Supplementary Information for

Sulfur K-edge XAS and DFT Calculations on Nitrile Hydratase: Geometric and Electronic Structure of the Non-heme Iron Active Site

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Complete Reference 47

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Optimized Coordinates

(**1**) Fe(III)(ADIT)$_2$

C	5.416480	5.340387	9.164817
C	5.567788	5.423677	7.679549
C	6.494733	6.454528	7.090311
C	4.921914	4.566591	5.505796
C	3.540248	4.189993	4.986911
C	0.910781	3.782488	9.059984
C	1.268113	2.331036	9.080983
C	0.304906	1.344856	9.688214
C	2.875602	0.601209	8.551481
C	4.397679	0.599791	8.605946
N	3.063049	2.996152	5.743854
N	4.862843	4.585210	6.978195
N	2.418258	2.003693	8.568196
N	4.903750	1.595880	7.617597
S	4.629732	3.764852	9.688394
S	1.983697	4.745724	7.920864
Fe	3.640968	3.295418	7.777168
H	4.779125	6.179723	9.495248
H	6.387574	5.457709	9.666765
H	6.930983	7.080214	7.876796
H	5.967186	7.114483	6.385469
H	7.319454	5.976906	6.539042
H	5.239190	5.529445	5.084102
H	5.666806	3.813054	5.197781
H	3.557722	4.013880	3.901681
H	2.832766	5.003202	5.194780

H	1.022442	4.181786	10.083565
H	-0.143113	3.921027	8.778207
H	-0.605380	1.848638	10.031451
H	0.751373	0.827480	10.551220
H	0.014687	0.573781	8.958240
H	2.466849	0.019686	9.388671
H	2.521647	0.127496	7.619875
H	4.799940	-0.407636	8.424747
H	4.735696	0.935272	9.594939
H	3.369759	2.136418	5.276302
H	2.038403	2.988426	5.748117
H	4.978443	1.162034	6.691208
H	5.847198	1.890273	7.887609

(**2**) Fe(III)(ADIT)(ADIT-O)

H	-1.363045	-2.890914	-5.571435
H	-1.752508	-1.180992	-5.247823
C	-1.403833	-2.119556	-4.789919
H	0.632046	-1.371426	-4.835617
C	-3.472152	-3.088387	-4.016232
C	-0.041496	-1.900882	-4.144764
H	0.425849	-2.865590	-3.897825
N	-2.367185	-2.478903	-3.724293
C	-4.490396	-3.286424	-2.957654
O	-1.698929	1.091803	-3.113137
H	-0.533704	-0.130363	-3.100173
N	-0.257216	-1.132699	-2.888582
S	-2.826578	0.269535	-2.445031
H	0.608807	-1.092868	-2.343332
Fe	-1.967384	-1.821317	-1.967540
H	-1.345876	-4.353137	-1.500710
H	0.089773	-3.561879	-1.565493
S	-3.900336	-2.637926	-1.333864
N	-0.873514	-3.488842	-1.221547
C	-2.893345	0.839746	-0.660438
N	-1.551420	-1.097854	-0.220780
C	-0.878363	-3.374039	0.267448
C	-1.995966	0.037672	0.208160
H	-1.869915	-3.693212	0.612060
H	0.388399	-1.620813	0.387950
H	-0.119334	-4.017222	0.735874
C	-0.649199	-1.911049	0.619983
H	-0.816785	-1.726601	1.690072
H	-5.416211	-2.755305	-3.239578
H	-4.766323	-4.348447	-2.856915
H	-2.641292	1.909882	-0.660195
H	-3.943487	0.736752	-0.339216
H	-3.675614	-3.417563	-5.043550
H	-1.721573	0.401850	1.206948

(**3**) CoIII((η^2-SO)(SO_2)N_3(Pr,Pr))

C	1.991146	3.385327	2.163664
C	2.149987	2.666798	3.453502
C	-3.124389	3.173057	3.523622
C	-3.185172	2.269709	2.353120
H	1.350160	1.524872	4.814382

H	0.115512	-0.610895	4.026101
H	-2.224007	1.021463	1.172533
H	-1.295492	-0.763612	3.205344
Co	-0.459195	1.686996	2.937809
O	0.570475	1.270284	1.184593
O	-0.991055	4.034399	4.914283
O	-1.987165	1.775476	5.494972
S	0.446038	2.828203	1.321658
S	-1.567812	2.762593	4.473060
N	1.185106	1.940469	3.892264
N	-2.140279	1.594420	2.019712
N	-0.751567	-0.123516	3.787854
H	-1.284081	0.069815	4.651394
H	-3.045081	4.223824	3.200260
H	-3.986641	3.074570	4.197758
H	1.889140	4.471176	2.335558
H	2.844655	3.233867	1.486103
H	3.079291	2.772469	4.023988
H	-4.105138	2.193375	1.763553

