -2.1787  1.2651  2.9808
H -3.2780  0.5755 -1.6705

H -3.0928  2.9780 -1.9768
H -3.8261  3.1882 -0.3948
H -0.9328  2.3177 -1.0352
H -1.4507  3.7820 -0.1944
H -3.4746  2.4261  1.7640
H -0.3920 -0.0033  3.2023
N -4.2249 -1.4828 -1.2409
C -4.9315 -0.7233 -0.2268
C -4.5805  0.7566 -0.1208
O -5.1374  1.4316  0.7350
H -3.2799 -1.7965 -1.0580
H -5.9989 -0.7967 -0.4535
H -4.7881 -1.1497  0.7735
H -4.3302 -2.8402 -2.8106
C -4.9585 -2.1873 -2.1764
O -6.1523 -2.0824 -2.2988
C  0.4570 -0.5161 -3.1030
S -0.3801 -0.4026 -1.4750
H -0.1081 -1.2162 -3.7217
H  1.4848 -0.8702 -3.0038
H  0.4391  0.4639 -3.5882
C  0.2407 -3.7903  1.8144
N  1.2720 -3.3842  2.6429
C -0.0693 -2.6824  1.0761
C  1.5582 -2.0928  2.3854
N  0.7607 -1.6298  1.4289
C -0.2955 -5.1721  1.7847
H -0.8187 -2.5823  0.3073
H  2.3361 -1.5332  2.8791
N  4.7618 -1.3786 -1.2387
C  3.9420 -2.4777 -1.4362
C  4.0321 -0.3860 -0.6823
C  2.7194 -2.0853 -0.9674
N  2.7784 -0.7809 -0.5030
H  5.7476 -1.3299 -1.4732
H  4.4389  0.5840 -0.4373
H  1.8074 -2.6600 -0.9343
N  2.7938  3.6389 -1.4649
C  2.5969  4.1122 -0.1791
C  2.2878  2.3891 -1.5504
C  1.9525  3.0988  0.4704
N  1.7772  2.0245 -0.3818
H  3.2221  4.1561 -2.2252
H  2.3142  1.7909 -2.4489
H  1.5861  3.0885  1.4832
O  2.2637  0.7257  2.2552

C  4.3816 -3.7574 -2.0528
H -2.8061  1.1637  3.8531
C  3.0642  5.4243  0.3215
H  1.7291 -3.9630  3.3388
H -1.0962 -5.2482  1.0452
H -0.7109 -5.4729  2.7539
H  0.4784 -5.9009  1.5154
H  3.5420 -4.4551 -2.0957
H  5.1848 -4.2341 -1.4783
H  4.7468 -3.6117 -3.0763
H  2.7548  5.5581  1.3608
H  2.6503  6.2591 -0.2566
H  4.1571  5.5085  0.2842
H  3.1312  1.1540  2.2234
H  1.7765  1.1205  2.9943

9. $Fe^{II}$ 5C
Fe  0.8038  0.0154 -0.1207
N -3.5487 -1.5403  0.6346
C -3.0113 -2.8162  0.1964
C -1.5833 -2.7139 -0.3924
C -1.5106 -1.7845 -1.5744
N -0.6358 -0.7019 -1.6526
C -2.2994 -1.7925 -2.6979
C -0.9032 -0.0858 -2.7955
N -1.8956 -0.7186 -3.4571
H -0.9022 -2.3519  0.3813
H -1.2540 -3.7249 -0.6693
H -2.9956 -3.5083  1.0462
H -3.7096 -3.2155 -0.5432
H -3.1472 -1.1095  1.4583
H -2.3129 -0.4213 -4.3285
H -3.1420 -2.4044 -2.9761
H -0.4124  0.8016 -3.1627
N -4.1744  0.9820  1.6615
C -4.8703  0.5374  0.4917
C -4.4510 -0.8246 -0.0910
O -4.9278 -1.2023 -1.1523
H -3.1707  1.1380  1.6488
H -5.9309  0.4735  0.7518
H -4.7886  1.2577 -0.3326
C -4.8621  1.2885  2.7959
O -6.0578  1.1794  2.9582
H -4.1714  1.6666  3.5486
C  0.2327 -0.2158  3.2834
S -0.5990  0.3428  1.7349

H -0.3433  0.1569  4.1328
H  1.2510  0.1772  3.3549
H  0.2669 -1.3071  3.3363
C -0.6193  5.4660 -1.2559
C  0.0624  4.1423 -1.3489
N  1.2555  3.9436 -2.0257
C -0.2447  2.9117 -0.8281
C  1.6193  2.6441 -1.8853
N  0.7307  1.9887 -1.1613
H -1.5316  5.3712 -0.6615
H -0.9044  5.8532 -2.2419
H  0.0157  6.2182 -0.7726
H  1.7673  4.6482 -2.5400
H -1.0858  2.6374 -0.2092
H  2.5279  2.2338 -2.3030
C  6.3917  1.3946  0.8461
C  4.9052  1.3077  0.8991
N  4.1153  2.1323  1.6832
C  4.0122  0.4838  0.2639
C  2.8160  1.7917  1.4972
N  2.7189  0.7909  0.6415
H  6.7843  0.6427  0.1566
H  6.8485  1.2146  1.8274
H  6.7351  2.3765  0.4968
H  4.4506  2.8544  2.3071
H  4.2229 -0.3210 -0.4247
H  1.9850  2.2868  1.9800
C  3.8293 -4.7597  1.0024
C  2.9920 -3.7341  0.3150
N  2.4712 -3.9033 -0.9587
C  2.5595 -2.4916  0.6974
C  1.7612 -2.7974 -1.2869
N  1.7949 -1.9166 -0.3025
H  2.7508 -1.9734  1.6252
H  1.2329 -2.6788 -2.2210
H  2.5948 -4.7192 -1.5437
H  4.1209 -4.3983  1.9916
H  4.7468 -4.9804  0.4432
H  3.2873 -5.7034  1.1404

10. $Fe^{III}$ 6C + $H_2O$
Fe -0.8063  0.1534 -0.0372
N  3.7821 -1.5137 -1.0345
C  3.0416 -2.7305 -1.3278
C  1.5400 -2.6390 -0.9405
C  1.3513 -2.1972  0.4823

N  0.4134 -1.3681  0.9515
N  2.0985 -2.6620  1.5148
C  0.5616 -1.3356  2.3299
C  1.6180 -2.1196  2.6887
H  3.5645 -0.6836 -1.5719
H  3.1187 -2.9559 -2.3968
H  3.5417 -3.5436 -0.7949
H  1.0274 -1.9297 -1.5884
H  1.0760 -3.6235 -1.0910
H  3.0028 -3.1263  1.4187
H -0.1008 -0.7546  2.9508
N  4.8502  1.0509 -0.7035
C  5.2071  0.0240  0.2549
C  4.6489 -1.3776  0.0046
O  4.9692 -2.2818  0.7684
H  3.9086  1.4273 -0.7154
H  6.2975 -0.0491  0.2594
H  4.8970  0.3014  1.2699
H  5.4194  2.5327 -2.0242
C  5.8300  1.7237 -1.3906
O  7.0098  1.4639 -1.3264
C  0.5028  0.9711 -3.2193
S  1.0317  0.8413 -1.4659
H  1.2829  1.4914 -3.7795
H -0.4274  1.5394 -3.3092
H  0.3698 -0.0227 -3.6576
C  0.5051  3.5750  2.2977
N -0.5704  3.0846  3.0206
C  0.6757  2.6761  1.2828
C -1.0129  1.9495  2.4454
N -0.2754  1.6732  1.3759
C  1.2208  4.8344  2.6297
H  1.3996  2.6932  0.4835
H -1.8657  1.3770  2.8025
N -3.8966  2.7566 -1.6132
C -2.8485  3.6618 -1.6129
C -3.4138  1.5449 -1.2503
C -1.7517  2.9303 -1.2530
N -2.1138  1.6182 -1.0237
H -4.8619  2.9735 -1.8330
H -4.0241  0.6613 -1.1510
H -0.7325  3.2614 -1.1298
N -2.8772 -2.4358 -2.7743
C -2.8479 -3.2018 -1.6188
C -2.0941 -1.3470 -2.5874
C -2.0204 -2.5246 -0.7728

