

Supporting Information

for

Solvation Effects on S K-edge XAS Spectra of Fe-S Proteins: Normal and Inverse Effects on WT and Mutant Rubredoxin

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Complete reference for Gaussian 03:

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

Derivation of the wavefunction coefficients:

We consider the bonding of one Fe 3d orbital $|Fe\rangle$ to three thiolate S and one alkoxide O orbital. The wavefunction of the Fe based orbital Ψ^*_{Fe} can be expressed as a linear combination of these orbitals:

$$\Psi^*_{Fe} = (c_{Fe}|Fe\rangle + c_S|S\rangle + c_S|S\rangle + c_S|S\rangle + c_O|O\rangle) \quad (S1)$$

The energy of Ψ^*_{Fe} (E^*_{Fe}) is obtained by solving the secular determinant (Eq. S2)

using relevant values of H_{FeFe} , H_{SS} , H_{OO} , H_{FeO} and H_{FeS} (see Table 6).

$$\begin{vmatrix} H_{FeFe} - E & H_{FeS} - ES_{FeS} & H_{FeS} - ES_{FeS} & H_{FeS} - ES_{FeS} & H_{FeO} - ES_{FeO} \\ H_{FeS} - ES_{FeS} & H_{SS} - E & 0 & 0 & 0 \\ H_{FeS} - ES_{FeS} & 0 & H_{SS} - E & 0 & 0 \\ H_{FeS} - ES_{FeS} & 0 & 0 & H_{SS} - E & 0 \\ H_{FeO} - ES_{FeO} & 0 & 0 & 0 & H_{OO} - E \end{vmatrix} = 0 \quad (S2)$$

Having calculated the value of E^*_{Fe} (the energy of the Fe d orbital after bonding),

the coefficients of the associated wavefunction, Ψ^*_{Fe} , can be calculated from the

secular equations of the variational principle:

$$c_{Fe}(H_{FeS} - E^*_{Fe}S_{FeS}) + c_S(H_{SS} - E^*_{Fe}) = 0 \quad (S3)$$

$$c_{Fe}(H_{FeO} - E^*_{Fe}S_{FeO}) + c_O(H_{OO} - E^*_{Fe}) = 0 \quad (S4)$$

and the normalization:

$$c_{\text{Fe}}^2 + 3c_{\text{S}}^2 + c_{\text{O}}^2 = 1 \quad (\text{S5})$$

Similarly, an FeS₄ molecule was calculated by replacing the alkoxide O with

another thiolate S in Eq. S1-5, i.e. the wavefunction of the Fe based orbital Ψ_{Fe}^*

for the FeS₄ model can be expressed as:

$$\Psi_{\text{Fe}}^* = (c_{\text{Fe}}|\text{Fe}\rangle + c_{\text{S}}|\text{S}\rangle + c_{\text{S}}|\text{S}\rangle + c_{\text{S}}|\text{S}\rangle + c_{\text{S}}|\text{S}\rangle) \quad (\text{S6})$$

and the determinant to obtain the energy of Ψ_{Fe}^* (E_{Fe}^*) becomes

$$\begin{vmatrix} H_{\text{FeFe}} - E & H_{\text{FeS}} - ES_{\text{FeS}} & H_{\text{FeS}} - ES_{\text{FeS}} & H_{\text{FeS}} - ES_{\text{FeS}} & H_{\text{FeS}} - ES_{\text{FeS}} \\ H_{\text{FeS}} - ES_{\text{FeS}} & H_{\text{SS}} - E & 0 & 0 & 0 \\ H_{\text{FeS}} - ES_{\text{FeS}} & 0 & H_{\text{SS}} - E & 0 & 0 \\ H_{\text{FeS}} - ES_{\text{FeS}} & 0 & 0 & H_{\text{SS}} - E & 0 \\ H_{\text{FeS}} - ES_{\text{FeS}} & 0 & 0 & 0 & H_{\text{SS}} - E \end{vmatrix} = 0 \quad (\text{S7})$$

The coefficients again can be calculated using the variational principal:

$$c_{\text{Fe}}(H_{\text{FeS}} - E_{\text{Fe}}^* S_{\text{FeS}}) + c_{\text{S}}(H_{\text{SS}} - E_{\text{Fe}}^*) = 0 \quad (\text{S8})$$

and normalization:

