ELECTRONIC SUPPORTING INFORMATION

Neutral Diiron(III) Complexes with $Fe_2(\mu\text{-}E)_2$ (E = O, S, Se) Core Structures: Reactivity of an Iron(I) Dimer Towards Chalcogens

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Contents

1. Solution State Spectra

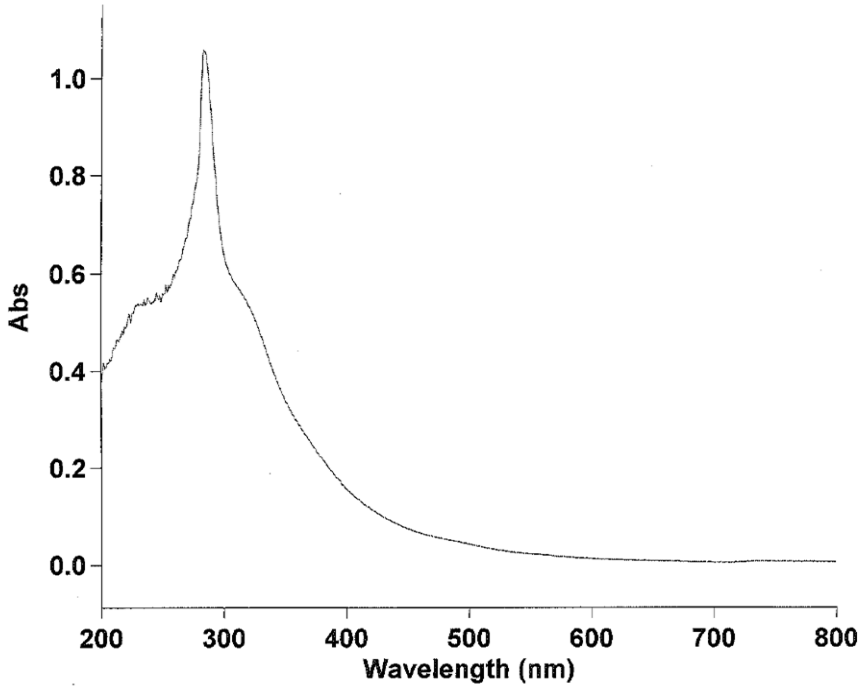


Figure S1. UV/visible spectrum of **3** recorded at room temperature in toluene (1.9 x 10^{-4} M).

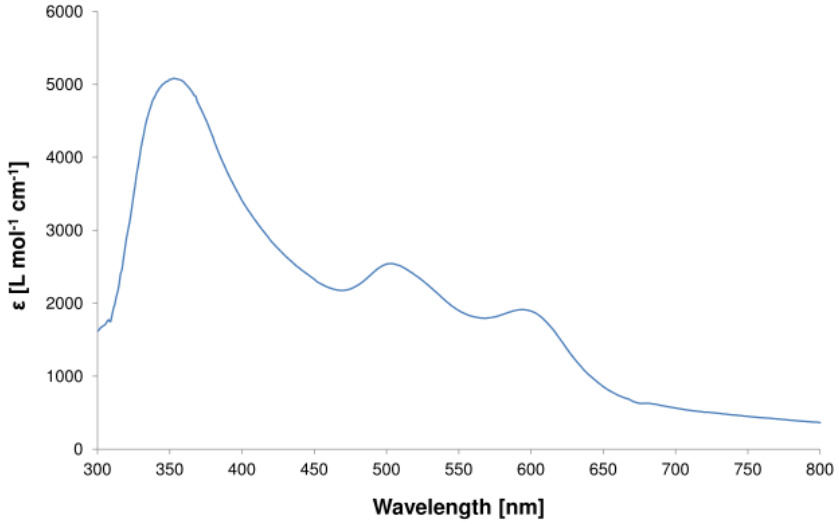
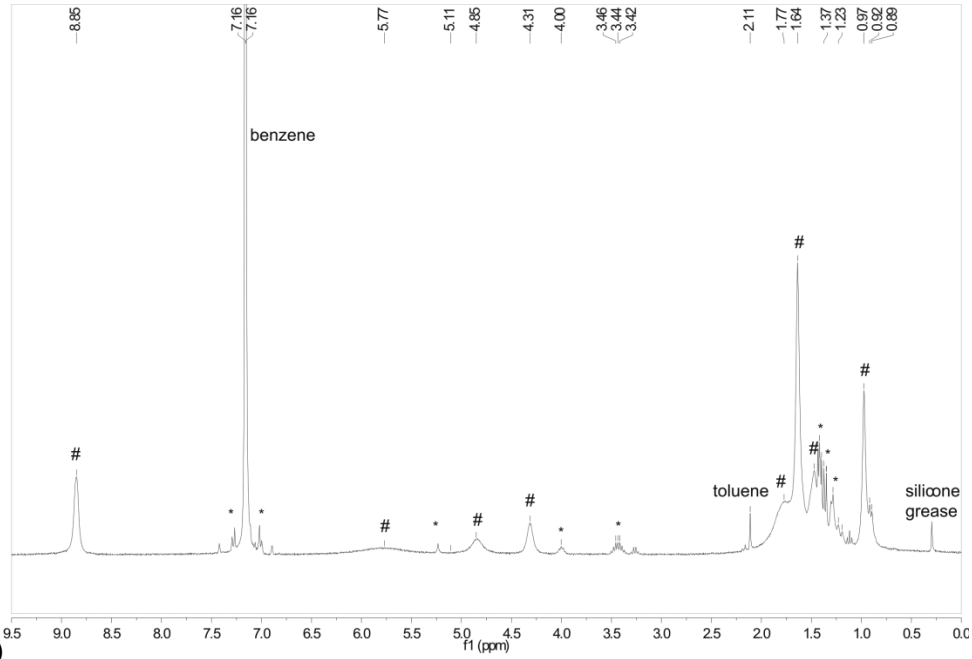
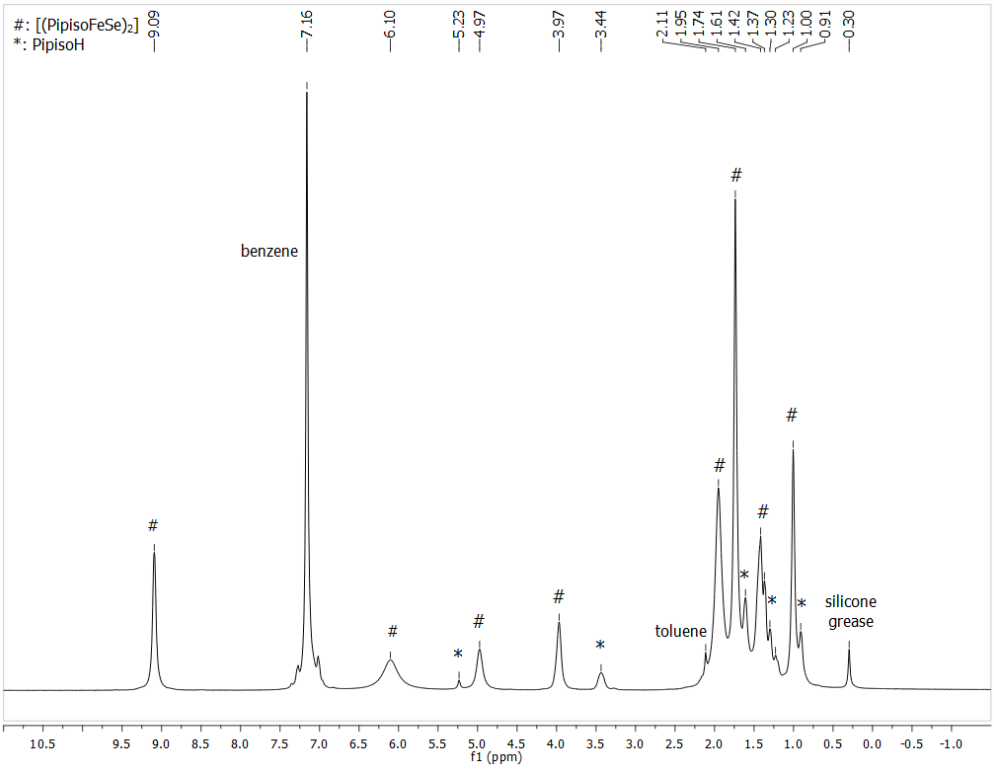


Figure S2. UV/visible spectrum of **4** recorded at room temperature in toluene (2.5 x 10^{-4} M).