N -1.5683 -1.3698 -1.3767
H -3.3993 -2.6415 -3.6135
H -1.9519 -0.5760 -3.3290
H -1.7595 -2.7634  0.2450
C -4.4465 -1.2338  1.8430
C -3.0200 -0.7522  2.0605
O -2.4741 -0.8944  3.1590
O -2.4388 -0.2194  1.0300
H -4.4054 -2.2934  1.5653
H -4.9445 -0.6812  1.0425
H -5.0159 -1.1521  2.7719
C -3.0016  5.1038 -1.9201
H  2.0657 -2.3386  3.6455
C -3.6370 -4.4353 -1.3933
H -0.9896  3.5051  3.8377
H  2.0226  5.0086  1.9075
H  1.6756  4.7993  3.6274
H  0.5522  5.7039  2.6017
H -2.0280  5.5980 -1.8727
H -3.6648  5.6062 -1.2049
H -3.4093  5.2730 -2.9246
H -3.4269 -4.8257 -0.3945
H -3.3972 -5.2255 -2.1156
H -4.7164 -4.2484 -1.4561
O -2.0885 -3.6778  2.3197
H -1.8860 -4.4358  2.8826
H -2.1261 -2.8973  2.9002

11. $Fe^{III}$-OOH + $H_2O$
Fe -0.8257  0.1659  0.3727
N  3.6953 -1.7253 -0.7974
C  2.9906 -2.9629 -0.5150
C  1.5623 -2.7319  0.0321
C  1.5496 -1.9387  1.3117
N  0.6402 -0.9170  1.5909
C  2.3745 -2.0867  2.3982
C  0.9104 -0.4866  2.8147
N  1.9533 -1.1636  3.3313
H  0.9660 -2.2096 -0.7158
H  1.0945 -3.7145  0.1880
H  2.9275 -3.5647 -1.4294
H  3.6044 -3.5180  0.1983
H  3.3220 -1.1200 -1.5166
H  2.3693 -1.0095  4.2398
H  3.2443 -2.7044  2.5561
H  0.3713  0.2853  3.3395

N  4.6676  0.8018 -1.5365
C  5.2092  0.1657 -0.3509
C  4.7047 -1.2441 -0.0229
O  5.1999 -1.8438  0.9190
H  3.7016  1.1112 -1.5486
H  6.2916  0.1055 -0.4847
H  5.0261  0.7767  0.5419
C  5.4887  1.1786 -2.5674
O  6.6810  0.9711 -2.6117
H  4.9347  1.6988 -3.3730
C  0.1307 -0.3640 -3.0292
S  0.7747  0.3739 -1.4723
H  0.8556 -0.1852 -3.8268
H -0.8244  0.0826 -3.3259
H -0.0063 -1.4435 -2.9187
C  1.3960  5.4896  1.0147
C  0.6692  4.2108  1.2160
N -0.3079  4.0241  2.1806
C  0.7418  3.0146  0.5572
C -0.7841  2.7634  2.0752
N -0.1655  2.1230  1.0958
H  2.1111  5.3846  0.1950
H  1.9584  5.7909  1.9073
H  0.7157  6.3118  0.7591
H -0.6213  4.7166  2.8479
H  1.3698  2.7423 -0.2766
H -1.5743  2.3448  2.6794
C -5.7407  2.2484 -1.9366
C -4.3139  1.9570 -1.6187
N -3.2597  2.5429 -2.3026
C -3.7138  1.1328 -0.7021
C -2.0978  2.0670 -1.8034
N -2.3386  1.2046 -0.8300
H -6.3950  1.6821 -1.2688
H -5.9940  1.9687 -2.9666
H -5.9792  3.3119 -1.8115
H -3.3437  3.2113 -3.0571
H -4.1690  0.5012  0.0447
H -1.1168  2.3538 -2.1531
C -3.8540 -4.1471 -1.9893
C -2.9805 -3.3225 -1.1167
N -2.5725 -3.7228  0.1451
C -2.4210 -2.0857 -1.2859
C -1.8107 -2.7464  0.6851
N -1.6983 -1.7366 -0.1609
H -2.5025 -1.4250 -2.1343

H -1.3914 -2.7829  1.6770
H -2.8080 -4.5987  0.5925
H -4.0419 -3.6241 -2.9306
H -4.8260 -4.3489 -1.5218
H -3.3969 -5.1139 -2.2343
O -2.4074 -0.8471  2.7215
O -1.9863  0.3039  1.9563
H -2.5789 -0.4428  3.5872
O -4.8542 -1.2356  1.2962
H -4.0448 -1.1685  1.8390
H -5.6049 -1.1729  1.9018

12. $Fe^{III}$-$O_2H_2$ + $H_2O$
Fe -0.6286  0.0477  0.0589
N  3.9734 -1.5101 -0.4554
C  3.3818 -2.7760 -0.0715
C  1.8832 -2.6614  0.2828
C  1.6145 -1.7921  1.4831
N  0.6588 -0.7663  1.5467
C  2.2530 -1.8470  2.6946
C  0.7421 -0.2412  2.7707
N  1.6876 -0.8731  3.4824
H  1.3404 -2.2766 -0.5827
H  1.5004 -3.6756  0.4677
H  3.4955 -3.4867 -0.8963
H  3.9517 -3.1650  0.7764
H  3.9311 -1.2121 -1.4213
H  1.9782 -0.6363  4.4233
H  3.0894 -2.4373  3.0310
H  0.1433  0.5681  3.1562
N  4.8052  0.9170 -1.4918
C  5.3206  0.5159 -0.2134
C  4.6906 -0.7353  0.4051
O  4.8498 -0.9970  1.5872
H  3.9573  1.4673 -1.5304
H  6.3890  0.3111 -0.3428
H  5.2346  1.3165  0.5295
C  5.6394  0.9769 -2.5799
O  6.7502  0.5115 -2.6370
H  5.1367  1.5014 -3.3920
C  0.1027 -0.2595 -3.2846
S  0.8517  0.2106 -1.6785
H  0.7528  0.1203 -4.0749
H -0.8956  0.1698 -3.3986
H  0.0501 -1.3485 -3.3622
C  0.9243  5.5584  0.5995