(**4**) Fe(ADIT)(ADIT-O-$ZnCl_3$)

H	1.472606	2.663736	-3.723373
H	1.250850	0.083909	-3.085569
H	-0.133315	3.055112	-3.035388
C	0.932343	2.895545	-2.797612
Cl	-2.639519	1.831689	-2.579701
H	2.789085	0.748262	-2.526380
H	1.332709	3.835075	-2.385124
C	1.759404	0.519152	-2.209428
C	1.044116	1.768946	-1.809926
Cl	-5.856349	0.069039	-1.219304
Zn	-4.068817	1.309760	-0.839403
S	1.793716	-0.736894	-0.864654
H	-0.772155	-2.969600	-0.466994
H	-1.273909	2.902696	-0.767938
N	0.495186	1.793354	-0.631961
H	0.176017	3.904234	-0.472577
S	-1.414121	-0.634094	-0.474446
C	-0.316845	2.956299	-0.213682
O	-2.694790	-0.092574	0.232399
C	-1.238280	-2.319235	0.292848
Cl	-3.922477	2.839341	0.866127
H	-2.264223	-2.675548	0.464068
Fe	0.431974	0.258458	0.548580
C	-0.569656	2.867274	1.280901
H	2.750212	1.232798	1.298132
H	-1.835543	1.213819	1.248189
H	-1.422671	3.506150	1.553786
C	-0.418192	-2.321179	1.543485
N	-0.871629	1.443076	1.596683
H	0.317805	3.177512	1.856910
N	0.346151	-1.286717	1.742148
H	-0.997397	-4.350663	1.955569
H	3.055595	-0.939713	1.883804
N	1.986579	0.855920	1.865592

C	-0.534378	-3.502002	2.472483
H	1.717046	1.589651	2.528845
C	2.430760	-0.368448	2.582367
H	-0.924245	1.314901	2.612315
H	0.438960	-3.826285	2.865350
C	1.193677	-1.180954	2.943459
H	-1.174482	-3.250965	3.334290
H	1.488587	-2.161403	3.341485
H	3.026617	-0.139806	3.479446
H	0.616116	-0.670512	3.733214

CH_3SO^-

C -1.3780457326 -0.5196224867 0
S 0.4670169964 -0.3252520474 0
O 0.7619359749 1.2517309319 0
H -1.6324736329 -1.591638675 0
H -1.8335058567 -0.050220551 -0.8875861821
H -1.8335058567 -0.050220551 0.8875861821

CH_3SOH

C -1.2532 -0.6015 0.0000
O 0.2307 -0.3822 0.0000
H -1.3313 -1.6964 0.0000
H -1.7093 -0.1910 -0.9111
H -1.7093 -0.1910 0.9111
H 0.4231 0.5991 0.0000

$CH_3SO\text{-}C(NH_2)^+$

N -1.5685 1.0613 0.1731
C -2.2524 -0.0677 0.0095
N -3.5961 -0.0676 -0.0518
N -1.5623 -1.2064 -0.0763
H -4.1166 -0.9303 -0.1202
H -4.1204 0.7940 0.0047
H -2.0150 -2.0641 -0.3619
H -0.5214 -1.1041 -0.0941
H -2.0409 1.9482 0.2765
H -0.5194 0.9724 0.1433
C 3.3374 0.0666 0.9117
S 2.3105 0.1195 -0.5894
O 0.7887 -0.0344 0.0054
H 4.3839 0.1601 0.6042
H 3.2034 -0.8809 1.4407
H 3.0877 0.8906 1.5861

$CH_3SO_2^-$

C	-1.589229	-0.000252	0.113548
S	0.239246	0.000027	-0.385425
O	0.715552	1.280201	0.300918
H	-2.074690	-0.909166	-0.277422
H	-2.074732	0.908966	-0.276663
H	-1.583930	-0.000712	1.215188
O	0.716017	-1.279954	0.300922

CH_3SO_2H

C	-1.253198	-0.601545	0.000000

S	0.528325	-0.338219	0.000000
O	1.725233	-1.313492	0.000000
O	0.766213	1.354375	0.000000
H	-1.331282	-1.696421	0.000000
H	-1.709315	-0.190981	-0.911121
H	-1.709315	-0.190981	0.911121
H	1.743654	1.445710	0.000000

