Supporting Information for

Spectroscopic and Computational Characterization of the NO Adduct of Substrate-Bound Fe(II) Cysteine Dioxygenase: Insights into the Mechanism of O_2 Activation

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Table S1. Experimentally observed vs. computationally predicted EPR parameters. The computed parameters were obtained from single-point DFT calculations (B3LYP, TZVP/CP(PPP)/IGLO-III) on the published crystal structures.

Species	$\mathbf{g_1}$	$\mathbf{g_2}$	$\mathbf{g_3}$	$\mathbf{A_1}$	$\mathbf{A_2}$	$\mathbf{A_3}$	**Ref.**
$[Fe(NO)(S_2C_2(p\text{-tolyl})_2)]^{2-}$,expt	2.050	2.030	2.010	0	14.4	15.6	*a*
$[Fe(NO)(S_2C_2(p\text{-tolyl})_2)]^{2-}$,calc	2.090	2.072	2.054	1	6	69	This work
$[(PaPy_3)Fe(NO)]^{-}$, expt	2.004	2.004	1.938	42	72	11	*b*
$[(PaPy_3)Fe(NO)]^{-}$, calc	2.074	2.032	2.024	38	46	11	This work
$[Fe(NO)(cyclam\text{-}ac)]^{+}$, expt	2.042	2.022	1.977	3	75	30	*c*
$[Fe(NO)(cyclam\text{-}ac)]^{+}$, calc	2.008	1.992	1.926	17	8	85	This work

[a] Crystal structure from the one-electron-reduced complex reported in reference 63 was used to generate starting coordinates for the geometry optimization of the $\{FeNO\}^7$ species. These optimized coordinates were utilized for the DFT calculation.
[b] From ref 59, where PaPy = *N*,*N*-bis(2-pyridylmethyl)amine-*N*-ethyl-2-pyridine-2-carboxamide
[c] From ref 58, where cyclam-ac = 1,4,8,11-tetraazacyclotetradecane-1-acetic acid

Table S2. Experimentally observed vs. computationally predicted electronic transition energies (nm). The computed values were obtained from INDO/S-CI calculations on the published crystal structures.

Species	Expt	Calc
$[Fe(NO)(S_2C_2(p\text{-tolyl})_2)]^{2-}$ [a]	316 (sh), 420, 710	350, 450, 640
$[(PaPy_3)Fe(NO)]^{-}$ [b]	476-500	350-450
$[Fe(NO)(cyclam\text{-}ac)]^{+}$ [c]	400, 560	350-400

[a] Crystal structure from the one-electron reduced complex reported in reference 63 was used to generate starting coordinates for the geometry optimization of the $[FeNO]^7$ species. These optimized coordinates were utilized for the INDO calculation.
[b] From ref 59, where PaPy = *N*,*N*-bis(2-pyridylmethyl)amine-*N*-ethyl-2-pyridine-2-carboxamide
[c] From ref 58, where cyclam-ac = 1,4,8,11-tetraazacyclotetradecane-1-acetic acid

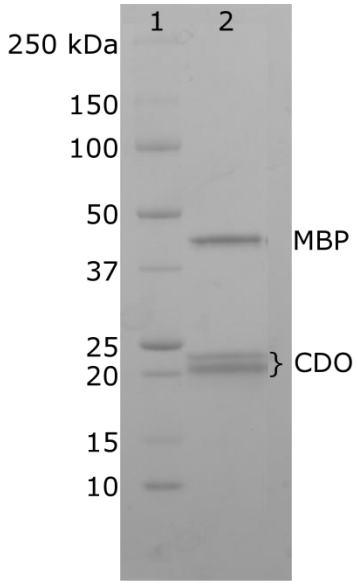

Figure S1. SDS-PAGE gel illustrating protein purity and degree of crosslink. Lane 1 is a protein ladder, lane 2 is a typical end-product of the protein purification.

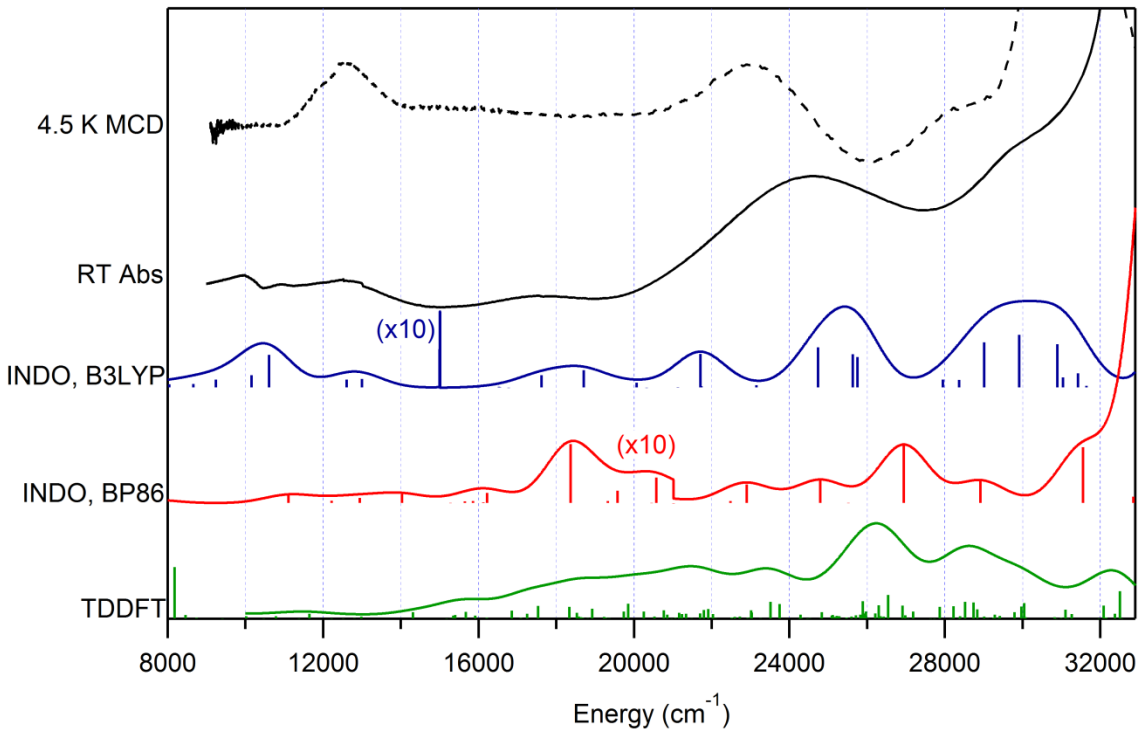

Figure S2. Comparison of computationally predicted Abs spectra versus the experimentally observed RT Abs and 4.5K MCD spectra of the NO adduct of Cys-Fe(II)CDO. For experimental and computational parameters, see the Experimental Section of this work.

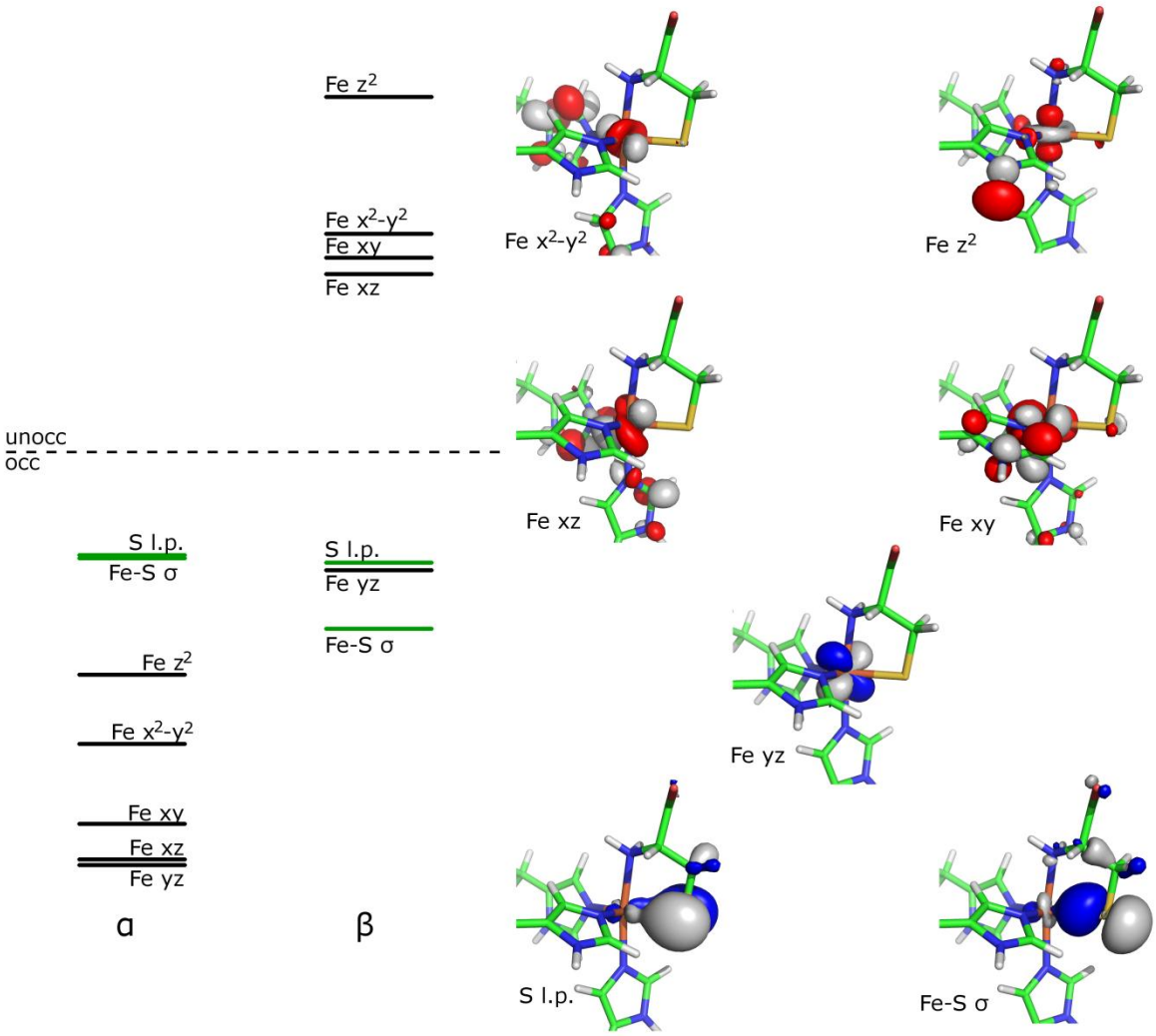

Figure S3. MO energy level diagram of species ^{5}**A**. Boundary surface plots of relevant β orbitals are shown. Relevant Loewdin spin densities: Fe = 3.640, S = 0.180.