$$c_{\text{Fe}}^2 + 4c_{\text{S}}^2 = 1 \quad (\text{S9})$$

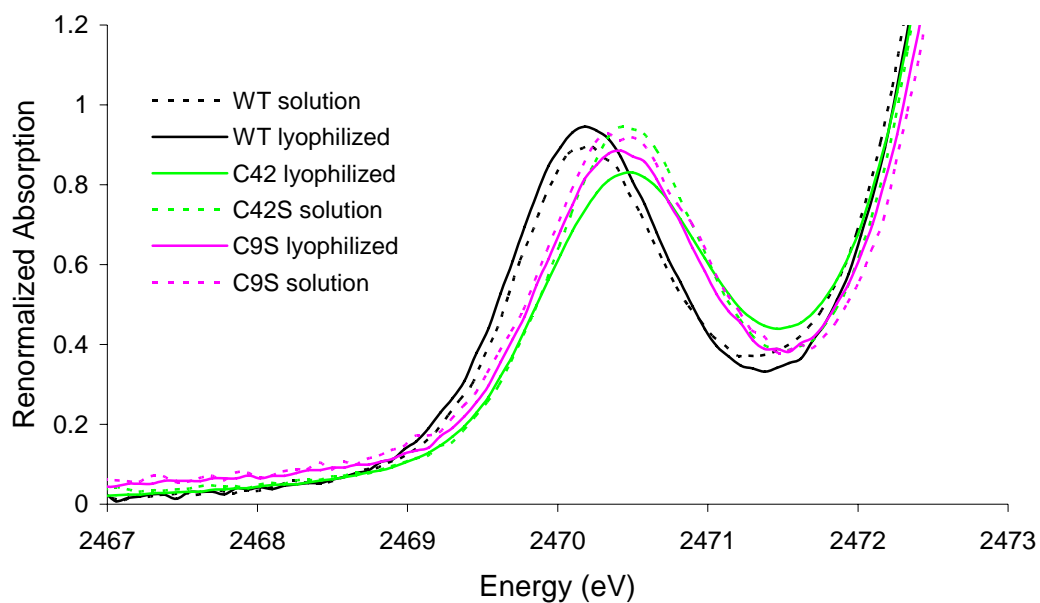


Figure S1. Comparison of S K-edge data for surface mutants and WT Rd with and without solvent.

Table S1. Calculated Fe-S-C-C dihedral angles of WT Rd and C42S with and without water.

	C42	C9	C6	C39
WT	85.8°	87.0°	167.2°	172.7°
WT+2water	87.6°	87.0°	167.7°	171.6°
C42S	-	89.6°	169.9°	168.8°
C42S+2water	-	88.8°	169.5°	170.6°

Optimized geometries:WT (Fe^{III})

C	5.41466	4.33904	3.28523
C	4.84132	2.95776	3.48556
O	5.17543	2.24277	4.43652
H	4.87979	4.94074	2.53068
H	6.47024	4.24876	2.97186
H	5.40552	4.87542	4.24822
N	3.92348	2.55103	2.54408
C	3.51019	1.14782	2.51810
C	4.68175	0.30295	1.97673
O	5.08432	0.45709	0.81185
C	2.29688	1.01348	1.59391
S	1.73090	-0.73683	1.48737
H	3.89344	3.04089	1.64636
H	3.25358	0.85392	3.54982
H	1.47237	1.64649	1.96299
H	2.58811	1.36572	0.58776
N	5.24695	-0.60568	2.82274
C	6.37735	-1.42470	2.38356
C	6.02663	-2.53321	1.35703
O	6.92232	-3.11654	0.73435
H	5.01922	-0.53717	3.81460
H	7.14333	-0.79218	1.90349
H	6.82865	-1.89827	3.27122
N	4.69218	-2.82187	1.24910
C	4.22012	-3.72116	0.20648
C	4.22127	-3.11942	-1.21507
O	4.68332	-3.75396	-2.16571
H	4.00841	-2.20047	1.69308
H	4.88223	-4.59860	0.16065
H	3.19745	-4.04897	0.46617
N	3.66571	-1.86495	-1.35604
C	3.53129	-1.30084	-2.69230
C	4.29866	0.00547	-2.96159
O	4.40413	0.42242	-4.12126
C	2.06922	-1.09711	-3.13372
S	1.20160	0.26771	-2.22405
H	3.16666	-1.44161	-0.56294
H	3.97248	-2.06290	-3.36201
H	2.07244	-0.79256	-4.19229
H	1.50939	-2.04052	-3.02239
N	4.76563	0.68705	-1.88111
C	5.42837	1.96168	-2.05258

C	4.56000	3.22369	-1.89782
O	5.07832	4.33522	-2.04666
H	4.73419	0.28664	-0.93882
H	6.25660	2.05069	-1.32887
H	5.85265	1.99705	-3.07045
N	3.24005	3.06499	-1.54861
C	2.38125	4.25006	-1.52987
H	2.79882	2.15040	-1.72286
H	2.96876	5.09335	-1.13629
H	1.50665	4.05837	-0.88657
H	2.02706	4.52346	-2.54274
C	-5.75707	0.07337	4.71469
C	-5.20377	0.94371	3.59735
O	-5.72522	2.00455	3.21707
H	-5.64577	-1.00476	4.50302
H	-6.82411	0.30158	4.85863
H	-5.22530	0.29120	5.65891
N	-4.01302	0.47126	3.09411
C	-3.34529	1.16153	1.99671
C	-4.32077	1.31528	0.81211
O	-4.89753	0.31968	0.32126
C	-2.12577	0.33128	1.57449
S	-1.23432	1.12621	0.17154
H	-3.79714	-0.52157	3.21093
H	-3.01736	2.14966	2.35937
H	-1.43394	0.21835	2.42756
H	-2.47117	-0.67149	1.26576
N	-4.50485	2.56275	0.30343
C	-5.51495	2.74223	-0.74959
C	-5.10319	2.14997	-2.10988
O	-5.97357	1.96249	-2.96298
C	-5.73217	4.27584	-0.78942
C	-4.39686	4.84737	-0.27062
C	-3.98441	3.84535	0.82478
H	-6.43511	2.20087	-0.47437
H	-6.00436	4.61964	-1.80025
H	-6.55537	4.54492	-0.10290
H	-3.64330	4.84658	-1.07889
H	-4.48273	5.87628	0.11791
H	-2.89067	3.79726	0.95912
H	-4.46447	4.06668	1.79764
N	-3.76488	1.91801	-2.31449
C	-3.32800	1.23424	-3.52774
C	-3.38825	-0.31004	-3.47531