(a)



(b)

Figure S3. Representative ^{1}H NMR spectra: C_6D_6 solution of (a) [{(*N,N'*-Pipiso)Fe(μ-S)}$_2$] **4** and (b) [{(*N,N'*-Pipiso)Fe(μ-Se)}$_2$] **5**. Signals denoted # are due to **4** and **5**, whereas signals denoted * represent contamination with small quantities of PipisoH.

2. X-ray Crystallography

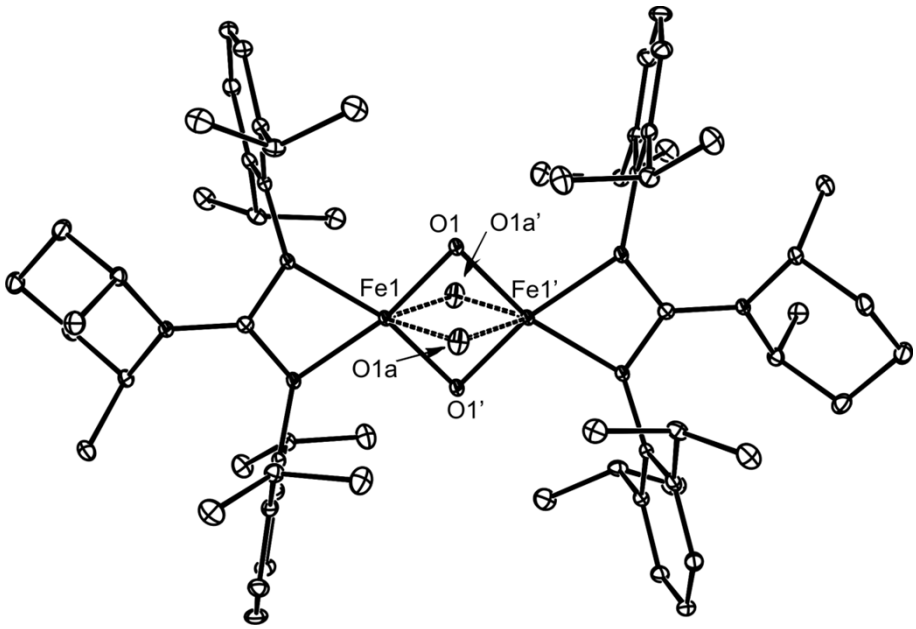


Figure S4. Displacement ellipsoid plot (25% probability surface) of the molecular structure of **3** showing minor disordered set (*ca.* 8% occupancy) of O atoms (O1a and O1a'). Hydrogen atoms are omitted. Selected metrical parameters are given in Table 1 (main text). Additional interatomic distances (Å) and angles (°) are as follows: Fe(1)-O(1A) 1.784(8), Fe(1)-O(1A)' 1.795(8), O(1A)-Fe(1)-O(1A)' 92.5(3), Fe(1)-O(1A)-Fe(1)' 87.5(3).
Symmetry transformations used to generate equivalent atoms (‘): -x+1,-y+1,-z+1.

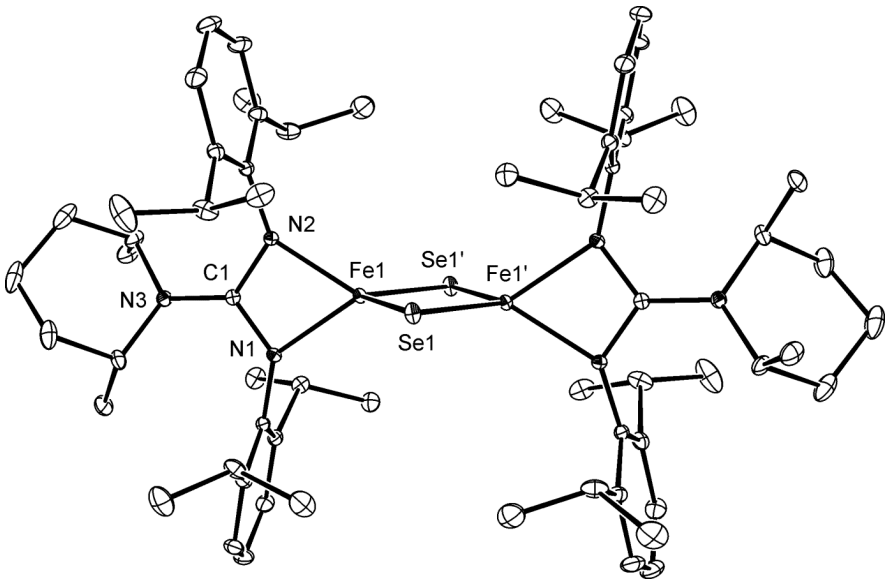


Figure S5. Displacement ellipsoid plot (25% probability surface) of the molecular structure of **5**. Hydrogen atoms are omitted. Selected metrical parameters are given in Table 1 (main text). Symmetry transformations used to generate equivalent atoms (‘): -x+1, -y, -z+1.

3. Magnetochemistry

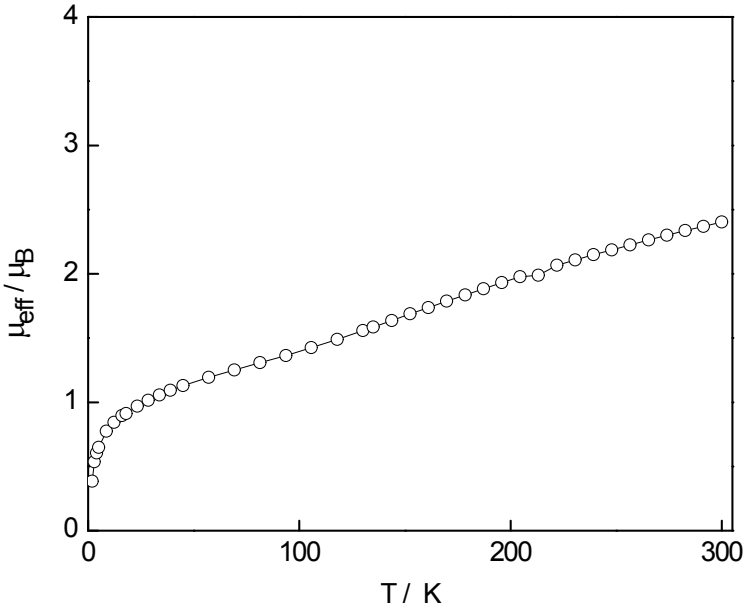


Figure S6. Plot of μ_{eff} (per two Fe centres) *vs. T* for **5**, in an applied field of 1 T. The solid line is a guide to the eye.