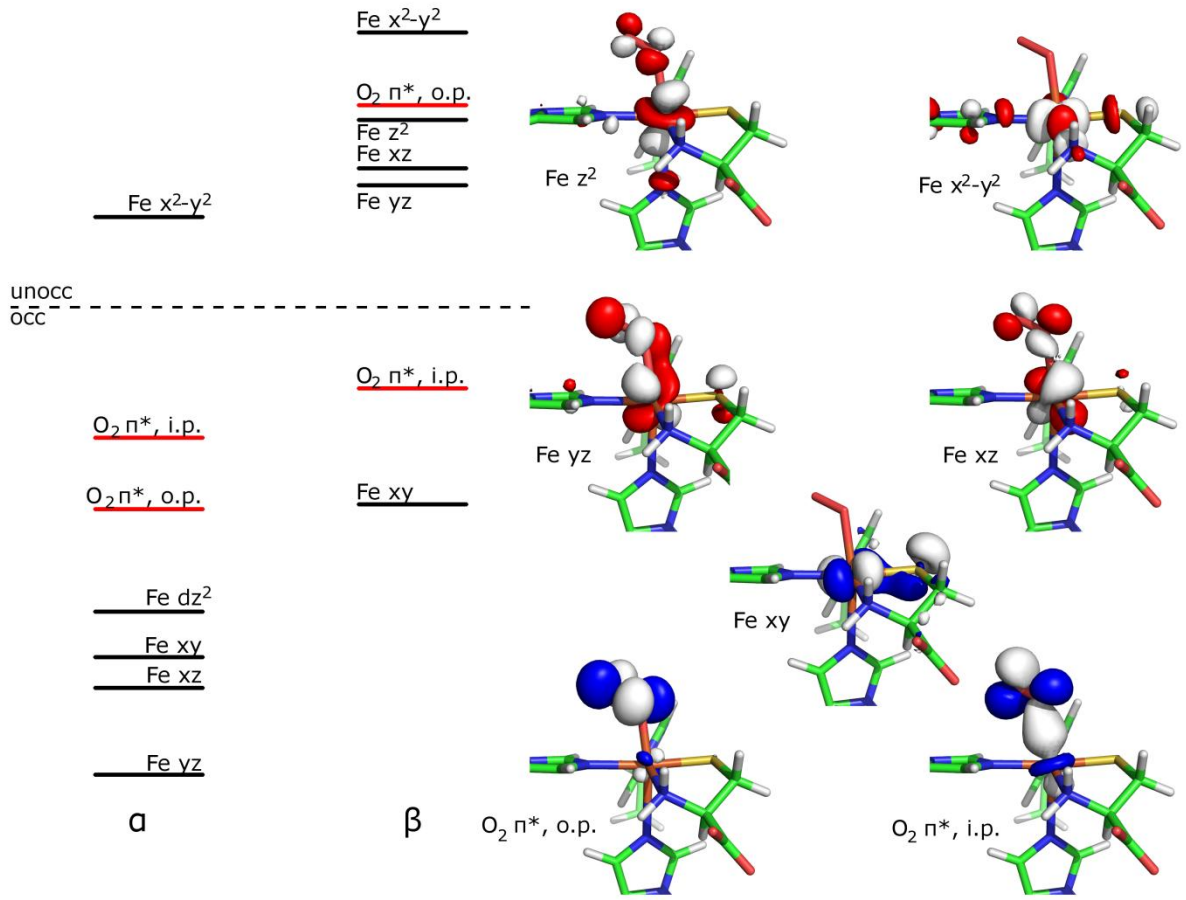

Figure S4. MO energy level diagram of species ^{5}**B**. Boundary surface plots are of relevant β orbitals, except the in plane O_2 π* (O_2 π*, i.p.). Relevant Loewdin spin densities: Fe = 2.775, S = -0.040, O_p = 0.635, O_d = 0.675.

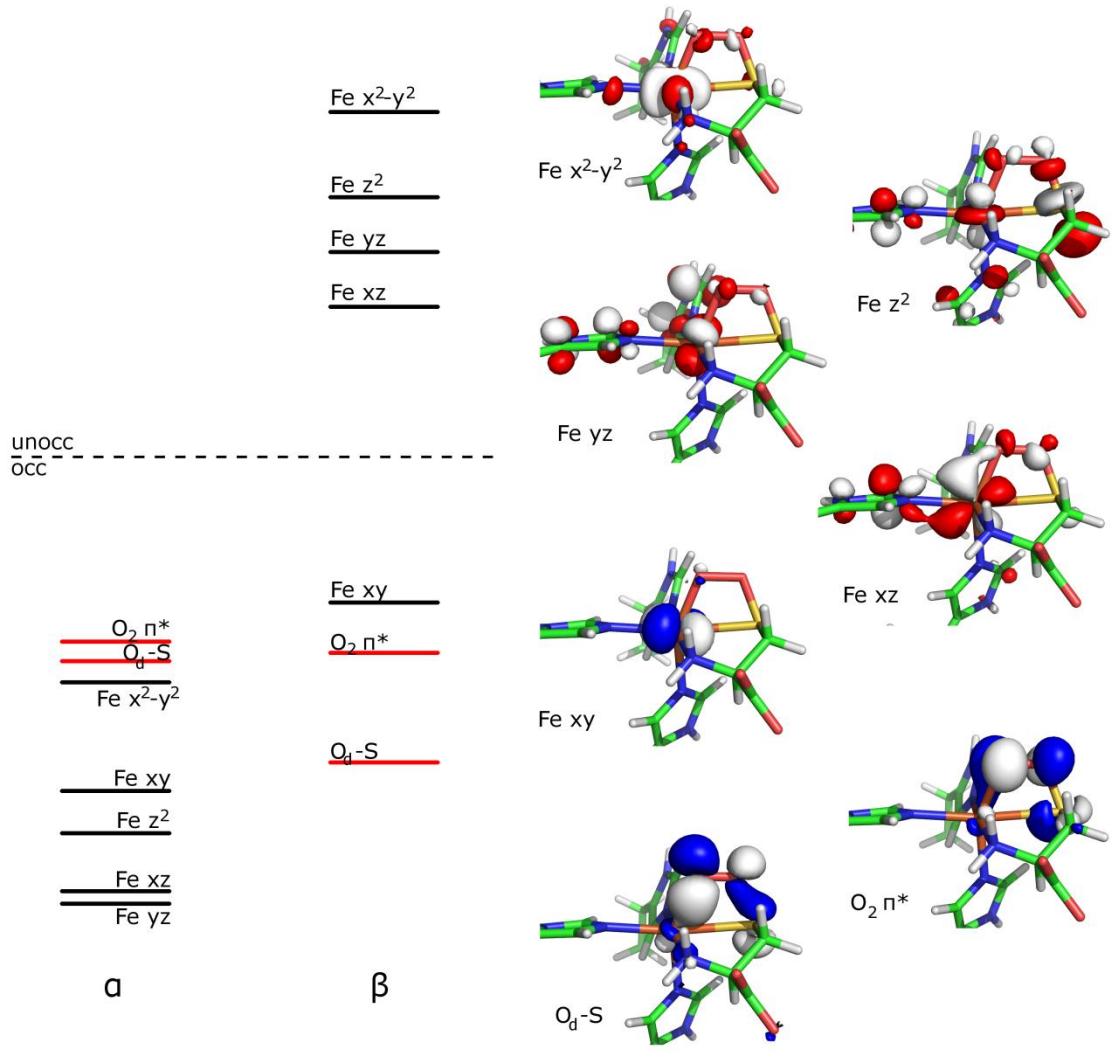

Figure S5. MO energy level diagram of species ^{5}**C**. Boundary surface plots are of relevant β orbitals. Relevant Loewdin spin densities: Fe = 3.672, S = 0.036, O_p = 0.018, O_d = 0.135

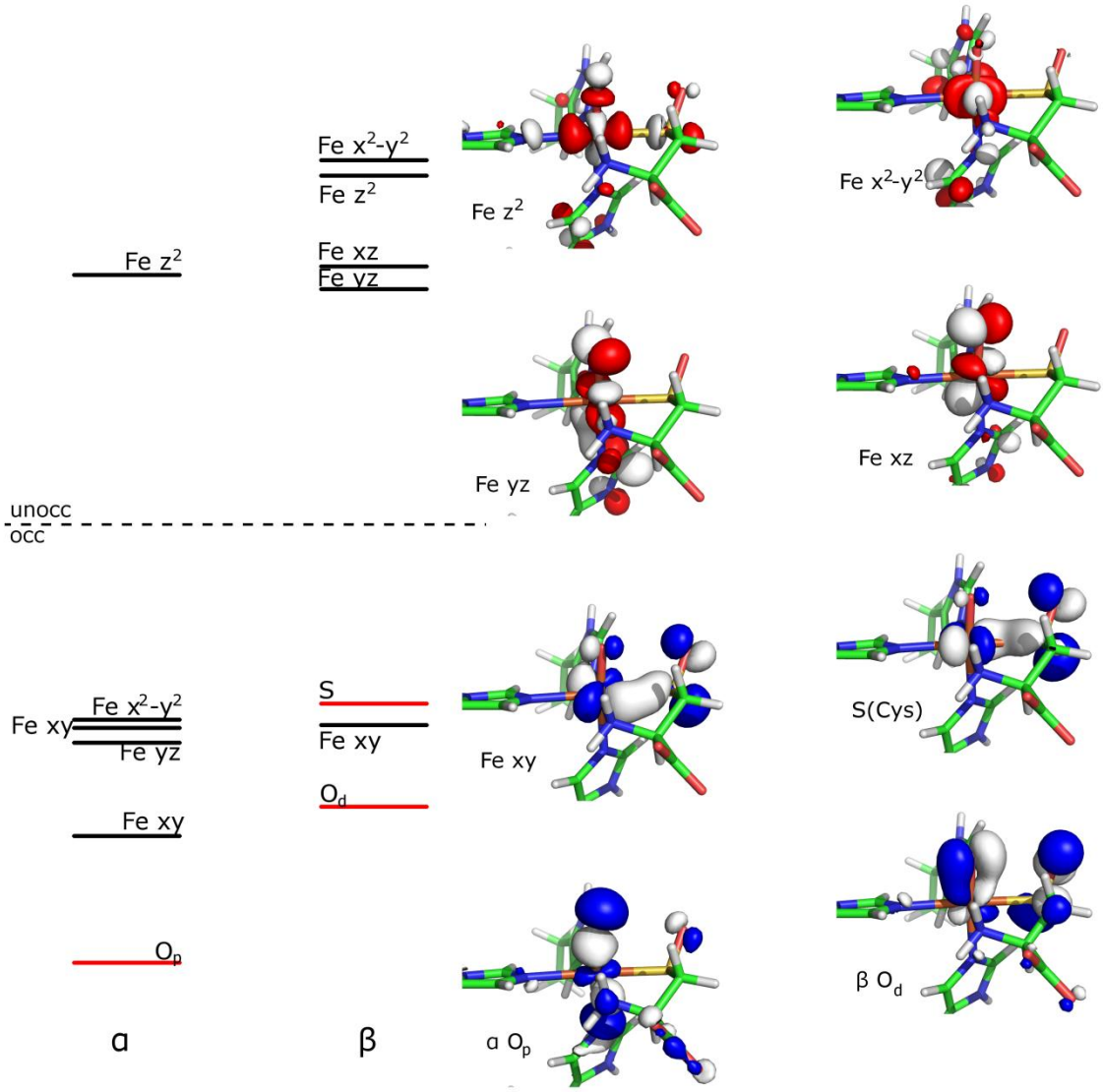

Figure S6. MO energy level diagram of species ^{3}**D**. Boundary surface plots are of relevant β orbitals, except where noted. Relevant Loewdin spin densities: Fe = 2.074, S = -0.303, O_p = 0.563, O_d = -0.294

