Supplementary Information for

S K-edge XAS and DFT Calculations on Cytochrome P450: Covalent and Ionic Contributions to the Cysteine-Fe Bond and Their Contribution to Reactivity

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Full reference 25:
Frisch, M. J. T., 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.; C02 ed.; Gaussian, Inc.: Wallingford CT, 2004.

Optimized co-ordinates for

1) Resting state model A, B, C
2) Substrate bound high-spin state models A, B, C and model A with Imidazole and Fluoride axial ligands
3) Compound O models A, B, C and model A with Imidazole and Fluoride axial ligands
4) Compound I models A, B, C and model A with Imidazole and Fluoride axial ligands
5) Compound II models A, B, C and model A with Imidazole and Fluoride axial ligands
6) Fe(IV)=O models A, B and model A with Imidazole and Fluoride axial ligands

1A)

Fe	1.6760	0.2547	0.5091
C	3.7194	-1.8289	-1.3183
C	2.7691	2.9210	-1.3225
C	-0.0708	2.4026	2.5626
C	0.6949	-2.3715	2.4224
N	2.9968	0.4933	-1.0034
C	3.7222	-0.4797	-1.6535
C	4.4750	0.0983	-2.7381
C	4.1912	1.4310	-2.7461
C	3.2710	1.6701	-1.6621
N	1.4374	2.2658	0.6360
C	1.9198	3.1933	-0.2573
C	1.4324	4.5096	0.0778
C	0.6422	4.3688	1.1776
C	0.6427	2.9659	1.5121
N	0.5574	0.0647	2.1698
C	-0.1081	1.0466	2.8604
C	-0.8701	0.4714	3.9441
C	-0.6626	-0.8716	3.8964
C	0.2292	-1.1155	2.7861
N	2.1120	-1.7022	0.5317
C	1.5808	-2.6359	1.3855
C	2.1004	-3.9480	1.0790
C	2.9614	-3.7960	0.0362
C	2.9632	-2.3920	-0.2978
H	4.3451	-2.4939	-1.9057
H	3.0726	3.7604	-1.9409
H	-0.6584	3.0699	3.1856
H	0.3536	-3.2176	3.0110
H	5.1280	-0.4564	-3.4000
H	4.5653	2.1951	-3.4157
H	1.6717	5.4127	-0.4693
H	0.0979	5.1314	1.7200
H	-1.4786	1.0377	4.6376
H	-1.0640	-1.6409	4.5437
H	1.8357	-4.8540	1.6093
H	3.5500	-4.5507	-0.4700
C	-0.4430	-2.4435	-1.9429
C	0.1610	-1.0571	-2.1700
S	-0.1140	0.1085	-0.7725
H	-1.5172	-2.3734	-1.7411
H	1.2309	-1.1263	-2.3793

H -0.3052 -0.5818 -3.0408
O 3.3937 0.5642 1.7954
H 3.3162 1.4633 2.1483
H 4.1720 0.5483 1.2181
H 0.0265 -2.9479 -1.0933
H -0.3043 -3.0715 -2.8339

1B)
Fe 1.6430 0.2369 0.4669
C 3.6236 -1.8586 -1.4149
C 2.7813 2.9105 -1.3171
C -0.1034 2.3769 2.5318
C 0.6218 -2.4050 2.3476
N 2.9565 0.4725 -1.0465
C 3.6497 -0.5041 -1.7258
C 4.4070 0.0782 -2.8047
C 4.1595 1.4175 -2.7790
C 3.2549 1.6557 -1.6819
N 1.4307 2.2455 0.6245
C 1.9340 3.1796 -0.2506
C 1.4606 4.4974 0.0984
C 0.6540 4.3516 1.1847
C 0.6325 2.9442 1.4989
N 0.5065 0.0367 2.1173
C -0.1568 1.0180 2.8138
C -0.9301 0.4385 3.8864
C -0.7298 -0.9054 3.8303
C 0.1669 -1.1467 2.7235
N 2.0401 -1.7298 0.4565
C 1.5077 -2.6671 1.3073
C 2.0095 -3.9813 0.9827
C 2.8599 -3.8286 -0.0695
C 2.8745 -2.4225 -0.3902
H 4.2289 -2.5256 -2.0208
H 3.1018 3.7544 -1.9203
H -0.6890 3.0436 3.1568
H 0.2855 -3.2521 2.9383
H 5.0386 -0.4783 -3.4853
H 4.5470 2.1866 -3.4349
H 1.7164 5.4045 -0.4341
H 0.1093 5.1128 1.7281
H -1.5388 1.0024 4.5814
H -1.1387 -1.6756 4.4720
H 1.7430 -4.8898 1.5078
H 3.4342 -4.5853 -0.5885
N -4.1947 1.1977 -1.8658
C -4.5817 1.7631 -3.1349
H -3.8828 0.2370 -1.8269
H -4.0733 1.2231 -3.9378
H -4.2961 2.8175 -3.1682
H -5.6660 1.7013 -3.2967
N -3.4777 -0.1916 0.4201
C -4.0536 1.1346 0.5764
C -4.4439 1.8694 -0.7190
O -4.9318 2.9919 -0.6903
H -2.4764 -0.2707 0.2628

H -4.9602 1.0504 1.1813
H -3.3426 1.7695 1.1133
N -2.1923 -2.6613 -0.2463
C -3.5578 -2.6633 0.2375
C -4.2674 -1.3000 0.3379
O -5.4839 -1.2624 0.3832
H -1.4263 -2.6541 0.4144
H -4.1738 -3.2739 -0.4258
H -3.5778 -3.1205 1.2323
C -0.4430 -2.4435 -1.9429
C -1.9219 -2.5028 -1.5774
O -2.8140 -2.3972 -2.4091
C 0.0258 -1.0052 -2.2332
S -0.1489 0.1817 -0.8396
H 0.1765 -2.8946 -1.1633
H -0.3204 -3.0362 -2.8574
H 1.0632 -1.0152 -2.5760
H -0.5852 -0.5872 -3.0400
O 3.3342 0.4806 1.7642
H 3.2974 1.3722 2.1420
H 4.1453 0.4194 1.2378

1C)
O -3.9907 1.8490 2.0908
O -1.5731 0.7748 1.5331
Fe 0.0295 0.7763 0.1927
C 2.2043 1.4455 2.7457
C -0.2200 4.1235 -0.4739
C -2.1441 0.1073 -2.3617
C 0.1421 -2.5611 0.9630
N 0.7952 2.4473 1.0107
C 1.7107 2.5310 2.0369
C 2.1070 3.9134 2.2731
C 1.3929 4.6508 1.3747
C 0.5921 3.7378 0.5906
C 3.1197 4.3850 3.2829
N -1.0374 1.9019 -1.1021
C -0.9471 3.2643 -1.2874
C -1.6854 3.6641 -2.4790
C -2.1825 2.5117 -3.0083
C -1.7882 1.4308 -2.1489
C -1.8948 5.0477 -3.0126
N -0.8528 -0.8857 -0.5296
C -1.7200 -0.9645 -1.5900
C -2.1179 -2.3260 -1.8169
C -1.4905 -3.0931 -0.8862
C -0.6888 -2.1790 -0.0845
C -1.5904 -4.5729 -0.7319
N 0.9868 -0.3394 1.5747
C 0.9303 -1.7068 1.7298
C 1.8092 -2.1361 2.8128
C 2.3825 -0.9909 3.2904
C 1.8608 0.1148 2.5288
C 2.0310 -3.5395 3.3148
H 2.9191 1.6460 3.5380
H -0.2518 5.1831 -0.7081

H -2.7732 -0.1103 -3.2197
H 0.1968 -3.6215 1.1891
H 1.4117 5.7251 1.2351
H 3.2137 5.4747 3.2509
H 4.1117 3.9581 3.0890
H -2.7850 2.4015 -3.9023
H -2.4825 5.0146 -3.9342
H -0.9483 5.5534 -3.2353
H -2.8012 -2.6495 -2.5921
H -1.9803 -4.8604 0.2547
H -0.6145 -5.0628 -0.8435
H 3.0888 -0.8982 4.1072
H 2.7762 -3.5435 4.1165
H 2.3875 -4.2072 2.5214
H 1.1086 -3.9799 3.7162
H -2.4335 5.6831 -2.2949
H 2.8405 4.1024 4.3063
H -2.2594 -4.9933 -1.4886
N 2.5604 -2.6758 -1.7728
C 1.6143 -3.0955 -2.7927
H 2.4149 -1.7545 -1.3689
H 1.3848 -4.1598 -2.6822
H 2.0188 -2.9477 -3.8017
N 4.5594 -1.3588 -0.2326
C 4.8245 -2.6782 -0.7730
C 3.8105 -3.2023 -1.8043
O 4.1216 -4.1136 -2.5601
H 4.0416 -1.2718 0.6312
H 5.7946 -2.6766 -1.2736
H 4.8724 -3.3942 0.0542
C 4.2398 1.0626 -0.4376
C 4.7046 -0.2594 -1.0377
O 5.1634 -0.3489 -2.1722
C 3.0626 1.6462 -1.2332
S 1.6034 0.5286 -1.3608
H 3.9689 0.9506 0.6165
H 5.0833 1.7642 -0.4961
C -5.0499 2.5095 -1.2405
O -5.0268 1.3591 -0.3910
H -5.7535 3.2114 -0.7855
H -4.4539 0.6695 -0.7721
N -5.0391 -3.5008 1.4720
C -5.6452 -4.1232 0.3182
H -4.9581 -4.0443 2.3188
H -5.0419 -4.9622 -0.0524
H -5.7132 -3.3672 -0.4652
H -6.6509 -4.4889 0.5543
C -3.7774 -1.8971 2.7486
C -4.4584 -2.2682 1.4523
O -4.4537 -1.5205 0.4743
H -4.2546 -2.3353 3.6311
H -3.7708 -0.8087 2.8410
H -2.7294 -2.2247 2.7205
H -4.5719 1.3747 2.7019
H -4.3774 1.6770 1.1966
H -5.4155 2.2564 -2.2438