C  0.3227  4.2190  0.8545
N -0.6568  3.9939  1.8054
C  0.5224  2.9945  0.2726
C -1.0183  2.6951  1.7723
N -0.3220  2.0486  0.8433
H  1.6638  5.4916 -0.2020
H  1.4320  5.9508  1.4883
H  0.1662  6.2906  0.2974
H -1.0353  4.6895  2.4377
H  1.2096  2.7360 -0.5176
H -1.7625  2.2684  2.4271
C -5.7254  1.4483 -2.4070
C -4.3227  1.4154 -1.9124
N -3.4087  2.4166 -2.1838
C -3.6201  0.5014 -1.1686
C -2.2249  2.0981 -1.6250
N -2.3114  0.9332 -0.9953
H -6.2643  0.5576 -2.0753
H -5.7649  1.4732 -3.5023
H -6.2670  2.3249 -2.0327
H -3.5954  3.2511 -2.7277
H -3.9595 -0.4541 -0.7977
H -1.3470  2.7237 -1.6833
C -3.2693 -4.7274 -1.8645
C -2.5786 -3.6957 -1.0371
N -2.2796 -3.8789  0.3044
C -2.1165 -2.4368 -1.3199
C -1.6739 -2.7742  0.7791
N -1.5575 -1.8660 -0.1824
H -2.1560 -1.9091 -2.2599
H -1.3351 -2.6623  1.7965
H -2.4768 -4.7155  0.8411
H -3.3929 -4.3663 -2.8882
H -4.2641 -4.9619 -1.4680
H -2.6960 -5.6608 -1.9072
O -2.4553  0.5129  3.3550
O -2.4626 -0.2360  2.1162
H -2.4577 -0.1873  4.0303
H -3.4362 -0.2615  1.9107
O -5.1218 -0.3632  1.7637
H -5.6405  0.4528  1.7930
H -5.6482 -1.0464  2.2022

13. $Fe^{III}$-CN
Fe  1.1000  0.1838  0.3024
N -3.7474  1.2714 -0.8673

C -3.2353  2.6291 -0.7944
C -1.7563  2.6971 -0.3295
C -1.5067  1.8801  0.9174
N -0.4528  1.1168  1.2836
N -2.3823  1.9402  1.9521
C -0.6841  0.7379  2.6024
C -1.8884  1.2189  3.0147
H -3.3177  0.6355 -1.5280
H -3.3134  3.1095 -1.7756
H -3.8957  3.1786 -0.1187
H -1.1007  2.3216 -1.1159
H -1.4880  3.7448 -0.1378
H -3.3494  2.2535  1.8620
H  0.0337  0.1603  3.1564
N -4.3019 -1.4516 -1.1699
C -4.9031 -0.7447 -0.0568
C -4.6191  0.7517  0.0386
O -5.1464  1.3981  0.9462
H -3.3039 -1.6320 -1.1769
H -5.9846 -0.8763 -0.1418
H -4.5996 -1.1771  0.9051
H -4.5172 -2.6959 -2.8059
C -5.1020 -2.1356 -2.0526
O -6.3173 -2.1229 -2.0227
C  0.1528 -0.0671 -3.1270
S -0.4789 -0.4066 -1.4362
H -0.5123 -0.5667 -3.8366
H  1.1624 -0.4648 -3.2807
H  0.1448  1.0022 -3.3625
C  0.2459 -3.7678  1.6877
N  1.1326 -3.2681  2.6284
C  0.0177 -2.7174  0.8355
C  1.4175 -1.9862  2.3331
N  0.7542 -1.6083  1.2397
C -0.2270 -5.1857  1.7258
H -0.5998 -2.6757 -0.0473
H  2.1001 -1.3722  2.8989
N  4.6191 -1.6595 -0.9823
C  3.7491 -2.5230 -1.6405
C  3.9105 -0.6751 -0.3876
C  2.5065 -1.9835 -1.4141
N  2.6133 -0.8351 -0.6308
H  5.6252 -1.7550 -0.9360
H  4.3406  0.0931  0.2365
H  1.5398 -2.3386 -1.7349
N  2.6589  3.5391 -1.6233

C 2.4986 4.0727 -0.3499
C 2.1497 2.2848 -1.6456
C 1.8727 3.0831 0.3577
N 1.6649 1.9704 -0.4512
H 3.0811 4.0083 -2.4135
H 2.1610 1.6460 -2.5135
H 1.5994 3.0771 1.3992
N 3.1067 0.8419 2.5916
C 2.3244 0.6157 1.7522
C 4.2202 -3.7567 -2.3710
H -2.4245 1.1206 3.9454
C 3.0029 5.4222 0.0668
H 1.5101 -3.7774 3.4167
H -0.9100 -5.3777 0.8945
H -0.7633 -5.4104 2.6556
H 0.6095 -5.8899 1.6410
H 3.3639 -4.2784 -2.8048
H 4.7323 -4.4499 -1.6935
H 4.9097 -3.5056 -3.1853
H 2.7662 5.5907 1.1199
H 2.5462 6.2305 -0.5166
H 4.0909 5.4950 -0.0476

14. $Fe^{III}$-CN +$H_2O$
Fe 0.9243 0.1768 0.1830
N -3.9768 1.2768 -0.7211
C -3.4576 2.6331 -0.6788
C -1.9551 2.6975 -0.2958
C -1.6399 1.8818 0.9370
N -0.5697 1.1159 1.2462
N -2.4572 1.9461 2.0181
C -0.7294 0.7399 2.5764
C -1.9079 1.2251 3.0533
H -3.5858 0.6385 -1.4032
H -3.5880 3.1121 -1.6551
H -4.0784 3.1856 0.0312
H -1.3447 2.3188 -1.1163
H -1.6737 3.7447 -0.1209
H -3.4269 2.2621 1.9806
H 0.0161 0.1610 3.0912
N -4.5548 -1.4451 -0.9880
C -5.0921 -0.7346 0.1552
C -4.7990 0.7611 0.2322
O -5.2739 1.4105 1.1662
H -3.5592 -1.6284 -1.0493
H -6.1770 -0.8631 0.1298

H -4.7375 -1.1663  1.0998
H -4.8631 -2.6914 -2.6075
C -5.4041 -2.1281 -1.8242
O -6.6159 -2.1118 -1.7278
C -0.2102 -0.0769 -3.1888
S -0.7050 -0.3813 -1.4396
H -0.9146 -0.5757 -3.8600
H  0.7883 -0.4778 -3.3969
H -0.2281  0.9920 -3.4254
C  0.1362 -3.7700  1.6201
N  1.0746 -3.2714  2.5099
C -0.1354 -2.7204  0.7798
C  1.3465 -1.9909  2.1971
N  0.6253 -1.6128  1.1411
C -0.3380 -5.1865  1.6866
H -0.8003 -2.6783 -0.0679
H  2.0609 -1.3780  2.7236
N  4.3624 -1.6790 -1.2894
C  3.4552 -2.5410 -1.8974
C  3.6903 -0.6915 -0.6585
C  2.2284 -1.9975 -1.6041
N  2.3813 -0.8481 -0.8299
H  5.3693 -1.7774 -1.2982
H  4.1562  0.0764 -0.0603
H  1.2445 -2.3502 -1.8708
N  2.3849  3.5243 -1.8312
C  2.2962  4.0605 -0.5519
C  1.8716  2.2715 -1.8233
C  1.7072  3.0739  0.1907
N  1.4522  1.9605 -0.6036
H  2.7644  3.9910 -2.6442
H  1.8335  1.6313 -2.6894
H  1.4914  3.0704  1.2457
N  3.0388  0.8671  2.3951
C  2.2035  0.6453  1.6059
C  3.8820 -3.7773 -2.6504
H -2.3924  1.1299  4.0121
C  2.8264  5.4091 -0.1659
H  1.4933 -3.7806  3.2772
H -1.0661 -5.3778  0.8943
H -0.8231 -5.4081  2.6448
H  0.4906 -5.8933  1.5573
H  3.0017 -4.2971 -3.0357
H  4.4285 -4.4709 -2.0008
H  4.5265 -3.5295 -3.5017
H  2.6483  5.5800  0.8983