NO/Cys-Fe(II)CDO QM/MM-Optimized Active Site (QM Region E=-4742.70683861 Eh, $\langle S^2 \rangle$ = 0.75)

Fe	5.086439	-1.032835	0.353754
N	3.533691	-1.299464	-0.450148
O	2.952816	-1.309886	-1.466051
N	4.086670	-0.552368	2.154851
C	3.943772	0.924487	2.396863
C	2.955713	1.269906	3.522285
O	1.877313	0.535100	3.628215
C	3.491024	1.588011	1.087906
S	4.707045	1.228025	-0.243878
O	3.176420	2.296357	4.242122
C	10.988866	-1.633311	2.734030
C	9.897750	-0.800364	3.437389
C	8.755721	-0.427737	2.553765
C	7.535812	-1.029166	2.345308
N	8.793320	0.616138	1.628769
C	7.633329	0.600510	0.907478
N	6.844992	-0.380999	1.327508
C	6.025207	-6.335389	3.868129
C	5.028783	-6.353404	2.679495
C	5.171504	-5.158067	1.777817
C	4.640872	-3.880202	1.765127
N	6.167892	-5.113973	0.807225
C	6.242845	-3.853663	0.289916
N	5.329623	-3.068603	0.852572
C	10.368356	-1.591663	-2.897988
C	9.044860	-1.891694	-3.622242
C	7.796647	-1.606925	-2.855616
C	7.486111	-1.532073	-1.516732
N	6.590959	-1.356757	-3.502385
C	5.617429	-1.158619	-2.576311
N	6.128269	-1.250773	-1.355211
H	11.427289	-1.062756	1.925391
H	10.551872	-2.597202	2.356054
H	11.762364	-1.871550	3.456778
H	9.523085	-1.396379	4.275424
H	10.368163	0.084150	3.878372
H	9.593357	1.195851	1.412631
H	7.089019	-1.843661	2.884078
H	7.391545	1.300585	0.128266
H	7.033792	-6.203767	3.477314
H	5.966361	-7.227085	4.589271
H	5.774839	-5.467740	4.475213
H	5.198287	-7.276161	2.113319
H	4.015443	-6.417671	3.081581
H	6.830483	-5.863873	0.597539
H	3.758261	-3.524736	2.270789
H	6.960759	-3.603946	-0.470994
H	10.646759	-2.461728	-2.281516
H	10.335590	-0.576163	-2.368167
H	11.111190	-1.480033	-3.686171
H	9.036928	-1.288807	-4.538890
H	9.073849	-2.941233	-3.947318
H	6.376678	-1.404209	-4.496202
H	8.138667	-1.680743	-0.673818
H	4.598032	-0.940522	-2.835054
H	3.413601	2.668068	1.224746
H	4.525491	-0.976333	2.975795
H	4.929862	1.300810	2.672012
H	2.507182	1.205011	0.797878
H	3.152942	-0.961614	2.071357

NO/Sec-Fe(II)CDO QM/MM-Optimized Active Site (QM Region E=-6746.07745037 Eh, $\langle S^2 \rangle$ = 0.75)

Fe	5.069759	-1.051890	0.325508
N	3.518095	-1.293015	-0.502178
O	2.964044	-1.451933	-1.522868
N	4.044627	-0.541357	2.122288
C	3.893803	0.929401	2.400357
C	2.930637	1.244633	3.558707
O	1.859464	0.501995	3.673516
C	3.379333	1.635940	1.141222
Se	4.623596	1.317361	-0.356892
O	3.157378	2.265739	4.284506
C	10.978561	-1.637854	2.726472
C	9.877192	-0.809428	3.421063
C	8.737235	-0.441126	2.531534
C	7.513792	-1.036579	2.323364
N	8.782221	0.597870	1.601812
C	7.624812	0.584006	0.876951
N	6.828039	-0.390166	1.299264
C	6.016177	-6.338982	3.870011
C	5.013421	-6.353274	2.686465
C	5.153338	-5.159469	1.781651
C	4.622376	-3.881591	1.764282
N	6.143187	-5.121243	0.804227
C	6.213844	-3.864889	0.277294
N	5.304016	-3.075801	0.840530
C	10.352909	-1.602112	-2.905014
C	9.037908	-1.903635	-3.640780
C	7.786524	-1.626435	-2.879630
C	7.471587	-1.555548	-1.541835
N	6.582946	-1.380636	-3.530622
C	5.605173	-1.190533	-2.608138
N	6.111784	-1.282689	-1.384183
H	11.430333	-1.052228	1.918518
H	10.535443	-2.630527	2.347094
H	11.748666	-1.871521	3.454390
H	9.500425	-1.405837	4.257995
H	10.340821	0.078139	3.863474
H	9.585722	1.172240	1.384271
H	7.060513	-1.844726	2.866616
H	7.393148	1.282092	0.093009
H	7.023135	-6.205038	3.474373
H	5.958933	-7.231000	4.591258
H	5.769949	-5.471382	4.478909
H	5.177126	-7.276762	2.119647
H	4.002212	-6.414788	3.094277
H	6.804593	-5.872377	0.595258
H	3.743422	-3.522526	2.273727
H	6.928025	-3.620362	-0.488684
H	10.629376	-2.472300	-2.287844
H	10.320306	-0.586410	-2.375716
H	11.100705	-1.489817	-3.688446
H	9.034269	-1.296835	-4.554846
H	9.073073	-2.951792	-3.969837
H	6.372609	-1.428192	-4.525321
H	8.122279	-1.702546	-0.697236
H	4.584679	-0.987373	-2.873168
H	3.307067	2.710365	1.312549
H	4.470504	-0.979111	2.942760
H	4.883389	1.309251	2.658370
H	2.395422	1.252822	0.859509
H	3.112645	-0.950608	2.017715

^{5}A QM/MM-Optimized Active Site (QM Region E=-4612.77465483 Eh, $\langle S^2 \rangle$ = 6.00)

Fe	5.095898	-1.382175	0.685725
N	3.973409	-0.767530	2.535915
C	3.854779	0.725344	2.566983
C	2.956362	1.208316	3.716605
O	1.806190	0.596454	3.860775
C	3.281744	1.252273	1.232355
S	4.141986	0.571164	-0.252393
O	3.309627	2.200914	4.430236
C	11.014828	-1.944546	2.442852
C	10.068347	-1.055707	3.274034
C	8.874907	-0.586284	2.521863
C	7.599502	-1.091173	2.503330
N	8.877552	0.401952	1.536127
C	7.638652	0.437979	0.954909
N	6.846162	-0.455338	1.529159
C	5.961185	-6.452690	3.918957
C	4.881366	-6.739189	2.857370
C	4.822218	-5.610627	1.865836
C	4.320956	-4.322174	1.953125
N	5.601627	-5.600179	0.720253
C	5.588456	-4.352015	0.192214
N	4.818458	-3.536523	0.911435
C	10.152623	-2.035196	-3.157015
C	8.758392	-2.154913	-3.809583
C	7.585557	-1.967374	-2.905811
C	7.416109	-1.938667	-1.539340
N	6.299919	-1.784339	-3.415363
C	5.426617	-1.651662	-2.378355
N	6.075999	-1.729848	-1.226815
H	11.445953	-1.351832	1.626375
H	10.512600	-2.881959	2.090968
H	11.832621	-2.265343	3.074962
H	9.729079	-1.647270	4.130704
H	10.652159	-0.224789	3.684755
H	9.674840	0.953446	1.245733
H	7.156050	-1.826302	3.148427
H	7.353679	1.095442	0.150775
H	6.962698	-6.403485	3.458557
H	5.971677	-7.112215	4.826740
H	5.723187	-5.472481	4.323469
H	5.113847	-7.691816	2.369946
H	3.923955	-6.860407	3.372335
H	6.125969	-6.357844	0.269825
H	3.560174	-3.946870	2.617079
H	6.144710	-4.090274	-0.688105
H	10.329469	-2.900713	-2.497524
H	10.257088	-1.041662	-2.658870
H	10.897860	-2.067663	-3.950619
H	8.712113	-1.416873	-4.619072
H	8.700914	-3.135135	-4.298057
H	6.009105	-1.825030	-4.392453
H	8.156869	-2.041886	-0.762808
H	4.370889	-1.476323	-2.500057
H	3.359372	2.341247	1.224401
H	4.362477	-1.086071	3.425232
H	4.860562	1.121027	2.722305
H	2.226527	0.988529	1.150659
H	3.037214	-1.166763	2.440295

^{5}A' QM/MM-Optimized Active Site (QM Region E=-6616.13405203 Eh, $\langle S^2 \rangle$ = 6.00)