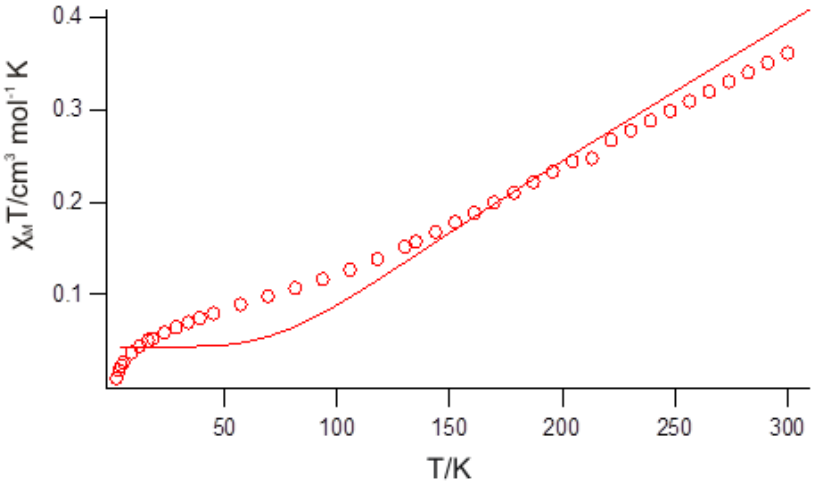


Figure S7. Plot of $\chi_M T$ (per Fe) *vs.* *T* for **5** (open circles). The solid line is that calculated for an S = 5/2 dimer model using the parameters: g = 2.0, J = -118 cm^{-1} and 1 % monomer impurity. Zero field splitting for S = 5/2 is not included.

4. Computational Studies

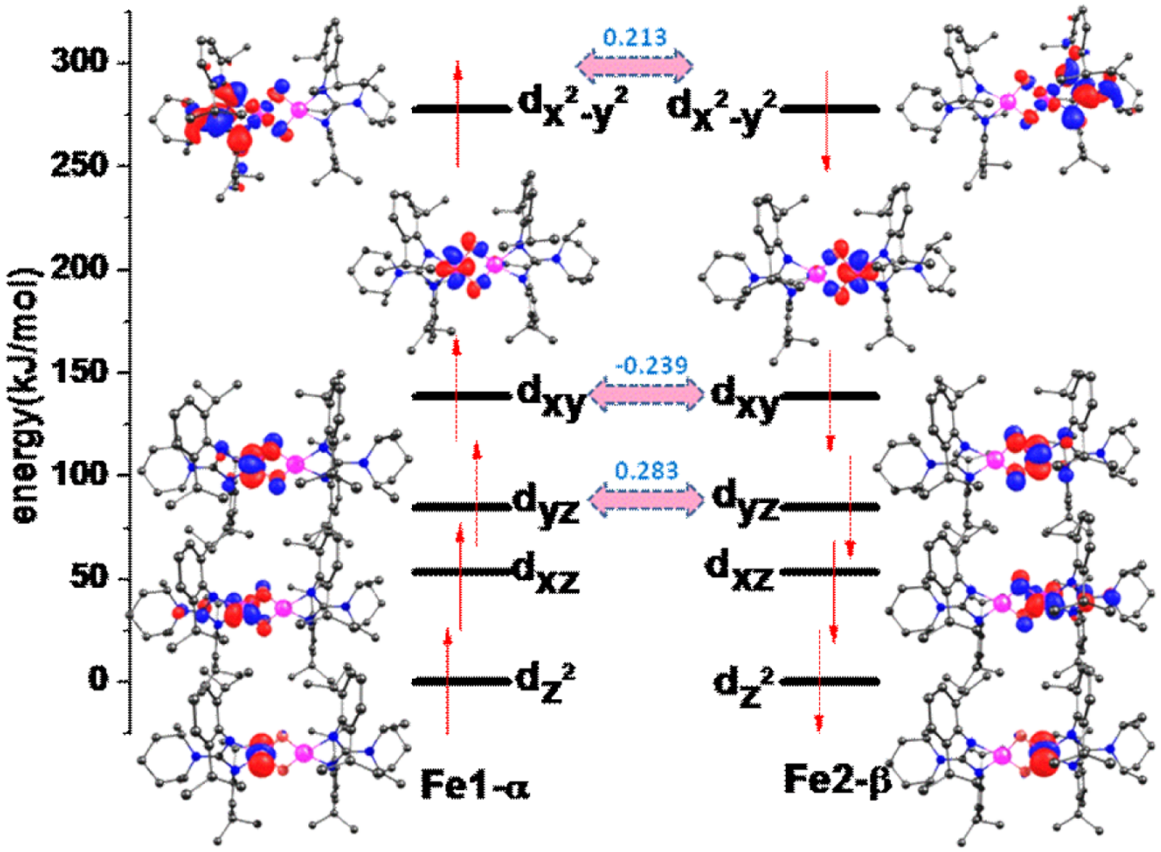


Figure S8. Computed molecular orbital energy level diagram incorporating BS orbitals for Fe(1) and Fe(2) atoms in complex **3**.

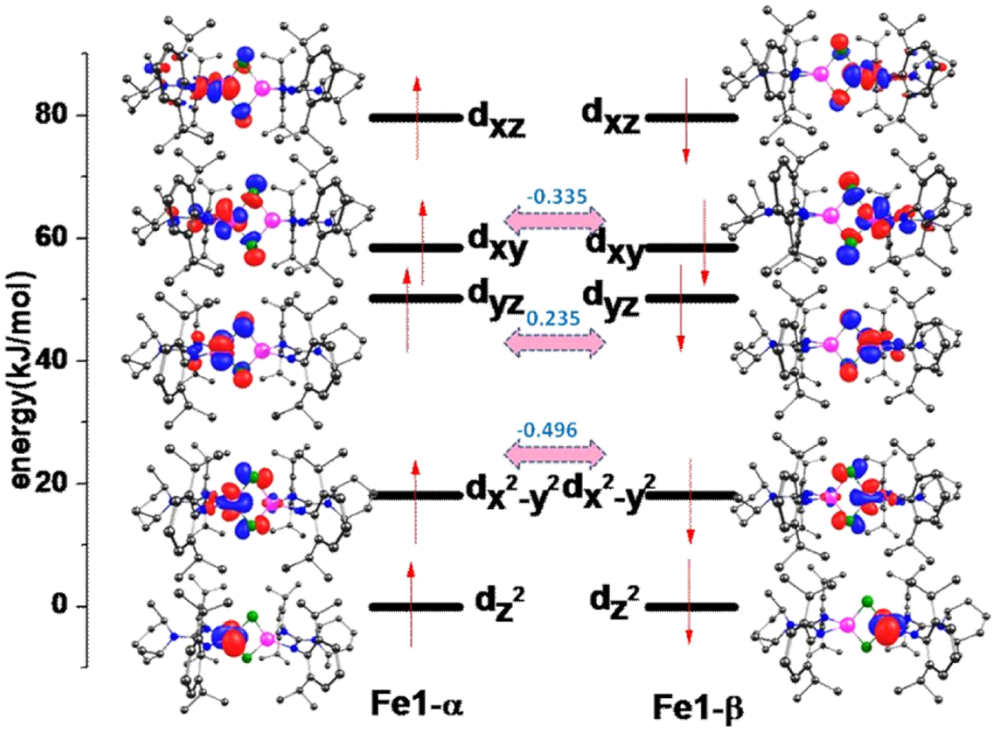


Figure S9. Computed molecular orbital energy level diagram incorporating BS orbitals for Fe(1) and Fe(2) atoms in complex **4**.