H 2.3407 6.2178 -0.7248
H 3.9067 5.4785 -0.3399
O 5.7170 -0.0569 1.5795
H 6.3217 0.5257 2.0621
H 4.8308 0.2525 1.8495

15. SOD $Fe^{III}$ 5C

| | | | |
|---|---|---|---|
| O | -0.366581 | -2.470108 | -0.721809 |
| Fe | -0.114181 | -0.740302 | -0.171826 |
| C | 5.603334 | -0.188878 | -0.906453 |
| C | 4.173550 | -0.625477 | -0.923485 |
| N | 3.759394 | -1.871535 | -1.374670 |
| C | 3.018024 | -0.002448 | -0.534725 |
| C | 2.420896 | -1.966748 | -1.245946 |
| N | 1.933134 | -0.841872 | -0.737724 |
| H | 5.675779 | 0.826215 | -0.508255 |
| H | 6.040265 | -0.185894 | -1.912273 |
| H | 6.218356 | -0.840774 | -0.274557 |
| H | 2.898838 | 0.987970 | -0.125709 |
| H | 1.823558 | -2.830387 | -1.499475 |
| H | 4.362086 | -2.600590 | -1.734146 |
| C | -1.151429 | -1.610902 | 3.823718 |
| C | -0.907415 | -1.978996 | 2.375327 |
| O | -1.174315 | -3.069730 | 1.899190 |
| O | -0.381052 | -0.978619 | 1.689802 |
| H | -1.567549 | -2.458680 | 4.370582 |
| H | -1.846331 | -0.765558 | 3.876247 |
| H | -0.211159 | -1.299354 | 4.291054 |
| C | -5.293884 | 1.548062 | -1.273134 |
| C | -4.048125 | 0.720856 | -1.255054 |
| N | -3.986698 | -0.560669 | -1.785660 |
| C | -2.791349 | 0.944128 | -0.756407 |
| C | -2.751306 | -1.062130 | -1.591593 |
| N | -1.993769 | -0.170297 | -0.966171 |
| H | -5.103347 | 2.517856 | -0.806833 |
| H | -6.106787 | 1.063992 | -0.718777 |
| H | -5.645457 | 1.731904 | -2.295405 |
| H | -2.411721 | 1.820766 | -0.255308 |
| H | -2.424753 | -2.051364 | -1.876228 |
| H | -4.749877 | -1.050832 | -2.234290 |
| C | 1.503031 | 4.880168 | 0.242316 |
| C | 0.986935 | 3.506863 | 0.480477 |
| N | 0.737279 | 3.010511 | 1.748877 |
| C | 0.678500 | 2.471130 | -0.362672 |
| C | 0.307877 | 1.735131 | 1.642100 |
| N | 0.264042 | 1.372219 | 0.369940 |

| | | | |
|---|---|---|---|
| H | 1.626322 | 5.054429 | -0.829642 |
| H | 2.478522 | 5.036193 | 0.719112 |
| H | 0.819161 | 5.647250 | 0.625837 |
| H | 0.736838 | 2.446733 | -1.441363 |
| H | 0.053770 | 1.094829 | 2.471941 |
| H | 0.855760 | 3.519107 | 2.615507 |
| H | -0.663490 | -3.061364 | 0.003024 |

16. SOD $Fe^{II}$ 5C

| | | | |
|---|---|---|---|
| O | -0.370260 | -2.772000 | -0.683259 |
| Fe | -0.053034 | -0.602592 | -0.259331 |
| C | 5.616758 | -0.105315 | -0.941684 |
| C | 4.203541 | -0.596141 | -0.976237 |
| N | 3.857889 | -1.924523 | -1.180678 |
| C | 3.004212 | 0.043587 | -0.809782 |
| C | 2.513133 | -2.042182 | -1.125893 |
| N | 1.956227 | -0.861540 | -0.899986 |
| H | 5.629002 | 0.971433 | -0.754487 |
| H | 6.135405 | -0.285419 | -1.891059 |
| H | 6.194371 | -0.590416 | -0.145662 |
| H | 2.829494 | 1.090992 | -0.620689 |
| H | 1.973308 | -2.972250 | -1.222752 |
| H | 4.504731 | -2.687395 | -1.332660 |
| C | -1.138695 | -1.644244 | 3.750762 |
| C | -0.885751 | -1.954413 | 2.291050 |
| O | -1.280673 | -3.014476 | 1.770055 |
| O | -0.262985 | -1.027570 | 1.652183 |
| H | -1.598137 | -2.491838 | 4.262457 |
| H | -1.800697 | -0.773885 | 3.825077 |
| H | -0.195785 | -1.383976 | 4.242389 |
| C | -5.267222 | 1.728523 | -1.218805 |
| C | -4.117223 | 0.798592 | -0.989151 |
| N | -4.282953 | -0.486522 | -0.497300 |
| C | -2.760075 | 0.925881 | -1.150566 |
| C | -3.070865 | -1.071516 | -0.379848 |
| N | -2.115241 | -0.240076 | -0.767210 |
| H | -4.901453 | 2.687763 | -1.594514 |
| H | -5.821350 | 1.921008 | -0.292505 |
| H | -5.972358 | 1.328130 | -1.956809 |
| H | -2.209128 | 1.788289 | -1.495316 |
| H | -2.923711 | -2.059399 | 0.032814 |
| H | -5.165389 | -0.915712 | -0.251320 |
| C | 1.558987 | 4.950814 | 0.398998 |
| C | 1.059669 | 3.565681 | 0.584433 |
| N | 0.877489 | 2.991888 | 1.827992 |
| C | 0.709097 | 2.583331 | -0.305550 |

| | | | |
|---|---|---|---|
| C | 0.445625 | 1.720525 | 1.659689 |
| N | 0.337024 | 1.438374 | 0.373813 |
| H | 1.621949 | 5.187965 | -0.666243 |
| H | 2.559279 | 5.085359 | 0.828353 |
| H | 0.897256 | 5.692241 | 0.863590 |
| H | 0.712739 | 2.633153 | -1.385631 |
| H | 0.233950 | 1.028406 | 2.459413 |
| H | 1.035312 | 3.446597 | 2.717499 |
| H | -0.950503 | -3.150879 | -1.357016 |
| H | -0.693064 | -3.078035 | 0.224432 |

