

SUPPORTING INFORMATION FOR

DFT Calculations on Mössbauer Parameters of Nonheme Iron Nitrosyls

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Coordinates for geometry-optimized complexes (ADF, OLYP/STO-TZP,
COSMO)

[Fe(SEt)₄]¹⁻			
C	3.478202	-5.023087	-11.793611
C	2.062875	-5.522838	-12.069808
S	1.378595	-6.628782	-10.755448
Fe	-0.015698	-5.304920	-9.443107
S	-1.418964	-3.955626	-10.720033
C	-2.153101	-5.026537	-12.036211
C	-3.552635	-5.544173	-11.720516
S	-1.343927	-6.715992	-8.152534
C	-0.264983	-7.407887	-6.819887
C	0.225328	-8.828169	-7.082125
S	1.339944	-3.910172	-8.162013
C	0.253709	-3.153516	-6.871170
C	-0.191349	-1.728341	-7.183176
H	-3.925162	-6.140465	-12.564298
H	-3.553957	-6.181492	-10.830704
H	-4.255908	-4.721581	-11.553650
H	3.812628	-4.380387	-12.619083
H	3.522259	-4.435574	-10.871440
H	4.186383	-5.853943	-11.704839
H	-0.805913	-1.343133	-6.358708
H	0.666491	-1.058444	-7.304969
H	-0.790106	-1.686366	-8.098182
H	0.832394	-9.172433	-6.234180
H	-0.610674	-9.525295	-7.201945
H	0.845110	-8.878709	-7.982975
H	0.580388	-6.728743	-6.682826
H	-0.861182	-7.377072	-5.901690
H	0.829499	-3.172927	-5.939920
H	-2.173217	-4.414858	-12.944399
H	-1.467176	-5.858059	-12.217187
H	-0.612635	-3.805824	-6.732239
H	1.373468	-4.683609	-12.196848
H	2.043662	-6.106999	-12.996507

[FeS₄C₈O₄]²⁻

C	4.418189	4.398211	0.303530
C	4.200192	5.749145	0.859027
C	2.700142	5.463451	0.824248
C	3.019599	4.126289	0.290129
S	2.177980	2.725828	-0.176964
Fe	4.252450	1.567730	-0.502983
S	5.735380	3.420984	-0.138610
S	4.524003	0.315679	-2.527597
C	4.643269	-1.130115	-1.641540
C	4.777724	-2.573828	-1.919311
C	4.773369	-2.810004	-0.410231
C	4.620396	-1.353371	-0.234699
S	4.465817	-0.254280	1.050324
O	1.680987	6.084201	1.128044
O	4.905650	6.693296	1.213459
O	4.854945	-3.794410	0.324701
O	4.853716	-3.288734	-2.918506

[Fe(SPh)₄]²⁻

C	0.164096	5.083546	-0.799287
C	-0.276744	6.417463	-0.662956
C	-1.666800	6.635678	-0.541931
C	-2.569644	5.568035	-0.550534
C	-2.116069	4.249353	-0.679737
C	-0.740822	4.019558	-0.805917
S	0.844524	7.797763	-0.653396
Fe	3.023436	7.168035	-0.025977
S	3.913215	9.341337	0.146865
C	5.681911	9.385489	0.317372
C	6.470053	8.216359	0.341523
C	7.861257	8.285024	0.439662
C	8.512228	9.521559	0.521807
C	7.741663	10.691253	0.511121
C	6.349058	10.626298	0.412244
S	4.069272	5.617776	-1.458937
C	4.571610	6.276073	-3.032963
C	4.729327	5.415877	-4.141754
C	5.171625	5.902847	-5.375686
C	5.467909	7.261363	-5.543197
C	5.305829	8.125693	-4.453639
C	4.863064	7.643498	-3.220122
S	3.239922	5.880699	1.930209
C	2.473147	6.604507	3.361257
C	1.768140	7.826987	3.318217
C	1.183390	8.364906	4.467486
C	1.279131	7.703113	5.697379
C	1.973763	6.488306	5.756031
C	2.561753	5.947361	4.609457
H	4.504945	4.357167	-4.032695
H	5.284268	5.214583	-6.211534
H	5.817811	7.639038	-6.501667

H	5.532131	9.185904	-4.559388
H	4.748704	8.327019	-2.385328
H	1.673268	8.354927	2.375268
H	0.646994	9.310164	4.397590
H	0.821657	8.124426	6.590152
H	2.060425	5.955591	6.701529
H	3.097466	5.002909	4.678198
H	5.986490	7.247740	0.262388
H	8.439277	7.362013	0.445009
H	9.596862	9.572244	0.591551
H	8.227171	11.663441	0.577280
H	5.769779	11.547315	0.402162
H	-2.040908	7.651724	-0.435880
H	-3.635031	5.769415	-0.451518
H	-2.818666	3.418575	-0.682495
H	-0.364595	3.002897	-0.910292
H	1.224826	4.882089	-0.905983