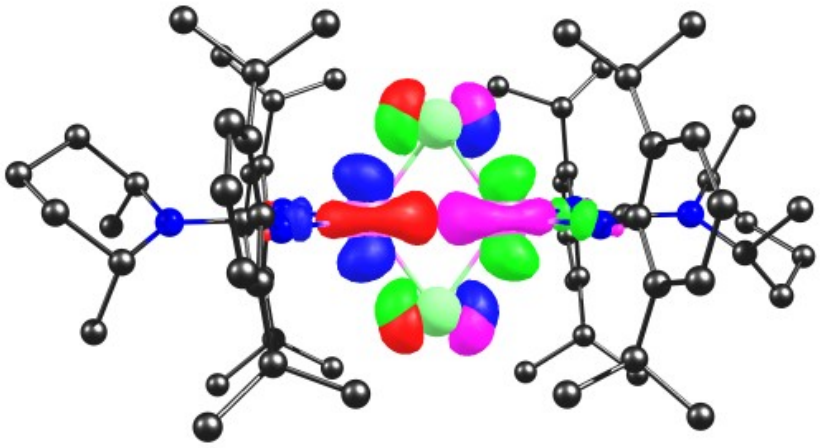


Figure S10. Superimposing the α and β $d_{x^2-y^2}$ orbitals on the Fe(I) and Fe(2) centres to demonstrate the nature of overlap in complex **5**.

Table S1. Overlap integral values corresponding to complex **3** (significant values highlighted in yellow).

Alpha/Beta	dxy	dxz	dyz	dx2-y2	dz2
dxy	-0.2389	0.0007	-0.0378	0.0107	-0.1202
dxz	0.0007	-0.1757	-0.0227	0.0066	0.0004
dyz	-0.0378	-0.0227	0.2827	0.0054	-0.0222
dx2-y2	-0.0107	-0.0065	-0.0054	0.2130	0.0363
dz2	-0.1202	0.0004	-0.0222	-0.0363	0.0170

Table S2. Overlap integral values corresponding to complex **4** (significant values highlighted in yellow).

Alpha/Beta	dxy	dxz	dyz	dx2-y2	dz2
dxy	-0.3354	-0.1305	0.0096		0.0109
dxz	-0.1305	-0.1720	0.0046	0.0059	-0.0053
dyz	0.0096	0.0047	0.2346	-0.0329	0.0587
dx2-y2	-0.0029	0.0059	-0.0329	-0.4963	-0.0361
dz2	0.0109	-0.0053	0.0587	-0.0361	0.0370

Table S3. Overlap integral values corresponding to complex **5** (significant values highlighted in yellow).

Alpha/Beta	dxy	dxz	dyz	dx2-y2	dz2
dxy	-0.3658	-0.1017	0.0114	0.0079	-0.0107
dxz	-0.1017	-0.1402	-0.0045	-0.0114	-0.0062
dyz	0.0114	-0.0045	0.0750	0.0693	-0.1010
dx2-y2	0.0079	-0.0114	0.0693	-0.4943	-0.0282
dz2	-0.0107	-0.0062	-0.1010	-0.0282	0.1878

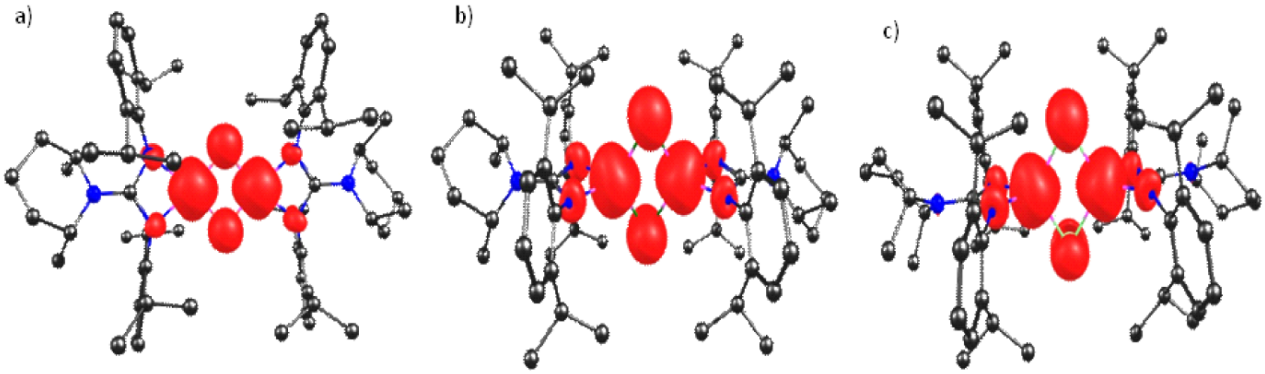


Figure S11. DFT computed spin density plot for complexes a) **3**, b) **4** and c) **5**. Plot cutoff employed is 0.01 e^- / $bohr^3$.

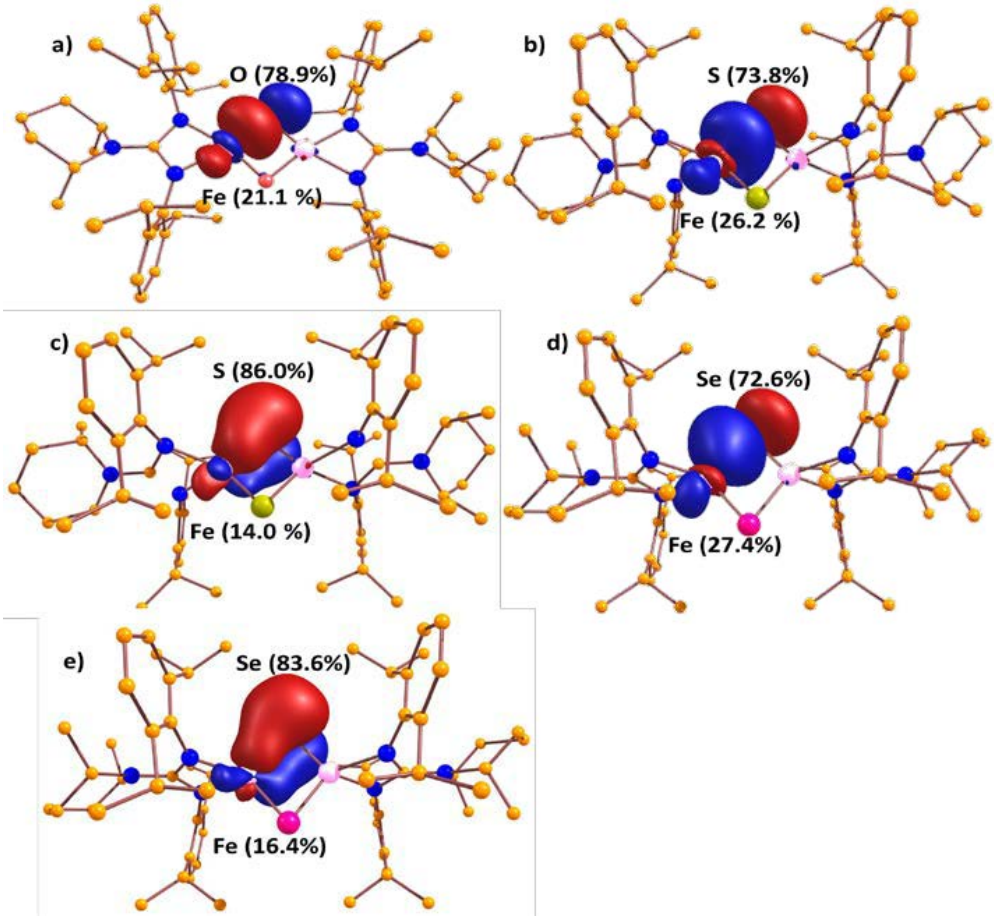


Figure S12. NBO computed Fe-E (E = O, S or Se) bond orbitals for complexes **3**-**5**. a) Fe-O σ interaction, b) Fe-S σ interaction, c) Fe- S π interaction, d) Fe-Se σ interaction, and e) Fe-Se π interaction. Computed percent contributions are given in parentheses.