Fe	5.225746	-1.144682	0.652964
N	3.871452	-0.634032	2.375276
C	3.752163	0.847097	2.541418
C	2.799125	1.258562	3.672900
O	1.672291	0.595981	3.777778
C	3.228876	1.504505	1.246854
Se	4.235168	0.947167	-0.365467
O	3.076076	2.269990	4.397449
C	10.988154	-1.573878	2.756638
C	10.012324	-0.688619	3.558186
C	8.842088	-0.229629	2.759894
C	7.573901	-0.751083	2.686070
N	8.878868	0.743141	1.758869
C	7.670627	0.746741	1.114544
N	6.858265	-0.143298	1.664795
C	6.036095	-6.280716	3.922044
C	5.001198	-6.469770	2.793846
C	5.037411	-5.341959	1.815020
C	4.526395	-4.064463	1.845317
N	5.891529	-5.350043	0.712414
C	5.897143	-4.109355	0.146654
N	5.062431	-3.304427	0.804314
C	10.367543	-1.571498	-2.875905
C	9.054396	-1.854306	-3.627286
C	7.816324	-1.654447	-2.824257
C	7.575906	-1.622275	-1.470720
N	6.561148	-1.465270	-3.402232
C	5.634093	-1.339363	-2.412129
N	6.227013	-1.415941	-1.228691
H	11.436847	-0.988588	1.943136
H	10.469867	-2.483286	2.370085
H	11.788171	-1.895716	3.412484
H	9.650549	-1.287093	4.401199
H	10.569895	0.146653	3.991300
H	9.693673	1.257697	1.451687
H	7.121677	-1.502877	3.306361
H	7.417429	1.382394	0.282769
H	7.022314	-6.152588	3.484610
H	6.014164	-7.093158	4.696212
H	5.764467	-5.369554	4.452608
H	5.199864	-7.426503	2.300389
H	4.010307	-6.549032	3.248225
H	6.564095	-6.086621	0.491579
H	3.819380	-3.648504	2.540285
H	6.534681	-3.865188	-0.686000
H	10.630808	-2.453515	-2.268085
H	10.346054	-0.585707	-2.354100
H	11.120206	-1.461003	-3.654569
H	9.031190	-1.197405	-4.505622
H	9.109244	-2.882304	-4.012653
H	6.307586	-1.482956	-4.389096
H	8.272208	-1.763419	-0.661619
H	4.586489	-1.164680	-2.589207
H	3.293979	2.588429	1.343524
H	4.149932	-1.074782	3.255804
H	4.749321	1.226934	2.774251
H	2.187549	1.228919	1.076868
H	2.957101	-1.015304	2.124406

^{1}B QM/MM-Optimized Active Site (QM Region E=-4763.11352134 Eh, $\langle S^2 \rangle$ = 0.00)

Fe	5.128840	-0.966077	0.384472
O	3.535746	-1.395749	-0.234540
O	3.061374	-1.035894	-1.366663
N	4.122866	-0.533504	2.173632
C	3.953976	0.939104	2.400893
C	2.961388	1.286295	3.523771
O	1.893117	0.543661	3.637927
C	3.490801	1.556715	1.072339
S	4.742193	1.199033	-0.221439
O	3.183149	2.319426	4.233809
C	10.990183	-1.648147	2.726327
C	9.917710	-0.807135	3.446994
C	8.779184	-0.411735	2.571119
C	7.553575	-0.999390	2.359031
N	8.831790	0.634225	1.649920
C	7.675632	0.635193	0.925950
N	6.875552	-0.339696	1.340306
C	6.020760	-6.344134	3.860418
C	5.032314	-6.345218	2.663226
C	5.184885	-5.135417	1.780881
C	4.658518	-3.855447	1.785717
N	6.198686	-5.073892	0.828441
C	6.289500	-3.802698	0.342926
N	5.370116	-3.026583	0.907299
C	10.367717	-1.603546	-2.905453
C	9.031736	-1.894353	-3.614563
C	7.791255	-1.600108	-2.836703
C	7.504964	-1.481889	-1.496048
N	6.569059	-1.384381	-3.468205
C	5.610116	-1.159964	-2.532872
N	6.148276	-1.202201	-1.320564
H	11.442394	-1.061896	1.917823
H	10.528432	-2.633229	2.351959
H	11.767916	-1.897949	3.440677
H	9.539214	-1.406014	4.281012
H	10.403088	0.066024	3.893843
H	9.636736	1.210488	1.442430
H	7.099261	-1.814754	2.890228
H	7.448431	1.339681	0.146438
H	7.031714	-6.212105	3.477442
H	5.955731	-7.240676	4.570403
H	5.770315	-5.480041	4.472895
H	5.205298	-7.260007	2.085248
H	4.015603	-6.413729	3.055684
H	6.855017	-5.825589	0.605936
H	3.762648	-3.511243	2.276216
H	7.018844	-3.539995	-0.402570
H	10.644451	-2.473834	-2.288968
H	10.347328	-0.587367	-2.375652
H	11.103402	-1.500392	-3.701357
H	9.019014	-1.293843	-4.532972
H	9.049163	-2.944668	-3.937923
H	6.339966	-1.455634	-4.457733
H	8.173401	-1.601918	-0.661069
H	4.573597	-0.963923	-2.745561
H	3.355122	2.634424	1.171406
H	4.567181	-0.953345	2.993825
H	4.931284	1.340021	2.672992
H	2.539637	1.105783	0.769011
H	3.196457	-0.959351	2.077114

^{3}B QM/MM-Optimized Active Site (QM Region E=-4763.13221319 Eh, $\langle S^2 \rangle$ = 2.00)

Fe	5.145346	-0.962849	0.404198
O	3.583685	-1.551887	-0.491301
O	2.811890	-0.877982	-1.271700
N	4.028118	-0.550555	2.101023
C	3.911833	0.921063	2.374427
C	2.935462	1.288991	3.504749
O	1.852914	0.570047	3.639741
C	3.496724	1.586851	1.057170
S	4.740302	1.152709	-0.225478
O	3.186617	2.321081	4.205766
C	10.988787	-1.637404	2.726612
C	9.922420	-0.797512	3.458793
C	8.776124	-0.396553	2.595280
C	7.539962	-0.969972	2.403994
N	8.830094	0.643140	1.667374
C	7.665315	0.655076	0.957719
N	6.857363	-0.306401	1.389578
C	6.021733	-6.333871	3.869070
C	5.030794	-6.347721	2.674176
C	5.175886	-5.144003	1.783119
C	4.646312	-3.866130	1.784215
N	6.184972	-5.084784	0.824354
C	6.269102	-3.816804	0.331271
N	5.350772	-3.040837	0.897540
C	10.365659	-1.602458	-2.905163
C	9.028932	-1.886408	-3.615274
C	7.794443	-1.597419	-2.827781
C	7.527423	-1.475987	-1.483280
N	6.560998	-1.396227	-3.442195
C	5.613577	-1.180286	-2.491760
N	6.174007	-1.210162	-1.289242
H	11.409010	-1.049529	1.918233
H	10.552800	-2.619311	2.351250
H	11.770136	-1.893300	3.434862
H	9.550348	-1.398955	4.293849
H	10.412534	0.073451	3.904821
H	9.639449	1.208493	1.447322
H	7.078904	-1.771382	2.951028
H	7.438436	1.353368	0.172693
H	7.031367	-6.201370	3.482447
H	5.960563	-7.227757	4.486887
H	5.769777	-5.467764	4.477708
H	5.205880	-7.266155	2.102750
H	4.015248	-6.417272	3.069622
H	6.842563	-5.835869	0.603473
H	3.753840	-3.520481	2.279783
H	6.995335	-3.554114	-0.417649
H	10.638916	-2.474872	-2.289983
H	10.352323	-0.586374	-2.374440
H	11.101444	-1.502908	-3.701333
H	9.014561	-1.279381	-4.529342
H	9.044580	-2.934642	-3.945259
H	6.320370	-1.468348	-4.429241
H	8.205645	-1.591331	-0.655182
H	4.577727	-0.990154	-2.710474
H	3.442784	2.670101	1.170605
H	4.393119	-1.014641	2.936266
H	4.903977	1.270583	2.664018
H	2.519927	1.213978	0.732622
H	3.093623	-0.935653	1.925855

^{5}B QM/MM-Optimized Active Site (QM Region E=-4763.17143114 Eh, $\langle S^2 \rangle$ = 6.00)

Fe	4.842868	-2.154089	-0.223197
O	3.450618	-3.221962	-1.531797
O	3.804763	-4.362601	-2.019453
N	3.950852	-1.259659	1.441065
C	4.124371	0.231637	1.421863
C	3.545463	1.010166	2.611709
O	2.515857	0.544640	3.255732
C	3.561215	0.710771	0.086057
S	4.483335	-0.195407	-1.227541
O	4.129953	2.113843	2.843305
C	11.075076	-2.203174	3.015773
C	9.796147	-1.482686	3.496816
C	8.759228	-1.230254	2.447816
C	7.707854	-1.992963	1.983490
N	8.682351	-0.055501	1.702993
C	7.618566	-0.159130	0.841785
N	6.994908	-1.316339	1.004361
C	5.913750	-6.709893	4.056843
C	4.837636	-6.970005	2.979675
C	4.898091	-5.943504	1.883490
C	4.379823	-4.669438	1.729781
N	5.796802	-6.068695	0.831698
C	5.829185	-4.912397	0.113324
N	4.989155	-4.031920	0.636308
C	10.526094	-2.099697	-2.622873
C	9.431028	-2.569608	-3.593152
C	8.058221	-2.544493	-3.021766
C	7.570907	-2.586543	-1.736635
N	6.931815	-2.391726	-3.823733
C	5.827921	-2.348255	-3.031603
N	6.187039	-2.461660	-1.757721
H	11.574014	-1.577703	2.281387
H	10.807055	-3.226567	2.599882
H	11.730770	-2.345583	3.866422
H	9.358298	-2.087072	4.299010
H	10.094333	-0.541504	3.970664
H	9.375470	0.681726	1.692214
H	7.443546	-3.002407	2.242352
H	7.346374	0.606583	0.135351
H	6.902807	-6.622408	3.608112
H	5.893814	-7.386557	4.981717
H	5.660473	-5.734065	4.459566
H	4.982319	-7.978455	2.581775
H	3.860381	-6.948628	3.469223
H	6.459406	-6.834519	0.710016
H	3.537181	-4.228121	2.239435
H	6.502909	-4.766926	-0.708975
H	10.710212	-2.919960	-1.907732
H	10.319704	-1.062488	-2.157096
H	11.425294	-1.976393	-3.224338
H	9.454471	-1.919011	-4.470600
H	9.705448	-3.570880	-3.956296
H	6.875545	-2.381616	-4.841411
H	8.112459	-2.703862	-0.816325
H	4.822454	-2.246554	-3.398762
H	3.720439	1.782255	-0.046443
H	4.319532	-1.625855	2.321269
H	5.195378	0.423704	1.447944
H	2.492200	0.495419	0.015195
H	2.945399	-1.482142	1.425217

^{1}B' QM/MM-Optimized Active Site (QM Region E=-6766.48307313 Eh, $\langle S^2 \rangle$ = 0.00)