[Fe(H₂O)₅NO]²⁺

O	-0.076634	-0.019741	2.135507
Fe	-0.008480	0.221409	-0.000766
N	-0.000551	1.998857	0.003823
O	0.030761	3.149486	-0.001820
O	2.187030	-0.123121	-0.051369
O	0.062232	0.017726	-2.152850
O	0.011840	-2.001570	0.084410
O	-2.196393	-0.145460	-0.002366
H	2.600368	0.224469	-0.859876
H	2.688163	0.297656	0.667141
H	-0.264896	-0.796312	-2.569307
H	0.246947	0.660158	2.748142
H	-0.771482	-2.487942	-0.218494
H	0.770531	-2.475276	-0.290907
H	0.222080	-0.867796	2.498941
H	-2.606425	0.100160	0.843919
H	-2.699321	0.361664	-0.662000
H	-0.237712	0.739150	-2.729481

[Fe(NO)(dtci-Pr₂)₂]

Fe	1.309084	-2.114228	3.733927
S	2.553738	-0.482662	4.764665
S	-0.174369	-0.387185	4.097926
S	2.477291	-3.865161	4.625129
S	-0.242821	-3.792628	3.940076
O	2.027636	-2.191505	0.987638
N	1.713717	-2.085350	2.129713
N	1.052781	1.783331	5.225208
N	0.852974	-6.063150	5.008392
C	1.145178	0.529169	4.774163
C	-0.269420	2.484990	5.160171
C	-0.212041	3.756501	4.305928
C	-0.860410	2.715245	6.555719
C	2.194618	2.548519	5.836633

C	3.307670	2.875101	4.831271
C	2.713622	1.931633	7.142907
C	1.018634	-4.804529	4.592512
C	1.938759	-6.902085	5.626848
C	3.056771	-7.265398	4.639897
C	2.457743	-6.345510	6.960104
C	-0.502991	-6.693116	4.901307
C	-0.490873	-7.954272	4.029774
C	-1.139519	-6.912933	6.278581
H	-0.929166	1.786408	4.642156
H	1.734852	3.499638	6.109254
H	1.422322	-7.832856	5.865858
H	-1.112573	-5.953717	4.377958
H	-1.231715	4.138057	4.187382
H	0.186163	3.547038	3.308515
H	0.385051	4.552289	4.762333
H	-1.874005	3.115179	6.445145
H	-0.283270	3.434125	7.146138
H	-0.927773	1.776870	7.114799
H	2.902577	3.339390	3.927252
H	3.883927	1.992587	4.542550
H	3.994081	3.590888	5.297236
H	3.378708	2.657987	7.623309
H	1.893839	1.718849	7.835318
H	3.281275	1.012175	6.979515
H	3.685916	-6.408902	4.384508
H	2.649688	-7.688064	3.716688
H	3.693114	-8.026342	5.105286
H	3.065699	-7.120708	7.439584
H	3.081770	-5.457600	6.834012
H	1.633621	-6.100698	7.636630
H	0.047447	-8.788325	4.491048
H	-0.053398	-7.754126	3.047146
H	-1.526271	-8.276844	3.877171
H	-2.168721	-7.260048	6.137282
H	-0.613256	-7.668603	6.870512
H	-1.174064	-5.980680	6.850624

[Fe(SPh)₂(NO)₂]¹⁻

C	8.482454	8.683762	2.491821
C	8.961358	7.530949	3.151532
C	10.282239	7.551652	3.643609
C	11.084692	8.685810	3.494330
C	10.598010	9.824830	2.843964
C	9.291501	9.811793	2.339986
S	7.878140	6.128706	3.288992
Fe	8.549056	4.702507	4.981823
N	8.997545	5.522159	6.357028
O	9.104544	5.952921	7.460782
H	11.225104	10.706748	2.731751
S	10.457910	3.495651	4.469943
C	10.145319	2.283879	3.208290
C	11.090947	1.251517	3.022568
C	10.912993	0.284798	2.030723

C	9.786576	0.315243	1.199066
C	8.843952	1.333873	1.373456
C	9.019235	2.307441	2.360394
H	9.646761	-0.440512	0.429094
N	7.213750	3.731099	5.176552
O	6.247245	3.165311	5.578889
H	10.686061	6.676403	4.141569
H	12.099460	8.673659	3.887823
H	7.467653	8.693154	2.101052
H	8.279994	3.094048	2.467009
H	8.894527	10.687502	1.830099
H	11.658236	-0.499288	1.911227
H	11.969203	1.208859	3.662571
H	7.963724	1.378600	0.734684

[Fe(SC₂H₃N₃)(SC₂H₂N₃)(NO)₂]