H -4.0714 2.9879 -1.3251
H 2.7639 2.6130 -0.8218
H 3.3792 1.7997 -2.2693
H 0.6992 -2.5130 -2.6814
H -2.3035 0.1931 1.2649
H -2.0639 1.5614 1.8516

2A)
Fe 0.0661 -0.0044 0.1171
S 0.0029 -0.0324 2.4235
N 1.4373 1.5290 -0.2774
N 1.6264 -1.3429 -0.2639
N -1.2569 -1.5354 -0.4139
N -1.4451 1.3372 -0.4156
C 1.1493 2.8713 -0.3212
C 2.8058 1.4226 -0.2721
C 2.9695 -1.0580 -0.2590
C 1.5164 -2.7122 -0.2991
C -0.9629 -2.8775 -0.4379
C -2.6182 -1.4293 -0.5661
C -2.7813 1.0522 -0.5677
C -1.3305 2.7070 -0.4466
C 2.3745 3.6356 -0.3333
C 3.4004 2.7385 -0.3049
C 3.7306 -2.2844 -0.2812
C 2.8308 -3.3088 -0.3041
C -2.1777 -3.6414 -0.5935
C -3.2023 -2.7450 -0.6753
C -3.5329 2.2788 -0.6806
C -2.6351 3.3031 -0.6026
C 3.5173 0.2241 -0.2509
C 0.3183 -3.4219 -0.3625
C -3.3271 -0.2297 -0.6238
C -0.1319 3.4166 -0.3810
C -1.7761 0.0647 2.8707
H 4.6008 0.2955 -0.2442
H 0.3919 -4.5050 -0.3882
H -4.4039 -0.3004 -0.7459
H -0.2023 4.4998 -0.4128
H 4.8117 -2.3417 -0.2852
H 3.0270 -4.3731 -0.3325
H 2.4295 4.7162 -0.3693
H 4.4648 2.9364 -0.3113
H -2.2268 -4.7217 -0.6452
H -4.2584 -2.9445 -0.8064
H -4.6061 2.3371 -0.8120
H -2.8262 4.3673 -0.6593
H -1.8486 -0.0326 3.9567
H -2.3458 -0.7439 2.4054
H -2.2025 1.0255 2.5718
2B)
Fe 1.721278 0.236156 0.483280
C 2.604705 -3.093572 0.346747
C 4.327219 0.960853 -1.646181
C 1.172432 3.598565 0.967566
C -0.455064 -0.435775 3.063252

N	3.116159	-0.845419	-0.499470
C	3.292741	-2.227849	-0.456030
C	4.365436	-2.613837	-1.346818
C	4.854586	-1.472304	-1.896018
C	4.081335	-0.379418	-1.353071
N	2.626257	1.937599	-0.158076
C	3.658969	2.039661	-1.078946
C	3.915802	3.407644	-1.387136
C	3.010647	4.150856	-0.658006
C	2.233758	3.223065	0.081281
N	0.642858	1.353163	1.795354
C	0.455322	2.737446	1.741655
C	-0.600291	3.126660	2.654208
C	-1.039647	1.993990	3.256791
C	-0.266944	0.897883	2.708338
N	1.198861	-1.431305	1.521243
C	0.227720	-1.521823	2.513958
C	0.033595	-2.879433	2.890316
C	0.909093	-3.631945	2.128749
C	1.610481	-2.717304	1.301802
H	2.846198	-4.149465	0.280781
H	5.118783	1.178544	-2.355740
H	0.931339	4.655086	1.020948
H	-1.204177	-0.648924	3.818836
H	4.699197	-3.632462	-1.496828
H	5.671633	-1.355855	-2.596185
H	4.669632	3.755950	-2.080810
H	2.894910	5.225813	-0.624124
H	-0.939691	4.143962	2.799191
H	-1.818013	1.882904	4.000480
H	-0.651465	-3.218785	3.656356
H	1.052786	-4.704187	2.133434
N	-4.244159	1.195744	-1.931632
C	-4.655249	1.711088	-3.213815
H	-3.862534	0.262362	-1.869404
H	-4.433006	0.966457	-3.981293
H	-4.123496	2.639342	-3.449815
H	-5.729377	1.928290	-3.224568
N	-3.411961	-0.083349	0.382644
C	-4.002752	1.242664	0.499769
C	-4.447659	1.920095	-0.810596
O	-4.947393	3.039034	-0.813751
H	-2.423286	-0.157237	0.152161
H	-4.888643	1.169816	1.135771
H	-3.286755	1.908983	0.989492
N	-2.133912	-2.583525	-0.214157
C	-3.484838	-2.566320	0.303518
C	-4.194321	-1.201710	0.367248
O	-5.407872	-1.171929	0.455794
H	-1.354895	-2.605304	0.429388
H	-4.120432	-3.205908	-0.312477
H	-3.474499	-2.978508	1.317721
C	-0.427731	-2.447530	-1.957205
C	-1.897058	-2.477289	-1.555305
O	-2.809109	-2.391991	-2.367487
C	0.027056	-1.041582	-2.384869

S -0.111595 0.256736 -1.084202
H 0.208180 -2.817526 -1.147126
H -0.314974 -3.124781 -2.812687
H 1.060939 -1.084463 -2.740158
H -0.595874 -0.699867 -3.216402

2C)

Fe -0.8996 0.3390 -0.5434
C -0.7172 -2.8949 -1.7653
C -4.1480 -0.2079 0.3815
C -1.4135 3.7403 -0.2390
C 2.1855 0.9890 -1.9898
N -2.2153 -1.2352 -0.7480
C -1.9146 -2.5143 -1.1648
C -3.0101 -3.4133 -0.8546
C -3.9658 -2.6434 -0.2481
C -3.4701 -1.2922 -0.1843
C -3.0277 -4.8879 -1.1275
N -2.5366 1.5600 -0.1462
C -3.7094 1.1137 0.4192
C -4.4144 2.2223 1.0502
C -3.6580 3.3314 0.8074
C -2.4830 2.9114 0.0869
C -5.6661 2.1334 1.8654
N 0.1589 2.0431 -1.0805
C -0.1872 3.3367 -0.7644
C 0.9278 4.2124 -1.0045
C 1.9682 3.4512 -1.4580
C 1.4653 2.0880 -1.5236
C 3.3590 3.9063 -1.7752
N 0.4633 -0.7368 -1.7140
C 1.7172 -0.3205 -2.1066
C 2.4654 -1.4377 -2.6675
C 1.6222 -2.5144 -2.6071
C 0.3839 -2.0748 -2.0176
C 3.8624 -1.4055 -3.2210
H -0.6182 -3.9380 -2.0500
H -5.1119 -0.4229 0.8329
H -1.5231 4.7962 -0.0108
H 3.2048 1.1750 -2.3129
H -4.9290 -2.9669 0.1280
H -3.9766 -5.3315 -0.8114
H -2.2230 -5.4061 -0.5906
H -3.8571 4.3464 1.1294
H -5.9890 3.1274 2.1889
H -5.5123 1.5230 2.7643
H 0.9242 5.2812 -0.8279
H 3.6515 3.6532 -2.8024
H 4.0930 3.4408 -1.1057
H 1.8225 -3.5237 -2.9472
H 4.1746 -2.4054 -3.5363
H 4.5872 -1.0447 -2.4805
H 3.9367 -0.7424 -4.0923
H -6.4943 1.6798 1.3056
H -2.8973 -5.1060 -2.1949
H 3.4456 4.9910 -1.6628
N 3.2033 0.5919 1.5037

C 3.2027 2.0054 1.8390
H 2.2957 0.1771 1.3172
H 4.1598 2.4511 1.5533
H 3.0663 2.1712 2.9150
N 2.7612 -2.2094 1.4512
C 4.0803 -1.7032 1.7850
C 4.1666 -0.1916 2.0590
O 5.1128 0.2684 2.6824
H 2.4952 -2.3048 0.4808
H 4.4420 -2.2005 2.6868
H 4.7667 -1.9431 0.9660
C 0.3972 -2.6435 1.9566
C 1.7987 -2.2690 2.4237
O 2.0478 -2.0084 3.5940
C -0.5959 -1.5425 2.3451
S -0.1679 0.1092 1.6427
H 0.3626 -2.8334 0.8791
H 0.1101 -3.5716 2.4695
H -1.6131 -1.8146 2.0534
H -0.5677 -1.4041 3.4285
H 2.3944 2.4980 1.2954

2Imz)
Fe 1.6430 0.2369 0.4669
C 3.6236 -1.8586 -1.4149
C 2.7813 2.9105 -1.3171
C -0.1034 2.3769 2.5318
C 0.6218 -2.4050 2.3476
N 2.9565 0.4725 -1.0465
C 3.6497 -0.5041 -1.7258
C 4.4070 0.0782 -2.8047
C 4.1595 1.4175 -2.7790
C 3.2549 1.6557 -1.6819
N 1.4307 2.2455 0.6245
C 1.9340 3.1796 -0.2506
C 1.4606 4.4974 0.0984
C 0.6540 4.3516 1.1847
C 0.6325 2.9442 1.4989
N 0.5065 0.0367 2.1173
C -0.1568 1.0180 2.8138
C -0.9301 0.4385 3.8864
C -0.7298 -0.9054 3.8303
C 0.1669 -1.1467 2.7235
N 2.0401 -1.7298 0.4565
C 1.5077 -2.6671 1.3073
C 2.0095 -3.9813 0.9827
C 2.8599 -3.8286 -0.0695
C 2.8745 -2.4225 -0.3902
H 4.2289 -2.5256 -2.0208
H 3.1018 3.7544 -1.9203
H -0.6890 3.0436 3.1568
H 0.2855 -3.2521 2.9383
H 5.0386 -0.4783 -3.4853
H 4.5470 2.1866 -3.4349
H 1.7164 5.4045 -0.4341
H 0.1093 5.1128 1.7281