17. SOD $Fe^{III} – O_2^-$

| | | | |
|---|---|---|---|
| O | 1.182635 | 0.333019 | -2.348741 |
| Fe | 0.358726 | 0.039752 | -0.708952 |
| O | -0.235830 | -1.961406 | -0.536713 |
| O | 0.501216 | -2.586922 | -1.409697 |
| C | -5.239915 | -0.356366 | -2.091653 |
| C | -3.777482 | -0.080303 | -2.107256 |
| N | -3.023663 | 0.062132 | -3.264042 |
| C | -2.874868 | 0.051492 | -1.088630 |
| C | -1.728320 | 0.258584 | -2.910021 |
| N | -1.613297 | 0.259361 | -1.597961 |
| H | -5.586961 | -0.431403 | -1.057411 |
| H | -5.485928 | -1.302272 | -2.591984 |
| H | -5.822108 | 0.436759 | -2.579660 |
| H | -3.049972 | -0.014277 | -0.026126 |
| H | -0.893492 | 0.363524 | -3.588795 |
| H | -3.370476 | 0.006278 | -4.211046 |
| C | 1.362085 | 4.141634 | 0.399347 |
| C | 1.257587 | 2.931843 | -0.530814 |
| O | 1.834968 | 2.940759 | -1.620662 |
| O | 0.538361 | 1.971938 | -0.048824 |
| H | 1.972254 | 4.927632 | -0.051219 |
| H | 1.806276 | 3.836219 | 1.353984 |
| H | 0.361590 | 4.535504 | 0.613909 |
| C | 4.570085 | -1.982366 | 2.706347 |
| C | 3.764870 | -1.441773 | 1.577791 |
| N | 4.211283 | -1.395962 | 0.264013 |
| C | 2.502077 | -0.917158 | 1.532414 |
| C | 3.229054 | -0.865633 | -0.505420 |
| N | 2.186961 | -0.565235 | 0.240732 |
| H | 3.996995 | -1.908796 | 3.634767 |
| H | 5.507915 | -1.429807 | 2.851751 |
| H | 4.828444 | -3.039580 | 2.560648 |
| H | 1.797674 | -0.779739 | 2.338592 |
| H | 3.268807 | -0.719178 | -1.575350 |

| | | | |
|---|---|---|---|
| H | 5.108762 | -1.716787 | -0.070249 |
| C | -2.997915 | -1.294366 | 4.066347 |
| C | -2.101412 | -0.612806 | 3.087216 |
| N | -1.789035 | 0.738184 | 3.160341 |
| C | -1.433177 | -1.060332 | 1.975375 |
| C | -0.973219 | 1.046256 | 2.118198 |
| N | -0.742453 | -0.020473 | 1.381987 |
| H | -3.097106 | -2.350603 | 3.801466 |
| H | -4.005936 | -0.858911 | 4.076541 |
| H | -2.607016 | -1.245702 | 5.091384 |
| H | -1.404111 | -2.050470 | 1.544371 |
| H | -0.578252 | 2.027066 | 1.900719 |
| H | -2.112679 | 1.384663 | 3.866007 |
| H | 1.502367 | 1.258957 | -2.403359 |

18. SOD $Fe^{III}$-$OH_2$

| | | | |
|---|---|---|---|
| O | -0.3575 | -2.4826 | -0.7268 |
| Fe | -0.0864 | -0.7329 | -0.1786 |
| C | 5.6033 | -0.1889 | -0.9065 |
| C | 4.2103 | -0.6984 | -0.7886 |
| N | 3.7928 | -1.9572 | -1.1986 |
| C | 3.0792 | -0.1060 | -0.2970 |
| C | 2.4741 | -2.0851 | -0.9483 |
| N | 2.0104 | -0.9708 | -0.4065 |
| H | 5.6532 | 0.8343 | -0.5259 |
| H | 5.9499 | -0.1752 | -1.9473 |
| H | 6.3123 | -0.7940 | -0.3284 |
| H | 2.9675 | 0.8845 | 0.1150 |
| H | 1.8702 | -2.9552 | -1.1636 |
| H | 4.3486 | -2.6745 | -1.6379 |
| C | -1.1514 | -1.6109 | 3.8237 |
| C | -0.9006 | -1.9713 | 2.3744 |
| O | -1.1748 | -3.0623 | 1.8952 |
| O | -0.3667 | -0.9756 | 1.7011 |
| H | -1.5691 | -2.4599 | 4.3679 |
| H | -1.8478 | -0.7666 | 3.8768 |
| H | -0.2138 | -1.2987 | 4.2959 |
| C | -5.2939 | 1.5481 | -1.2731 |
| C | -4.0977 | 0.6706 | -1.1533 |
| N | -4.0448 | -0.6408 | -1.6044 |
| C | -2.8596 | 0.8970 | -0.6134 |
| C | -2.8296 | -1.1522 | -1.3275 |
| N | -2.0838 | -0.2379 | -0.7292 |
| H | -5.0711 | 2.5338 | -0.8569 |
| H | -6.1541 | 1.1424 | -0.7268 |
| H | -5.5988 | 1.6880 | -2.3175 |

H -2.4797  1.7955 -0.1522
H -2.5023 -2.1577 -1.5495
H -4.7722 -1.1573 -2.0740
C  1.5030  4.8802  0.2423
C  0.9871  3.5091  0.4914
N  0.6844  3.0392  1.7591
C  0.7216  2.4544 -0.3424
C  0.2658  1.7584  1.6594
N  0.2792  1.3715  0.3948
H  1.6718  5.0282 -0.8275
H  2.4556  5.0582  0.7566
H  0.7978  5.6517  0.5755
H  0.8256  2.3948 -1.4154
H -0.0187  1.1312  2.4896
H  0.7650  3.5654  2.6193
H -0.6448 -3.0465  0.0245
O  0.2030 -0.0535 -2.3738
H  0.8571 -0.5794 -2.8547
H -0.6240 -0.0804 -2.8747

19. non H-bonded $Fe^{III}$ 6C S=5/2
Fe  0.2078 -0.1606 -0.2154
C -0.3403 -3.3733 -2.0315
C  0.4983 -3.3976 -0.7910
N  0.7405 -2.2671  0.0222
C  1.1590 -4.4800 -0.2325
C  1.5231 -2.6713  1.0429
N  1.7997 -4.0033  0.9154
H -0.5403 -4.3957 -2.3709
H  0.1686 -2.8355 -2.8394
H -1.2985 -2.8737 -1.8583
H  1.2223 -5.5066 -0.5533
H  1.8519 -2.0566  1.8700
H  2.3653 -4.5469  1.5545
C -1.2366 -0.0341 -3.4484
S  0.4575 -0.1235 -2.6311
H -1.0972 -0.1697 -4.5238
H -1.6869  0.9467 -3.2665
H -1.8908 -0.8158 -3.0581
C  5.4728  2.0861 -1.1745
C  4.2703  1.4546 -0.5482
N  4.1527  1.2015  0.8279
C  3.0815  1.0106 -1.0945
C  2.9316  0.6315  1.0757
N  2.2537  0.5026 -0.0787
H  5.3287  2.1699 -2.2557

H 6.3815 1.4926 -1.0075
H 5.6553 3.0960 -0.7833
H 2.7790 1.0127 -2.1279
H 2.5856 0.3125 2.0503
H 4.8537 1.4029 1.5301
C -2.3565 4.8231 1.1388
C -1.5510 3.7821 0.4329
N -0.9257 3.9924 -0.8074
C -1.2611 2.4713 0.7626
C -0.3012 2.8300 -1.1866
N -0.4918 1.8891 -0.2515
H -2.7420 4.4200 2.0798
H -3.2175 5.1513 0.5410
H -1.7599 5.7127 1.3812
H -1.5376 1.9094 1.6370
H 0.2594 2.7002 -2.0977
H -0.9275 4.8590 -1.3308
C -5.6330 -0.2846 -0.3602
C -4.1914 -0.6413 -0.1816
N -3.7492 -1.7596 0.5423
C -3.0343 -0.0295 -0.6281
C -2.3769 -1.7864 0.5145
N -1.9127 -0.7489 -0.1933
H -5.7193 0.6303 -0.9536
H -6.1329 -0.1055 0.6010
H -6.1890 -1.0727 -0.8851
H -2.9424 0.8732 -1.2052
H -1.7730 -2.5304 1.0050
H -4.3432 -2.4355 1.0065
C -0.8397 0.0046 4.0309
C 0.2822 -0.2779 3.0450
O 1.4195 -0.6934 3.4335
O -0.0053 -0.0345 1.7784
H -1.8086 -0.2793 3.6067
H -0.8673 1.0811 4.2492
H -0.6645 -0.5266 4.9699