C	3.710155	4.628970	8.164163
N	3.776250	5.796952	7.536359
N	3.531491	5.437042	6.250425
C	3.335961	4.103366	6.130830
N	3.450311	3.563702	7.360835
S	3.039522	3.311474	4.607943
Fe	1.662190	1.509555	5.104599
N	0.565869	1.943345	6.283827
O	-0.395701	2.229314	6.908835
S	2.839417	-0.433238	5.779159
C	3.208345	-0.231383	7.445146
N	3.410167	-1.238758	8.341323
C	3.707274	-0.682536	9.547394
N	3.704334	0.626280	9.471403
N	3.394365	0.884922	8.167712
N	0.922384	1.091028	3.662915
O	0.105557	0.903007	2.830559
H	3.856398	4.547022	9.233450
H	3.333228	-2.225894	8.133647
H	3.914535	-1.253571	10.439852
H	3.382428	1.883236	7.829275
H	3.508366	6.133041	5.517916

[Fe₂S₂(S₂-o-xy)₂]²⁻

C	-6.291789	-0.359609	1.381940
C	-5.096291	-0.675831	0.710519
C	-5.096291	-0.675831	-0.710519
C	-6.291789	-0.359609	-1.381940
C	-7.468544	-0.051641	-0.698642
C	-7.468544	-0.051641	0.698642
C	-3.893949	-1.031428	1.549382
S	-2.717235	0.378629	1.871105
Fe	-1.336563	0.218544	0.000000
S	-2.717235	0.378629	-1.871105
C	-3.893949	-1.031428	-1.549382
Fe	1.349542	-0.212367	0.000000
S	0.244547	1.760855	0.000000

S	2.731826	-0.376459	-1.870070
C	3.914457	1.028457	-1.548616
C	5.115402	0.666355	-0.710504
C	5.115402	0.666355	0.710504
C	6.308867	0.343034	1.381986
C	7.483751	0.027919	0.698641
C	7.483751	0.027919	-0.698641
C	6.308867	0.343034	-1.381986
C	3.914457	1.028457	1.548616
S	2.731826	-0.376459	1.870070
S	-0.231288	-1.754453	0.000000
H	-6.297660	-0.371852	2.470412
H	-8.377538	0.172741	1.252348
H	-8.377538	0.172741	-1.252348
H	-6.297660	-0.371852	-2.470412
H	-4.227882	-1.360776	-2.535004
H	6.314807	0.355054	2.470465
H	8.391268	-0.202230	1.252382
H	8.391268	-0.202230	-1.252382
H	6.314807	0.355054	-2.470465
H	4.249361	1.357106	2.534034
H	3.342986	1.847598	1.111642
H	-3.318545	-1.848472	1.113448
H	-4.227882	-1.360776	2.535004
H	-3.318545	-1.848472	-1.113448
H	3.342986	1.847598	-1.111642
H	4.249361	1.357106	-2.534034

[Fe₂S₂(OPh-*p*-CH₃)₄]²⁻

C	-3.222671	0.323142	-5.570280
C	-4.181654	-0.313404	-4.764221
C	-4.005685	-0.460134	-3.386751
C	-2.845047	0.032031	-2.739854
C	-1.886125	0.687551	-3.547677
C	-2.077620	0.820788	-4.922703
O	-2.717020	-0.125873	-1.421102
Fe	-1.405228	-0.011721	0.000000
O	-2.717020	-0.125873	1.421102
C	-2.845047	0.032031	2.739854
C	-4.005685	-0.460134	3.386751
C	-4.181654	-0.313404	4.764221
C	-3.222671	0.323142	5.570280
C	-2.077620	0.820788	4.922703
C	-1.886125	0.687551	3.547677
C	-3.396173	0.447336	7.067275
C	-3.396173	0.447336	-7.067275
Fe	1.404978	0.033776	0.000000
S	0.049321	-1.759428	0.000000
S	-0.049409	1.782502	0.000000
O	2.715916	0.149692	-1.423306
C	2.836700	-0.024007	-2.740973
C	3.995089	0.455687	-3.400707
C	4.160744	0.292548	-4.777742
C	3.193174	-0.348152	-5.570386

C	2.049711	-0.832852	-4.909932
C	1.869885	-0.684173	-3.535207
C	3.356713	-0.490467	-7.066863
O	2.715916	0.149692	1.423306
C	2.836700	-0.024007	2.740973
C	3.995089	0.455687	3.400707
C	4.160744	0.292548	4.777742
C	3.193174	-0.348152	5.570386
C	2.049711	-0.832852	4.909932
C	1.869885	-0.684173	3.535207
C	3.356713	-0.490467	7.066863
H	4.762136	0.955669	-2.812008
H	5.067416	0.676054	-5.244872
H	1.274973	-1.340195	-5.484774
H	0.974560	-1.072343	-3.059765
H	4.370202	-0.229270	-7.384735
H	2.663374	0.165227	-7.610165
H	3.150571	-1.513848	-7.401062
H	4.762136	0.955669	2.812008
H	5.067416	0.676054	5.244872
H	1.274973	-1.340195	5.484774
H	0.974560	-1.072343	3.059765
H	4.370202	-0.229270	7.384735
H	3.150571	-1.513848	7.401062
H	2.663374	0.165227	7.610165
H	-4.766108	-0.957264	2.787232
H	-0.989256	1.085243	3.083172
H	-4.766108	-0.957264	-2.787232
H	-0.989256	1.085243	-3.083172
H	-5.089349	-0.706987	5.220872
H	-1.308907	1.325102	5.508429
H	-5.089349	-0.706987	-5.220872
H	-1.308907	1.325102	-5.508429
H	-4.409590	0.175198	7.376001
H	-2.701263	-0.209539	7.607137
H	-3.199366	1.468285	7.414289
H	-4.409590	0.175198	-7.376001
H	-3.199366	1.468285	-7.414289
H	-2.701263	-0.209539	-7.607137