O	-3.88820	-0.97623	-4.38903
H	-3.13138	1.93696	-1.50719
H	-3.99009	1.54284	-4.34971
H	-2.29001	1.54139	-3.75383
N	-2.81100	-0.88921	-2.36497
C	-2.70256	-2.33639	-2.29892
C	-3.57969	-3.03088	-1.24768
O	-3.60734	-4.26579	-1.21917
C	-1.26272	-2.85925	-2.13861
S	-0.58174	-2.60204	-0.43253
H	-2.33293	-0.30507	-1.66639
H	-3.07762	-2.68637	-3.28036
H	-1.28153	-3.95016	-2.28518
H	-0.60501	-2.39502	-2.89134
N	-4.25642	-2.25667	-0.35576
C	-5.19574	-2.87054	0.56497
C	-4.63418	-3.50190	1.85233
O	-5.40549	-4.09914	2.61224
H	-4.29035	-1.23273	-0.43695
H	-5.91871	-2.09781	0.87390
H	-5.74834	-3.67868	0.05459
N	-3.30004	-3.31150	2.13924
C	-2.71715	-4.02793	3.27678
H	-2.67914	-3.07653	1.35502
H	-3.48440	-4.09373	4.06270
H	-1.83477	-3.48034	3.64706
H	-2.41112	-5.05625	3.00413
Fe	0.30024	-0.53895	-0.32066
WT+2water (Fe ^{III})			
C	5.38167	3.28046	4.40724
C	4.82106	1.89482	4.20703
O	5.16632	0.94013	4.91081
H	4.83206	4.06823	3.86440
H	6.43349	3.29580	4.06933
H	5.38227	3.51610	5.48400
N	3.89975	1.76528	3.19137
C	3.50360	0.42195	2.76973
C	4.67752	-0.21975	2.00041
O	5.07150	0.26596	0.92688
C	2.27563	0.54419	1.86358
S	1.76888	-1.09258	1.18855
H	3.86958	2.48734	2.46703
H	3.26514	-0.15644	3.67811
H	1.43524	0.99348	2.41831

H	2.53232	1.20514	1.01621
N	5.25359	-1.32738	2.54926
C	6.38811	-1.97876	1.89193
C	6.04163	-2.74939	0.59092
O	6.93942	-3.11802	-0.17518
H	5.03419	-1.54466	3.52147
H	7.14786	-1.22943	1.61181
H	6.84509	-2.68279	2.60687
N	4.71198	-3.00732	0.40631
C	4.23049	-3.58158	-0.84182
C	4.22959	-2.59835	-2.03301
O	4.69082	-2.92020	-3.13059
H	4.02607	-2.57149	1.02865
H	4.88874	-4.41244	-1.13710
H	3.21156	-3.96994	-0.65665
N	3.67284	-1.35489	-1.80863
C	3.53938	-0.43954	-2.93215
C	4.27748	0.90510	-2.81503
O	4.36588	1.63830	-3.80791
C	2.07748	-0.15059	-3.31888
S	1.18909	0.87682	-2.05413
H	3.18661	-1.16946	-0.92201
H	4.00185	-0.97608	-3.78247
H	2.07294	0.44483	-4.24538
H	1.53284	-1.09517	-3.48121
N	4.73881	1.25438	-1.58475
C	5.39116	2.53046	-1.38059
C	4.51442	3.68320	-0.86057
O	5.01755	4.79982	-0.70169
H	4.72493	0.59481	-0.80072
H	6.22449	2.40922	-0.66764
H	5.80663	2.86663	-2.34565
N	3.20176	3.41935	-0.56009
C	2.32404	4.54426	-0.22399
H	2.78385	2.56093	-0.94079
H	2.89772	5.47037	-0.38214
H	1.99758	4.49952	0.83239
H	1.42655	4.52582	-0.86841
C	-5.74571	-1.32353	4.58429
C	-5.20755	-0.16523	3.75985
O	-5.73813	0.95575	3.70216
H	-5.61653	-2.29713	4.07940
H	-6.81624	-1.16229	4.78269
H	-5.21694	-1.37046	5.55379

