Supporting information for

Reactivity Studies on $[Cp'Fe(\mu\text{-}I)]_2$: Nitrido-, Sulfido-, and Diselenido Iron Complexes Derived from Pseudohalide Activation

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1. Crystallographic details

Table S1. Crystallographic data.

Compound	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Chemical formula	$C_{36}H_{58}Fe_2N_2O_2$	$C_{34}H_{58}Fe_2S_2$	$C_{34}H_{58}Fe_2Se_4$	$C_{34}H_{58}Fe_2N_2$	$C_{36}H_{44}FeNO_2P$	$C_{20}H_{29}FeNO_3$	$C_{44}H_{56}FeN_4$
Formula Mass	662.54	642.62	894.34	606.52	609.54	387.29	696.78
Crystal system	Monoclinic	Monoclinic	Monoclinic	Tetragonal	Triclinic	Orthorhombic	Monoclinic
a/Å	10.3424(4)	11.8548(2)	13.0954(4)	8.9474(3)	10.7445(8)	15.0303(3)	11.35137(10)
b/Å	9.2633(2)	10.3648(2)	18.8412(6)	8.9474(3)	11.3344(8)	10.4122(2)	23.7261(2)
c/Å	18.3885(6)	28.0527(4)	15.8088(6)	41.253(4)	15.2795(9)	12.7073(3)	13.9429(2)
α/°	90	90	90	90	109.628(6)	90	90
β/°	91.346(2)	91.796(2)	107.643(4	90	90.508(6)	90	93.494(2)
γ/°	90	90	90	90	109.886(7)	90	90
Unit cell volume/Å^3	1761.22(10)	3445.21(10)	3717.1(2)	3302.6(3)	1632.14(19)	1988.67(7)	3748.17(7)
Temperature/K	100(2)	130(2)	100(2)	100(2)	100(2)	100(2)	100(2)
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P4_12_12$	$P\bar{1}$	$Pca2_1$	$P2_1/n$
No. of formula units per unit cell, *Z*	2	4	4	4	2	4	4
Radiation type	Cu *K*α	Cu *K*α	Mo *K*α	Mo *K*α	Cu *K*α	Cu *K*α	Cu *K*α
Absorption coefficient, μ/mm^{-1}	6.8	8.0	4.7	0.9	4.4	6.2	3.5
No. of reflections measured	17685	73668	126169	19222	59261	33186	84181
No. of independent reflections	3658	7177	7605	2957	6742	3888	7838
R_{int}	0.0335	0.0783	0.1059	0.0486	0.0902	0.0601	0.0532
Final R_1 values ($I > 2\sigma(I)$)	0.0269	0.0407	0.0356	0.0328	0.0420	0.0343	0.0310
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.0692	0.0977	0.0683	0.0616	0.0995	0.0806	0.0749
Final R_1 values (all data)	0.0302	0.0427	0.0547	0.0399	0.0453	0.0376	0.0327
Final $wR(F^2)$ values (all data)	0.0702	0.0990	0.0742	0.0636	0.1013	0.0825	0.0759
Goodness of fit on F^2	1.08	1.11	1.04	1.06	1.07	1.03	1.03
Flack parameter	-	-	-	0.01(2)	-	0.017(4)	-
Largest diff. peak and hole/e Å^3	0.24/-0.37	0.41/-0.61	1.02/-0.48	0.25/-0.26	0.39/-0.44	0.23/-0.39	0.23/-0.37

2. Experimental and Structural Details [Cp'FeI(OPPh$_3$)], [Cp'Fe(CO)(μ-CO)]$_2$ and [Cp'Fe(μ-S$_2$)]$_2$

Synthesis of [Cp'FeI(OPPh$_3$)]. A mixture of [Cp'FeI]$_2$ (0.43 g, 0.5 mmol) and Ph$_3$PO (0.28 g, 1 mmol) was dissolved in *ca.* 10 mL of toluene to form a green solution, which was concentrated and overlayered with pentane (*ca.* 5 mL). Large green crystals formed at the bottom of the Schlenk flask after 7 d at ambient temperature. The crystals were isolated and dried under dynamic vacuum. Yield: 0.55 g (0.79 mmol, 79 %). The green crystals changed color to yellow at 115 °C and to orange-red at 185 °C. Mp.: 198-200 °C (dec.). ^{1}H NMR (C_6D_6, 289K): δ 32.9 (6H, *o*-C*H*, $\nu_{1/2}$= 950 Hz), 12.3 (6H, *m*-C*H*, $\nu_{1/2}$= 80 Hz), 8.2 (3 H, *p*-C*H*, $\nu_{1/2}$= 50 Hz), –13.3 (18H, CMe_3, $\nu_{1/2}$= 590 Hz), –22.0 (9H, CMe_3, $\nu_{1/2}$= 480 Hz. IR (Nujol mull; KBr windows; cm^{-1}): 3080(w), 3061(w), 1590(m), 1440(s), 1312(w), 1262(w), 1239(s), 1201(w), 1191(sh), 1143(vs), 1123(vs), 1085(vs), 1026(m), 1000(m), 957(w), 926(w), 826(s), 798(sh), 745(m), 695(s), 677(m). Anal. calcd. for $C_{35}H_{44}IOPFe$ (694.42): C, 60.53; H, 6.39. Found: C, 60.67; H, 6.23.