NHase-NO optimized in gas phase

N	27.895401	78.897970	55.472124
N	29.653306	79.612015	56.763005
C	28.346000	79.649000	56.463000
N	29.170732	75.991510	58.712687
C	27.965000	75.425000	59.004000
N	27.556381	75.641406	60.330356
N	27.273316	74.799752	58.103292
H	26.761118	75.070216	60.607160
H	28.318652	75.558239	61.004743
H	26.487389	74.285181	58.508158
H	27.386331	74.544679	56.492462
H	29.427437	76.823553	59.226336
H	29.539709	75.935439	57.752564
N	30.115582	73.774474	54.668329
O	30.178585	73.122209	55.637898
Fe	29.739869	74.892879	53.497295
N	28.946019	73.613312	52.268769
C	27.636715	73.064171	52.585149
C	26.733716	74.196622	53.037369
S	27.618416	75.197516	54.313613
O	27.287327	74.110637	55.557170
H	26.508137	74.899511	52.227048
H	25.813462	73.852632	53.524510
H	27.222487	72.569419	51.691409
H	27.703346	72.302562	53.382152
N	31.283011	74.719597	52.259675
C	31.157746	73.554018	51.377218
C	29.771741	72.938540	51.441394
O	29.454274	71.935207	50.778835
H	31.387974	73.822468	50.334540
H	31.885702	72.772692	51.652502
C	32.569844	76.760093	52.857029
C	32.442541	76.566583	54.362466
S	30.696773	76.495595	54.864714
C	32.348415	75.509458	52.001900
O	33.172777	75.265448	51.094366
O	30.240527	77.956443	54.675513
O	30.707171	76.115729	56.321057
H	31.883321	77.555035	52.526027
H	33.592303	77.089499	52.626603
H	32.887639	75.620828	54.705562
H	32.866376	77.403510	54.938807
C	28.833000	76.056000	50.400000
S	28.867503	76.631655	52.165306
N	27.529772	80.488826	57.151427
H	26.915403	78.650226	55.397492
H	28.629448	78.372913	54.921671

H	30.084033	80.455743	57.125271
H	30.211195	78.991215	56.127862
H	27.755288	80.684307	58.123891
H	26.543727	80.496055	56.920626
H	28.385884	76.882847	49.834012
H	28.234424	75.145819	50.287199
H	29.859377	75.880834	50.061444

NHase-NO optimized in PCM 4.0

N	2.7939	1.6427	2.1135
N	3.7166	2.7245	0.2944
C	3.8707	2.1698	1.5058
N	3.4997	-1.1812	-2.0138
C	4.2654	-1.9402	-1.2138
N	5.5334	-2.2662	-1.6150
N	3.8236	-2.3159	-0.0075
H	5.9353	-3.1294	-1.2357
H	5.7813	-2.0900	-2.5937
H	4.4370	-2.9086	0.5587
H	2.7652	-2.3084	0.2327
H	3.8449	-0.9117	-2.9378
H	2.6371	-0.6943	-1.6948
N	-0.8184	-1.2516	-1.4053
O	-0.5271	-1.9067	-2.3424
Fe	-1.1410	-0.2938	-0.1333
N	-2.4138	-1.5021	0.6674
C	-1.9380	-2.6605	1.4215
C	-0.7490	-2.2287	2.2716
S	0.4692	-1.2988	1.2118
O	1.2211	-2.4619	0.4151
H	-1.0493	-1.5252	3.0652
H	-0.1871	-3.0756	2.7026
H	-2.7605	-3.0528	2.0496
H	-1.6299	-3.4817	0.7383
N	-2.7765	0.5806	-0.8455
C	-3.9489	-0.2980	-0.7359
C	-3.6778	-1.4930	0.1799
O	-4.5583	-2.3516	0.4302
H	-4.8265	0.2643	-0.3634
H	-4.2504	-0.6945	-1.7299
C	-1.8888	2.8555	-1.3350
C	-0.6301	2.3521	-2.0462
S	0.3362	1.2326	-0.9650
C	-3.0485	1.8487	-1.2443
O	-4.2084	2.2464	-1.5363
O	0.9968	2.1958	0.0497
O	1.3725	0.5988	-1.8974
H	-1.6175	3.1983	-0.3179
H	-2.2840	3.7277	-1.8842
H	-0.8669	1.7715	-2.9553
H	0.0696	3.1675	-2.3081
C	-3.0477	1.0329	2.3722
S	-1.3022	1.1208	1.7925
N	5.0942	2.1087	2.0957

H 2.9052 0.9961 2.8985
H 1.9108 1.6193 1.5647
H 4.4540 3.2885 -0.1328
H 2.7687 2.6759 -0.1312
H 5.8505 2.6802 1.7074
H 5.1293 1.9804 3.1119
H -3.1132 1.6465 3.2876
H -3.3460 -0.0023 2.6002
H -3.7275 1.4483 1.6108