N	-4.01589	-0.46347	3.13689
C	-3.35898	0.52033	2.28424
C	-4.34087	1.00005	1.19493
O	-4.91125	0.17840	0.44309
C	-2.13725	-0.14772	1.63900
S	-1.21930	1.03739	0.56691
H	-3.79815	-1.44626	2.95524
H	-3.03624	1.36400	2.91663
H	-1.45769	-0.52558	2.42311
H	-2.48554	-1.00085	1.03054
N	-4.53572	2.33908	1.06594
C	-5.55326	2.80542	0.11148
C	-5.14375	2.63116	-1.36238
O	-6.01837	2.68212	-2.23060
C	-5.78693	4.28207	0.51703
C	-4.45787	4.69447	1.18167
C	-4.02921	3.42208	1.93794
H	-6.46614	2.19704	0.22100
H	-6.06380	4.90001	-0.35218
H	-6.61263	4.33254	1.24991
H	-3.70533	4.94219	0.41131
H	-4.55732	5.56272	1.85489
H	-2.93448	3.35375	2.05267
H	-4.50849	3.34322	2.93292
N	-3.81050	2.47302	-1.63310
C	-3.37362	2.18318	-2.99448
C	-3.42065	0.68788	-3.38087
O	-3.91552	0.29485	-4.44363
H	-3.14965	2.34940	-0.86031
H	-4.05389	2.70057	-3.68692
H	-2.34670	2.57933	-3.11656
N	-2.83975	-0.18383	-2.48027
C	-2.72325	-1.58804	-2.83108
C	-3.59153	-2.56788	-2.02730
O	-3.59012	-3.76156	-2.34895
C	-1.28139	-2.12536	-2.81754
S	-0.63688	-2.33441	-1.08971
H	-2.38902	0.17755	-1.63178
H	-3.09222	-1.64151	-3.87427
H	-1.28595	-3.13435	-3.25701
H	-0.61654	-1.46287	-3.39464
N	-4.28201	-2.08768	-0.95864
C	-5.19768	-2.95289	-0.23690
C	-4.61301	-3.91212	0.81809

O	-5.36961	-4.71600	1.37441
H	-4.32956	-1.08293	-0.74686
H	-5.92673	-2.30925	0.28202
H	-5.74611	-3.59523	-0.94772
N	-3.28105	-3.79907	1.14405
C	-2.67853	-4.81206	2.02462
H	-2.66912	-3.33449	0.46309
H	-3.05046	-5.81849	1.76471
H	-2.93882	-4.61887	3.08059
H	-1.58335	-4.77563	1.90314
Fe	0.27350	-0.39302	-0.43114
O	-0.35617	3.72693	-2.52106
H	0.07066	2.83797	-2.43718
H	0.06209	4.08545	-3.33076
O	1.03648	-4.42333	0.94049
H	0.59137	-4.10646	0.12114
H	1.12977	-3.59754	1.46426
C42S (Fe ^{III})			
C	5.38638	4.09906	3.53677
C	4.81304	2.69955	3.65685
O	5.15368	1.93862	4.56412
H	4.83790	4.74807	2.83310
H	6.43531	4.02667	3.19816
H	5.39341	4.56707	4.53440
N	3.89398	2.33915	2.69263
C	3.48328	0.93472	2.56602
C	4.67027	0.13737	1.98752
O	5.07960	0.36544	0.84191
C	2.28391	0.84900	1.60896
S	1.68908	-0.88944	1.37662
H	3.85247	2.89065	1.83178
H	3.21194	0.57105	3.57156
H	1.45562	1.46481	1.99835
H	2.59636	1.25879	0.63130
N	5.23656	-0.81654	2.78190
C	6.37695	-1.59885	2.30327
C	6.03732	-2.64727	1.21084
O	6.93376	-3.18972	0.56271
H	4.99891	-0.81218	3.77384
H	7.14023	-0.93340	1.86524
H	6.82746	-2.12099	3.16355
N	4.70337	-2.93003	1.07868
C	4.23536	-3.77011	-0.01259
C	4.23212	-3.08943	-1.40063

O	4.70488	-3.66783	-2.37554
H	4.01731	-2.33674	1.55615
H	4.90241	-4.63973	-0.10967
H	3.21605	-4.11975	0.23131
N	3.65634	-1.83822	-1.47334
C	3.52882	-1.18462	-2.77042
C	4.30550	0.13363	-2.95703
O	4.41187	0.61354	-4.08679
C	2.06868	-0.93511	-3.19809
S	1.21613	0.38989	-2.21744
H	3.16883	-1.45585	-0.65095
H	3.96468	-1.90042	-3.49211
H	2.07687	-0.57268	-4.23809
H	1.49542	-1.87575	-3.14828
N	4.77070	0.75042	-1.83749
C	5.42883	2.03693	-1.92803
C	4.55235	3.28554	-1.70488
O	5.06335	4.40252	-1.78729
H	4.73941	0.29530	-0.91992
H	6.24921	2.08563	-1.19186
H	5.86363	2.13721	-2.93701
N	3.23324	3.10047	-1.36982
C	2.36541	4.27591	-1.28371
H	2.79651	2.19559	-1.59888
H	2.92757	5.08974	-0.80066
H	1.47168	4.02480	-0.68904
H	2.04422	4.63003	-2.28229
C	-5.76966	-0.29052	4.68619
C	-5.22075	0.64689	3.61783
O	-5.74273	1.72426	3.30298
H	-5.60720	-1.35427	4.43993
H	-6.84886	-0.11074	4.80734
H	-5.27432	-0.08299	5.65216
N	-4.02748	0.21019	3.08551
C	-3.36685	0.97944	2.03628
C	-4.34334	1.18760	0.86130
O	-4.90028	0.21349	0.31677
C	-2.12571	0.21717	1.55535
S	-1.21456	1.19499	0.28127
H	-3.81177	-0.78844	3.13286
H	-3.06283	1.94830	2.46498
H	-1.45236	0.01675	2.40732
H	-2.44041	-0.74601	1.11623
N	-4.54110	2.46063	0.42872