Table S4. DFT computed spin density values for complexes **3**-**5** in both high-spin and broken symmetry states.

Atoms	Complex **3** (E = O)		Complex **4** (E = S)		Complex **5** (E = Se)	
	HS	BS	HS	BS	HS	BS
Fe(1)	4.03	3.98	3.84	3.9	3.82	3.9
Fe(2)	4.03	-3.98	3.84	-3.9	3.82	-3.9
E(1)	0.6	-0.034	0.10	-0.004	0.73	0.005
E(2)	0.6	0.034	0.10	0.004	0.73	-0.005
N	0.10-0.11	(-)0.10-0.11	0.17-0.14	(-)0.15-0.14	0.16-0.14	(-)0.15-0.14

Table S5. Absolute energies (high spin, HS, and broken symmetry, BS, states) and cartesian coordinates for the structures of **3**, $\mathbf{3}_{tet}$, **4** and **5** used for the calculations.

Absolute energies:

Complexes	E_{HS}	E_{BS}
Fe_2O_2(**3**)	-5502.731387 a.u.	-5502.734362 a.u.
Fe_2S_2(**4**)	-6148.739141 a.u.	-6148.771624 a.u.
Fe_2Se_2(**5**)	-10155.51136 a.u.	-10155.54323 a.u.
Fe_2O_2($\mathbf{3}_{tet}$)	-5502.794081 a.u.	-5502.806058 a.u.

XYZ Coordinates for **3:**

Fe	1.237020	0.035760	-0.018490
Fe	-1.237030	-0.035760	0.018490
H	-4.189000	-1.717070	-5.691330
H	3.660770	-2.501250	-5.657590
H	3.421800	-0.206450	-5.371690
H	3.706650	1.947260	-5.015630
H	-4.277660	0.458240	-4.874250
C	-3.975370	-1.538050	-4.783210
C	3.516580	-2.145630	-4.788620
C	3.378610	-0.777990	-4.614070
H	-3.591910	-3.456000	-4.258100
C	-4.013240	-0.244820	-4.292500
H	-4.422820	2.543200	-4.152280
H	1.329880	1.517410	-4.366780
C	3.937570	2.101120	-4.075670
H	4.866060	1.829870	-3.918730
C	-3.620450	-2.566020	-3.927310
H	3.835260	3.052900	-3.865800
H	3.537150	-3.930580	-3.824820
C	3.444210	-2.993710	-3.697160
H	-2.027260	2.119540	-3.669170
H	-5.561970	1.926140	-3.212860
C	-4.696080	2.384800	-3.224650
C	1.557950	1.680020	-3.427540
C	3.178260	-0.223030	-3.353930
H	1.443820	2.631880	-3.223750
C	3.006370	1.277650	-3.179600
H	-1.719060	-4.472760	-3.021930
H	5.757210	-0.300580	-2.778100
C	-3.679320	0.061440	-2.981890
H	-4.774130	3.241990	-2.756130
H	6.687790	-1.583910	-2.557910
H	-4.217420	-4.896610	-2.609400
H	0.968390	1.149710	-2.851780
C	-2.250970	2.111110	-2.715110
C	-3.304430	-2.326440	-2.593130

C	-3.645080	1.512200	-2.523510
H	7.208620	-0.133980	-2.124580
C	6.422270	-0.715290	-2.189740
C	3.236610	-2.491470	-2.411650
H	-2.238750	3.027720	-2.368650
H	-6.341650	-0.681980	-2.058220
H	3.735700	-5.218100	-2.039770
C	3.109420	-1.098930	-2.249920
H	3.224760	1.499860	-2.229380
C	-1.644950	-4.127530	-2.107730
H	-1.593330	1.569780	-2.230190
C	-3.318400	-0.999550	-2.115720
H	-0.941580	-3.446000	-2.071870
H	-8.371180	0.321850	-1.362720
C	-4.090800	-4.562840	-1.696730
H	-7.308930	-1.823380	-1.487600
H	4.966520	-4.354550	-1.491520
H	1.383580	-4.376290	-1.730980
H	5.553960	2.493900	-1.547970
H	6.983450	1.797230	-1.367390
C	-2.976570	-3.507590	-1.688000
H	-4.925120	-4.159560	-1.377740
H	-1.419950	-4.861560	-1.498610
C	-6.777510	-1.026030	-1.238640
H	-3.847090	1.524370	-1.544140
C	4.047220	-4.642000	-1.310730
H	-3.841450	-5.306040	-1.108740
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H	-2.879490	-3.165510	-0.753300
H	4.020400	-5.139590	-0.466900
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C	6.891280	-1.282990	0.227210
C	3.658330	0.113660	-0.163600
C	5.706530	1.429610	0.230490
H	-1.635060	4.363830	0.150600
H	-6.629680	-3.122910	0.543740

H	-4.020410	5.139590	0.466900
N	-5.014090	-0.221150	0.283200
C	7.715590	-0.052600	0.671450
C	-3.658330	-0.113660	0.163600
H	-3.431060	2.890240	0.406620
H	5.028570	1.981250	0.716310
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H	-5.202110	1.697850	0.865440
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H	3.841450	5.306040	1.108740
N	2.908380	0.735180	0.772860
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H	4.925110	4.159560	1.377740
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H	-5.553960	-2.493900	1.547970
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H	-3.735700	5.218100	2.039770
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C	1.644950	4.127530	2.107720
H	0.941580	3.446000	2.071870
C	3.318400	0.999550	2.115720
H	-6.687790	1.583910	2.557900
H	-3.224770	-1.499860	2.229380
H	4.217410	4.896610	2.609400
C	-3.109430	1.098930	2.249920
H	1.593330	-1.569780	2.230190
H	2.238750	-3.027720	2.368640
C	-3.236610	2.491470	2.411650
C	3.645080	-1.512200	2.523500
H	4.774120	-3.241990	2.756130
H	-5.757210	0.300580	2.778090
C	3.304430	2.326440	2.593130
C	2.250960	-2.111110	2.715110
H	1.719050	4.472760	3.021930
H	5.561960	-1.926150	3.212850
C	3.679320	-0.061440	2.981890
H	-0.968390	-1.149710	2.851780
C	4.696070	-2.384800	3.224650
C	-3.006380	-1.277650	3.179600

H	-1.443830	-2.631880	3.223740
C	-3.178270	0.223030	3.353920
C	-1.557950	-1.680020	3.427540
C	-3.444220	2.993700	3.697160
H	-3.537160	3.930580	3.824820
H	2.027250	-2.119540	3.669160
H	-3.835260	-3.052900	3.865800
H	-4.866060	-1.829870	3.918730
C	3.620450	2.566020	3.927310
C	-3.937570	-2.101130	4.075670
H	4.422820	-2.543210	4.152280
H	3.591900	3.456000	4.258100
C	4.013240	0.244810	4.292500
H	-1.329890	-1.517410	4.366780
C	-3.378610	0.777990	4.614070
C	3.975360	1.538050	4.783200
C	-3.516580	2.145630	4.788620
H	4.277650	-0.458240	4.874240
H	-3.706660	-1.947260	5.015620
H	-3.421800	0.206450	5.371680
H	-3.660770	2.501250	5.657580
H	4.188990	1.717070	5.691330