H -1.5388 1.0024 4.5814
H -1.1387 -1.6756 4.4720
H 1.7430 -4.8898 1.5078
H 3.4342 -4.5853 -0.5885
H -2.9566 -0.5948 -1.6106
H -1.7140 -0.4439 0.6691
C -1.2717 -0.2841 -0.3106
H 1.1832 0.4046 -2.3395
N 0.0157 0.0247 -0.5521
H -1.2993 -0.0924 -3.5536
C 0.2149 0.1523 -1.9163
C -1.0044 -0.0909 -2.5076
N -1.9055 -0.3567 -1.4904
2 F)
Fe 1.7004 0.2931 0.5265
C 3.6690 -1.8182 -1.3493
C 2.8104 2.9638 -1.3093
C -0.0360 2.4390 2.5895
C 0.7616 -2.3503 2.5066
N 2.9789 0.5220 -1.0513
C 3.6961 -0.4636 -1.6816
C 4.4765 0.1146 -2.7499
C 4.2268 1.4560 -2.7438
C 3.2951 1.7060 -1.6691
N 1.4404 2.3251 0.6288
C 1.9533 3.2481 -0.2463
C 1.4770 4.5657 0.1063
C 0.6804 4.4191 1.2039
C 0.6640 3.0111 1.5268
N 0.5869 0.0871 2.2426
C -0.0673 1.0840 2.9201
C -0.8041 0.5153 4.0248
C -0.5838 -0.8306 3.9985
C 0.2914 -1.0913 2.8790
N 2.1252 -1.7111 0.5599
C 1.6122 -2.6345 1.4377
C 2.1057 -3.9479 1.1005
C 2.9276 -3.7996 0.0209
C 2.9390 -2.3955 -0.3100
H 4.2817 -2.4840 -1.9494
H 3.1446 3.8060 -1.9078
H -0.6113 3.1119 3.2180
H 0.4392 -3.1923 3.1117
H 5.1272 -0.4453 -3.4095
H 4.6328 2.2187 -3.3963
H 1.7272 5.4742 -0.4268
H 0.1444 5.1828 1.7529
H -1.4108 1.0840 4.7181
H -0.9721 -1.5891 4.6665
H 1.8523 -4.8569 1.6313
H 3.4807 -4.5631 -0.5114
F 0.0714 0.0493 -0.7130

3A)
Anti
Fe 0.0488 0.0852 -0.1518

C -0.4236 3.4802 -0.1753
C 3.4284 0.5607 -0.0412
C 0.5245 -3.3025 0.1090
C -3.3035 -0.3919 -0.4360
N 1.2611 1.7070 -0.1139
C 0.8868 3.0200 -0.1222
C 2.0541 3.8744 -0.1008
C 3.1372 3.0499 -0.0873
C 2.6266 1.6960 -0.0906
N 1.6644 -1.1406 -0.0212
C 2.9754 -0.7526 0.0149
C 3.8331 -1.9075 0.1583
C 3.0179 -2.9956 0.2245
C 1.6632 -2.5044 0.1117
N -1.1515 -1.5278 -0.1409
C -0.7802 -2.8379 -0.0303
C -1.9423 -3.6957 -0.1114
C -3.0168 -2.8783 -0.2907
C -2.5074 -1.5247 -0.3065
N -1.5492 1.3081 -0.2567
C -2.8520 0.9225 -0.3979
C -3.7131 2.0831 -0.4792
C -2.9053 3.1725 -0.3831
C -1.5530 2.6736 -0.2528
H -0.5762 4.5561 -0.1809
H 4.5037 0.7145 -0.0089
H 0.6651 -4.3759 0.2032
H -4.3726 -0.5468 -0.5546
H 2.0269 4.9574 -0.0996
H 4.1881 3.3130 -0.0695
H 4.9148 -1.8707 0.2104
H 3.2897 -4.0383 0.3381
H -1.9171 -4.7768 -0.0455
H -4.0611 -3.1461 -0.3990
H -4.7903 2.0466 -0.5910
H -3.1773 4.2211 -0.4027
C -1.6433 -0.3507 2.8693
S 0.0498 0.0954 2.3139
H -1.6731 -0.2884 3.9640
H -1.9163 -1.3708 2.5781
O 0.1695 0.0841 -1.9868
O 0.2877 -1.2066 -2.6288
H 1.1067 -1.5524 -2.2346
H -2.3964 0.3378 2.4702

Syn
Fe 1.878208 0.293283 0.140210
C 3.460173 -1.298888 -2.405747
C 2.697557 3.332493 -1.249337
C 0.297739 1.906435 2.699382
C 1.103411 -2.733691 1.570262
N 2.871916 0.905679 -1.512301
C 3.452471 0.090986 -2.441078
C 4.079285 0.883072 -3.479500
C 3.868793 2.186727 -3.153727
C 3.113258 2.186217 -1.918228

N	1.558650	2.242947	0.621875
C	1.973858	3.349002	-0.061947
C	1.548898	4.552017	0.622781
C	0.871485	4.147922	1.730910
C	0.886277	2.699131	1.719749
N	0.895783	-0.304327	1.812404
C	0.297914	0.514881	2.733948
C	-0.328970	-0.276282	3.767412
C	-0.102298	-1.584252	3.455352
C	0.661708	-1.590603	2.229589
N	2.194490	-1.636744	-0.331679
C	1.823638	-2.743357	0.380058
C	2.279845	-3.944121	-0.286928
C	2.937280	-3.538913	-1.407104
C	2.881410	-2.092438	-1.420609
H	3.971190	-1.811784	-3.216346
H	2.959092	4.291108	-1.689361
H	-0.211597	2.419648	3.510908
H	0.863144	-3.694303	2.017978
H	4.606479	0.474874	-4.333655
H	4.185208	3.077351	-3.683642
H	1.751104	5.560717	0.282488
H	0.400042	4.754497	2.495172
H	-0.867860	0.131287	4.614634
H	-0.417095	-2.471361	3.992126
H	2.111102	-4.952301	0.072530
H	3.423837	-4.144345	-2.162666
C	-1.089308	-1.147462	-0.806328
S	-0.120012	0.374174	-1.131719
H	-2.011518	-1.102594	-1.396869
H	-1.362001	-1.236836	0.250546
O	3.483792	0.422026	1.047544
O	3.817531	-0.678214	1.926803
H	3.089378	-0.642830	2.569520
H	-0.538189	-2.048027	-1.097112

3B)
Anti

Fe	1.7697	0.2403	0.3237
C	3.2717	-1.4540	-2.2274
C	2.4294	3.2117	-1.2592
C	0.3907	1.9462	2.9384
C	1.0140	-2.7321	1.8588
N	2.6644	0.7764	-1.4106
C	3.2322	-0.0663	-2.3259
C	3.7830	0.6919	-3.4290
C	3.5340	2.0038	-3.1614
C	2.8372	2.0439	-1.8948
N	1.4812	2.1999	0.7588
C	1.8035	3.2752	-0.0200
C	1.4197	4.5051	0.6407
C	0.8630	4.1497	1.8297
C	0.8992	2.7031	1.8878
N	0.8762	-0.2950	2.0555
C	0.3790	0.5551	3.0049
C	-0.1855	-0.1984	4.1026

C -0.0220 -1.5156 3.7980
C 0.6490 -1.5614 2.5171
N 2.0565 -1.7079 -0.1089
C 1.6936 -2.7894 0.6474
C 2.1275 -4.0145 0.0137
C 2.7754 -3.6523 -1.1273
C 2.7254 -2.2085 -1.1932
H 3.7600 -1.9965 -3.0326
H 2.6269 4.1517 -1.7664
H -0.0463 2.4876 3.7733
H 0.7812 -3.6747 2.3460
H 4.2848 0.2594 -4.2864
H 3.7878 2.8766 -3.7507
H 1.5694 5.4978 0.2337
H 0.4516 4.7885 2.6021
H -0.6430 0.2409 4.9809
H -0.3094 -2.3854 4.3766
H 1.9577 -5.0087 0.4093
H 3.2448 -4.2882 -1.8684
N -4.8008 1.0808 -1.6232
C -5.4559 1.4748 -2.8437
H -4.3674 0.1684 -1.5559
H -5.0465 0.8980 -3.6770
H -5.2910 2.5411 -3.0235
H -6.5415 1.3069 -2.7985
N -3.5630 0.0000 0.6023
C -4.1852 1.3058 0.7326
C -4.8707 1.8692 -0.5259
O -5.4372 2.9571 -0.5175
H -2.5777 -0.0326 0.3056
H -4.9516 1.2600 1.5109
H -3.4216 2.0258 1.0439
N -2.2520 -2.4650 -0.0242
C -3.4947 -2.4696 0.7145
C -4.2718 -1.1422 0.7990
O -5.4647 -1.1683 1.0752
H -1.3949 -2.2330 0.4639
H -4.1809 -3.1951 0.2725
H -3.2887 -2.7841 1.7434
C -0.8797 -2.2096 -2.0234
C -2.2464 -2.4079 -1.3891
O -3.2816 -2.4743 -2.0459
C -0.5069 -0.7171 -2.2287
S -0.4364 0.3562 -0.7363
H -0.1092 -2.6905 -1.4148
H -0.9129 -2.7058 -3.0014
H 0.4621 -0.6795 -2.7347
H -1.2417 -0.2657 -2.9066
O 3.3792 0.3928 1.1557
O 3.8396 -0.8061 1.8383
H 4.5972 -0.4234 2.3109