C	-5.54208	2.69518	-0.62001
C	-5.11369	2.18345	-2.00745
O	-5.97548	2.03904	-2.86980
C	-5.76929	4.22685	-0.57417
C	-4.43967	4.77547	-0.01726
C	-4.02372	3.71476	1.01986
H	-6.46122	2.13273	-0.38645
H	-6.03824	4.62633	-1.56520
H	-6.59774	4.45106	0.12201
H	-3.68354	4.82806	-0.82142
H	-4.53425	5.77913	0.43063
H	-2.92970	3.66216	1.14889
H	-4.50314	3.88130	2.00374
N	-3.77391	1.96803	-2.21845
C	-3.32952	1.35347	-3.46641
C	-3.38922	-0.19548	-3.50369
O	-3.87342	-0.80313	-4.45786
H	-3.13932	1.95900	-1.41121
H	-3.98430	1.70860	-4.27547
H	-2.28976	1.67209	-3.66684
N	-2.82111	-0.81771	-2.41068
C	-2.61375	-2.25695	-2.36818
C	-3.54082	-3.03884	-1.41963
O	-3.58573	-4.26947	-1.48300
C	-1.14655	-2.59232	-1.99384
O	-0.78300	-2.00321	-0.76317
H	-2.32749	-0.25211	-1.70989
H	-2.81993	-2.64323	-3.38242
H	-1.06519	-3.69489	-1.91999
H	-0.49445	-2.24193	-2.82118
N	-4.22202	-2.32009	-0.48142
C	-5.18306	-2.97836	0.38260
C	-4.63207	-3.67678	1.63769
O	-5.39417	-4.33272	2.34669
H	-4.27096	-1.29377	-0.52292
H	-5.91063	-2.22276	0.72146
H	-5.72697	-3.75936	-0.17728
N	-3.30320	-3.48446	1.95182
C	-2.70783	-4.28849	3.02162
H	-2.69673	-3.14660	1.19881
H	-3.49287	-4.48606	3.76659
H	-1.87213	-3.73788	3.48496
H	-2.33231	-5.25990	2.64622
Fe	0.21133	-0.50470	-0.39727

C42S+water (Fe^{III})

C	5.49306	4.39259	3.31340
C	4.90572	3.00913	3.53570
O	5.24424	2.31431	4.49496
H	4.97204	4.98251	2.54036
H	6.55167	4.28555	3.01766
H	5.47168	4.94387	4.26749
N	3.97478	2.59299	2.60239
C	3.53726	1.18962	2.56465
C	4.71462	0.33352	2.05189
O	5.13211	0.47795	0.89629
C	2.34309	1.06844	1.59806
S	1.72382	-0.67283	1.45181
H	3.94579	3.08432	1.70533
H	3.24713	0.89723	3.58819
H	1.51992	1.71469	1.94659
H	2.67028	1.42088	0.60332
N	5.26335	-0.57298	2.91202
C	6.40092	-1.39617	2.49439
C	6.05642	-2.51835	1.47781
O	6.94805	-3.10759	0.86462
H	5.02739	-0.49334	3.90135
H	7.16985	-0.76859	2.01283
H	6.84414	-1.85796	3.39211
N	4.72053	-2.80220	1.37241
C	4.23581	-3.70933	0.34409
C	4.23642	-3.12373	-1.08550
O	4.69712	-3.77232	-2.02000
H	4.04437	-2.17910	1.82298
H	4.89080	-4.59249	0.30331
H	3.21378	-4.02939	0.61509
N	3.67914	-1.87170	-1.24730
C	3.55555	-1.32233	-2.59223
C	4.32826	-0.02085	-2.87432
O	4.43802	0.37746	-4.03398
C	2.10052	-1.13572	-3.06194
S	1.22321	0.30028	-2.26417
H	3.20519	-1.41963	-0.45347
H	4.00424	-2.09111	-3.24935
H	2.10494	-0.91124	-4.13962
H	1.52462	-2.05976	-2.89445
N	4.79482	0.67595	-1.80167
C	5.47593	1.93936	-1.99363
C	4.61897	3.21216	-1.85891

O	5.14188	4.31510	-2.01700
H	4.77842	0.28312	-0.85553
H	6.30172	2.02987	-1.26750
H	5.90530	1.95499	-3.00992
N	3.29702	3.06371	-1.50988
C	2.44573	4.25388	-1.49175
H	2.84959	2.15512	-1.69656
H	3.00740	5.07939	-1.02812
H	1.53526	4.03878	-0.90865
H	2.15334	4.57361	-2.51061
C	-5.70055	0.21637	4.83345
C	-5.14646	1.06888	3.69772
O	-5.66101	2.12589	3.30847
H	-5.57978	-0.86484	4.64584
H	-6.76968	0.44121	4.96653
H	-5.17429	0.46119	5.77392
N	-3.96068	0.57840	3.19174
C	-3.29230	1.25038	2.08176
C	-4.27664	1.39641	0.90394
O	-4.85174	0.39501	0.43468
C	-2.07810	0.41584	1.64395
S	-1.21978	1.22670	0.22176
H	-3.75584	-0.41649	3.31541
H	-2.95417	2.23983	2.43110
H	-1.36675	0.31276	2.48163
H	-2.41998	-0.59152	1.34693
N	-4.46308	2.63861	0.38360
C	-5.47635	2.81465	-0.66698
C	-5.06560	2.21115	-2.02193
O	-5.92687	1.99757	-2.86968
C	-5.68855	4.34873	-0.71692
C	-4.34645	4.91825	-0.21422
C	-3.92943	3.92431	0.88670
H	-6.39741	2.27715	-0.38726
H	-5.96823	4.68755	-1.72743
H	-6.50473	4.62430	-0.02493
H	-3.59979	4.90849	-1.02886
H	-4.42539	5.95048	0.16648
H	-2.83471	3.87021	1.01014
H	-4.39828	4.15861	1.86156
N	-3.72653	1.98736	-2.23924
C	-3.33741	1.26350	-3.44293
C	-3.41646	-0.27759	-3.34084
O	-3.86342	-0.97379	-4.25951