Crystallographic details:

Empirical formula	$C_{35}H_{44}FeIOP$	
Formula weight	694.42	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.8125(8) Å	α= 95.729(4)°
	b = 11.9887(10) Å	β= 90.970(4)°
	c = 14.0481(12) Å	γ = 97.250(3)°
Volume	1630.5(2) Å^3	
Z	2	
Density (calculated)	1.414 Mg/m^3	
Absorption coefficient	11.783 mm^{-1}	
F(000)	712	
Crystal size	0.15 x 0.15 x 0.05 mm^3	
Theta range for data collection	3.16 to 66.55°	
Index ranges	-11<=h<=11, -14<=k<=13, -16<=l<=15	
Reflections collected	14579	
Independent reflections	5451 [R(int) = 0.0239]	
Completeness to theta = 66.55°	94.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5903 and 0.2709	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5451 / 0 / 361	
Goodness-of-fit on F^2	1.085	
Final R indices [I>2sigma(I)]	R1 = 0.0246, wR2 = 0.0593	
R indices (all data)	R1 = 0.0255, wR2 = 0.0598	
Largest diff. peak and hole	0.522 and -0.365 e.Å^{-3}	

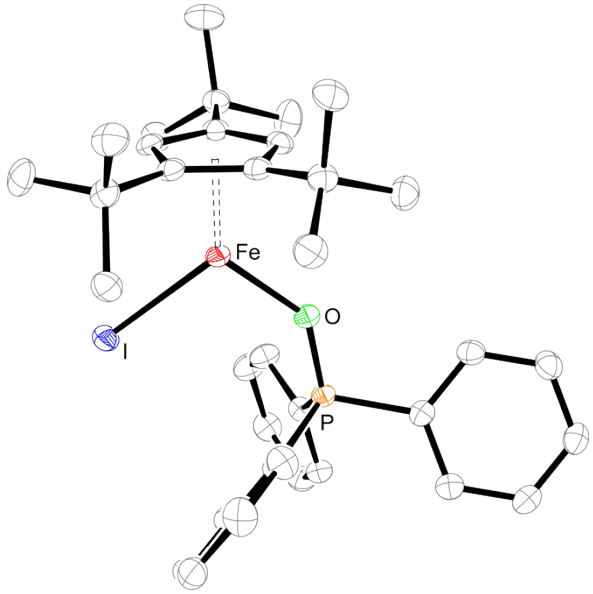

Figure S1. ORTEP diagram of **[Cp'FeI(OPPh$_3$)]**. Thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms have been omitted for clarity. Selected bond distances (Å) and angles (deg): Cp(cent)-Fe 1.97, Fe-I 2.6309(4), Fe-O 1.9908(15), Cp(cent)-Fe-O 128.8, Cp(cent)-Fe-I 128.1, I-Fe-O 102.65(5).