20. non H-bonded $Fe^{III}$ 6C S=1/2
Fe -0.0691 -0.0813 -0.0879
C 0.3627 -3.5097 1.3109
C -0.5418 -3.2207 0.1572
N -0.7820 -1.9620 -0.4059
C -1.2969 -4.1408 -0.5219
C -1.6555 -2.1433 -1.3927
N -1.9908 -3.4445 -1.4905
H 0.4801 -4.5920 1.4224

H -0.0471 -3.0986  2.2378
H  1.3533 -3.0675  1.1692
H -1.3976 -5.2069 -0.3912
H -2.0064 -1.3633 -2.0530
H -2.6386 -3.8338 -2.1604
C  1.0461 -0.6004  3.4859
S -0.3407 -0.3165  2.2746
H  0.5646 -0.7346  4.4573
H  1.7225  0.2590  3.5478
H  1.6273 -1.4969  3.2505
C -5.6592  0.7607  0.7858
C -4.2080  0.8546  0.3977
N -3.7052  1.9266 -0.3293
C -3.1154  0.0485  0.6074
C -2.3815  1.7417 -0.5322
N -1.9839  0.6063  0.0205
H -5.8332 -0.1576  1.3520
H -6.3124  0.7426 -0.0948
H -5.9630  1.6043  1.4168
H -3.0529 -0.8726  1.1653
H -1.7614  2.4136 -1.1015
H -4.2414  2.7132 -0.6683
C  2.1507  5.0132 -1.0253
C  1.5249  3.8149 -0.3851
N  1.0985  3.7989  0.9350
C  1.2273  2.5627 -0.8581
C  0.5737  2.5825  1.2150
N  0.6376  1.8057  0.1432
H  2.3923  4.7930 -2.0681
H  3.0806  5.3050 -0.5221
H  1.4783  5.8797 -1.0137
H  1.3741  2.1444 -1.8404
H  0.1562  2.2829  2.1651
H  1.1676  4.5656  1.5903
C  5.5617 -1.0813  0.2190
C  4.0954 -1.0412 -0.1187
N  3.5777 -1.6844 -1.2342
C  3.0001 -0.4485  0.4654
C  2.2432 -1.4673 -1.2918
N  1.8535 -0.7185 -0.2711
H  5.7499 -0.5101  1.1314
H  6.1698 -0.6448 -0.5821
H  5.9088 -2.1074  0.3886
H  2.9590  0.1541  1.3589
H  1.6009 -1.8313 -2.0765
H  4.1091 -2.2249 -1.9030

O -1.1859  0.4424 -2.7061
H -0.8243  0.4148 -3.6088
O  0.0523  0.1824 -1.9641

21. non H-bonded $Fe^{III}$-OOH S=5/2
Fe -0.1865 -0.1626 -0.1244
C  0.4893 -3.5866  1.3065
C -0.4705 -3.4727  0.1686
N -0.7765 -2.2718 -0.4678
C -1.2007 -4.4729 -0.4186
C -1.6692 -2.5541 -1.4074
N -1.9545 -3.8727 -1.4096
H  0.6137 -4.6359  1.5903
H  0.1224 -3.0279  2.1732
H  1.4726 -3.1819  1.0458
H -1.2519 -5.5317 -0.2174
H -2.0936 -1.8369 -2.0906
H -2.6065 -4.3353 -2.0272
C  1.0164 -0.4064  3.3724
S -0.4557 -0.2897  2.2792
H  0.6618 -0.5849  4.3904
H  1.5861  0.5293  3.3693
H  1.6784 -1.2278  3.0837
C -5.6197  1.4511  1.1813
C -4.3321  1.1736  0.4889
N -4.0163  1.6496 -0.7765
C -3.2269  0.4724  0.8834
C -2.7684  1.2352 -1.0982
N -2.2593  0.5188 -0.1053
H -5.6221  0.9659  2.1604
H -6.4826  1.0714  0.6199
H -5.7753  2.5253  1.3424
H -3.0548 -0.0453  1.8142
H -2.2523  1.4721 -2.0185
H -4.6145  2.2164 -1.3620
C  2.5466  4.9022 -0.9302
C  1.6932  3.8015 -0.3969
N  1.0120  3.8828  0.8105
C  1.3867  2.5591 -0.8833
C  0.3422  2.7240  1.0102
N  0.5489  1.8964 -0.0034
H  2.9779  4.6040 -1.8891
H  3.3753  5.1438 -0.2530
H  1.9734  5.8228 -1.0964
H  1.6819  2.1053 -1.8149
H -0.2552  2.4982  1.8814

H 1.0154 4.6730 1.4411
C 5.5218 -0.8223 0.6130
C 4.1254 -0.9011 0.1049
N 3.7583 -1.5774 -1.0497
C 2.9552 -0.3832 0.5881
C 2.4211 -1.4449 -1.2217
N 1.9035 -0.7300 -0.2365
H 5.5459 -0.2383 1.5365
H 6.1946 -0.3373 -0.1052
H 5.9342 -1.8138 0.8371
H 2.8079 0.2226 1.4667
H 1.8676 -1.8540 -2.0524
H 4.3832 -2.0794 -1.6660
O -0.2732 1.0531 -2.8251
H -0.2396 0.6961 -3.7296
O -0.2616 -0.1872 -2.0702

22. non H-bonded $Fe^{III}$-OOH S=1/2
Fe -0.0691 -0.0813 -0.0879
C 0.3627 -3.5097 1.3109
C -0.5418 -3.2207 0.1572
N -0.7820 -1.9620 -0.4059
C -1.2969 -4.1408 -0.5219
C -1.6555 -2.1433 -1.3927
N -1.9908 -3.4445 -1.4905
H 0.4801 -4.5920 1.4224
H -0.0471 -3.0986 2.2378
H 1.3533 -3.0675 1.1692
H -1.3976 -5.2069 -0.3912
H -2.0064 -1.3633 -2.0530
H -2.6386 -3.8338 -2.1604
C 1.0461 -0.6004 3.4859
S -0.3407 -0.3165 2.2746
H 0.5646 -0.7346 4.4573
H 1.7225 0.2590 3.5478
H 1.6273 -1.4969 3.2505
C -5.6592 0.7607 0.7858
C -4.2080 0.8546 0.3977
N -3.7052 1.9266 -0.3293
C -3.1154 0.0485 0.6074
C -2.3815 1.7417 -0.5322
N -1.9839 0.6063 0.0205
H -5.8332 -0.1576 1.3520
H -6.3124 0.7426 -0.0948
H -5.9630 1.6043 1.4168
H -3.0529 -0.8726 1.1653