Syn
Fe 1.7702 0.2219 0.3448
C 3.2035 -1.5427 -2.2264
C 2.4601 3.1406 -1.2694

C 0.3917 2.0061 2.9509
C 1.0896 -2.6802 1.9775
N 2.6262 0.6958 -1.4191
C 3.1704 -0.1575 -2.3388
C 3.7190 0.5862 -3.4510
C 3.5048 1.9022 -3.1797
C 2.8269 1.9580 -1.9029
N 1.4768 2.1890 0.7628
C 1.8392 3.2403 -0.0303
C 1.4853 4.4920 0.6053
C 0.9047 4.1746 1.7935
C 0.9054 2.7296 1.8800
N 0.8912 -0.2400 2.1154
C 0.3919 0.6192 3.0533
C -0.1383 -0.1210 4.1776
C 0.0548 -1.4399 3.9019
C 0.7065 -1.5011 2.6102
N 2.0625 -1.7255 -0.0681
C 1.7376 -2.7745 0.7481
C 2.1621 -4.0212 0.1505
C 2.7599 -3.7040 -1.0312
C 2.6971 -2.2657 -1.1531
H 3.6733 -2.1010 -3.0313
H 2.6868 4.0691 -1.7864
H -0.0415 2.5685 3.7732
H 0.8851 -3.6110 2.4996
H 4.2012 0.1415 -4.3132
H 3.7745 2.7682 -3.7722
H 1.6639 5.4721 0.1798
H 0.5046 4.8382 2.5505
H -0.5947 0.3272 5.0518
H -0.2049 -2.3021 4.5046
H 2.0164 -4.9989 0.5937
H 3.2080 -4.3666 -1.7618
N -4.9321 0.9168 -1.7422
C -5.6250 1.1499 -2.9846
H -4.4824 0.0256 -1.5765
H -5.2320 0.4720 -3.7470
H -5.4707 2.1848 -3.3024
H -6.7070 0.9844 -2.8878
N -3.6164 0.1371 0.5566
C -4.2649 1.4357 0.5534
C -4.9939 1.8267 -0.7441
O -5.5797 2.8989 -0.8521
H -2.6237 0.0973 0.2964
H -5.0079 1.4691 1.3555
H -3.5118 2.2048 0.7482
N -2.2540 -2.3471 0.1871
C -3.4744 -2.2989 0.9608
C -4.2881 -0.9909 0.9125
O -5.4721 -1.0070 1.2189
H -1.3999 -1.9859 0.6004
H -4.1506 -3.0850 0.6188
H -3.2288 -2.4946 2.0105
C -0.9452 -2.2636 -1.8639
C -2.2920 -2.4381 -1.1775

O -3.3415 -2.6328 -1.7862
C -0.5810 -0.7803 -2.1231
S -0.4216 0.2934 -0.6369
H -0.1553 -2.7310 -1.2698
H -1.0109 -2.7871 -2.8251
H 0.3567 -0.7502 -2.6854
H -1.3543 -0.3325 -2.7576
O 3.3507 0.3481 1.2438
O 4.4841 -0.2988 0.5966
H 5.1691 -0.0805 1.2464

3C)
O -6.2174 -0.0876 -0.6977
O -1.1697 1.1219 1.5380
O -2.5140 1.0128 1.0030
Fe 0.1602 0.8300 0.3091
C 2.5774 1.1319 2.7345
C 0.3099 4.1770 -0.2666
C -1.9181 0.4328 -2.3624
C -0.0871 -2.5233 1.0017
N 1.2139 2.3547 1.1118
C 2.1848 2.2925 2.0798
C 2.7521 3.6117 2.3347
C 2.0687 4.4599 1.5112
C 1.1239 3.6703 0.7477
C 3.8824 3.9211 3.2859
N -0.6877 2.0736 -1.0187
C -0.5029 3.4268 -1.1124
C -1.2132 3.9520 -2.2774
C -1.7819 2.8717 -2.8795
C -1.4640 1.7139 -2.0815
C -1.3208 5.3798 -2.7155
N -0.8258 -0.7318 -0.5057
C -1.6438 -0.6968 -1.6049
C -2.2077 -1.9983 -1.8490
C -1.7449 -2.8308 -0.8774
C -0.8521 -2.0284 -0.0518
C -2.1114 -4.2649 -0.6651
N 1.0599 -0.4479 1.6248
C 0.8337 -1.7954 1.7550
C 1.7201 -2.3667 2.7675
C 2.4674 -1.3209 3.2286
C 2.0444 -0.1364 2.5217
C 1.8109 -3.8045 3.2031
H 3.3598 1.2167 3.4836
H 0.3641 5.2472 -0.4470
H -2.5599 0.3087 -3.2297
H -0.1770 -3.5837 1.2197
H 2.2050 5.5305 1.4036
H 4.1065 4.9933 3.2833
H 4.8013 3.3871 3.0092
H -2.3806 2.8564 -3.7832
H -1.8972 5.4534 -3.6436
H -0.3377 5.8349 -2.8967
H -2.9069 -2.2309 -2.6436
H -2.6203 -4.4146 0.2973

H -1.2338 -4.9245 -0.6718
H 3.2379 -1.3451 3.9915
H 2.5758 -3.9228 3.9779
H 2.0718 -4.4702 2.3696
H 0.8601 -4.1702 3.6150
H -1.8239 6.0014 -1.9609
H 3.6413 3.6332 4.3182
H -2.7881 -4.6081 -1.4548
N 2.2023 -2.8350 -1.9144
C 1.1452 -3.1390 -2.8621
H 2.2000 -1.8875 -1.5236
H 0.7342 -4.1369 -2.6707
H 1.5197 -3.1296 -3.8937
N 4.4504 -1.8621 -0.4167
C 4.4849 -3.1769 -1.0244
C 3.3595 -3.5265 -2.0110
O 3.5134 -4.4668 -2.7867
H 3.9078 -1.7319 0.4277
H 5.4187 -3.2882 -1.5796
H 4.4755 -3.9302 -0.2279
C 4.4707 0.5849 -0.5283
C 4.6825 -0.7606 -1.2046
O 5.0376 -0.8731 -2.3732
C 3.3599 1.3667 -1.2437
S 1.7856 0.4308 -1.3977
H 4.2246 0.4615 0.5314
H 5.4180 1.1410 -0.5918
C -4.6759 3.2039 -0.8325
O -4.8563 2.2706 0.2227
H -5.6400 3.3187 -1.3440
H -3.9630 1.9491 0.4855
N -5.2864 -2.9109 1.7863
C -6.0194 -3.3453 0.6107
H -5.6332 -3.1607 2.6997
H -6.7145 -4.1362 0.9004
H -5.3276 -3.7385 -0.1390
H -6.5716 -2.5093 0.1666
C -3.7667 -1.4382 2.9854
C -4.3731 -1.9091 1.6945
O -4.0388 -1.4326 0.6078
H -4.1728 -1.9353 3.8725
H -3.9108 -0.3571 3.0703
H -2.6833 -1.6003 2.9512
H -5.4268 -0.6469 -0.6247
H -5.8863 0.7635 -0.3389
H -2.6299 0.0582 0.8303
H -3.9291 2.8811 -1.5618
H -4.3725 4.1912 -0.4514
H 3.1873 2.3187 -0.7330
H 3.6898 1.5831 -2.2643
H 0.3564 -2.3975 -2.7546

3 Imz)
Fe 1.8203 0.2195 0.5303
C 3.6097 -1.8715 -1.4774
C 2.8460 2.9063 -1.3556

C 0.0177 2.3287 2.5301
C 0.7132 -2.4643 2.3547
N 2.9750 0.4699 -1.1078
C 3.6653 -0.5138 -1.7689
C 4.4532 0.0596 -2.8363
C 4.2357 1.4030 -2.8065
C 3.3165 1.6502 -1.7194
N 1.4752 2.2137 0.5566
C 1.9911 3.1608 -0.2898
C 1.5374 4.4784 0.0937
C 0.7469 4.3152 1.1886
C 0.7176 2.8978 1.4723
N 0.6027 -0.0235 2.1232
C -0.0279 0.9713 2.8332
C -0.7670 0.4028 3.9344
C -0.5751 -0.9468 3.8844
C 0.2824 -1.2043 2.7536
N 2.0742 -1.7703 0.4349
C 1.5560 -2.7172 1.2796
C 2.0219 -4.0330 0.9043
C 2.8390 -3.8652 -0.1697
C 2.8684 -2.4475 -0.4520
H 4.2048 -2.5373 -2.0954
H 3.1902 3.7575 -1.9355
H -0.5362 3.0008 3.1791
H 0.3814 -3.3158 2.9416
H 5.0879 -0.5063 -3.5066
H 4.6541 2.1694 -3.4469
H 1.8052 5.3955 -0.4158
H 0.2293 5.0707 1.7667
H -1.3478 0.9740 4.6480
H -0.9665 -1.7078 4.5481
H 1.7564 -4.9504 1.4146
H 3.3852 -4.6160 -0.7270
O 3.2743 0.4800 1.5311
H -2.9294 -0.5472 -1.3726
H -1.4150 -0.4512 0.6724
C -1.1045 -0.2848 -0.3464
H 0.9576 0.3733 -2.6817
N 0.1246 0.0043 -0.7382
H -1.6458 -0.0634 -3.5333
C 0.0738 0.1375 -2.1119
C -1.2046 -0.0762 -2.5491
N -1.9418 -0.3442 -1.4118
O 3.4199 -0.4363 2.6337
H 2.9221 0.0345 3.3263
3 Fluoride)
Fe 1.8681 0.3509 0.6524
C 3.6700 -1.7848 -1.3391
C 2.8450 2.9810 -1.2647
C -0.0990 2.4448 2.5329
C 0.8725 -2.2926 2.5779
N 3.0369 0.5549 -0.9740
C 3.7009 -0.4287 -1.6492
C 4.4472 0.1361 -2.7551
C 4.2220 1.4774 -2.7285

C 3.3347 1.7253 -1.6103
N 1.4459 2.3258 0.6375
C 1.9610 3.2510 -0.2249
C 1.4410 4.5682 0.0823
C 0.6038 4.4167 1.1441
C 0.6195 3.0081 1.4833
N 0.6335 0.1270 2.2499
C -0.0829 1.0996 2.8864
C -0.8282 0.5344 3.9929
C -0.5450 -0.7963 4.0098
C 0.3692 -1.0386 2.9115
N 2.2378 -1.6477 0.6430
C 1.7194 -2.5737 1.5093
C 2.1588 -3.9011 1.1412
C 2.9370 -3.7631 0.0305
C 2.9754 -2.3507 -0.2746
H 4.2346 -2.4567 -1.9806
H 3.1708 3.8234 -1.8698
H -0.7180 3.1108 3.1287
H 0.5546 -3.1324 3.1907
H 5.0559 -0.4351 -3.4462
H 4.6054 2.2414 -3.3947
H 1.6935 5.4738 -0.4569
H 0.0244 5.1716 1.6628
H -1.4760 1.0974 4.6546
H -0.9124 -1.5577 4.6881
H 1.8910 -4.8093 1.6686
H 3.4418 -4.5336 -0.5406
F 0.4553 0.0629 -0.4323
O 3.2329 0.7077 1.8140
O 4.4890 0.0143 1.5416
H 4.1764 -0.9074 1.5226