[Fe₂S₂(C₄H₄N₄)₄]²⁻

C	-0.714494	-3.207038	-4.065443
C	-1.107250	-2.227591	-3.160710
N	0.000000	-1.623483	-2.600501
C	1.107250	-2.227591	-3.160710
C	0.714494	-3.207038	-4.065443
Fe	0.000000	0.000000	-1.390144
N	0.000000	1.623483	-2.600501
C	-1.107250	2.227591	-3.160710
C	-0.714494	3.207038	-4.065443
C	0.714494	3.207038	-4.065443
C	1.107250	2.227591	-3.160710
Fe	0.000000	0.000000	1.372140
S	1.748463	0.000000	-0.009022

S	-1.748463	0.000000	-0.009022
N	0.000000	-1.623071	2.582317
C	1.107270	-2.227101	3.142528
C	0.714511	-3.206352	4.047460
C	-0.714511	-3.206352	4.047460
C	-1.107270	-2.227101	3.142528
N	0.000000	1.623071	2.582317
C	-1.107270	2.227101	3.142528
C	-0.714511	3.206352	4.047460
C	0.714511	3.206352	4.047460
C	1.107270	2.227101	3.142528
H	2.107864	-1.922059	2.860906
H	1.371871	-3.842790	4.631951
H	-1.371871	-3.842790	4.631951
H	-2.107864	-1.922059	2.860906
H	-2.107901	1.922643	-2.879105
H	2.107901	1.922643	-2.879105
H	-1.371894	3.843637	-4.649713
H	1.371894	3.843637	-4.649713
H	2.107901	-1.922643	-2.879105
H	1.371894	-3.843637	-4.649713
H	-1.371894	-3.843637	-4.649713
H	-2.107901	-1.922643	-2.879105
H	-2.107864	1.922059	2.860906
H	-1.371871	3.842790	4.631951
H	1.371871	3.842790	4.631951
H	2.107864	1.922059	2.860906

[Fe₂(NO)₂(Et-HPTB)(O₂CPh)]²⁺

C	5.114793	0.087244	1.209500
C	4.416139	-0.070354	0.000966
C	5.113610	0.090478	-1.207770
C	6.469960	0.420840	-1.208993
C	7.151392	0.592176	0.000469
C	6.471135	0.417189	1.210142
C	2.925718	-0.354712	0.001060
O	2.365759	-0.449326	-1.139139
Fe	0.237302	-0.376157	-1.778566
N	0.009082	-2.107876	-1.443063
O	0.182164	-3.266925	-1.543376
O	-0.022180	0.617525	0.000139
C	0.080010	2.030831	-0.000025
C	0.844827	2.548340	1.238692
N	0.468184	1.833607	2.483721
C	-0.796841	2.335914	3.083958
C	-1.921399	1.348565	2.980835
N	-1.779406	0.140948	2.452728
C	-3.023013	-0.474437	2.562555
C	-3.917355	0.423302	3.188430
N	-3.181971	1.578960	3.444884
C	-5.248839	0.088117	3.452310
C	-5.665301	-1.185170	3.065927
C	-4.784952	-2.086896	2.435842
C	-3.459581	-1.747269	2.175688