XYZ Coordinates for **4:**

Fe	-1.32253	-0.01443	-0.04916
Fe	1.32254	0.01443	0.04916
H	-4.02789	-0.54596	-5.30111
H	-4.18608	-2.13264	-5.16441
H	4.29365	-1.94628	-5.05331
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H	-1.67888	-2.25458	-4.54170
H	-5.12785	-1.15820	-4.31317
H	5.16473	-1.02725	-4.07481
H	3.73113	-3.76648	-3.94636
H	-3.74061	-3.86474	-3.89320
C	-1.79649	-1.38704	-4.10156
C	1.81888	-1.30244	-4.09857
C	-3.21265	-1.28375	-3.55473
C	3.19249	-1.22638	-3.44057
H	1.12386	-1.27283	-3.40833
H	-1.15518	-1.30471	-3.36507
H	-6.92358	0.27366	-2.89340
H	-4.07747	3.72614	-3.00745
H	4.68801	3.25536	-2.96758
C	3.63567	-3.65208	-3.00810
C	-3.72817	-3.67560	-2.96237
H	-3.28824	-0.40770	-3.07842
H	3.22290	-0.38715	-2.89759
H	3.96278	-5.59640	-2.53747
H	2.23398	3.49787	-2.76493

H	-4.15064	-5.56679	-2.38440
H	7.48438	-0.18288	-2.25840
H	-5.74965	1.26223	-2.43988
H	-1.67171	3.91971	-2.59113
C	-3.46754	-2.37965	-2.53792
C	3.37421	-2.38962	-2.49665
C	-6.48322	0.69350	-2.12529
C	3.75872	-4.74183	-2.17601
C	-3.96792	-4.68877	-2.07069
C	-4.26583	3.82275	-2.05055
H	6.49035	1.03249	-1.94512
C	4.79220	3.43885	-2.01067
H	4.90523	4.40261	-1.87312
H	-4.37720	4.77187	-1.83365
H	6.85951	-2.45975	-1.67889
H	-5.08833	3.33817	-1.82899
H	-7.13262	1.23948	-1.63490
H	5.21923	-0.84686	-1.80549
H	5.58038	2.96573	-1.67123
H	-7.61456	-1.56138	-1.44528
H	-5.30172	-0.94040	-1.75098
C	6.93954	0.24348	-1.55032
C	2.32858	3.68958	-1.80858
H	2.43868	4.65463	-1.67811
C	-1.81521	3.98959	-1.62432
H	-1.89394	4.93358	-1.37315
H	-2.99845	2.28445	-1.48356
H	3.43602	1.98337	-1.44237
C	-5.92993	-0.38577	-1.20523
H	8.49733	1.36209	-0.76844
C	3.55048	2.96048	-1.26280
H	1.52720	3.38503	-1.33354
S	0.04306	0.95222	-1.45054
C	-3.10477	3.24939	-1.24357
C	5.88203	-0.74705	-1.06331
C	-3.42808	-2.12179	-1.15387
C	6.49178	-2.12173	-0.83566
H	-1.05633	3.58813	-1.15165
C	3.26015	-2.23165	-1.10541
C	-7.01657	-1.31959	-0.69420
C	3.58573	-4.59004	-0.82051
C	-3.94300	-4.43006	-0.72337
C	7.84882	0.69722	-0.42576
H	5.80054	-2.73612	-0.51128
H	-6.59711	-2.15207	-0.36095
N	-3.04030	-0.81567	-0.72342
H	8.35614	-0.07663	-0.07400
H	7.20804	-2.05517	-0.17025
N	2.96883	-0.93831	-0.59322
H	3.63968	-5.35433	-0.25896
H	-8.35613	0.07663	0.07400
H	-4.11937	-5.13518	-0.11160
C	3.33448	-3.34950	-0.25172
C	-3.66420	-3.15405	-0.23222
H	-7.20803	2.05518	0.17025
N	-5.14702	0.17764	-0.08784

H	4.11938	5.13518	0.11160
C	-3.78607	0.10258	-0.07453
C	-7.84882	-0.69722	0.42576
N	5.14703	-0.17764	0.08785
H	-3.63967	5.35433	0.25897
H	6.59712	2.15207	0.36095
C	3.78608	-0.10258	0.07453
C	3.66420	3.15405	0.23223
H	-8.49732	-1.36209	0.76845
C	-3.33447	3.34950	0.25173
H	-5.80053	2.73612	0.51128
C	7.01658	1.31960	0.69420
C	-6.49178	2.12173	0.83566
C	3.94300	4.43006	0.72337
C	-3.58572	4.59004	0.82052
N	-2.96882	0.93831	0.59323
N	3.04031	0.81567	0.72342
C	-5.88203	0.74705	1.06331
H	7.61457	1.56138	1.44528
C	5.92994	0.38577	1.20523
C	-3.26014	2.23165	1.10541
C	3.42809	2.12179	1.15387
H	1.05634	-3.58813	1.15165
C	3.10477	-3.24939	1.24357
C	-6.93953	-0.24348	1.55032
C	-3.55048	-2.96048	1.26280
H	7.13262	-1.23948	1.63490
H	1.89395	-4.93358	1.37316
H	-6.85950	2.45975	1.67889
H	-1.52719	-3.38503	1.33354
H	-5.58037	-2.96572	1.67124
H	-3.43601	-1.98337	1.44237
H	2.99846	-2.28445	1.48357
H	-2.43867	-4.65462	1.67811
H	4.37720	-4.77187	1.83365
H	-4.90522	-4.40261	1.87313
C	1.81522	-3.98959	1.62432
H	5.08834	-3.33817	1.82900
H	5.30173	0.94040	1.75098
S	-0.04305	-0.95222	1.45054
H	-6.49034	-1.03249	1.94513
H	-5.21922	0.84686	1.80549
C	-2.32857	-3.68958	1.80858
C	-4.79220	-3.43885	2.01067
H	-7.48438	0.18288	2.25841
C	3.96793	4.68877	2.07069
C	6.48322	-0.69350	2.12529
C	4.26584	-3.82275	2.05055
C	-3.75871	4.74183	2.17601
H	4.15065	5.56679	2.38441
H	-3.96277	5.59640	2.53747
H	5.74965	-1.26223	2.43988
C	-3.37420	2.38962	2.49666
C	3.46755	2.37965	2.53793
H	6.92358	-0.27366	2.89340
H	1.67172	-3.91971	2.59113

H	-2.23397	-3.49787	2.76494
H	-4.68801	-3.25536	2.96758
C	3.72818	3.67560	2.96237
H	4.07747	-3.72614	3.00745
C	-3.63566	3.65208	3.00811
H	-3.22289	0.38715	2.89759
H	3.28825	0.40770	3.07843
C	-3.19248	1.22638	3.44057
H	1.15519	1.30471	3.36508
H	-1.12385	1.27283	3.40833
C	3.21266	1.28375	3.55473
H	3.74061	3.86474	3.89321
H	-3.73113	3.76648	3.94637
H	-5.16472	1.02725	4.07481
H	5.12786	1.15820	4.31318
C	-1.81887	1.30244	4.09857
C	1.79650	1.38704	4.10156
C	-4.29323	1.13013	4.51099
H	1.67889	2.25458	4.54170
C	4.22880	1.27977	4.68338
H	-1.74381	2.13994	4.60199
H	-1.70631	0.54363	4.70842
H	1.64342	0.66825	4.74988
H	-4.29364	1.94628	5.05331
H	-4.12243	0.35543	5.08629
H	4.18609	2.13264	5.16441
H	4.02790	0.54596	5.30111