Fe	5.122676	-0.961568	0.368087
O	3.519322	-1.382858	-0.250837
O	3.050955	-0.989381	-1.378402
N	4.098365	-0.503524	2.153749
C	3.909459	0.962530	2.411220
C	2.936374	1.273692	3.563760
O	1.878039	0.518764	3.681222
C	3.385085	1.614604	1.125478
Se	4.689061	1.309018	-0.318468
O	3.157869	2.300069	4.284047
C	10.984710	-1.641842	2.721907
C	9.907864	-0.804699	3.441319
C	8.771495	-0.407340	2.563167
C	7.541461	-0.986238	2.349917
N	8.833577	0.636045	1.640129
C	7.679567	0.643132	0.913623
N	6.869365	-0.323641	1.327597
C	6.019028	-6.339372	3.865916
C	5.023410	-6.337363	2.674551
C	5.171773	-5.127407	1.790999
C	4.646136	-3.846742	1.795399
N	6.179577	-5.068866	0.832133
C	6.267953	-3.799129	0.342325
N	5.352123	-3.020566	0.909354
C	10.358857	-1.605982	-2.909557
C	9.027023	-1.897170	-3.625388
C	7.784098	-1.610240	-2.849961
C	7.498398	-1.483720	-1.509971
N	6.559216	-1.412826	-3.482063
C	5.598874	-1.191508	-2.547362
N	6.139517	-1.216380	-1.334997
H	11.436950	-1.055217	1.913877
H	10.525419	-2.627605	2.345867
H	11.761633	-1.890430	3.437513
H	9.527663	-1.406144	4.272824
H	10.390718	0.068171	3.891776
H	9.642371	1.207132	1.433281
H	7.080060	-1.796506	2.883358
H	7.462981	1.349493	0.132843
H	7.028109	-6.206612	3.477806
H	5.957143	-7.236389	4.579699
H	5.772428	-5.475712	4.480663
H	5.191481	-7.252066	2.094859
H	4.009144	-6.404952	3.073493
H	6.834291	-5.821604	0.608294
H	3.754311	-3.500417	2.291896
H	6.994465	-3.539383	-0.407136
H	10.633074	-2.476383	-2.292054
H	10.339545	-0.588985	-2.381261
H	11.097561	-1.503948	-3.702855
H	9.016041	-1.292878	-4.541431
H	9.048660	-2.946157	-3.953010
H	6.330906	-1.489906	-4.471504
H	8.168120	-1.591845	-0.674370
H	4.559116	-1.010727	-2.759791
H	3.233647	2.685416	1.258473
H	4.538897	-0.929770	2.972680
H	4.885709	1.375286	2.669899
H	2.444959	1.146549	0.819062
H	3.177004	-0.937928	2.044665

^{3}B' QM/MM-Optimized Active Site (QM Region E=-6766.50082484 Eh, $\langle S^2 \rangle$ = 2.00)

Fe	5.127849	-0.976473	0.382668
O	3.558051	-1.548886	-0.519038
O	2.775325	-0.866569	-1.268384
N	4.005850	-0.532108	2.084086
C	3.878527	0.932018	2.396947
C	2.918285	1.257985	3.555664
O	1.843846	0.526743	3.684342
C	3.403897	1.654871	1.133331
Se	4.672426	1.255756	-0.324047
O	3.164662	2.280484	4.272920
C	10.978473	-1.644247	2.711262
C	9.904581	-0.806251	3.435909
C	8.760808	-0.407119	2.567220
C	7.520649	-0.972677	2.375647
N	8.822883	0.629011	1.636274
C	7.659564	0.645199	0.924434
N	6.842281	-0.308280	1.357087
C	6.012896	-6.335762	3.880136
C	5.013809	-6.347591	2.692018
C	5.156131	-5.146102	1.796710
C	4.629701	-3.866597	1.795256
N	6.157515	-5.093918	0.829815
C	6.239899	-3.828506	0.328993
N	5.327505	-3.046858	0.897526
C	10.343773	-1.628613	-2.919303
C	9.011143	-1.913239	-3.634991
C	7.774404	-1.626419	-2.851689
C	7.504135	-1.499234	-1.508337
N	6.541576	-1.437138	-3.469842
C	5.590959	-1.223826	-2.521704
N	6.148747	-1.241922	-1.317029
H	11.429664	-1.058640	1.902041
H	10.515074	-2.628457	2.336794
H	11.757168	-1.895579	3.424159
H	9.529795	-1.407221	4.270252
H	10.390424	0.066698	3.883118
H	9.636276	1.187801	1.414587
H	7.054259	-1.769630	2.925060
H	7.442080	1.343873	0.137156
H	7.020400	-6.204610	3.486889
H	5.954291	-7.228067	4.600439
H	5.766470	-5.468140	4.488989
H	5.181885	-7.267631	2.120922
H	4.000944	-6.413299	3.095013
H	6.813318	-5.846714	0.609331
H	3.743105	-3.516038	2.297842
H	6.962187	-3.571706	-0.425730
H	10.616419	-2.499644	-2.302328
H	10.331676	-0.611249	-2.390367
H	11.081787	-1.530059	-3.713633
H	8.999930	-1.305670	-4.548820
H	9.029244	-2.961359	-3.965312
H	6.304595	-1.513047	-4.457555
H	8.181634	-1.605644	-0.678504
H	4.554208	-1.049097	-2.747208
H	3.360004	2.731766	1.293443
H	4.371240	-1.006980	2.913075
H	4.872554	1.285620	2.675308
H	2.420270	1.292525	0.821912
H	3.072142	-0.918731	1.908432

^{5}B' QM/MM-Optimized Active Site (QM Region E=-6766.48728517 Eh, $\langle S^2 \rangle$ = 6.00)

Fe	5.104944	-1.180683	0.490107
O	3.287251	-0.699539	-0.567062
O	2.819829	-1.150502	-1.709251
N	3.869910	-0.513582	2.249810
C	3.758823	0.963851	2.461422
C	2.847330	1.353024	3.639967
O	1.748180	0.663279	3.809651
C	3.189826	1.652437	1.210112
Se	4.302681	1.420741	-0.382267
O	3.146370	2.381405	4.326423
C	10.989953	-1.619028	2.732740
C	9.945900	-0.750652	3.468113
C	8.789510	-0.337000	2.621686
C	7.515609	-0.847296	2.535111
N	8.851591	0.623366	1.608947
C	7.656032	0.636370	0.948448
N	6.820298	-0.234768	1.497202
C	6.027108	-6.314114	3.898881
C	4.999381	-6.496182	2.756716
C	5.032283	-5.370010	1.774201
C	4.420495	-4.135188	1.730671
N	5.977256	-5.318250	0.752213
C	5.941986	-4.085461	0.170173
N	5.000789	-3.336996	0.741461
C	10.364474	-1.610503	-2.898871
C	9.057780	-1.900604	-3.656377
C	7.810582	-1.675575	-2.875162
C	7.545075	-1.600003	-1.528197
N	6.567891	-1.504369	-3.482472
C	5.617719	-1.346594	-2.521912
N	6.187898	-1.382837	-1.322309
H	11.449989	-1.039451	1.923631
H	10.497999	-2.578568	2.337999
H	11.766714	-1.901571	3.435346
H	9.569835	-1.339746	4.310593
H	10.458008	0.112829	3.903963
H	9.678468	1.121327	1.305188
H	7.032637	-1.566242	3.172725
H	7.439464	1.264464	0.102358
H	7.019134	-6.181436	3.468972
H	6.007431	-7.157928	4.684241
H	5.754099	-5.411575	4.440927
H	5.206665	-7.451031	2.262848
H	4.004815	-6.583910	3.200972
H	6.684008	-6.031435	0.559742
H	3.552462	-3.801718	2.275470
H	6.619844	-3.812427	-0.621668
H	10.624988	-2.486908	-2.282070
H	10.340341	-0.594198	-2.369477
H	11.122239	-1.503884	-3.673260
H	9.046805	-1.261312	-4.547847
H	9.110243	-2.935702	-4.023050
H	6.326833	-1.563236	-4.470591
H	8.226979	-1.723044	-0.703043
H	4.556323	-1.250630	-2.708843
H	3.082608	2.724710	1.384992
H	4.181622	-0.941535	3.123967
H	4.762082	1.337651	2.675251
H	2.214814	1.235217	0.944321
H	2.938315	-0.889033	2.042634

^{1}C QM/MM-Optimized Active Site (QM Region E=-4763.13683160 Eh, $\langle S^2 \rangle$ = 0.00)

Fe	5.066707	-0.894054	0.384850
O	3.312164	0.212233	-1.259888
O	3.428627	-1.149333	-0.646976
N	3.925353	-0.527342	2.075084
C	3.818847	0.931609	2.361647
C	2.996994	1.338165	3.602734
O	1.877261	0.707056	3.859313
C	3.248960	1.613619	1.111691
S	4.316885	1.198136	-0.335565
O	3.434966	2.330491	4.257181
C	10.989999	-1.648000	2.726000
C	9.831616	-0.880137	3.389252
C	8.727390	-0.483217	2.478768
C	7.466296	-1.006810	2.335305
N	8.807444	0.541426	1.536173
C	7.617297	0.592660	0.863755
N	6.782078	-0.328987	1.331627
C	6.021000	-6.344000	3.860000
C	5.016512	-6.277334	2.677958
C	5.167220	-5.057806	1.804398
C	4.624447	-3.781822	1.797703
N	6.130536	-5.014774	0.802314
C	6.158684	-3.763474	0.254256
N	5.263263	-2.972920	0.842309
C	10.368000	-1.604000	-2.905000
C	9.028478	-1.903562	-3.615352
C	7.777018	-1.615061	-2.847664
C	7.500203	-1.401510	-1.516964
N	6.535904	-1.512959	-3.477944
C	5.577492	-1.266872	-2.537650
N	6.133775	-1.171192	-1.334360
H	11.465638	-1.020462	1.968055
H	10.700403	-2.653592	2.327063
H	11.727170	-1.836941	3.495280
H	9.419542	-1.513426	4.180625
H	10.258704	-0.006776	3.897033
H	9.643627	1.056691	1.289884
H	7.002859	-1.777509	2.929859
H	7.422001	1.261076	0.044228
H	7.030169	-6.239880	3.469361
H	5.914792	-7.227511	4.539306
H	5.799537	-5.485513	4.488739
H	5.147922	-7.187841	2.078836
H	4.006516	-6.323375	3.092993
H	6.741152	-5.792627	0.540769
H	3.777092	-3.424506	2.359418
H	6.849609	-3.522443	-0.532348
H	10.631659	-2.469967	-2.277311
H	10.358066	-0.611671	-2.393461
H	11.106193	-1.511985	-3.698658
H	9.015953	-1.310416	-4.538694
H	9.053153	-2.955863	-3.935406
H	6.329216	-1.642101	-4.469635
H	8.187030	-1.430694	-0.688729
H	4.526842	-1.173321	-2.745953
H	3.197298	2.696826	1.228944
H	4.266636	-1.005613	2.909728
H	4.832869	1.293783	2.543798
H	2.255571	1.227876	0.858260
H	2.996476	-0.908039	1.853326