Fe	0.235261	-0.374358	1.778654
N	0.007511	-2.106448	1.444430
O	0.178749	-3.265406	1.547898
C	-3.677968	2.786599	4.123343
C	-4.364381	3.787490	3.197461
N	0.471290	1.832372	-2.483283
C	-0.793708	2.334518	-3.084137
C	-1.918490	1.347325	-2.981337
N	-1.776974	0.139497	-2.453036
C	-3.020805	-0.475476	-2.563418
C	-3.914558	0.422729	-3.189519
N	-3.178762	1.578049	-3.445851
C	-5.246411	0.088657	-3.453036
C	-5.663775	-1.184230	-3.066211
C	-4.783797	-2.086765	-2.436544
C	-3.458144	-1.748138	-2.176683
C	-3.674311	2.786040	-4.123942
C	-4.358512	3.787375	-3.196894
N	0.932451	-0.525527	-3.842921
C	1.473342	0.592055	-4.323373
N	1.947269	0.444670	-5.590241
C	1.680500	-0.870912	-5.966024
C	1.035456	-1.470191	-4.860181
C	1.938562	-1.569141	-7.150049
C	1.519410	-2.896646	-7.201815
C	0.861724	-3.501824	-6.112491
C	0.610791	-2.804196	-4.933800
C	2.616406	1.456607	-6.426229
C	1.685092	2.157259	-7.411792
C	1.570061	1.830968	-3.480063
O	2.365505	-0.448754	1.141025
N	0.929812	-0.524363	3.843330
C	1.470510	0.593412	4.323634
N	1.946884	0.445175	5.589596
C	1.682776	-0.871101	5.964551
C	1.035823	-1.469926	4.859571
C	1.945263	-1.570329	7.147118
C	1.527771	-2.898426	7.198395
C	0.867649	-3.502982	6.110220
C	0.612766	-2.804443	4.932956
C	2.614724	1.457394	6.426128
C	1.682370	2.157090	7.411969
C	1.566337	1.832648	3.481119
C	0.847488	2.546310	-1.237682
H	1.909807	2.360818	-1.083415
H	0.712661	3.629521	-1.345596
H	-0.939319	2.449967	-0.001392
H	0.706799	3.630905	1.346787
H	1.907638	2.364775	1.086174
H	2.517303	1.811634	2.943811
H	1.563217	2.743110	4.086902
H	0.100317	-3.286331	4.109223
H	0.548188	-4.538376	6.191189
H	1.710011	-3.476450	8.100186
H	2.444456	-1.108031	7.992715
H	3.420974	0.944882	6.954771

S10

H	3.087660	2.179342	5.759351
H	1.215584	1.446703	8.100017
H	2.268601	2.867775	8.003109
H	0.893139	2.714225	6.897683
H	-0.630819	2.568399	4.140043
H	-1.081388	3.281858	2.613173
H	-2.794284	-2.449915	1.685327
H	-5.149520	-3.067829	2.143673
H	-6.693533	-1.483924	3.251944
H	-5.935299	0.778593	3.932792
H	-4.363420	2.450349	4.903823
H	-2.832996	3.252423	4.632620
H	-5.234034	3.347109	2.701421
H	-4.707433	4.637388	3.796130
H	-3.680557	4.167408	2.432182
H	1.567658	2.741036	-4.086371
H	2.520700	1.808915	-2.942156
H	0.099715	-3.286348	-4.109258
H	0.540786	-4.536643	-6.193710
H	1.698135	-3.473571	-8.105016
H	2.435148	-1.107255	-7.997630
H	3.089642	2.178024	-5.759290
H	3.423222	0.944062	-6.954409
H	1.217871	1.447774	-8.100533
H	0.896423	2.714493	-6.897058
H	2.272684	2.867778	-8.001533
H	-1.078509	3.280944	-2.613783
H	-0.627414	2.567318	-4.140083
H	-2.793622	-2.451610	-1.686443
H	-5.148843	-3.067557	-2.144420
H	-6.692187	-1.482357	-3.251760
H	-5.931476	0.780216	-3.933722
H	-2.829163	3.250903	-4.633655
H	-4.361372	2.450072	-4.902938
H	-5.227585	3.347396	-2.699759
H	-3.673242	4.167335	-2.432839
H	-4.701738	4.637373	-3.795239
H	4.586157	-0.043965	-2.146378
H	6.994318	0.549063	-2.153140
H	8.205878	0.859281	0.000371
H	6.996700	0.542460	2.154054
H	4.588111	-0.049123	2.148301

[Fe(NO)₂{Fe(NO)(N(CH₂CH₂S)₃)}-S,S']

C	3.942652	-1.560592	3.237982
S	4.070803	0.273741	3.344753
Fe	5.816153	0.690561	4.795436
N	5.804821	-0.413688	6.022738
O	5.770567	-1.040239	7.026691
C	4.773003	-2.160534	2.106713
N	6.166367	-1.647919	2.016812
C	6.996717	-2.131096	3.153637
C	8.189334	-1.235296	3.453941
S	7.760711	0.549075	3.568983

S11

C	6.793222	-2.060204	0.728967
C	6.251121	-1.315729	-0.477887
S	6.249092	0.500186	-0.223498
N	5.689911	2.257273	5.345867
O	5.594538	3.175984	6.084741
Fe	6.022117	0.677984	2.024500
N	5.982912	2.397502	1.918209
O	6.441792	3.407526	1.491112
H	4.193818	-1.976450	4.213826
H	2.890122	-1.787737	3.049877
H	4.773555	-3.256211	2.216914
H	4.280734	-1.930510	1.161426
H	8.965228	-1.297206	2.686972
H	8.643495	-1.532356	4.403162
H	7.355896	-3.152101	2.956869
H	6.367124	-2.186960	4.040046
H	5.239192	-1.633504	-0.739999
H	6.891511	-1.531719	-1.337720
H	6.668877	-3.144764	0.584410
H	7.863541	-1.862348	0.809624