XYZ Coordinates for **5:**

Fe	-1.36609	-0.03767	-0.03086
Fe	1.36609	0.03767	0.03085
H	-4.10725	1.78221	-4.49370
H	-4.08545	-3.10266	-4.31440
H	4.17288	-2.79022	-4.23963
H	4.76466	1.36632	-4.19954
H	2.34602	1.73580	-4.22192
H	-1.71771	2.16402	-4.21848
H	-4.44970	3.25102	-3.95857
H	4.97372	2.90699	-3.82065
H	-1.68097	-3.01887	-3.81435
C	-4.31164	2.31647	-3.69790
H	1.71892	-2.82467	-3.81032
H	2.48500	3.25966	-3.75313
H	-1.93902	3.64048	-3.64230
H	4.38365	-4.15161	-3.42512
H	-4.27753	-4.40089	-3.39851
C	4.85752	2.00302	-3.46044
C	-4.28365	-3.42093	-3.40897
C	4.34887	-3.17474	-3.35559
C	2.39306	2.33332	-3.44653
H	-5.12501	1.97205	-3.27344
C	-1.85805	2.69304	-3.40547
H	-5.16700	-3.09697	-3.13492
H	5.20636	-2.84050	-3.01880
H	5.63905	1.76396	-2.91961

H	1.87784	-4.20972	-3.02469
H	-6.93677	-1.22490	-2.68035
H	-5.78327	-0.11832	-2.75834
C	1.87679	-3.23394	-2.93398
H	-1.74967	-4.29026	-2.84483
C	-1.82707	-3.31450	-2.89151
H	1.57407	2.24472	-2.91577
H	-1.09631	2.57134	-2.80104
C	-3.14225	2.22869	-2.70910
H	4.16046	4.53737	-2.46063
H	-3.70745	4.79663	-2.43446
C	3.59983	1.95902	-2.58749
C	-3.22103	-2.89244	-2.43704
C	-6.51781	-0.47145	-2.21417
H	-3.25937	-1.89343	-2.45559
H	6.56128	-0.07226	-2.18889
C	3.22943	-2.77116	-2.39144
H	-3.02661	1.27108	-2.44524
H	-7.18338	0.23263	-2.06733
H	3.21461	-1.77280	-2.33672
H	1.16680	-2.96421	-2.31472
H	-1.15527	-2.90510	-2.30712
H	3.47551	1.02139	-2.26298
H	7.55528	-1.27599	-1.83678
H	8.55100	0.82208	-1.32566
H	3.78881	-5.22880	-1.56609
C	7.00336	-0.55337	-1.44511
C	3.97775	4.22840	-1.58103
C	-3.65044	4.40948	-1.56883
Se	0.04140	0.04715	-1.86100
H	-3.74128	-5.30748	-1.45992
C	-3.38484	3.04465	-1.44702
C	3.70322	2.87329	-1.37722
H	-7.24418	1.86364	-0.91029
H	5.27687	-1.62683	-1.14555
H	-5.34308	-1.69823	-1.05809
H	-5.84383	2.63816	-0.92250
C	7.90658	0.41143	-0.69629
C	-3.48426	-3.34164	-1.00853
C	-5.97286	-0.94486	-0.86947
H	4.16944	6.04500	-0.69949
H	6.65269	2.05182	-0.74507
C	3.43173	-3.31532	-0.98473
C	3.69763	-4.66661	-0.80567
H	-7.66401	-2.08201	-0.49352
C	-3.73944	-4.68370	-0.74338
H	-4.04865	6.12746	-0.56274
C	3.98974	5.12641	-0.53762
C	5.93469	-1.17249	-0.54490
C	-3.83207	5.20834	-0.45851
C	-6.54259	2.25724	-0.35065
H	6.92853	-2.96371	-0.20823
H	8.41885	-0.07883	-0.00550
H	-8.41885	0.07883	0.00549
C	7.06966	1.49656	-0.03942
C	-7.06966	-1.49656	0.03942

N	-5.19853	0.10005	-0.16673
H	-6.92853	2.96371	0.20823
C	-3.31251	2.49002	-0.15701
N	-3.08438	-1.07782	-0.20375
C	-3.83345	0.04432	-0.11222
C	3.46476	2.42913	-0.06699
N	3.01900	-1.10997	-0.04390
H	7.66401	2.08201	0.49351
C	6.54259	-2.25724	0.35064
C	-3.46476	-2.42913	0.06699
N	5.19853	-0.10005	0.16672
N	-3.01900	1.10997	0.04390
C	3.83345	-0.04432	0.11222
C	3.31251	-2.49002	0.15701
H	4.04865	-6.12746	0.56274
C	3.83207	-5.20835	0.45851
C	-7.90658	-0.41143	0.69628
N	3.08438	1.07782	0.20374
C	-3.98974	-5.12641	0.53762
H	-4.16944	-6.04500	0.69949
C	-5.93469	1.17249	0.54490
H	-6.65269	-2.05182	0.74507
H	7.24418	-1.86364	0.91029
C	3.73944	4.68370	0.74338
C	-3.69763	4.66661	0.80566
C	5.97286	0.94486	0.86947
H	5.84383	-2.63816	0.92250
H	-8.55100	-0.82208	1.32565
H	5.34308	1.69823	1.05809
C	-3.43173	3.31531	0.98473
C	3.48426	3.34164	1.00853
H	-5.27687	1.62683	1.14555
C	-7.00336	0.55337	1.44510
H	3.74128	5.30748	1.45992
H	-3.78881	5.22880	1.56609
C	-3.70322	-2.87329	1.37722
C	3.38483	-3.04465	1.44702
C	3.65043	-4.40948	1.56883
C	-3.97776	-4.22840	1.58103
H	-7.55528	1.27598	1.83678
H	7.18338	-0.23263	2.06733
H	-6.56128	0.07226	2.18889
C	6.51781	0.47145	2.21417
Se	-0.04141	-0.04715	1.86100
H	3.70745	-4.79663	2.43445
H	-4.16046	-4.53737	2.46063
H	-3.47551	-1.02139	2.26298
H	6.93677	1.22490	2.68035
H	-3.21461	1.77280	2.33672
H	1.15526	2.90510	2.30712
C	-3.22943	2.77116	2.39143
H	-1.16680	2.96421	2.31472
C	3.22102	2.89244	2.43704
H	3.25937	1.89343	2.45558
H	3.02661	-1.27109	2.44524
C	-3.59984	-1.95902	2.58749

H	5.78327	0.11832	2.75834
C	3.14225	-2.22869	2.70910
H	-5.63905	-1.76396	2.91961
H	1.74967	4.29026	2.84483
H	-5.20636	2.84050	3.01880
H	1.09630	-2.57134	2.80104
C	1.82706	3.31450	2.89151
H	5.16700	3.09697	3.13492
C	-1.87679	3.23394	2.93398
H	-1.87784	4.20972	3.02469
H	-1.57407	-2.24473	2.91576
H	5.12501	-1.97205	3.27344
H	4.27753	4.40089	3.39851
H	-4.38365	4.15161	3.42512
C	-4.34887	3.17474	3.35558
C	4.28365	3.42093	3.40897
C	-4.85752	-2.00302	3.46044
C	1.85804	-2.69304	3.40547
C	-2.39306	-2.33332	3.44653
C	4.31164	-2.31647	3.69790
H	1.93902	-3.64048	3.64230
H	-4.97372	-2.90699	3.82064
H	-2.48500	-3.25966	3.75313
H	4.44970	-3.25102	3.95857
H	1.68097	3.01887	3.81435
H	-1.71892	2.82467	3.81032
H	-4.76466	-1.36632	4.19954
H	-4.17289	2.79022	4.23963
H	4.08545	3.10266	4.31440
H	-2.34602	-1.73581	4.22192
H	1.71771	-2.16402	4.21848
H	4.10724	-1.78221	4.49369