4 A)
Fe 0.2931 0.0834 0.2815
C 2.0347 -2.0344 -1.7704
C 1.2324 2.7370 -1.6689
C -1.6667 2.1711 2.1613
C -0.9358 -2.6085 2.0070
N 1.3652 0.2995 -1.4145
C 2.0649 -0.6804 -2.0747
C 2.8363 -0.1057 -3.1499
C 2.6041 1.2352 -3.1259
C 1.6939 1.4797 -2.0341
N -0.1577 2.0502 0.2308
C 0.3784 2.9955 -0.6065
C -0.0790 4.3123 -0.2336
C -0.8928 4.1534 0.8450
C -0.9334 2.7398 1.1295
N -1.0634 -0.1728 1.7544
C -1.7204 0.8144 2.4477
C -2.4887 0.2422 3.5258
C -2.2835 -1.1022 3.4823
C -1.3890 -1.3507 2.3779
N 0.4646 -1.9208 0.1118
C -0.0661 -2.8652 0.9559

C 0.4139 -4.1784 0.6024
C 1.2562 -4.0168 -0.4547
C 1.2875 -2.6049 -0.7491
H 2.6436 -2.6979 -2.3767
H 1.5782 3.5853 -2.2513
H -2.2403 2.8397 2.7956
H -1.2770 -3.4565 2.5925
H 3.4696 -0.6701 -3.8227
H 3.0066 2.0025 -3.7748
H 0.1976 5.2265 -0.7432
H -1.4260 4.9095 1.4070
H -3.0998 0.8112 4.2147
H -2.6903 -1.8692 4.1290
H 0.1364 -5.0924 1.1119
H 1.8145 -4.7706 -0.9952
C -1.6397 -1.3398 -2.6537
S -2.0015 -0.1231 -1.3675
H -2.5049 -1.5273 -3.2919
H -1.3037 -2.2676 -2.1778
O 1.5494 0.2489 1.2677
H -0.8000 -0.9689 -3.2536

4B)

Fe	1.942222	0.236574	0.647847
C	2.517650	-3.114596	0.220744
C	4.143529	0.933401	-1.865303
C	1.120101	3.545976	0.852568
C	-0.469357	-0.492992	2.980130
N	3.064161	-0.869806	-0.606014
C	3.225838	-2.232450	-0.585909
C	4.231527	-2.634289	-1.539027
C	4.684423	-1.496388	-2.131837
C	3.957275	-0.402240	-1.536883
N	2.511970	1.899754	-0.313834
C	3.464576	2.000679	-1.293750
C	3.655719	3.380080	-1.672408
C	2.801683	4.114380	-0.910744
C	2.094475	3.181046	-0.067230
N	0.582955	1.307405	1.688497
C	0.424390	2.669557	1.673523
C	-0.569687	3.073124	2.637867
C	-1.004626	1.937164	3.247887
C	-0.281832	0.841604	2.647603
N	1.123016	-1.468751	1.387790
C	0.178722	-1.565369	2.384563
C	-0.038203	-2.947368	2.733399
C	0.805555	-3.687075	1.958013
C	1.536782	-2.756989	1.135006
H	2.753667	-4.170490	0.130203
H	4.879733	1.161854	-2.629602
H	0.886279	4.602304	0.939404
H	-1.186833	-0.715410	3.763856
H	4.537336	-3.657189	-1.717232
H	5.440568	-1.388541	-2.898700
H	4.351544	3.720403	-2.428288
H	2.646702	5.185461	-0.907950
H	-0.881176	4.095013	2.810632

H	-1.746110	1.831231	4.029256
H	-0.727796	-3.289942	3.494687
H	0.943004	-4.760829	1.946256
N	-3.955786	1.480086	-1.862408
C	-4.147545	2.127053	-3.137607
H	-3.792331	0.482935	-1.835957
H	-3.629628	1.555397	-3.911912
H	-3.738045	3.139292	-3.097707
H	-5.210412	2.201975	-3.402404
N	-3.667347	-0.059974	0.427326
C	-4.069253	1.330765	0.579238
C	-4.224787	2.147630	-0.716434
O	-4.554730	3.325826	-0.686948
H	-2.680756	-0.275497	0.326598
H	-5.036073	1.354863	1.088335
H	-3.339212	1.846884	1.209785
N	-2.677721	-2.665346	-0.225078
C	-4.071692	-2.490076	0.132789
C	-4.591149	-1.043304	0.223246
O	-5.788481	-0.835489	0.160167
H	-1.993649	-2.859237	0.494303
H	-4.701224	-2.989343	-0.606856
H	-4.248168	-2.966423	1.102632
C	-0.775532	-2.727080	-1.764070
C	-2.268113	-2.532516	-1.521934
O	-3.048336	-2.259501	-2.423797
C	-0.082539	-1.414308	-2.170975
S	-0.202728	-0.072686	-0.936048
H	-0.279057	-3.157390	-0.889642
H	-0.672975	-3.439241	-2.592062
H	0.966716	-1.597530	-2.414802
H	-0.574305	-1.016154	-3.067752
O	3.069266	0.304361	1.796691

4C)

O	-5.1718	-0.7369	-1.8649
O	-1.0688	1.0656	1.5863
O	-3.7729	1.5306	1.8722
Fe	0.0483	0.8556	0.4289
C	2.6055	1.2481	2.6726
C	0.2508	4.1718	-0.3799
C	-2.1484	0.3685	-2.1337
C	0.0737	-2.5311	1.0251
N	1.2048	2.3951	1.0233
C	2.1820	2.3831	1.9950
C	2.7277	3.7143	2.2023
C	2.0393	4.5238	1.3440
C	1.1003	3.7046	0.6204
C	3.8412	4.0803	3.1529
N	-0.8100	2.0445	-0.9456
C	-0.6162	3.3936	-1.1350
C	-1.3921	3.8689	-2.2749
C	-2.0283	2.7713	-2.7646
C	-1.6727	1.6546	-1.9346
C	-1.4861	5.2713	-2.7986
N	-0.8315	-0.7517	-0.3948
C	-1.7577	-0.7436	-1.4047

C -2.2757 -2.0611 -1.6378
C -1.6830 -2.8953 -0.7433
C -0.7724 -2.0632 0.0307
C -1.9449 -4.3564 -0.5745
N 1.1611 -0.4066 1.5715
C 0.9887 -1.7627 1.7395
C 1.8967 -2.2815 2.7535
C 2.6040 -1.1976 3.1927
C 2.1347 -0.0433 2.4734
C 2.0129 -3.7065 3.2298
H 3.3785 1.3763 3.4242
H 0.3019 5.2316 -0.6104
H -2.9088 0.2137 -2.8904
H 0.0325 -3.5918 1.2513
H 2.1630 5.5901 1.1977
H 4.0456 5.1548 3.1019
H 4.7707 3.5525 2.9042
H -2.6951 2.7138 -3.6155
H -2.1402 5.2977 -3.6794
H -0.5062 5.6597 -3.1061
H -3.0398 -2.2873 -2.3690
H -2.3720 -4.5854 0.4085
H -1.0222 -4.9553 -0.6710
H 3.3718 -1.1756 3.9570
H 2.8085 -3.7916 3.9797
H 2.2560 -4.3937 2.4080
H 1.0842 -4.0607 3.6860
H -1.8942 5.9599 -2.0570
H 3.5896 3.8347 4.1885
H -2.6431 -4.7102 -1.3362
N 2.2963 -2.8506 -1.8738
C 1.2448 -3.1676 -2.8358
H 2.2842 -1.9168 -1.4725
H 0.9147 -4.2036 -2.6997
H 1.6116 -3.0738 -3.8671
N 4.5608 -1.7637 -0.4643
C 4.6261 -3.0934 -1.0396
C 3.4880 -3.4932 -1.9935
O 3.6543 -4.4191 -2.7712
H 4.1591 -1.6390 0.4544
H 5.5479 -3.1936 -1.6160
H 4.6579 -3.8249 -0.2251
C 4.5435 0.6840 -0.5976
C 4.7651 -0.6697 -1.2600
O 5.0702 -0.7728 -2.4399
C 3.4287 1.4370 -1.3356
S 1.8648 0.4948 -1.4499
H 4.3009 0.5832 0.4651
H 5.4767 1.2571 -0.6762
C -4.7453 3.0247 -0.8322
O -5.2484 1.7508 -0.4690
H -5.3269 3.8378 -0.3813
H -4.8480 1.5302 0.4021
N -5.1379 -3.0165 1.8740
C -5.8623 -3.5371 0.7404
H -5.2130 -3.4884 2.7623

H -6.8350 -3.9182 1.0564
H -5.3126 -4.3597 0.2462
H -6.0068 -2.7421 0.0102
C -3.6389 -1.5199 3.0506
C -4.3228 -1.9350 1.7773
O -4.1445 -1.3201 0.7252
H -3.8898 -2.1445 3.9127
H -3.8924 -0.4789 3.2520
H -2.5520 -1.5519 2.8910
H -4.7846 -1.1307 -1.0615
H -5.3112 0.1833 -1.5567
H -2.9208 1.1221 1.5999
H -4.8217 3.1198 -1.9239
H -3.6937 3.1491 -0.5514
H 3.2494 2.4205 -0.8939
H 3.7330 1.5828 -2.3784
H 0.4081 -2.4962 -2.6806
H -3.4996 2.3932 2.2193