[Fe₄S₄(SPh)₄]²⁻

C	19.213904	27.079127	8.264361
C	18.054266	26.459330	8.773185
C	17.029878	26.120485	7.866857
C	17.169132	26.378181	6.501070
C	18.324973	26.990701	6.005022
C	19.343332	27.343072	6.898369
S	17.940541	26.179844	10.529284
Fe	16.552126	24.385817	10.933856
S	14.262544	24.737686	10.651112
Fe	14.625028	22.533168	10.424008
S	16.916086	22.374178	10.007349
Fe	16.550974	22.025357	12.286079
S	16.914303	24.036939	13.212609
Fe	14.623227	23.878152	12.793755
S	14.261283	21.673880	12.566909
S	13.227125	25.202390	14.061866
C	13.169299	24.496962	15.699059
C	14.312936	23.993049	16.349621
C	14.226188	23.463364	17.639081
C	13.002440	23.436891	18.316978
C	11.863569	23.949924	17.685646
C	11.942025	24.470596	16.390894
S	17.937991	20.231286	12.693126
C	18.057412	19.961563	14.450238
C	17.034873	20.303556	15.357546
C	17.178151	20.053233	16.724249
C	18.336309	19.445044	17.220217
C	19.352664	19.089149	16.325915
C	19.219327	19.346049	14.959027
S	13.231177	21.211984	9.150957
C	13.172423	21.928425	7.518561
C	14.317717	22.428393	6.867744
C	14.230954	22.967550	5.582459

S12

C	13.005305	23.007833	4.908651
C	11.864620	22.498695	5.540078
C	11.943315	21.968619	6.830894
H	20.020948	19.069024	14.278655
H	16.117935	20.758548	14.996568
H	20.016885	27.353595	8.944050
H	16.362594	26.103446	5.823595
H	16.114680	25.661906	8.227631
H	18.428849	27.193050	4.941283
H	20.248202	27.824277	6.532672
H	15.281885	22.391502	7.365501
H	15.130949	23.350842	5.104792
H	12.940869	23.425586	3.906342
H	10.904064	22.517188	5.029042
H	11.046811	21.584670	7.311542
H	15.275911	24.019587	15.848793
H	15.124776	23.076765	18.116692
H	12.938109	23.026616	19.322392
H	10.904433	23.941919	18.199637
H	11.046752	24.857464	15.910421
H	16.373052	20.330398	17.402569
H	18.443435	19.248446	18.284718
H	20.259049	18.610930	16.691696

[Fe₄S₄(OPh)₄]²⁻

C	2.981446	0.805113	8.586726
C	1.800088	1.492247	8.218719
C	1.505324	2.704559	8.886933
C	2.366425	3.214385	9.860079
C	3.537977	2.531506	10.209205
C	3.831641	1.321220	9.567110
O	0.987393	0.969976	7.283517
Fe	0.186924	1.906573	5.809307
S	1.456121	3.299815	4.572443
Fe	-0.639847	4.342122	4.801530
O	-0.402064	6.247646	4.880177
C	0.147338	7.016330	5.830217
C	0.092960	8.426984	5.699939
C	0.649290	9.258238	6.674094
C	1.279619	8.721853	7.805263
C	1.347283	7.330251	7.940956
C	0.794179	6.489100	6.974021
Fe	-0.003367	2.266547	3.069227
O	0.761049	1.929128	1.353001
C	1.134688	2.691872	0.317606
C	1.466046	2.066830	-0.910810
C	1.854603	2.823116	-2.017415
C	1.927927	4.220392	-1.941468
C	1.610654	4.848309	-0.730988
C	1.222645	4.102975	0.384505
Fe	-2.313967	2.147396	4.579132
O	-4.093594	1.499880	4.868613
C	-4.932966	0.725097	4.171617
C	-6.278682	0.610055	4.602774

C	-7.183441	-0.202778	3.918982
C	-6.784964	-0.926861	2.787226
C	-5.459902	-0.816992	2.348621
C	-4.544869	-0.004590	3.022172
S	-0.724086	0.448941	4.217781
S	-1.892314	3.651800	2.942627
S	-1.609084	3.250809	6.517354
H	1.408732	0.981829	-0.975686
H	2.100592	2.315819	-2.948666
H	2.226719	4.807260	-2.806961
H	1.664132	5.932739	-0.650778
H	0.982916	4.608261	1.316306
H	-0.394928	8.852427	4.824842
H	0.589160	10.337964	6.548340
H	1.709035	9.373767	8.562532
H	1.835608	6.890005	8.809602
H	0.861141	5.412922	7.094541
H	-6.593144	1.169356	5.482127
H	-8.210081	-0.271882	4.274795
H	-7.491638	-1.562646	2.258964
H	-5.129901	-1.371136	1.471308
H	-3.519021	0.063439	2.669618
H	0.591613	3.235662	8.635543
H	2.116031	4.153698	10.351306
H	4.207541	2.933483	10.966064
H	4.735433	0.773702	9.828590
H	3.218106	-0.132842	8.087838