^{3}C QM/MM-Optimized Active Site (QM Region E=-4763.13749575 Eh, $\langle S^2 \rangle$ = 2.00)

Fe	5.072150	-0.759389	0.331370
O	3.344749	0.562200	-1.307986
O	3.426114	-0.772128	-0.649989
N	3.895511	-0.362938	1.997638
C	3.759557	1.088614	2.311274
C	2.956842	1.413457	3.588233
O	1.863798	0.734807	3.838305
C	3.119060	1.833972	1.125226
S	4.136179	1.739741	-0.398068
O	3.374041	2.391928	4.277279
C	10.990003	-1.648011	2.725996
C	9.831700	-0.870805	3.379790
C	8.737764	-0.450907	2.465536
C	7.462703	-0.940128	2.328933
N	8.837827	0.577390	1.524446
C	7.649722	0.662480	0.858129
N	6.794482	-0.237569	1.331046
C	6.021012	-6.344007	3.860013
C	5.022702	-6.400969	2.678987
C	5.125227	-5.212147	1.769725
C	4.558012	-3.950021	1.778233
N	6.074007	-5.148341	0.754423
C	6.064563	-3.888351	0.216513
N	5.159897	-3.127334	0.819915
C	10.368011	-1.603996	-2.905003
C	9.025075	-1.901284	-3.611183
C	7.777114	-1.571562	-2.853901
C	7.497655	-1.359884	-1.524386
N	6.550972	-1.386430	-3.498567
C	5.599331	-1.084827	-2.570328
N	6.148428	-1.035066	-1.360489
H	11.471792	-1.023178	1.969013
H	10.697499	-2.650819	2.324881
H	11.723410	-1.839529	3.497867
H	9.403792	-1.503998	4.162669
H	10.263807	-0.006144	3.898465
H	9.683629	1.079156	1.281702
H	6.978882	-1.702743	2.920466
H	7.457575	1.342315	0.047145
H	7.028398	-6.239138	3.462898
H	5.930664	-7.196094	4.583726
H	5.770060	-5.456047	4.434210
H	5.201824	-7.332119	2.127261
H	4.012954	-6.472267	3.092889
H	6.711683	-5.905389	0.494940
H	3.717313	-3.609089	2.361281
H	6.741503	-3.619964	-0.575781
H	10.634036	-2.469408	-2.277696
H	10.363488	-0.609706	-2.395185
H	11.102467	-1.514401	-3.702638
H	9.024200	-1.324948	-4.545192
H	9.034499	-2.959612	-3.910354
H	6.345496	-1.513601	-4.490816
H	8.169177	-1.441106	-0.686921
H	4.560291	-0.912772	-2.789831
H	2.996727	2.890688	1.373061
H	4.218294	-0.853202	2.832970
H	4.766833	1.475921	2.480270
H	2.139792	1.416026	0.868328
H	2.978836	-0.754197	1.746779

^{5}C QM/MM-Optimized Active Site (QM Region E=-4763.15684571 Eh, $\langle S^2 \rangle$ = 6.00)

Fe	4.905920	-0.951054	0.368175
O	3.345019	0.696746	-1.278664
O	3.341579	-0.707190	-0.821588
N	3.779335	-0.435838	2.215089
C	3.691503	1.025692	2.471362
C	2.863006	1.415719	3.710011
O	1.740565	0.774884	3.941285
C	3.110474	1.759024	1.245823
S	4.218532	1.669932	-0.217467
O	3.287084	2.396008	4.391046
C	10.990013	-1.647993	2.726005
C	9.824037	-0.862949	3.355979
C	8.727814	-0.459015	2.435402
C	7.426430	-0.891607	2.371306
N	8.837543	0.505831	1.430357
C	7.627321	0.606962	0.803183
N	6.748361	-0.214471	1.361121
C	6.020987	-6.344001	3.859989
C	5.017045	-6.413269	2.685177
C	5.100494	-5.229291	1.769873
C	4.512296	-3.978562	1.768175
N	6.036695	-5.166240	0.741978
C	6.001527	-3.921642	0.180626
N	5.089051	-3.165499	0.784964
C	10.367997	-1.604003	-2.904999
C	9.066119	-1.927351	-3.668012
C	7.799394	-1.650190	-2.930087
C	7.502743	-1.495119	-1.595808
N	6.581031	-1.452841	-3.580521
C	5.617693	-1.201832	-2.645102
N	6.152789	-1.201178	-1.431437
H	11.477034	-1.033040	1.964650
H	10.700604	-2.653256	2.329455
H	11.715524	-1.830412	3.507534
H	9.393947	-1.483612	4.147990
H	10.251525	0.011603	3.862439
H	9.695937	0.944967	1.118425
H	6.933573	-1.603443	3.017787
H	7.441169	1.248529	-0.039903
H	7.026256	-6.233403	3.461496
H	5.933829	-7.194574	4.586836
H	5.765150	-5.455619	4.431400
H	5.200879	-7.344609	2.135526
H	4.010338	-6.491992	3.105323
H	6.683762	-5.916896	0.487752
H	3.676515	-3.637450	2.357237
H	6.664114	-3.653068	-0.622678
H	10.625956	-2.467636	-2.270843
H	10.335601	-0.609438	-2.397445
H	11.130767	-1.498794	-3.673591
H	9.074206	-1.331426	-4.588611
H	9.120105	-2.978153	-3.989243
H	6.383473	-1.549734	-4.577344
H	8.168581	-1.593898	-0.754078
H	4.578280	-1.026747	-2.865629
H	2.949532	2.812369	1.482435
H	4.112422	-0.902502	3.059408
H	4.706525	1.384896	2.657048
H	2.160515	1.315811	0.928072
H	2.843558	-0.805866	2.012959

^{1}C' QM/MM-Optimized Active Site (QM Region E=-6766.50716169 Eh, $\langle S^2 \rangle$ = 0.00)

Fe	5.074317	-0.881916	0.368025
O	3.226273	0.118644	-1.317695
O	3.442856	-1.184511	-0.648927
N	3.913792	-0.491986	2.052110
C	3.790587	0.961133	2.367705
C	2.977405	1.334779	3.626155
O	1.863931	0.691942	3.878200
C	3.184279	1.673848	1.154609
Se	4.306277	1.307041	-0.428879
O	3.409913	2.323425	4.290496
C	10.989999	-1.648000	2.726000
C	9.830388	-0.880699	3.388225
C	8.730209	-0.478536	2.475123
C	7.465110	-0.992158	2.329874
N	8.821463	0.541803	1.528844
C	7.634264	0.599195	0.852370
N	6.789421	-0.313026	1.320640
C	6.021000	-6.344000	3.860000
C	5.014081	-6.269632	2.680090
C	5.165776	-5.047811	1.809487
C	4.622603	-3.771683	1.801526
N	6.131250	-5.004460	0.809464
C	6.160434	-3.753240	0.261755
N	5.263710	-2.962531	0.847609
C	10.368000	-1.604000	-2.905000
C	9.033902	-1.907350	-3.622983
C	7.780532	-1.622808	-2.858564
C	7.505031	-1.404744	-1.528458
N	6.538600	-1.528604	-3.487955
C	5.580143	-1.282859	-2.547339
N	6.138632	-1.179913	-1.345054
H	11.466463	-1.020582	1.968411
H	10.700865	-2.653866	2.326843
H	11.726247	-1.836830	3.496237
H	9.414660	-1.515772	4.176254
H	10.257423	-0.009657	3.900125
H	9.662138	1.049702	1.282368
H	6.993720	-1.757215	2.925775
H	7.448905	1.265225	0.028860
H	7.030020	-6.105452	3.468630
H	5.913272	-7.228721	4.537240
H	5.802939	-5.486756	4.491857
H	5.141546	-7.178508	2.077545
H	4.004925	-6.314334	3.097080
H	6.740412	-5.783313	0.547487
H	3.772942	-3.414373	2.359917
H	6.852331	-3.513527	-0.524236
H	10.630918	-2.469016	-2.275693
H	10.355922	-0.610662	-2.395248
H	11.109588	-1.511381	-3.695481
H	9.023711	-1.313904	-4.546160
H	9.063323	-2.959495	-3.943156
H	6.331077	-1.661988	-4.478979
H	8.192769	-1.427343	-0.700795
H	4.528650	-1.193782	-2.754478
H	3.119577	2.751991	1.303118
H	4.249688	-0.980317	2.883150
H	4.801719	1.332808	2.546363
H	2.197753	1.277128	0.893674
H	2.989838	-0.878208	1.818656

^{3}C' QM/MM-Optimized Active Site (QM Region E=-6766.50919534 Eh, $\langle S^2 \rangle$ = 2.00)

Fe	5.069125	-0.753649	0.318586
O	3.312194	0.451829	-1.391119
O	3.422255	-0.808241	-0.635315
N	3.896956	-0.347595	1.993950
C	3.746440	1.099649	2.321477
C	2.953391	1.404514	3.611808
O	1.862617	0.722337	3.859440
C	3.067517	1.849076	1.164995
Se	4.125839	1.836588	-0.493309
O	3.372287	2.377784	4.307370
C	10.989996	-1.648007	2.725995
C	9.826439	-0.872732	3.373559
C	8.735896	-0.452178	2.454890
C	7.458403	-0.935251	2.317463
N	8.841880	0.573824	1.511614
C	7.655286	0.663220	0.843749
N	6.794521	-0.231212	1.317057
C	6.021015	-6.344011	3.860020
C	5.022466	-6.400981	2.679356
C	5.123724	-5.211082	1.771942
C	4.556172	-3.949153	1.783430
N	6.072293	-5.145053	0.756815
C	6.061857	-3.883800	0.221454
N	5.157585	-3.124188	0.826924
C	10.368003	-1.603994	-2.905004
C	9.029477	-1.904056	-3.617311
C	7.778618	-1.577651	-2.864296
C	7.495114	-1.363664	-1.536023
N	6.554585	-1.394700	-3.512929
C	5.600072	-1.091770	-2.588069
N	6.145414	-1.038929	-1.376476
H	11.472552	-1.023439	1.969281
H	10.700688	-2.652618	2.326292
H	11.720639	-1.835915	3.501466
H	9.395201	-1.506829	4.153968
H	10.254893	-0.007896	3.895149
H	9.690055	1.071410	1.268440
H	6.970685	-1.694830	2.909886
H	7.467398	1.342644	0.031591
H	7.028735	-6.238843	3.463502
H	5.929764	-7.196289	4.583587
H	5.770120	-5.455853	4.434208
H	5.202254	-7.331483	2.126744
H	4.012901	-6.473533	3.093631
H	6.709685	-5.901751	0.495750
H	3.715529	-3.609906	2.367628
H	6.737489	-3.613691	-0.571178
H	10.632373	-2.468997	-2.276473
H	10.361391	-0.608903	-2.396234
H	11.105631	-1.513833	-3.699688
H	9.030979	-1.326660	-4.550649
H	9.042904	-2.962056	-3.917575
H	6.351526	-1.524746	-4.505310
H	8.164535	-1.442166	-0.696658
H	4.563135	-0.915159	-2.813648
H	2.923194	2.898662	1.426957
H	4.226124	-0.841464	2.824699
H	4.749729	1.499455	2.482957
H	2.101640	1.407087	0.901048
H	2.982438	-0.744950	1.744915