4 Imz)
Fe 1.7627 0.2602 0.5769
C 3.6300 -1.8391 -1.3728
C 2.8152 2.9257 -1.2929
C -0.0927 2.3629 2.5242
C 0.6383 -2.4171 2.3769
N 2.9883 0.4984 -1.0178
C 3.6686 -0.4812 -1.6912
C 4.4426 0.0842 -2.7688
C 4.2074 1.4262 -2.7519
C 3.2969 1.6685 -1.6598
N 1.4556 2.2599 0.6302
C 1.9501 3.1984 -0.2335
C 1.4669 4.5142 0.1099
C 0.6495 4.3565 1.1871
C 0.6380 2.9450 1.4887
N 0.5325 0.0211 2.1629
C -0.1462 1.0023 2.8357
C -0.9309 0.4350 3.9033
C -0.7320 -0.9137 3.8573
C 0.1773 -1.1570 2.7654
N 2.0703 -1.7390 0.5093
C 1.5210 -2.6866 1.3315
C 2.0129 -4.0009 0.9943
C 2.8679 -3.8364 -0.0522
C 2.8842 -2.4242 -0.3494
H 4.2355 -2.5040 -1.9816
H 3.1422 3.7712 -1.8910
H -0.6851 3.0307 3.1427
H 0.2842 -3.2676 2.9522
H 5.0824 -0.4792 -3.4352
H 4.6147 2.1896 -3.4018
H 1.7325 5.4268 -0.4071
H 0.1061 5.1132 1.7372
H -1.5430 1.0018 4.5925
H -1.1467 -1.6776 4.5020
H 1.7426 -4.9148 1.5068

H 3.4411 -4.5878 -0.5791
O 3.0365 0.4224 1.5728
H -2.9289 -0.5828 -1.4702
H -1.5205 -0.4080 0.6290
C -1.1577 -0.2606 -0.3753
H 0.9822 0.3772 -2.6534
N 0.0869 0.0448 -0.7195
H -1.5680 -0.1222 -3.5842
C 0.0884 0.1374 -2.1019
C -1.1677 -0.1059 -2.5827
N -1.9434 -0.3600 -1.4714
4 Fluoride)
Fe -0.0040 0.0062 -0.0888
C 3.3926 0.3502 -0.0132
C 0.3484 -3.3912 0.0198
C -3.3959 -0.3491 -0.0139
C -0.3509 3.3955 0.0164
N 1.5721 -1.2769 -0.0126
C 2.8967 -0.9524 -0.0117
C 3.7151 -2.1446 0.0082
C 2.8560 -3.1994 0.0213
C 1.5225 -2.6398 0.0077
N -1.2810 -1.5698 -0.0117
C -0.9542 -2.8938 0.0127
C -2.1453 -3.7136 0.0315
C -3.2019 -2.8566 0.0169
C -2.6444 -1.5228 -0.0086
N -1.5717 1.2785 -0.0153
C -2.8969 0.9530 -0.0108
C -3.7153 2.1441 0.0137
C -2.8570 3.2000 0.0264
C -1.5238 2.6422 0.0079
N 1.2753 1.5731 -0.0149
C 0.9514 2.8982 0.0086
C 2.1433 3.7156 0.0296
C 3.1982 2.8561 0.0184
C 2.6388 1.5233 -0.0080
H 4.4733 0.4632 -0.0080
H 0.4590 -4.4719 0.0395
H -4.4768 -0.4589 -0.0091
H -0.4628 4.4760 0.0363
H 4.7974 -2.1543 0.0154
H 3.0847 -4.2572 0.0409
H -2.1531 -4.7957 0.0549
H -4.2594 -3.0870 0.0267
H -4.7975 2.1527 0.0243
H -3.0865 4.2575 0.0491
H 2.1533 4.7977 0.0527
H 4.2561 3.0843 0.0311
F 0.0075 -0.0154 1.7312
O 0.0058 -0.0171 -1.7339

5A)
Anti
Fe 1.5589 0.2396 0.4035
C 3.6516 -1.8299 -1.3583

C 2.6990 2.9093 -1.3775
C -0.0206 2.3896 2.5812
C 0.5524 -2.4005 2.3074
N 2.9000 0.4845 -1.0452
C 3.6428 -0.4721 -1.6813
C 4.4181 0.1037 -2.7693
C 4.1264 1.4229 -2.7949
C 3.1839 1.6643 -1.7118
N 1.4005 2.2277 0.5879
C 1.8825 3.1672 -0.2739
C 1.4657 4.5074 0.1206
C 0.7223 4.3671 1.2387
C 0.6731 2.9413 1.5276
N 0.5245 0.0425 2.1079
C -0.0919 1.0195 2.8411
C -0.8667 0.4490 3.9327
C -0.7284 -0.8911 3.8413
C 0.1438 -1.1440 2.7003
N 2.0173 -1.6966 0.4631
C 1.4588 -2.6473 1.2755
C 1.9745 -3.9709 0.9617
C 2.8631 -3.8116 -0.0438
C 2.8842 -2.3901 -0.3596
H 4.2918 -2.4842 -1.9400
H 3.0047 3.7539 -1.9852
H -0.5595 3.0576 3.2442
H 0.1806 -3.2538 2.8641
H 5.0885 -0.4553 -3.4086
H 4.5056 2.1882 -3.4592
H 1.7311 5.4131 -0.4087
H 0.2384 5.1305 1.8333
H -1.4318 1.0265 4.6522
H -1.1522 -1.6617 4.4718
H 1.6836 -4.8796 1.4719
H 3.4630 -4.5603 -0.5444
C 0.1350 -1.0796 -2.2308
S -0.1993 0.0881 -0.8690
H -0.7765 -1.0965 -2.8364
H 0.3280 -2.0902 -1.8636
H 0.9639 -0.7473 -2.8604

Syn
Fe -0.0493 0.0013 -0.2157
C 3.3513 -0.2906 -0.4112
C -0.3536 -3.4011 -0.2242
C -3.4799 0.2970 -0.1118
C 0.2317 3.4012 -0.0696
N 1.2431 -1.5334 -0.2638
C 2.6073 -1.4611 -0.3786
C 3.1684 -2.7876 -0.4505
C 2.1262 -3.6602 -0.3824
C 0.9256 -2.8695 -0.2767
N -1.6080 -1.2903 -0.1913
C -1.5259 -2.6603 -0.1859
C -2.8470 -3.2331 -0.1490
C -3.7270 -2.1941 -0.1285

C -2.9451 -0.9839 -0.1470
N -1.3656 1.5413 -0.1225
C -2.7343 1.4670 -0.0916
C -3.2993 2.7925 -0.0193
C -2.2550 3.6644 0.0033
C -1.0508 2.8736 -0.0612
N 1.4815 1.2864 -0.1993
C 1.3993 2.6577 -0.1507
C 2.7177 3.2326 -0.2252
C 3.5948 2.1971 -0.3378
C 2.8153 0.9856 -0.3238
H 4.4285 -0.3796 -0.5066
H -0.4461 -4.4823 -0.2293
H -4.5606 0.3889 -0.0794
H 0.3293 4.4812 -0.0270
H 4.2254 -3.0025 -0.5426
H 2.1473 -4.7421 -0.4088
H -3.0551 -4.2952 -0.1409
H -4.8086 -2.2249 -0.0976
H -4.3599 3.0061 0.0147
H -2.2772 4.7452 0.0572
H 2.9252 4.2947 -0.2030
H 4.6732 2.2313 -0.4251
C 1.5668 -0.0761 2.7428
S -0.1420 -0.0809 2.0973
H 1.4829 -0.1426 3.8322
H 2.0928 0.8463 2.4854
O -0.1292 0.0497 -2.0232
H -1.0331 0.0187 -2.3705
H 2.1367 -0.9357 2.3818
5 A)
Anti
Fe 1.7516 0.2580 0.5342
C 3.6505 -1.9360 -1.2665
C 2.8239 2.8332 -1.4250
C 0.0395 2.4709 2.5151
C 0.4687 -2.3534 2.3693
N 2.9531 0.4093 -1.0559
C 3.6865 -0.5983 -1.6336
C 4.4871 -0.0698 -2.7093
C 4.2302 1.2654 -2.7728
C 3.2833 1.5596 -1.7271
N 1.4798 2.2496 0.5412
C 2.0027 3.1470 -0.3537
C 1.6017 4.4874 -0.0015
C 0.8414 4.3878 1.1213
C 0.7665 2.9851 1.4514
N 0.5057 0.0909 2.1251
C -0.0889 1.1210 2.8110
C -0.9067 0.5969 3.8761
C -0.8080 -0.7598 3.8201
C 0.0791 -1.0687 2.7265
N 1.9857 -1.7463 0.5306
C 1.3819 -2.6568 1.3650
C 1.8656 -3.9831 1.0770
C 2.7802 -3.8613 0.0736

C 2.8492 -2.4633 -0.2633
H 4.2841 -2.6246 -1.8157
H 3.1677 3.6509 -2.0500
H -0.4888 3.1753 3.1490
H 0.0761 -3.1782 2.9559
H 5.1511 -0.6603 -3.3273
H 4.6429 2.0010 -3.4510
H 1.8791 5.3759 -0.5535
H 0.3576 5.1765 1.6827
H -1.4797 1.2043 4.5646
H -1.2787 -1.4978 4.4569
H 1.5463 -4.8792 1.5936
H 3.3615 -4.6378 -0.4066
N -4.1158 1.2858 -1.8429
C -4.4435 1.9111 -3.1012
H -3.8292 0.3167 -1.8329
H -3.9110 1.3980 -3.9060
H -4.1414 2.9611 -3.0769
H -5.5211 1.8738 -3.3079
N -3.5264 -0.2144 0.4134
C -4.0821 1.1169 0.5998
C -4.4006 1.9133 -0.6790
O -4.8674 3.0432 -0.6218
H -2.5219 -0.3092 0.2956
H -5.0160 1.0273 1.1606
H -3.3835 1.7134 1.1939
N -2.2631 -2.6781 -0.3126
C -3.6469 -2.6738 0.1178
C -4.3337 -1.3015 0.2501
O -5.5495 -1.2394 0.2447
H -1.5234 -2.7318 0.3752
H -4.2474 -3.2426 -0.5950
H -3.7145 -3.1730 1.0899
C -0.4437 -2.4528 -1.9333
C -1.9373 -2.4749 -1.6250
O -2.7921 -2.3142 -2.4856
C 0.0637 -1.0251 -2.2046
S -0.1243 0.1521 -0.8052
H 0.1357 -2.9179 -1.1317
H -0.2969 -3.0460 -2.8437
H 1.1088 -1.0501 -2.5212
H -0.5201 -0.5872 -3.0210
O 3.1468 0.4166 1.6462
H 3.1130 -0.2098 2.3861
Syn
Fe 1.7471 0.2483 0.5586
C 3.6492 -1.9073 -1.2989
C 2.8474 2.8674 -1.3512
C -0.0771 2.4176 2.4815
C 0.5230 -2.3864 2.3749
N 2.9580 0.4320 -1.0341
C 3.6815 -0.5634 -1.6409
C 4.4850 -0.0146 -2.7047
C 4.2436 1.3243 -2.7298
C 3.3000 1.5983 -1.6760
N 1.4740 2.2469 0.5830