H	-3.08137	2.00771	-1.44018
H	-4.01565	1.55955	-4.25634
H	-2.30188	1.54105	-3.71493
N	-2.88684	-0.82237	-2.19800
C	-2.67597	-2.26088	-2.11416
C	-3.55436	-2.97902	-1.07673
O	-3.59382	-4.21975	-1.04396
C	-1.17306	-2.58129	-1.93767
O	-0.64002	-2.04032	-0.73526
H	-2.41617	-0.21627	-1.51188
H	-2.98504	-2.67086	-3.09357
H	-1.05659	-3.68299	-1.92347
H	-0.64955	-2.18468	-2.83054
N	-4.25340	-2.21036	-0.20920
C	-5.18079	-2.82082	0.72542
C	-4.60481	-3.41238	2.02664
O	-5.38032	-3.98763	2.78956
H	-4.28226	-1.18480	-0.28493
H	-5.91732	-2.05469	1.01747
H	-5.71877	-3.64708	0.22975
N	-3.27095	-3.20738	2.30599
C	-2.68969	-3.92357	3.44573
H	-2.61958	-3.21079	1.50266
H	-3.29235	-3.72762	4.34696
H	-1.65947	-3.56664	3.59314
H	-2.66531	-5.01588	3.27749
Fe	0.25936	-0.46629	-0.35940
O	-0.61080	-0.86420	-4.96117
H	-0.36462	-0.26533	-4.22230
H	-1.58868	-0.92543	-4.95883
O	-1.19130	-4.29841	0.70664
H	-1.87298	-4.63643	0.08244
H	-0.80733	-3.49729	0.26195
C39S (Fe ^{III})			
C	5.47059	4.23403	3.35075
C	4.88877	2.84858	3.51825
O	5.21603	2.11131	4.44909
H	4.95815	4.84486	2.58834
H	6.53480	4.14447	3.06899
H	5.43268	4.75809	4.31998
N	3.96463	2.47342	2.56759
C	3.52720	1.07723	2.51152
C	4.68529	0.23339	1.93441
O	5.09415	0.41988	0.78038

C	2.28466	0.98333	1.61765
S	1.64992	-0.74445	1.52853
H	3.94386	2.98190	1.67984
H	3.28828	0.76338	3.54157
H	1.50360	1.65037	2.02051
H	2.55504	1.32488	0.60160
N	5.23995	-0.70564	2.75398
C	6.36608	-1.52030	2.29658
C	6.00845	-2.59729	1.23803
O	6.89804	-3.16759	0.60410
H	4.99949	-0.67609	3.74464
H	7.13683	-0.87986	1.83508
H	6.81220	-2.02082	3.17188
N	4.67025	-2.86495	1.12133
C	4.17480	-3.72946	0.06072
C	4.17467	-3.09198	-1.34901
O	4.64199	-3.70969	-2.30213
H	3.99794	-2.25847	1.60111
H	4.82204	-4.61606	-0.01440
H	3.14889	-4.04638	0.32083
N	3.60662	-1.83377	-1.44097
C	3.40788	-1.18991	-2.73691
C	4.24440	0.08837	-3.00200
O	4.39469	0.51778	-4.14919
C	1.91917	-0.89751	-3.04212
S	1.10043	0.41696	-2.00200
H	3.10697	-1.46165	-0.62232
H	3.74855	-1.92949	-3.48556
H	1.85337	-0.52677	-4.07777
H	1.34990	-1.83715	-2.95678
N	4.71804	0.73338	-1.90004
C	5.42933	1.98745	-2.02769
C	4.58824	3.26450	-1.84277
O	5.11372	4.36976	-1.97807
H	4.67992	0.30277	-0.97072
H	6.25024	2.02635	-1.29144
H	5.86717	2.04247	-3.03884
N	3.27144	3.11248	-1.48235
C	2.41798	4.29657	-1.45261
H	2.82176	2.19893	-1.63866
H	3.01269	5.14307	-1.07674
H	1.55633	4.11246	-0.78924
H	2.04026	4.56318	-2.45887
C	-5.73529	0.03760	4.71640