[Fe₄S₄(SPh)₂Cl₂]²⁻

C	-3.070711	18.020366	3.546725
C	-3.679213	17.323618	2.496018
C	-3.280653	16.022724	2.178085
C	-2.253721	15.383496	2.903865
C	-1.631107	16.105344	3.940916
C	-2.040922	17.401186	4.262967
S	-1.817438	13.715463	2.452854
Fe	-0.676451	12.636479	4.157897
S	-0.876517	10.355035	3.759626
Fe	1.177592	10.662960	4.631635
Cl	2.914582	9.426868	3.807376
Fe	0.690000	12.634330	6.525301
S	-1.522495	12.973740	6.300539
Fe	-1.177185	10.671395	6.056525
Cl	-2.923194	9.451049	6.885776
S	0.872789	10.351345	6.929614
S	1.538932	12.961130	4.381264
S	1.838601	13.702814	8.230809
C	2.252401	15.378514	7.786171
C	3.279165	16.024966	8.505525
C	3.661399	17.331443	8.190334
C	3.036076	18.026861	7.148621
C	2.006035	17.400567	6.439183
C	1.612733	16.098992	6.758561
H	3.783672	15.497733	9.311704

H	4.459000	17.804330	8.760243
H	3.347257	19.037915	6.894531
H	1.504812	17.925121	5.626710
H	0.806447	15.638917	6.199387
H	-3.771622	15.493902	1.364811
H	-0.825938	15.650560	4.505701
H	-4.476603	17.791107	1.921375
H	-1.552221	17.926659	5.082461
H	-3.394297	19.027134	3.801985

[Fe₄S₄(OPh)₂Cl₂]²⁻

C	-3.203072	17.676353	2.984072
C	-3.631970	16.749672	2.023890
C	-3.157083	15.437251	2.033357
C	-2.226930	15.007260	3.012001
C	-1.788217	15.958776	3.963495
C	-2.273911	17.267406	3.947404
O	-1.801389	13.736865	2.992991
Fe	-0.782843	12.658712	4.198468
S	-0.968886	10.359030	3.825986
Fe	1.135348	10.699231	4.574751
Cl	2.851198	9.471420	3.666655
Fe	0.720465	12.679732	6.520221
S	1.442622	12.998750	4.312328
Fe	-1.129521	10.663619	6.139933
Cl	-2.788797	9.373531	7.060500
S	0.982985	10.389833	6.888542
S	-1.515930	12.947575	6.409782
O	1.691515	13.777204	7.742266
C	2.199944	15.015911	7.699059
C	3.174312	15.395594	8.655790
C	3.728895	16.676270	8.643373
C	3.340713	17.617209	7.680096
C	2.373674	17.256400	6.734899
C	1.803303	15.982130	6.744137
H	3.484902	14.665998	9.401123
H	4.475280	16.943657	9.388393
H	3.783791	18.609895	7.662042
H	2.062001	17.972349	5.976344
H	1.054192	15.720451	6.003700
H	-3.498582	14.720828	1.288889
H	-1.072804	15.661170	4.722371
H	-4.347521	17.048670	1.259494
H	-1.920887	17.972502	4.698447
H	-3.584006	18.694886	2.983439

[Fe₄S₄Cl₄]²⁻

S	-1.836403	0.000000	1.257596
Fe	-1.406603	0.000000	-0.950455
Cl	-3.171858	0.000000	-2.393235
Fe	0.000000	1.407752	0.952912
Cl	0.000000	3.181897	2.386723
Fe	0.000000	-1.407752	0.952912
Cl	0.000000	-3.181897	2.386723

S15

Fe	1.406603	0.000000	-0.950455
Cl	3.171858	0.000000	-2.393235
S	1.836403	0.000000	1.257596
S	0.000000	1.836230	-1.254772
S	0.000000	-1.836230	-1.254772