C 1.9991 3.1611 -0.2950
C 1.5423 4.4854 0.0404
C 0.7290 4.3601 1.1246
C 0.6820 2.9570 1.4512
N 0.4749 0.0513 2.1175
C -0.1730 1.0649 2.7797
C -0.9875 0.5196 3.8373
C -0.8273 -0.8319 3.8018
C 0.0895 -1.1153 2.7262
N 2.0005 -1.7419 0.5139
C 1.4328 -2.6632 1.3631
C 1.9341 -3.9810 1.0679
C 2.8256 -3.8445 0.0471
C 2.8640 -2.4450 -0.2905
H 4.2814 -2.5863 -1.8615
H 3.1963 3.6951 -1.9597
H -0.6532 3.1064 3.0906
H 0.1587 -3.2223 2.9638
H 5.1436 -0.5951 -3.3376
H 4.6637 2.0750 -3.3864
H 1.8156 5.3833 -0.4984
H 0.1922 5.1327 1.6595
H -1.5975 1.1097 4.5088
H -1.2761 -1.5815 4.4407
H 1.6417 -4.8812 1.5931
H 3.4136 -4.6101 -0.4423
N -4.1086 1.2709 -1.8403
C -4.4434 1.9041 -3.0926
H -3.8143 0.3040 -1.8390
H -3.9110 1.3997 -3.9030
H -4.1465 2.9553 -3.0614
H -5.5215 1.8628 -3.2962
N -3.4955 -0.2399 0.4019
C -4.0603 1.0856 0.6004
C -4.3910 1.8886 -0.6710
O -4.8636 3.0156 -0.6034
H -2.4909 -0.3250 0.2741
H -4.9906 0.9852 1.1654
H -3.3630 1.6834 1.1947
N -2.2182 -2.6885 -0.3464
C -3.6001 -2.6976 0.0889
C -4.2959 -1.3312 0.2330
O -5.5123 -1.2776 0.2359
H -1.4757 -2.7261 0.3394
H -4.1986 -3.2656 -0.6261
H -3.6611 -3.2045 1.0576
C -0.4088 -2.4136 -1.9716
C -1.8999 -2.4720 -1.6584
O -2.7601 -2.3141 -2.5144
C 0.0671 -0.9726 -2.2276
S -0.1415 0.1910 -0.8189
H 0.1847 -2.8764 -1.1787
H -0.2557 -2.9927 -2.8904
H 1.1116 -0.9722 -2.5474
H -0.5266 -0.5389 -3.0392
O 3.1291 0.4245 1.7006

H 2.9932 1.1035 2.3788

5C)
O -5.2903 -0.7676 -1.8324
O -1.0281 1.1320 1.5961
O -3.6606 1.6777 1.8953
Fe 0.2338 0.8319 0.3006
C 2.6926 1.1632 2.6573
C 0.4319 4.1693 -0.4090
C -2.1641 0.4552 -2.0975
C 0.0264 -2.5412 1.0090
N 1.3632 2.3456 0.9620
C 2.3163 2.3006 1.9591
C 2.8754 3.6205 2.1852
C 2.2181 4.4513 1.3216
C 1.2783 3.6616 0.5719
C 3.9595 3.9647 3.1697
N -0.7282 2.0813 -0.9400
C -0.4864 3.4242 -1.1311
C -1.3047 3.9327 -2.2244
C -2.0109 2.8632 -2.6830
C -1.6515 1.7222 -1.8904
C -1.3744 5.3391 -2.7361
N -0.8030 -0.7339 -0.4310
C -1.7650 -0.6762 -1.4092
C -2.3415 -1.9719 -1.6223
C -1.7568 -2.8334 -0.7463
C -0.7906 -2.0436 0.0046
C -2.0817 -4.2864 -0.5684
N 1.1479 -0.4355 1.6016
C 0.9439 -1.7955 1.7407
C 1.8394 -2.3390 2.7475
C 2.5841 -1.2788 3.1900
C 2.1543 -0.1062 2.4803
C 1.9188 -3.7695 3.2115
H 3.4707 1.2681 3.4064
H 0.5122 5.2284 -0.6313
H -2.9615 0.3350 -2.8208
H -0.0441 -3.6011 1.2287
H 2.3557 5.5188 1.1976
H 4.1912 5.0330 3.1273
H 4.8851 3.4135 2.9614
H -2.7292 2.8394 -3.4927
H -2.0713 5.4030 -3.5767
H -0.3977 5.6994 -3.0836
H -3.1475 -2.1603 -2.3186
H -2.4969 -4.4897 0.4276
H -1.1979 -4.9258 -0.6887
H 3.3588 -1.2878 3.9477
H 2.7084 -3.8848 3.9597
H 2.1358 -4.4559 2.3837
H 0.9764 -4.1005 3.6660
H -1.7186 6.0380 -1.9625
H 3.6644 3.7273 4.1995
H -2.8230 -4.5991 -1.3093
N 2.1772 -2.9052 -1.8787

C 1.1236 -3.1710 -2.8451
H 2.1720 -1.9971 -1.4271
H 0.6937 -4.1653 -2.6821
H 1.5129 -3.1426 -3.8689
N 4.4392 -1.8538 -0.4917
C 4.4979 -3.1887 -1.0589
C 3.3520 -3.5700 -2.0117
O 3.4982 -4.4885 -2.8054
H 4.0231 -1.7187 0.4194
H 5.4188 -3.2969 -1.6350
H 4.5229 -3.9163 -0.2409
C 4.4135 0.5934 -0.6518
C 4.6652 -0.7670 -1.2934
O 5.0159 -0.8845 -2.4617
C 3.2709 1.3193 -1.3756
S 1.6930 0.3712 -1.4019
H 4.1972 0.5085 0.4173
H 5.3292 1.1882 -0.7649
C -4.6803 3.1701 -0.7604
O -4.8425 1.7777 -0.6087
H -5.4097 3.7427 -0.1615
H -4.5195 1.5495 0.2933
N -5.2597 -2.8462 1.9268
C -5.9659 -3.3685 0.7795
H -5.3533 -3.3145 2.8153
H -6.9314 -3.7752 1.0946
H -5.4007 -4.1628 0.2731
H -6.1389 -2.5624 0.0633
C -3.6719 -1.4278 3.0862
C -4.3854 -1.8134 1.8191
O -4.1697 -1.2281 0.7587
H -4.0514 -1.9336 3.9802
H -3.7570 -0.3434 3.2064
H -2.6071 -1.6631 2.9740
H -4.8739 -1.0937 -1.0136
H -5.3499 0.1868 -1.6310
H -2.7385 1.3989 1.6580
H -4.8472 3.4204 -1.8128
H -3.6716 3.5068 -0.4866
H 3.1064 2.3127 -0.9559
H 3.5328 1.4287 -2.4324
H 0.3417 -2.4204 -2.7310
H -3.5521 2.5938 2.1928
H -0.8119 0.5728 2.3608

5 Imz)
Fe 1.7021 0.2450 0.5527
C 3.6942 -1.7951 -1.3690
C 2.6892 2.9350 -1.2795
C -0.0791 2.3113 2.6289
C 0.6098 -2.4580 2.2976
N 2.9285 0.5068 -1.0323
C 3.6848 -0.4290 -1.6824
C 4.4557 0.1751 -2.7399
C 4.1530 1.5037 -2.7265
C 3.2086 1.6997 -1.6545

N 1.3265 2.2289 0.6288
C 1.8332 3.1859 -0.2011
C 1.4101 4.5038 0.2125
C 0.6507 4.3336 1.3289
C 0.6070 2.9126 1.5807
N 0.4543 -0.0202 2.1174
C -0.1547 0.9335 2.8770
C -0.8986 0.3351 3.9608
C -0.7258 -1.0103 3.8497
C 0.1319 -1.2212 2.7069
N 2.0682 -1.7389 0.4603
C 1.5263 -2.6994 1.2621
C 2.0487 -4.0024 0.9310
C 2.9353 -3.8182 -0.0873
C 2.9379 -2.4058 -0.3755
H 4.3454 -2.4324 -1.9601
H 3.0108 3.7963 -1.8578
H -0.6055 2.9656 3.3177
H 0.2724 -3.3247 2.8586
H 5.1335 -0.3551 -3.3960
H 4.5350 2.2872 -3.3675
H 1.6801 5.4265 -0.2841
H 0.1651 5.0868 1.9353
H -1.4664 0.8829 4.7014
H -1.1194 -1.7945 4.4828
H 1.7748 -4.9249 1.4258
H 3.5343 -4.5582 -0.6015
O 3.0539 0.4813 1.6926
H -2.8425 0.4846 -1.7993
H -1.3999 1.2418 0.1481
C -1.0884 0.5692 -0.6352
H 0.9135 -1.3515 -2.2136
N 0.1052 0.0016 -0.7445
H -1.5922 -1.1117 -3.3567
C 0.0630 -0.7749 -1.8886
C -1.1701 -0.6690 -2.4682
N -1.8863 0.1887 -1.6572
H 3.8285 -0.0298 1.4013

5 Fluoride)
Fe 0.0019 0.0016 -0.2861
N 1.3966 -1.4587 -0.2358
N 1.4507 1.3862 -0.2705
N -1.3937 1.4613 -0.2437
N -1.4538 -1.3896 -0.3002
C 1.1705 -2.8110 -0.2532
C 2.4264 -3.5221 -0.2511
C 3.4096 -2.5823 -0.2484
C 2.7565 -1.2955 -0.2491
C 3.4228 -0.0799 -0.2696
C 2.8050 1.1611 -0.2861
C 3.5133 2.4160 -0.3075
C 2.5731 3.3998 -0.3102
C 1.2873 2.7492 -0.2905
C 0.0756 3.4227 -0.2791
C -1.1690 2.8123 -0.2602