XYZ Coordinates for **3_{tet}:**

Fe	-1.23702	-0.03729	-0.01542
Fe	1.23702	0.03730	0.01543
H	3.66082	2.71015	-5.56061
H	-4.21694	-1.16503	-5.42511
H	3.53710	0.38808	-5.47066
H	-3.59207	1.02454	-5.38773
H	3.73570	-1.80746	-5.30315
H	-1.71920	-0.57655	-5.36732
H	-4.18910	3.24112	-4.98349
H	-3.84122	-2.57568	-4.76950
C	3.51650	2.27544	-4.72830
C	3.44428	0.89471	-4.67237
C	-4.09055	-1.64691	-4.58127
H	-1.41962	-1.99091	-4.68102
C	-3.62057	1.34584	-4.49412
C	4.04743	-1.99235	-4.39266
H	4.96668	-1.66832	-4.28999
C	-1.64489	-1.05192	-4.51362
H	1.38392	-1.50027	-4.46071
C	-3.97540	2.66260	-4.26083
H	4.02111	-2.95805	-4.22818

H	-4.92496	-1.63038	-4.06754
H	-0.94173	-0.63920	-3.97002
H	3.42156	3.97182	-3.62255
C	-2.97653	-0.97277	-3.76918
C	3.37845	3.02421	-3.57062
C	1.69239	-1.72956	-3.55923
C	3.23663	0.23602	-3.45946
C	-3.30434	0.48063	-3.45040
H	1.63564	-2.69955	-3.43128
C	3.13882	-1.27794	-3.38661
H	6.68821	0.93372	-2.85969
C	-4.01351	3.12192	-2.95612
H	-4.27796	4.01988	-2.79403
H	-2.87935	-1.46637	-2.90500
H	-7.30866	-0.04014	-2.35323
H	1.12821	-1.27916	-2.89649
H	3.43124	-1.55328	-2.47080
H	-6.62968	-2.43003	-2.03575
C	3.17812	2.41921	-2.33372
C	6.42224	1.21258	-1.95859
H	5.75697	1.92943	-2.02145
C	3.10949	1.01069	-2.29107
H	-6.34148	1.13234	-1.84908
C	-3.31843	0.97163	-2.12859
H	-5.02833	-0.73115	-1.97590
H	7.49983	-1.13695	-1.60235
H	3.70534	5.08980	-1.74609
H	5.20249	-0.43347	-1.85555
C	-6.77728	0.28409	-1.58335
C	-3.67941	2.31804	-1.87646
H	7.20822	1.53807	-1.47212
H	1.32951	4.31549	-1.65718
C	-6.26922	-2.17202	-1.16177
C	-5.70630	-0.74650	-1.24103
C	5.81974	0.02288	-1.21467
H	4.86564	4.17537	-1.13087
H	-8.37127	1.24815	-0.63324
C	3.93724	4.47006	-1.02323
C	6.89147	-1.00063	-0.83352
H	-5.55408	-2.79197	-0.90745
C	3.00632	3.25408	-1.07450
H	-4.42341	4.81314	-0.73514
N	2.84744	0.33534	-1.07087
N	-2.90845	0.11616	-1.06025
H	4.77465	-4.19703	-0.69946
H	6.45726	-1.86707	-0.63139
C	1.55750	3.70297	-0.92705
H	-5.56230	3.69704	-0.60071
H	-6.98333	-2.20448	-0.49142
C	-7.71563	0.54629	-0.39309
H	0.96808	2.92078	-0.96076
H	2.23924	-3.76292	-0.78572
H	-2.02767	4.17070	-0.74725
H	-8.21425	-0.28006	-0.17265
C	-3.64534	2.90354	-0.47234
C	-4.69652	4.00210	-0.25769

H	3.83617	4.92268	-0.15983
H	8.21425	0.28007	0.17265
H	3.22474	2.67131	-0.29177
H	3.84717	-2.16291	-0.16862
H	-1.59376	2.71660	-0.23883
C	-2.25129	3.43626	-0.13823
N	5.01406	0.35958	-0.01356
C	7.71563	-0.54629	0.39310
H	1.44336	4.16125	-0.06844
H	-3.83617	-4.92267	0.15984
O	0.03339	-1.26390	-0.26821
N	-5.01407	-0.35957	0.01356
H	8.37127	-1.24814	0.63325
C	4.69652	-4.00210	0.25769
C	3.65823	0.19864	-0.01845
H	-1.44336	-4.16125	0.06844
C	-3.65823	-0.19863	0.01846
H	6.98333	2.20448	0.49142
C	2.25129	-3.43625	0.13823
H	-3.84718	2.16291	0.16863
H	5.56230	-3.69704	0.60071
H	-3.22474	-2.67131	0.29177
H	-6.45726	1.86707	0.63139
H	1.59376	-2.71659	0.23883
C	3.64534	-2.90353	0.47234
H	-4.77465	4.19703	0.69946
H	4.42341	-4.81314	0.73515
O	-0.03340	1.26391	0.26821
C	-6.89147	1.00063	0.83353
H	5.55408	2.79197	0.90745
H	2.02767	-4.17070	0.74725
H	-2.23924	3.76293	0.78573
C	-3.93724	-4.47006	1.02323
C	6.26921	2.17203	1.16177
H	-4.86564	-4.17537	1.13088
C	-1.55750	-3.70296	0.92705
C	-5.81974	-0.02287	1.21468
H	-7.20822	-1.53806	1.47212
C	-3.00632	-3.25408	1.07450
H	-0.96809	-2.92078	0.96076
C	5.70630	0.74651	1.24103
H	-7.49983	1.13696	1.60235
N	2.90845	-0.11615	1.06025
N	-2.84744	-0.33534	1.07087
C	6.77727	-0.28408	1.58335
H	-3.70534	-5.08980	1.74610
H	6.34148	-1.13233	1.84908
H	-1.32951	-4.31549	1.65718
H	6.62968	2.43004	2.03576
C	-6.42224	-1.21258	1.95860
H	-5.20249	0.43348	1.85555
H	-5.75697	-1.92942	2.02145
C	3.67941	-2.31804	1.87647
H	5.02833	0.73115	1.97590
H	7.30866	0.04015	2.35324
C	3.31843	-0.97162	2.12859

C	-3.17812	-2.41920	2.33372
C	-3.10949	-1.01069	2.29107
H	-3.43124	1.55329	2.47080
H	-6.68821	-0.93371	2.85969
H	4.27796	-4.01987	2.79403
C	4.01351	-3.12191	2.95612
H	2.87935	1.46638	2.90500
H	-1.12821	1.27916	2.89649
C	-3.13882	1.27795	3.38661
H	-3.42156	-3.97181	3.62255
H	-1.63565	2.69955	3.43129
C	3.30434	-0.48062	3.45041
C	-3.37845	-3.02421	3.57062
C	-3.23663	-0.23601	3.45946
C	-1.69239	1.72957	3.55923
C	2.97653	0.97277	3.76919
H	4.92496	1.63039	4.06754
H	-4.02111	2.95806	4.22818
H	-4.96669	1.66832	4.28999
H	0.94172	0.63920	3.97002
C	3.97540	-2.66260	4.26084
C	-4.04743	1.99235	4.39266
C	3.62057	-1.34583	4.49412
C	4.09055	1.64691	4.58127
H	-1.38392	1.50027	4.46071
C	1.64489	1.05192	4.51362
H	3.84122	2.57569	4.76950
C	-3.51651	-2.27544	4.72830
C	-3.44428	-0.89471	4.67237
H	1.41962	1.99091	4.68102
H	4.18910	-3.24111	4.98349
H	-3.73570	1.80747	5.30316
H	4.21694	1.16504	5.42511
H	3.59207	-1.02454	5.38773
H	-3.66082	-2.71014	5.56061
H	-3.53710	-0.38807	5.47067
H	1.71920	0.57656	5.36733