^{5}C' QM/MM-Optimized Active Site (QM Region E=-6766.52804049 Eh, $\langle S^2 \rangle$ = 6.00)

Fe	4.905946	-0.951626	0.360064
O	3.281124	0.591677	-1.367766
O	3.336475	-0.765396	-0.823202
N	3.768942	-0.421206	2.198055
C	3.672984	1.035880	2.476359
C	2.852623	1.404913	3.729161
O	1.732588	0.759915	3.958604
C	3.062695	1.785454	1.279870
Se	4.218924	1.767670	-0.316256
O	3.277970	2.380362	4.416691
C	10.990013	-1.647993	2.726005
C	9.822419	-0.865693	3.356739
C	8.727944	-0.460397	2.434791
C	7.425050	-0.888450	2.369174
N	8.843639	0.500102	1.426282
C	7.635855	0.602332	0.795440
N	6.751825	-0.212994	1.354200
C	6.020987	-6.344001	3.859989
C	5.014535	-6.412762	2.687318
C	5.097145	-5.228568	1.772576
C	4.510787	-3.976968	1.773395
N	6.032833	-5.165271	0.744350
C	5.999380	-3.919530	0.185444
N	5.088606	-3.162996	0.791725
C	10.367997	-1.604003	-2.904999
C	9.069573	-1.931311	-3.672095
C	7.800865	-1.656157	-2.937252
C	7.502741	-1.501896	-1.603301
N	6.582880	-1.460342	-3.588920
C	5.618068	-1.211921	-2.654114
N	6.152199	-1.211171	-1.439865
H	11.476240	-1.031732	1.965245
H	10.701329	-2.653066	2.327974
H	11.715513	-1.830495	3.507484
H	9.391489	-1.488705	4.146467
H	10.248485	0.007886	3.866107
H	9.704000	0.934828	1.113488
H	6.928783	-1.597127	3.016682
H	7.455611	1.240564	-0.051210
H	7.025917	-6.234165	3.459710
H	5.933242	-7.194840	4.586876
H	5.767000	-5.455555	4.432100
H	5.196678	-7.344172	2.137238
H	4.008612	-6.490728	3.109481
H	6.678342	-5.916612	0.488087
H	3.675734	-3.635805	2.363507
H	6.661634	-3.650962	-0.618064
H	10.626385	-2.466375	-2.269399
H	10.331996	-0.608290	-2.385422
H	11.132534	-1.497375	-3.671712
H	9.079082	-1.336131	-4.593143
H	9.126961	-2.982274	-3.992338
H	6.385739	-1.557626	-4.585829
H	8.167959	-1.600222	-0.761042
H	4.578793	-1.039318	-2.876785
H	2.893529	2.832611	1.533248
H	4.095392	-0.898046	3.039330
H	4.686736	1.399969	2.658639
H	2.120321	1.334717	0.952124
H	2.835518	-0.791786	1.985074

^{1}D QM/MM-Optimized Active Site (QM Region E=-4763.13432261 Eh, $\langle S^2 \rangle$ = 0.00)

Fe	5.005662	-0.938074	0.357875
O	3.602823	-1.102911	-0.495083
O	4.256050	1.644776	-1.567043
N	3.916692	-0.539226	2.049796
C	3.832486	0.924704	2.330653
C	2.973693	1.331676	3.545479
O	1.859457	0.684409	3.781492
C	3.364102	1.604788	1.039565
S	4.765723	1.392797	-0.151898
O	3.388845	2.323938	4.214021
C	10.990000	-1.648000	2.726000
C	9.827601	-0.893625	3.398668
C	8.729793	-0.482673	2.484862
C	7.453888	-0.969697	2.345962
N	8.841626	0.518402	1.518687
C	7.662806	0.590826	0.838415
N	6.794229	-0.288930	1.324181
C	6.021000	-6.344000	3.860000
C	5.017363	-6.288394	2.679700
C	5.185616	-5.069650	1.815121
C	4.689535	-3.777856	1.843529
N	6.156857	-5.036636	0.820569
C	6.240234	-3.776353	0.308784
N	5.373142	-2.972165	0.920208
C	10.368000	-1.604000	-2.905000
C	9.022895	-1.891616	-3.617820
C	7.764014	-1.612451	-2.851695
C	7.478467	-1.442402	-1.516717
N	6.527498	-1.463945	-3.487207
C	5.566389	-1.224410	-2.549351
N	6.113941	-1.192934	-1.342199
H	11.458408	-1.011925	1.966273
H	10.691641	-2.651270	2.321226
H	11.739566	-1.837866	3.484545
H	9.414457	-1.541903	4.177137
H	10.250082	-0.028414	3.923352
H	9.685202	1.023236	1.274411
H	6.968065	-1.716636	2.953472
H	7.489884	1.258833	0.015445
H	7.032272	-6.242041	3.472176
H	5.911657	-7.227013	4.539801
H	5.799130	-5.482718	4.485119
H	5.149229	-7.200524	2.083811
H	4.006461	-6.330149	3.092719
H	6.728797	-5.834959	0.537117
H	3.847571	-3.405820	2.404125
H	6.933501	-3.542731	-0.477519
H	10.603242	-2.463984	-2.260773
H	10.356578	-0.608471	-2.397276
H	11.120974	-1.533255	-3.686720
H	9.010574	-1.286407	-4.532369
H	9.046368	-2.940111	-3.949174
H	6.320997	-1.563615	-4.482206
H	8.159844	-1.497560	-0.684903
H	4.523149	-1.063038	-2.757494
H	3.181197	2.672058	1.176547
H	4.242513	-1.024104	2.887051
H	4.845740	1.261636	2.566003
H	2.480931	1.120145	0.613369
H	2.983534	-0.901052	1.811190

^{3}D QM/MM-Optimized Active Site (QM Region E=-4763.17961518 Eh, $\langle S^2 \rangle$ = 2.02)

Fe	4.984098	-0.710493	0.366834
O	3.615090	-1.030223	-0.467434
O	4.083102	1.919103	-1.492529
N	3.941974	-0.358890	2.115429
C	3.800184	1.097824	2.399036
C	2.980324	1.495184	3.647286
O	1.918583	0.806539	3.978651
C	3.247993	1.764915	1.130344
S	4.632258	1.678148	-0.088883
O	3.399521	2.540520	4.230152
C	10.989985	-1.647990	2.726007
C	9.835772	-0.861335	3.376159
C	8.748546	-0.418389	2.465780
C	7.444575	-0.837012	2.371240
N	8.882626	0.578053	1.496359
C	7.685319	0.716859	0.859198
N	6.789794	-0.119463	1.372824
C	6.021006	-6.344013	3.859993
C	5.031364	-6.319153	2.667923
C	5.190939	-5.109718	1.793395
C	4.667222	-3.828649	1.824280
N	6.166289	-5.049801	0.804098
C	6.217277	-3.775970	0.304262
N	5.329176	-3.000160	0.912252
C	10.367983	-1.603999	-2.904997
C	8.998728	-1.861291	-3.579864
C	7.769134	-1.487758	-2.809945
C	7.494130	-1.303592	-1.474084
N	6.546391	-1.260324	-3.446789
C	5.601331	-0.964887	-2.511855
N	6.149129	-0.962768	-1.304471
H	11.495405	-1.028741	1.981499
H	10.692060	-2.649300	2.324179
H	11.707507	-1.855717	3.510063
H	9.395697	-1.494073	4.153104
H	10.276333	-0.005779	3.903197
H	9.748473	1.029581	1.226702
H	6.943344	-1.569825	2.985972
H	7.517202	1.393148	0.040947
H	7.033165	-6.248172	3.473804
H	5.911933	-7.227929	4.538351
H	5.790223	-5.476225	4.473556
H	5.177279	-7.239781	2.088546
H	4.016004	-6.359743	3.071143
H	6.775744	-5.824442	0.528416
H	3.815787	-3.479471	2.386635
H	6.913072	-3.515109	-0.473816
H	10.633577	-2.479782	-2.294139
H	10.404174	-0.619697	-2.374407
H	11.084557	-1.524323	-3.719078
H	9.000746	-1.306958	-4.527421
H	8.963975	-2.924133	-3.856261
H	6.331438	-1.354574	-4.440058
H	8.166632	-1.416662	-0.640894
H	4.567784	-0.752574	-2.724137
H	2.985889	2.811431	1.294090
H	4.344695	-0.834067	2.924214
H	4.806918	1.478021	2.596564
H	2.395328	1.219229	0.715469
H	3.020985	-0.777970	1.929007

^{5}D QM/MM-Optimized Active Site (QM Region E=-4763.17117216 Eh, $\langle S^2 \rangle$ = 6.01)