H -1.7614  2.4136 -1.1015
H -4.2414  2.7132 -0.6683
C  2.1507  5.0132 -1.0253
C  1.5249  3.8149 -0.3851
N  1.0985  3.7989  0.9350
C  1.2273  2.5627 -0.8581
C  0.5737  2.5825  1.2150
N  0.6376  1.8057  0.1432
H  2.3923  4.7930 -2.0681
H  3.0806  5.3050 -0.5221
H  1.4783  5.8797 -1.0137
H  1.3741  2.1444 -1.8404
H  0.1562  2.2829  2.1651
H  1.1676  4.5656  1.5903
C  5.5617 -1.0813  0.2190
C  4.0954 -1.0412 -0.1187
N  3.5777 -1.6844 -1.2342
C  3.0001 -0.4485  0.4654
C  2.2432 -1.4673 -1.2918
N  1.8535 -0.7185 -0.2711
H  5.7499 -0.5101  1.1314
H  6.1698 -0.6448 -0.5821
H  5.9088 -2.1074  0.3886
H  2.9590  0.1541  1.3589
H  1.6009 -1.8313 -2.0765
H  4.1091 -2.2249 -1.9030
O -1.1859  0.4424 -2.7061
H -0.8243  0.4148 -3.6088
O  0.0523  0.1824 -1.9641

23. non H-bonded $Fe^{III}$-$O_2^-$ S=5/2
Fe -0.1889 -0.1081 -0.4534
C -0.0148 -3.5856  1.3015
C -1.1357 -3.3754  0.3440
N -1.3003 -2.1762 -0.3263
C -2.1232 -4.2461 -0.0433
C -2.3552 -2.3201 -1.1049
N -2.8956 -3.5572 -0.9638
H -0.0875 -4.5701  1.7771
H -0.0425 -2.8027  2.0676
H  0.9556 -3.5196  0.7961
H -2.3411 -5.2634  0.2445
H -2.7237 -1.5717 -1.7880
H -3.7073 -3.9091 -1.4484
C  0.9861 -0.2745  3.3060
S -0.5233 -0.1565  2.2657

H 0.6986 -0.2586 4.3636
H 1.6747 0.5691 3.1445
H 1.5466 -1.2021 3.1315
C -5.3019 2.3071 1.1081
C -4.0917 1.8479 0.3619
N -3.6931 2.3731 -0.8636
C -3.1315 0.9207 0.6689
C -2.5333 1.7664 -1.2328
N -2.1716 0.8808 -0.3240
H -5.3873 1.7443 2.0415
H -6.2292 2.1529 0.5399
H -5.2470 3.3726 1.3683
H -3.0389 0.3072 1.5531
H -1.9700 1.9676 -2.1332
H -4.1695 3.0949 -1.3844
C 3.3039 4.4903 -0.9484
C 2.3188 3.5374 -0.3675
N 1.7762 3.6509 0.9075
C 1.7525 2.4054 -0.8855
C 0.9273 2.6020 1.1023
N 0.8949 1.8352 0.0315
H 3.5644 4.1702 -1.9611
H 4.2351 4.5384 -0.3671
H 2.9090 5.5133 -1.0175
H 1.8785 1.9551 -1.8582
H 0.3607 2.4050 2.0033
H 1.9765 4.3782 1.5786
C 5.3792 -1.6069 0.6395
C 4.0052 -1.4770 0.0575
N 3.5977 -2.0881 -1.1238
C 2.8952 -0.7988 0.4887
C 2.2949 -1.7638 -1.3489
N 1.8433 -0.9853 -0.3852
H 5.4368 -1.0289 1.5657
H 6.1547 -1.2279 -0.0390
H 5.6296 -2.6480 0.8818
H 2.7861 -0.1892 1.3704
H 1.7113 -2.0649 -2.2071
H 4.1685 -2.6699 -1.7199
O 0.0250 0.6785 -2.2424
O -0.3844 -0.6827 -2.2970

24. non H-bonded $Fe^{III}$-$O_2^-$ S=1/2

Fe -0.148441 -0.089228 -0.066311
C 0.444835 -3.623516 1.232781
C -0.535373 -3.294160 0.148451

| | | | |
|---|---|---|---|
| N | -0.820918 | -2.013364 | -0.336502 |
| C | -1.305078 | -4.204541 | -0.528871 |
| C | -1.732437 | -2.177622 | -1.282326 |
| N | -2.064667 | -3.480663 | -1.427266 |
| H | 0.416188 | -4.696483 | 1.448479 |
| H | 0.201035 | -3.062257 | 2.140728 |
| H | 1.467672 | -3.353442 | 0.947518 |
| H | -1.380219 | -5.277332 | -0.439351 |
| H | -2.143560 | -1.390211 | -1.888819 |
| H | -2.719325 | -3.849121 | -2.099575 |
| C | 1.063779 | -0.496871 | 3.410781 |
| S | -0.436175 | -0.201899 | 2.390967 |
| H | 0.751825 | -0.699987 | 4.441379 |
| H | 1.733171 | 0.374981 | 3.441168 |
| H | 1.650062 | -1.356065 | 3.063571 |
| C | -5.715850 | 1.341222 | 0.899153 |
| C | -4.310461 | 1.159364 | 0.378361 |
| N | -3.877858 | 1.757091 | -0.800270 |
| C | -3.208529 | 0.464431 | 0.825571 |
| C | -2.579833 | 1.412660 | -1.013334 |
| N | -2.138513 | 0.624748 | -0.047486 |
| H | -5.836756 | 0.785766 | 1.832899 |
| H | -6.465821 | 0.970272 | 0.188636 |
| H | -5.940681 | 2.395379 | 1.106280 |
| H | -3.092113 | -0.122195 | 1.725334 |
| H | -1.996100 | 1.709515 | -1.871391 |
| H | -4.430000 | 2.351053 | -1.401376 |
| C | 2.432173 | 4.814442 | -1.246410 |
| C | 1.652149 | 3.722346 | -0.569921 |
| N | 1.209668 | 3.804518 | 0.745556 |
| C | 1.226174 | 2.487864 | -0.993272 |
| C | 0.557066 | 2.650442 | 1.059151 |
| N | 0.551690 | 1.828925 | 0.024391 |
| H | 2.658430 | 4.519129 | -2.274504 |
| H | 3.385409 | 5.013697 | -0.739300 |
| H | 1.872961 | 5.758531 | -1.286194 |
| H | 1.340885 | 2.019337 | -1.958191 |
| H | 0.122329 | 2.407937 | 2.020497 |
| H | 1.346121 | 4.584387 | 1.371727 |
| C | 5.453813 | -0.827255 | 0.498332 |
| C | 4.016346 | -0.885972 | 0.071380 |
| N | 3.583246 | -1.599411 | -1.038895 |
| C | 2.870824 | -0.328637 | 0.581892 |
| C | 2.235913 | -1.449351 | -1.157624 |
| N | 1.771607 | -0.681656 | -0.184919 |
| H | 5.546043 | -0.211771 | 1.397398 |

| | | | |
|---|---|---|---|
| H | 6.095345 | -0.385345 | -0.275503 |
| H | 5.854763 | -1.821631 | 0.734841 |
| H | 2.763691 | 0.302100 | 1.449110 |
| H | 1.622027 | -1.803190 | -1.976663 |
| H | 4.166306 | -2.128226 | -1.670410 |
| O | -0.233641 | 0.218486 | -1.934348 |
| O | 0.103109 | -0.687848 | -2.863968 |