C -2.4249 3.5231 -0.2649
C -3.4083 2.5835 -0.2676
C -2.7549 1.2966 -0.2644
C -3.4232 0.0817 -0.2875
C -2.8106 -1.1632 -0.3033
C -3.5160 -2.4179 -0.3106
C -2.5746 -3.4030 -0.3079
C -1.2892 -2.7552 -0.2990
C -0.0734 -3.4236 -0.2780
H 2.5208 -4.6004 -0.2530
H 4.4826 -2.7255 -0.2479
H 4.5077 -0.1006 -0.2802
H 4.5916 2.5108 -0.3144
H 2.7168 4.4727 -0.3198
H 0.1041 4.5074 -0.2927
H -2.5192 4.6014 -0.2677
H -4.4812 2.7266 -0.2729
H -4.5081 0.1055 -0.2962
H -4.5941 -2.5147 -0.3083
H -2.7202 -4.4757 -0.3030
H -0.0988 -4.5085 -0.2836
F -0.0228 -0.0174 1.4507
O 0.0152 0.0095 -2.0576
H -0.6436 -0.6210 -2.3946

6 A)
Fe 0.0298 -0.0050 -0.3714
N 1.4335 -1.4637 -0.3273
N 1.4944 1.3886 -0.3139
N -1.3707 1.4513 -0.2976
N -1.4299 -1.4013 -0.3017
C 1.2085 -2.8118 -0.3081
C 2.4663 -3.5289 -0.3327
C 3.4489 -2.5894 -0.3740
C 2.7899 -1.3004 -0.3695
C 3.4546 -0.0801 -0.3880
C 2.8426 1.1684 -0.3578
C 3.5546 2.4278 -0.3534
C 2.6121 3.4081 -0.3049
C 1.3259 2.7455 -0.2848
C 0.1048 3.4087 -0.2635
C -1.1444 2.7996 -0.2799
C -2.4009 3.5168 -0.3048
C -3.3853 2.5782 -0.3491
C -2.7279 1.2889 -0.3459
C -3.3921 0.0673 -0.3771
C -2.7798 -1.1808 -0.3534
C -3.4907 -2.4402 -0.3667
C -2.5471 -3.4208 -0.3256
C -1.2615 -2.7584 -0.2936
C -0.0392 -3.4219 -0.2843
H 2.5612 -4.6082 -0.3192
H 4.5226 -2.7330 -0.3993
H 4.5406 -0.1029 -0.4177
H 4.6334 2.5266 -0.3786
H 2.7527 4.4823 -0.2842

H 0.1288 4.4950 -0.2467
H -2.4953 4.5962 -0.2909
H -4.4588 2.7235 -0.3774
H -4.4779 0.0900 -0.4150
H -4.5692 -2.5398 -0.3997
H -2.6875 -4.4952 -0.3206
H -0.0628 -4.5084 -0.2753
S 0.1619 0.0352 2.1338
O 0.0133 -0.0018 -2.0121
C -1.5314 -0.2266 2.7948
H -1.4943 -0.1837 3.8896
H -1.9357 -1.2031 2.5058
H -2.2265 0.5464 2.4483
6B)
Fe 2.1204 0.1770 0.2658
C 2.9598 -1.2757 -2.7193
C 2.3243 3.2650 -1.1755
C 1.2768 1.6273 3.2525
C 1.6540 -2.9183 1.6421
N 2.5238 0.8581 -1.5951
C 2.8887 0.1124 -2.6819
C 3.1797 0.9773 -3.8039
C 2.9859 2.2533 -3.3723
C 2.5836 2.1662 -1.9862
N 1.8413 2.0737 0.9112
C 1.9883 3.2129 0.1713
C 1.7599 4.3770 0.9993
C 1.4792 3.9179 2.2484
C 1.5309 2.4737 2.1799
N 1.5566 -0.5094 2.0870
C 1.2849 0.2384 3.1979
C 0.9791 -0.6248 4.3172
C 1.0697 -1.9031 3.8601
C 1.4385 -1.8183 2.4637
N 2.2455 -1.7245 -0.4175
C 2.0487 -2.8659 0.3096
C 2.3280 -4.0282 -0.5039
C 2.7106 -3.5664 -1.7263
C 2.6567 -2.1235 -1.6598
H 3.2671 -1.7352 -3.6544
H 2.4074 4.2484 -1.6295
H 1.0368 2.0881 4.2064
H 1.5277 -3.9023 2.0845
H 3.4854 0.6332 -4.7844
H 3.1011 3.1788 -3.9230
H 1.8103 5.4009 0.6498
H 1.2482 4.4844 3.1421
H 0.7247 -0.2780 5.3113
H 0.9098 -2.8284 4.4001
H 2.2399 -5.0532 -0.1651
H 2.9999 -4.1328 -2.6031
N -5.1095 0.9802 -1.4515
C -5.8782 1.2103 -2.6508
H -4.6591 0.0854 -1.3072
H -5.5397 0.5221 -3.4298
H -5.7349 2.2409 -2.9874

H -6.9532 1.0563 -2.4840
N -3.6741 0.2040 0.7791
C -4.3340 1.4957 0.8142
C -5.1252 1.8854 -0.4465
O -5.7192 2.9555 -0.5207
H -2.6803 0.1826 0.5211
H -5.0412 1.5190 1.6487
H -3.5801 2.2713 0.9788
N -2.3175 -2.2636 0.3193
C -3.4945 -2.2339 1.1601
C -4.3182 -0.9312 1.1674
O -5.4851 -0.9538 1.5333
H -1.4720 -1.7987 0.6529
H -4.1821 -3.0207 0.8442
H -3.1944 -2.4421 2.1935
C -1.1552 -2.0731 -1.8089
C -2.4450 -2.3324 -1.0430
O -3.5205 -2.5677 -1.5890
C -0.7869 -0.5691 -1.8913
S -0.4038 0.2639 -0.2913
H -0.3268 -2.6193 -1.3470
H -1.3081 -2.4636 -2.8217
H 0.0792 -0.4694 -2.5518
H -1.6147 -0.0282 -2.3645
O 3.6966 0.1925 0.6835
6Imz)
Fe 1.7951 0.2536 0.6166
C 3.6893 -1.7926 -1.3710
C 2.7237 2.9499 -1.2720
C -0.1021 2.3020 2.6057
C 0.6344 -2.4748 2.3217
N 2.9422 0.5183 -1.0233
C 3.6878 -0.4346 -1.6687
C 4.4611 0.1703 -2.7288
C 4.1752 1.5003 -2.7115
C 3.2333 1.7097 -1.6360
N 1.3607 2.2276 0.6368
C 1.8686 3.1857 -0.2025
C 1.4058 4.4945 0.1970
C 0.6259 4.3158 1.2979
C 0.6061 2.8965 1.5669
N 0.4903 -0.0321 2.1336
C -0.1492 0.9365 2.8647
C -0.9091 0.3332 3.9352
C -0.7157 -1.0107 3.8431
C 0.1680 -1.2284 2.7212
N 2.0723 -1.7408 0.4734
C 1.5342 -2.7033 1.2880
C 2.0566 -4.0036 0.9360
C 2.9289 -3.8110 -0.0902
C 2.9340 -2.3937 -0.3706
H 4.3316 -2.4343 -1.9665
H 3.0465 3.8102 -1.8506
H -0.6588 2.9563 3.2700
H 0.2934 -3.3382 2.8849
H 5.1298 -0.3684 -3.3885

H 4.5626 2.2827 -3.3520
H 1.6634 5.4187 -0.3049
H 0.1074 5.0621 1.8867
H -1.5040 0.8823 4.6544
H -1.1167 -1.7951 4.4727
H 1.7863 -4.9297 1.4277
H 3.5223 -4.5461 -0.6194
O 3.0477 0.4377 1.6228
H -2.8735 0.5002 -1.7506
H -1.3893 1.2242 0.1908
C -1.0951 0.5661 -0.6124
H 0.8865 -1.3171 -2.2438
N 0.0917 0.0045 -0.7501
H -1.6441 -1.0688 -3.3554
C 0.0338 -0.7509 -1.9034
C -1.2086 -0.6405 -2.4662
N -1.9164 0.2034 -1.6303
6 Fluoride)
Fe 0.0008 0.0004 -0.3621
N 1.4013 -1.4652 -0.2868
N 1.4663 1.4010 -0.2883
N -1.4000 1.4660 -0.2946
N -1.4649 -1.4003 -0.2931
C 1.1747 -2.8111 -0.2829
C 2.4329 -3.5297 -0.2708
C 3.4168 -2.5895 -0.2692
C 2.7560 -1.2998 -0.2804
C 3.4200 -0.0771 -0.2784
C 2.8122 1.1744 -0.2817
C 3.5308 2.4327 -0.2715
C 2.5905 3.4166 -0.2752
C 1.3009 2.7557 -0.2859
C 0.0782 3.4198 -0.2877
C -1.1734 2.8119 -0.2913
C -2.4317 3.5306 -0.2865
C -3.4155 2.5903 -0.2863
C -2.7547 1.3006 -0.2939
C -3.4187 0.0779 -0.2933
C -2.8109 -1.1736 -0.2925
C -3.5295 -2.4319 -0.2848
C -2.5892 -3.4158 -0.2814
C -1.2996 -2.7550 -0.2883
C -0.0769 -3.4190 -0.2841
H 2.5285 -4.6094 -0.2620
H 4.4910 -2.7339 -0.2587
H 4.5069 -0.1020 -0.2714
H 4.6104 2.5283 -0.2608
H 2.7350 4.4908 -0.2681
H 0.1030 4.5066 -0.2842
H -2.5273 4.6102 -0.2802
H -4.4897 2.7347 -0.2801
H -4.5056 0.1027 -0.2912
H -4.6092 -2.5276 -0.2794
H -2.7337 -4.4900 -0.2728
H -0.1017 -4.5059 -0.2789
F -0.0032 0.0014 1.4651

O 0.0043 -0.0006 -2.0111