Fe	4.838275	-0.885758	0.303413
O	3.419228	-0.923377	-0.630617
O	3.968835	2.030065	-1.395305
N	3.842103	-0.452356	2.266267
C	3.738718	1.015699	2.491399
C	2.893753	1.439467	3.709394
O	1.779491	0.795497	3.957653
C	3.197810	1.690679	1.216296
S	4.551662	1.670462	-0.033961
O	3.315301	2.442434	4.357354
C	10.989998	-1.648000	2.726000
C	9.810814	-0.876770	3.350477
C	8.720772	-0.469896	2.423223
C	7.416975	-0.895406	2.340232
N	8.844122	0.507747	1.433265
C	7.640368	0.625426	0.799461
N	6.749441	-0.199375	1.334672
C	6.020998	-6.343997	3.859998
C	5.022239	-6.372495	2.676980
C	5.132642	-5.174589	1.779766
C	4.558593	-3.915937	1.782587
N	6.090518	-5.107720	0.773336
C	6.084893	-3.854015	0.230608
N	5.171163	-3.095266	0.827707
C	10.368005	-1.604000	-2.905001
C	9.054991	-1.913709	-3.656099
C	7.795532	-1.613510	-2.913714
C	7.509416	-1.435080	-1.581377
N	6.573294	-1.413499	-3.560961
C	5.618168	-1.139192	-2.628859
N	6.162264	-1.125010	-1.417842
H	11.477385	-1.028288	1.968886
H	10.709274	-2.655921	2.329194
H	11.711268	-1.825607	3.512622
H	9.378066	-1.505741	4.134448
H	10.227062	-0.002754	3.867196
H	9.706148	0.952247	1.139486
H	6.918027	-1.613920	2.973498
H	7.470025	1.284544	-0.032782
H	7.029593	-6.237393	3.468271
H	5.924015	-7.205512	4.571047
H	5.774596	-5.463184	4.447623
H	5.193564	-7.297104	2.111758
H	4.012004	-6.441737	3.089403
H	6.725639	-5.866749	0.513995
H	3.709634	-3.576746	2.353408
H	6.765853	-3.587897	-0.557883
H	10.625380	-2.470213	-2.274410
H	10.347921	-0.609841	-2.394560
H	11.124068	-1.504243	-3.680779
H	9.065296	-1.323413	-4.580292
H	9.090882	-2.966974	-3.970970
H	6.372209	-1.515473	-4.556818
H	8.178338	-1.526710	-0.741838
H	4.578952	-0.953814	-2.843840
H	2.925932	2.732289	1.398845
H	4.234598	-0.899151	3.095594
H	4.749251	1.380675	2.695749
H	2.349871	1.147352	0.788246
H	2.905640	-0.842213	2.105366

^{1}D' QM/MM-Optimized Active Site (QM Region E= -6766.49780660 Eh, $\langle S^2 \rangle$ = 0.00)

Fe	5.020928	-0.923464	0.363639
O	3.612532	-1.061339	-0.489933
O	4.051015	1.669899	-1.755672
N	3.915723	-0.495846	2.054992
C	3.803292	0.965513	2.351136
C	2.964156	1.346732	3.589959
O	1.860555	0.687127	3.840761
C	3.270929	1.664801	1.095239
Se	4.725730	1.496984	-0.244782
O	3.379716	2.344623	4.250546
C	10.989998	-1.648000	2.726000
C	9.834025	-0.864778	3.376463
C	8.745438	-0.452431	2.454661
C	7.451316	-0.897579	2.349660
N	8.882747	0.506629	1.450608
C	7.699925	0.593124	0.778859
N	6.805620	-0.236794	1.305910
C	6.020998	-6.343997	3.859998
C	5.025062	-6.277191	2.673690
C	5.201800	-5.049734	1.821246
C	4.698444	-3.760033	1.850308
N	6.189574	-5.002669	0.842953
C	6.275123	-3.738471	0.342839
N	5.393280	-2.942939	0.944216
C	10.368005	-1.604000	-2.905001
C	9.021710	-1.890159	-3.615367
C	7.767239	-1.590994	-2.852508
C	7.480774	-1.453851	-1.514954
N	6.538538	-1.390794	-3.488327
C	5.578058	-1.158596	-2.548422
N	6.121393	-1.178039	-1.338139
H	11.483315	-1.031604	1.970045
H	10.694168	-2.653088	2.330211
H	11.716534	-1.842447	3.504411
H	9.404753	-1.491518	4.163900
H	10.268226	0.002916	3.888212
H	9.745372	0.958229	1.170339
H	6.951051	-1.611932	2.985593
H	7.548688	1.230827	-0.072125
H	7.035013	-6.248744	3.478196
H	5.905981	-7.223051	4.543060
H	5.801859	-5.479524	4.482218
H	5.159044	-7.184342	2.070855
H	4.011481	-6.318582	3.079668
H	6.782442	-5.789736	0.567462
H	3.846863	-3.395629	2.401219
H	6.982740	-3.498879	-0.429088
H	10.628859	-2.472046	-2.279002
H	10.365949	-0.611318	-2.393006
H	11.104181	-1.515801	-3.701100
H	9.016282	-1.295463	-4.537457
H	9.037695	-2.941809	-3.937636
H	6.335471	-1.460241	-4.486457
H	8.159533	-1.553868	-0.685214
H	4.540805	-0.959544	-2.756239
H	3.076175	2.724663	1.262121
H	4.237672	-0.980066	2.894173
H	4.813824	1.322428	2.570305
H	2.388688	1.170985	0.680518
H	2.988825	-0.869224	1.809245

^{3}D' QM/MM-Optimized Active Site (QM Region E= -6766.54279896 Eh, $\langle S^2 \rangle$ = 2.02)

Fe	4.981035	-0.763453	0.298269
O	3.608458	-1.062580	-0.534609
O	3.927013	1.887156	-1.737442
N	3.930262	-0.370148	2.040277
C	3.786766	1.081922	2.356454
C	2.957312	1.419167	3.615060
O	1.868265	0.737432	3.860533
C	3.210120	1.787656	1.122119
Se	4.646886	1.720728	-0.244742
O	3.368717	2.406458	4.293717
C	10.989984	-1.647991	2.726003
C	9.819475	-0.871508	3.360055
C	8.739796	-0.444832	2.431283
C	7.441517	-0.877093	2.315326
N	8.881322	0.544960	1.456064
C	7.696264	0.664942	0.794677
N	6.797047	-0.173494	1.299383
C	6.020999	-6.344003	3.859999
C	5.027168	-6.358690	2.672808
C	5.165463	-5.155079	1.786301
C	4.640908	-3.874096	1.816231
N	6.131172	-5.099342	0.787800
C	6.176083	-3.828338	0.280915
N	5.292733	-3.049786	0.892040
C	10.367989	-1.604000	-2.905001
C	9.023871	-1.902462	-3.610256
C	7.773472	-1.570992	-2.856199
C	7.484460	-1.386155	-1.523922
N	6.556300	-1.353515	-3.506692
C	5.599601	-1.061227	-2.581871
N	6.136875	-1.052815	-1.368628
H	11.482055	-1.028915	1.971022
H	10.702398	-2.654961	2.329087
H	11.711853	-1.833783	3.510462
H	9.378285	-1.504844	4.135540
H	10.244319	-0.007764	3.886716
H	9.746804	0.999514	1.189166
H	6.935824	-1.607942	2.928851
H	7.544347	1.328374	-0.036787
H	7.032822	-6.244714	3.471999
H	5.917960	-7.205047	4.569768
H	5.781237	-5.461403	4.448299
H	5.190736	-7.282896	2.104685
H	4.014086	-6.416622	3.079979
H	6.743876	-5.872774	0.516954
H	3.796334	-3.522064	2.386990
H	6.867368	-3.571764	-0.501923
H	10.633750	-2.468971	-2.276839
H	10.361913	-0.608533	-2.396609
H	11.102441	-1.514720	-3.702649
H	9.022824	-1.327522	-4.544780
H	9.033412	-2.961093	-3.908211
H	6.356121	-1.457948	-4.502544
H	8.149377	-1.491439	-0.683920
H	4.566774	-0.854618	-2.804533
H	2.969802	2.832814	1.317161
H	4.319956	-0.859277	2.847450
H	4.791313	1.461065	2.567040
H	2.345028	1.264108	0.706967
H	3.007685	-0.781542	1.844070

^{5}D' QM/MM-Optimized Active Site (QM Region E=-6766.54661367 Eh, $\langle S^2 \rangle$ = 6.00)

Fe	4.987427	-0.899801	0.319911
O	3.629396	-0.810650	-0.613992
O	5.535840	2.833547	0.277074
N	3.909056	-0.490449	2.043293
C	3.802685	0.976819	2.315039
C	3.074687	1.363141	3.613701
O	1.946098	0.755257	3.902751
C	3.099471	1.665368	1.122787
Se	3.981715	3.353961	0.648140
O	3.570273	2.330661	4.263525
C	10.990024	-1.648017	2.725992
C	9.806369	-0.905348	3.379735
C	8.706430	-0.492107	2.464259
C	7.454742	-1.025626	2.286993
N	8.762694	0.593823	1.584895
C	7.573408	0.676503	0.921037
N	6.754503	-0.285571	1.337024
C	6.020997	-6.343993	3.859997
C	5.014479	-6.431445	2.688942
C	5.117692	-5.261148	1.756628
C	4.561442	-3.995187	1.755671
N	6.069822	-5.210993	0.743348
C	6.075900	-3.955195	0.198686
N	5.176041	-3.184788	0.796590
C	10.368039	-1.604001	-2.905001
C	9.026065	-1.902574	-3.609195
C	7.782033	-1.575820	-2.847563
C	7.496770	-1.417460	-1.510738
N	6.558756	-1.373898	-3.489297
C	5.601020	-1.119170	-2.555779
N	6.143852	-1.119435	-1.345765
H	11.444195	-1.002739	1.970103
H	10.713247	-2.649132	2.311494
H	11.737818	-1.835959	3.492836
H	9.387521	-1.556879	4.152365
H	10.212526	-0.037356	3.913222
H	9.579630	1.160094	1.390960
H	6.998030	-1.834494	2.833560
H	7.330540	1.431265	0.193308
H	7.025213	-6.244839	3.449000
H	5.938791	-7.179360	4.604147
H	5.768930	-5.445384	4.416055
H	5.190515	-7.375018	2.158326
H	4.007304	-6.490117	3.111867
H	6.715806	-5.966222	0.499586
H	3.717511	-3.645090	2.328318
H	6.761010	-3.694866	-0.590004
H	10.643140	-2.470537	-2.283678
H	10.363383	-0.616650	-2.378686
H	11.099714	-1.504170	-3.702462
H	9.022951	-1.340243	-4.551487
H	9.031767	-2.963662	-3.893775
H	6.349907	-1.469659	-4.483212
H	8.165560	-1.518385	-0.672921
H	4.558427	-0.949355	-2.761889
H	2.046615	1.886320	1.318929
H	4.298161	-0.954086	2.866732
H	4.829419	1.333578	2.408201
H	3.160326	1.015458	0.238042
H	2.979724	-0.887915	1.866912

^{2}NO QM-Optimized Structure (E=-129.939747427 Eh)

N	0.000000	0.000000	-0.611833
O	0.000000	0.000000	0.535353

$^{3}O_2$ QM-Optimized Structure (E=-150.382047430 Eh)

O	0.000000	0.000000	0.604043
O	0.000000	0.000000	-0.604043