25. $Fe^{III}$-OMe OOH

| | | | |
|---|---|---|---|
| Fe | -0.118627 | -0.347683 | 0.007254 |
| C | 1.535650 | -3.216094 | 1.796278 |
| C | 0.656467 | -3.519217 | 0.622443 |
| N | -0.005826 | -2.549717 | -0.128459 |
| C | 0.354896 | -4.750736 | 0.100819 |
| C | -0.681573 | -3.191428 | -1.070820 |
| N | -0.493766 | -4.524259 | -0.966792 |
| H | 2.023036 | -4.129675 | 2.148395 |
| H | 0.953559 | -2.794383 | 2.621321 |
| H | 2.310226 | -2.488290 | 1.534871 |
| H | 0.661180 | -5.743638 | 0.391710 |
| H | -1.276108 | -2.716191 | -1.834425 |
| H | -0.902349 | -5.228388 | -1.564659 |
| O | -0.183991 | -0.363814 | 1.848727 |
| C | -5.810297 | 0.423892 | 0.919443 |
| C | -4.459157 | 0.204716 | 0.323932 |
| N | -4.195755 | 0.416463 | -1.022527 |
| C | -3.256180 | -0.191893 | 0.851367 |
| C | -2.889205 | 0.153250 | -1.260437 |
| N | -2.291027 | -0.219920 | -0.139484 |
| H | -5.785847 | 0.209844 | 1.991127 |
| H | -6.567974 | -0.229347 | 0.468981 |
| H | -6.147323 | 1.460501 | 0.794160 |
| H | -3.012512 | -0.461395 | 1.868116 |
| H | -2.391055 | 0.293576 | -2.209057 |
| H | -4.867074 | 0.725096 | -1.712338 |
| C | 0.736751 | 5.455088 | -0.541987 |
| C | 0.286619 | 4.085355 | -0.151498 |
| N | -0.491006 | 3.845451 | 0.972845 |
| C | 0.491547 | 2.844411 | -0.699974 |
| C | -0.713696 | 2.512513 | 1.066453 |
| N | -0.130671 | 1.875153 | 0.065213 |
| H | 1.325787 | 5.404717 | -1.461412 |
| H | 1.365532 | 5.914298 | 0.231088 |
| H | -0.109702 | 6.128098 | -0.727001 |
| H | 1.020401 | 2.579070 | -1.601445 |
| H | -1.291081 | 2.048391 | 1.850172 |

| | | | |
|---|---|---|---|
| H | -0.828261 | 4.545963 | 1.618634 |
| C | 5.553349 | 0.962132 | 0.471147 |
| C | 4.226509 | 0.427187 | 0.058981 |
| N | 4.008313 | -0.190719 | -1.163732 |
| C | 3.001393 | 0.420677 | 0.672820 |
| C | 2.700264 | -0.529618 | -1.249835 |
| N | 2.061160 | -0.173066 | -0.148334 |
| H | 5.484741 | 1.400430 | 1.470193 |
| H | 5.908318 | 1.744812 | -0.211072 |
| H | 6.320723 | 0.178676 | 0.505812 |
| H | 2.737149 | 0.815890 | 1.641427 |
| H | 2.234592 | -0.999501 | -2.101404 |
| H | 4.708028 | -0.357452 | -1.873877 |
| O | -0.285725 | 0.672467 | -2.737809 |
| H | -0.041668 | 0.334221 | -3.616482 |
| O | -0.092434 | -0.540615 | -1.946721 |
| C | 0.401430 | 0.004192 | 3.052528 |
| H | -0.270449 | -0.205334 | 3.900367 |
| H | 0.639375 | 1.083611 | 3.082744 |
| H | 1.341715 | -0.540401 | 3.240802 |

26. $Fe^{III}$-OMe $O_2H_2$

| | | | |
|---|---|---|---|
| Fe | -0.117570 | -0.297911 | 0.307012 |
| C | 0.790782 | -3.475838 | 1.795282 |
| C | -0.014387 | -3.487764 | 0.534274 |
| N | -0.386739 | -2.344376 | -0.187055 |
| C | -0.519871 | -4.582415 | -0.115217 |
| C | -1.095164 | -2.768192 | -1.235347 |
| N | -1.193426 | -4.108527 | -1.222749 |
| H | 0.985113 | -4.500304 | 2.121929 |
| H | 0.259348 | -2.957451 | 2.599745 |
| H | 1.754540 | -2.974492 | 1.656345 |
| H | -0.460812 | -5.634843 | 0.115997 |
| H | -1.519340 | -2.142596 | -2.005247 |
| H | -1.689641 | -4.671311 | -1.902053 |
| C | 0.265773 | -0.007997 | 3.362371 |
| O | -0.195778 | -0.311773 | 2.072494 |
| H | -0.437680 | -0.394525 | 4.109650 |
| H | 0.354383 | 1.079936 | 3.493143 |
| H | 1.248563 | -0.465633 | 3.536607 |
| C | -5.673629 | 1.212886 | 1.047695 |
| C | -4.352000 | 0.819551 | 0.452474 |
| N | -4.112248 | 0.891622 | -0.911076 |
| C | -3.166295 | 0.360342 | 0.978733 |
| C | -2.846179 | 0.498924 | -1.165587 |
| N | -2.229125 | 0.165825 | -0.035325 |

| | | | |
|---|---|---|---|
| H | -5.650994 | 1.087139 | 2.132683 |
| H | -6.488136 | 0.592816 | 0.656349 |
| H | -5.911845 | 2.261000 | 0.833262 |
| H | -2.924277 | 0.144371 | 2.008337 |
| H | -2.427727 | 0.462377 | -2.159216 |
| H | -4.786191 | 1.180553 | -1.609712 |
| C | 1.775879 | 5.080322 | -0.872780 |
| C | 1.015521 | 3.896140 | -0.384601 |
| N | -0.066452 | 3.982817 | 0.474373 |
| C | 1.172894 | 2.551354 | -0.603666 |
| C | -0.516981 | 2.738116 | 0.744929 |
| N | 0.214048 | 1.834747 | 0.103529 |
| H | 2.578519 | 4.761311 | -1.541889 |
| H | 2.231541 | 5.636017 | -0.044791 |
| H | 1.134091 | 5.774861 | -1.427466 |
| H | 1.952148 | 2.060641 | -1.167325 |
| H | -1.364835 | 2.529390 | 1.379616 |
| H | -0.451386 | 4.840764 | 0.851473 |
| C | 5.664860 | 0.370412 | 0.455240 |
| C | 4.272664 | -0.115136 | 0.174412 |
| N | 3.994892 | -1.088285 | -0.776656 |
| C | 3.039847 | 0.228880 | 0.672679 |
| C | 2.661370 | -1.290635 | -0.830428 |
| N | 2.037536 | -0.499482 | 0.036447 |
| H | 5.644142 | 1.134535 | 1.235788 |
| H | 6.121723 | 0.811167 | -0.438274 |
| H | 6.313180 | -0.442883 | 0.800755 |
| H | 2.810573 | 0.956998 | 1.435481 |
| H | 2.189825 | -2.001632 | -1.490623 |
| H | 4.684976 | -1.580897 | -1.330712 |
| O | -0.734298 | -0.284694 | -3.309449 |
| O | 0.198138 | 0.059669 | -2.252577 |
| H | -0.125924 | -0.556108 | -4.024730 |
| H | 0.228541 | 1.034767 | -2.324393 |