C	-5.16425	0.94004	3.61370
O	-5.69099	2.00608	3.26850
H	-5.66250	-1.03405	4.46057
H	-6.79201	0.29934	4.87490
H	-5.18660	0.20404	5.66108
N	-3.97421	0.46752	3.09444
C	-3.26621	1.10207	1.97713
C	-4.25477	1.33605	0.82340
O	-4.89036	0.38821	0.32722
C	-2.13003	0.12997	1.53636
O	-1.38588	0.58750	0.43132
H	-3.76054	-0.52082	3.24924
H	-2.82507	2.05217	2.32244
H	-1.47468	-0.02354	2.42431
H	-2.62043	-0.84285	1.31313
N	-4.39171	2.60279	0.33376
C	-5.44178	2.83675	-0.67583
C	-5.08140	2.28007	-2.06834
O	-5.96349	2.12447	-2.90955
C	-5.63910	4.37427	-0.65442
C	-4.29425	4.91377	-0.12486
C	-3.87806	3.86116	0.91950
H	-6.35841	2.29794	-0.38414
H	-5.91437	4.76263	-1.64820
H	-6.45410	4.62588	0.04781
H	-3.54962	4.94800	-0.94098
H	-4.37084	5.92415	0.31113
H	-2.78519	3.81522	1.05890
H	-4.36060	4.03252	1.90095
N	-3.74539	2.04129	-2.29443
C	-3.31130	1.37850	-3.51852
C	-3.39602	-0.16524	-3.49520
O	-3.91142	-0.79614	-4.41872
H	-3.12128	2.05110	-1.48417
H	-3.96523	1.71182	-4.33764
H	-2.26852	1.67625	-3.73424
N	-2.82069	-0.77843	-2.40015
C	-2.73217	-2.22932	-2.36385
C	-3.62334	-2.93812	-1.33556
O	-3.64941	-4.16820	-1.33511
C	-1.30089	-2.77784	-2.20948
S	-0.60745	-2.62173	-0.49622
H	-2.35433	-0.22933	-1.66906
H	-3.10568	-2.55488	-3.35369

H	-1.33600	-3.86078	-2.40407
H	-0.63416	-2.29616	-2.94291
N	-4.31113	-2.18824	-0.43382
C	-5.23497	-2.83441	0.47979
C	-4.65875	-3.49785	1.74589
O	-5.43117	-4.08285	2.50663
H	-4.34028	-1.16208	-0.47559
H	-5.95966	-2.07728	0.82103
H	-5.78911	-3.63080	-0.04723
N	-3.31805	-3.34929	2.01433
C	-2.73974	-4.05375	3.16178
H	-2.69467	-3.12000	1.22988
H	-3.48373	-4.05651	3.97268
H	-1.82242	-3.53515	3.48555
H	-2.49023	-5.10470	2.91964
Fe	0.06485	-0.48582	-0.17449
C6S (Fe ^{III})			
C	5.72881	3.93452	3.47969
C	4.53271	3.06843	3.83967
O	3.52051	3.51516	4.38973
H	6.66144	3.36020	3.34312
H	5.87909	4.69305	4.26440
H	5.51509	4.46793	2.53588
N	4.65434	1.76785	3.43023
C	3.57798	0.80138	3.50615
C	4.21995	-0.57240	3.16228
O	5.44013	-0.67573	2.98999
C	2.44185	1.26575	2.57538
O	2.02529	-0.90997	0.28576
H	5.54041	1.37612	3.09336
H	3.17231	0.75343	4.53770
H	2.82064	1.33209	1.53564
H	2.12874	2.26788	2.91484
N	3.37315	-1.64285	3.12590
C	3.89362	-3.00890	3.08430
C	4.32237	-3.63613	1.73250
O	5.07628	-4.61358	1.77664
H	2.37578	-1.46419	3.26581
H	4.79278	-3.06468	3.71940
H	3.12921	-3.67455	3.52254
N	3.79927	-3.11272	0.58610
C	4.07095	-3.77761	-0.68554
C	4.24832	-2.90253	-1.93562
O	4.77309	-3.38418	-2.94431

H	3.07730	-2.36587	0.61705
H	4.98432	-4.37913	-0.55703
H	3.25585	-4.48895	-0.93589
N	3.73336	-1.62082	-1.90190
C	3.62136	-0.89882	-3.16327
C	4.35863	0.44289	-3.24617
O	4.45396	1.01046	-4.33319
C	2.17052	-0.69343	-3.65121
S	1.17460	0.55831	-2.70494
H	3.19085	-1.30721	-1.07879
H	4.11584	-1.55489	-3.90547
H	2.21580	-0.30311	-4.68021
H	1.64463	-1.66262	-3.65436
N	4.84408	0.97101	-2.07614
C	5.53891	2.24873	-2.07527
C	4.69097	3.50592	-1.77734
O	5.21809	4.62100	-1.79378
H	4.78567	0.40422	-1.22969
H	6.36502	2.22975	-1.34325
H	5.97683	2.39266	-3.07754
N	3.37852	3.30788	-1.45291
C	2.53895	4.47355	-1.20308
H	2.93196	2.42011	-1.71122
H	3.11352	5.19977	-0.60797
H	1.64010	4.16057	-0.64698
H	2.22654	4.97239	-2.14103
C	-5.41432	-0.46425	4.71600
C	-4.90203	0.54116	3.69174
O	-5.42046	1.64442	3.48041
H	-5.29169	-1.50946	4.38274
H	-6.48078	-0.27330	4.91054
H	-4.86266	-0.33978	5.66553
N	-3.74306	0.11253	3.08028
C	-3.06544	0.90404	2.05749
C	-4.07183	1.25543	0.94203
O	-4.69775	0.34720	0.36522
C	-1.92365	0.04842	1.48227
S	-0.82356	1.04837	0.38224
H	-3.55295	-0.89217	3.07538
H	-2.65634	1.81294	2.53034
H	-1.33109	-0.36423	2.31849
H	-2.35399	-0.79314	0.91342
N	-4.22754	2.56127	0.59546
C	-5.28759	2.90399	-0.36999