[Fe₄S₄(SCH₂CO₂Et)₄]²⁻

C	-4.037315	3.615560	-6.741024
C	-5.080733	2.956340	-5.858797
O	-4.502033	2.556191	-4.573232
C	-4.185172	1.258402	-4.377747
C	-3.650894	1.075201	-2.963634
S	-2.832691	-0.540730	-2.689044
Fe	-1.335252	-0.140182	-0.986638
S	-1.901070	-0.202646	1.195760
Fe	-0.138893	1.333156	0.991496
S	-0.535495	2.828330	2.696693
C	1.077773	3.658256	2.956258
C	1.257203	4.216756	4.361147
O	2.560559	4.499176	4.571399
C	2.957767	5.086981	5.853727
C	3.577534	4.039157	6.759571
S	0.204037	-1.899773	-1.190336
Fe	1.335252	0.140182	-0.986638
S	1.901070	0.202646	1.195760
Fe	0.138893	-1.333156	0.991496
S	0.535495	-2.828330	2.696693
C	-1.077773	-3.658256	2.956258
C	-1.257203	-4.216756	4.361147
O	-2.560559	-4.499176	4.571399
C	-2.957767	-5.086981	5.853727
C	-3.577534	-4.039157	6.759571
S	-0.204037	1.899773	-1.190336
O	-4.333342	0.373765	-5.206473
S	2.832691	0.540730	-2.689044
C	3.650894	-1.075201	-2.963634
C	4.185172	-1.258402	-4.377747
O	4.502033	-2.556191	-4.573232
C	5.080733	-2.956340	-5.858797
C	4.037315	-3.615560	-6.741024
O	4.333342	-0.373765	-5.206473
O	0.364205	4.409813	5.171587
O	-0.364205	-4.409813	5.171587
H	-2.962750	1.894630	-2.746206
H	-4.504092	1.187567	-2.286389
H	-5.870374	3.661773	-5.587594
H	-5.526633	2.082293	-6.335052
H	-4.522911	3.971403	-7.657002
H	-3.582824	4.477019	-6.240292
H	-3.247070	2.912833	-7.023790
H	4.522911	-3.971403	-7.657002
H	3.582824	-4.477019	-6.240292
H	3.247070	-2.912833	-7.023790
H	5.870374	-3.661773	-5.587594

S16

H	5.526633	-2.082293	-6.335052
H	2.962750	-1.894630	-2.746206
H	4.504092	-1.187567	-2.286389
H	3.934315	4.528242	7.673364
H	4.433578	3.555782	6.276785
H	2.850858	3.271406	7.043856
H	3.687228	5.854194	5.581565
H	2.088908	5.561750	6.311226
H	1.899800	2.970252	2.748848
H	1.183533	4.500713	2.264029
H	-3.934315	-4.528242	7.673364
H	-4.433578	-3.555782	6.276785
H	-2.850858	-3.271406	7.043856
H	-3.687228	-5.854194	5.581565
H	-2.088908	-5.561750	6.311226
H	-1.899800	-2.970252	2.748848
H	-1.183533	-4.500713	2.264029

[Fe₄(NO)₄(μ₃-S)₄]

S	0.000000	1.750676	-1.226917
Fe	-1.301659	0.000000	-0.954228
N	-2.641345	0.000000	-1.919577
O	-3.573818	0.000000	-2.640431
Fe	1.301659	0.000000	-0.954228
N	2.641345	0.000000	-1.919577
O	3.573818	0.000000	-2.640431
Fe	0.000000	1.302053	0.952364
N	0.000000	2.637802	1.922669
O	0.000000	3.566439	2.648219
Fe	0.000000	-1.302053	0.952364
N	0.000000	-2.637802	1.922669
O	0.000000	-3.566439	2.648219
S	1.749730	0.000000	1.224927
S	0.000000	-1.750676	-1.226917
S	-1.749730	0.000000	1.224927

[Fe₄(NO)₄(μ₃-S)₄]¹⁻

S	0.000000	-1.742821	1.229587
Fe	-1.401454	0.000000	0.938337
N	-2.746001	0.000000	1.908862
O	-3.665900	0.000000	2.668337
Fe	1.401454	0.000000	0.938337
N	2.746001	0.000000	1.908862
O	3.665900	0.000000	2.668337
Fe	0.000000	-1.299297	-0.936562
N	0.000000	-2.648644	-1.880685
O	0.000000	-3.590004	-2.604430
Fe	0.000000	1.299297	-0.936562
N	0.000000	2.648644	-1.880685
O	0.000000	3.590004	-2.604430
S	1.764647	0.000000	-1.277004
S	0.000000	1.742821	1.229587
S	-1.764647	0.000000	-1.277004

[Fe₄(NO)₇(μ₃-S)₃]¹⁻

S	-1.018069	-1.763347	-0.611453
Fe	-2.097067	0.000000	0.288316
N	-2.063602	0.000000	1.938531
O	-2.356837	0.000000	3.087513
Fe	0.000000	0.000000	-1.412003
N	0.000000	0.000000	-3.056584
O	0.000000	0.000000	-4.241518
Fe	1.048534	-1.816114	0.288316
N	1.031801	-1.787132	1.938531
O	1.178419	-2.041081	3.087513
Fe	1.048534	1.816114	0.288316
N	1.031801	1.787132	1.938531
O	1.178419	2.041081	3.087513
S	2.036138	0.000000	-0.611453
S	-1.018069	1.763347	-0.611453
N	1.821886	-3.155599	-0.290114
O	2.414297	-4.181684	-0.364913
N	-3.643771	0.000000	-0.290114
O	-4.828593	0.000000	-0.364913
N	1.821886	3.155599	-0.290114
O	2.414297	4.181684	-0.364913