C	-4.96258	2.48090	-1.81810
O	-5.87133	2.40264	-2.64159
C	-5.45457	4.43572	-0.19892
C	-4.08277	4.90012	0.33262
C	-3.65522	3.75133	1.26530
H	-6.20900	2.35493	-0.11517
H	-5.75291	4.91964	-1.14285
H	-6.24252	4.63427	0.54984
H	-3.36336	4.99315	-0.50105
H	-4.12375	5.86845	0.85892
H	-2.55922	3.66215	1.34966
H	-4.09529	3.84884	2.27620
N	-3.63385	2.27178	-2.10569
C	-3.22747	1.74792	-3.40505
C	-3.30628	0.21074	-3.54328
O	-3.85059	-0.32981	-4.50401
H	-2.97480	2.22132	-1.32354
H	-3.90180	2.16201	-4.16906
H	-2.19179	2.07431	-3.61359
N	-2.71366	-0.51955	-2.53220
C	-2.63734	-1.96442	-2.67845
C	-3.45991	-2.77957	-1.67463
O	-3.48489	-4.00229	-1.79708
C	-1.20779	-2.52872	-2.70284
S	-0.36841	-2.49939	-1.05575
H	-2.11885	-0.05261	-1.83990
H	-3.09264	-2.16697	-3.66693
H	-1.27262	-3.59150	-2.98254
H	-0.60383	-1.98636	-3.44953
N	-4.09958	-2.12600	-0.66328
C	-5.01171	-2.85479	0.20198
C	-4.41028	-3.64700	1.37862
O	-5.15565	-4.33012	2.08141
H	-4.16220	-1.10063	-0.63966
H	-5.71858	-2.12795	0.63458
H	-5.58742	-3.58999	-0.38747
N	-3.06484	-3.49605	1.64146
C	-2.44665	-4.34934	2.65994
H	-2.47384	-3.17267	0.86648
H	-3.20689	-4.55984	3.42676
H	-1.58460	-3.82952	3.11117
H	-2.10111	-5.31178	2.23715
Fe	0.55558	-0.45764	-0.78527
H	1.92508	-0.64319	1.23336

O	1.34169	0.33927	2.66091
H	0.61550	0.71584	2.08752
Fe ^{III} (SCH ₃) ₄			
Fe	0.00001	0.00001	-0.00028
S	-1.33393	-1.44669	-1.20154
S	1.33444	1.20114	-1.44653
S	1.33421	-1.20124	1.44616
S	-1.33468	1.44600	1.20087
C	-2.35207	0.26620	2.19616
H	-1.72740	-0.26824	2.92655
H	-3.12714	0.83292	2.73664
H	-2.83241	-0.47474	1.54018
C	2.35449	-2.19428	0.26707
H	3.13036	-2.73306	0.83431
H	1.73178	-2.92600	-0.26783
H	2.83383	-1.53712	-0.47348
C	2.35085	2.19657	-0.26637
H	3.15907	2.69533	-0.82494
H	1.73554	2.96182	0.22899
H	2.78818	1.54677	0.50599
C	-2.35334	-0.26722	-2.19459
H	-1.74037	0.22775	-2.96195
H	-3.16303	-0.82613	-2.69058
H	-2.78869	0.50542	-1.54380
Fe ^{III} (SCH ₂ CH ₃) ₄			
Fe	-0.09492	0.04453	0.00990
S	-1.03178	1.21411	-1.73997
S	0.92874	1.53057	1.44006
S	-1.71301	-1.09514	1.18398
S	1.39081	-1.48307	-0.86001
C	-2.26466	2.32891	-0.90898
C	1.59753	0.45349	2.79876
C	-2.40084	-2.19594	-0.14389
C	2.56236	-0.37230	-1.77640
C	-1.67201	3.68262	-0.50653
C	3.02095	-0.04060	2.52448
C	-3.52678	-3.08121	0.39971
C	3.67119	-1.18003	-2.45871
H	-3.09233	2.46669	-1.62852
H	-2.67714	1.80557	-0.02772
H	1.56777	1.06602	3.71830
H	0.91327	-0.39988	2.95218
H	-2.76873	-1.55880	-0.96768
H	-1.58325	-2.81872	-0.54771

H	1.99205	0.20366	-2.52638
H	2.99170	0.35132	-1.06023
H	-0.86503	3.55136	0.23545
H	-1.24833	4.20338	-1.38378
H	-2.45195	4.33149	-0.05798
H	3.03913	-0.68735	1.62932
H	3.70472	0.80982	2.35161
H	3.40447	-0.62798	3.38382
H	-3.16160	-3.72509	1.21965
H	-4.35389	-2.46676	0.79833
H	-3.93184	-3.73317	-0.40009
H	4.25793	-1.75032	-1.71644
H	3.24594	-1.90295	-3.17747
H	4.36238	-0.50923	-3.00747