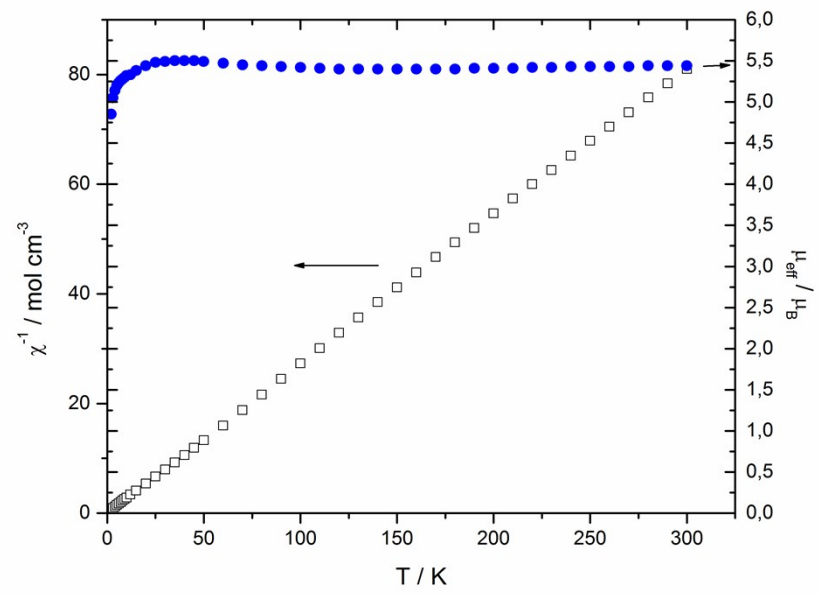

Figure S2. μ_{eff} and χ^{-1} vs. T plots for **[Cp'FeI(OPPh$_3$)]** recorded with an applied magnetic field of 5 kG between T = 2 – 300 K.

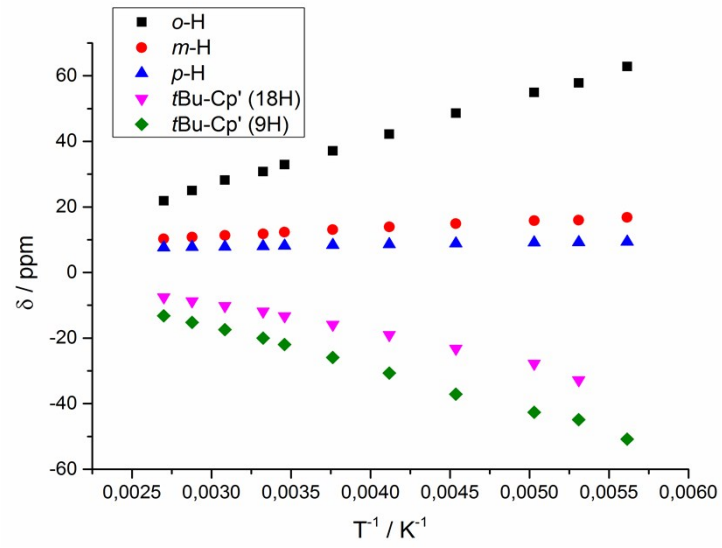

Figure S3. δ vs. T^{-1} plot for **[Cp'FeI(OPPh$_3$)]** recorded in C_7D_8 at temperatures T = 178 – 370 K.

Synthesis of [Cp'Fe(CO)(μ-CO)]$_2$. A Schlenk flask was charged with [Cp'Fe(CO)$_2$I] (0.236 g, 0.50 mmol) dissolved in toluene (10 mL), and a toluene solution (10 mL) of [(η^5-C_5H_5)$_2$Co] (0.110 g, 0.58 mmol) was added slowly (within 5 min). After 15 min the solvent was removed under dynamic vacuum. The dark residue was extracted with pentane (3 x 15 mL) and the wine-red extracts were combined and filtered; the solvent was evaporated. The residue was dissolved in toluene (15 mL), filtered and concentrated to 3 mL. On cooling to –30 °C dark red crystals formed. Yield: 0.098 g (0.14 mmol, 56%)**.** Mp.: 201-209 °C.

^{1}H NMR (300 MHz, C_6D_6, 297 K): δ = 4.53 (s, 4H, ring-C*H*), 1.52 (s, 36H, C*Me*$_3$), 1.22 (s, 18H, C*Me*$_3$) ppm. ^{13}C{^{1}H} NMR (75.5 MHz, C_6D_6, 298 K): δ = 244.8 (2C, CO), 176.6 (2C, CO), 108.4 (4C, ring-*C*$_{ipso}$), 107.9 (2C, ring-*C*$_{ipso}$), 88.6 (4C, ring-*C*H), 33.4 (12C, *C*H$_3$), 32.6 (4C, *C*Me$_3$), 32.0 (6C, *C*H$_3$), 31.2 (2C, *C*Me$_3$). IR (ATR, cm^{-1}): 2958(m), 2908(w), 2869(w), 1953(m), 1928(s), 1786(w), 1751(s), 1726(sh), 1460(w), 1393(w), 1372(sh), 1360(w), 1246(w), 1167(w), 1021(vw), 993(vw), 952(vw), 921(vw), 899(w), 877(w), 832(vw), 811(vw), 676(vw), 622(s). UV/vis (*n*-hexane, 22 °C): λ (ε, L mol^{-1} cm^{-1}) = 215 (25560), 219 (25650), 306 (sh, 8550), 367 (8870), 439 (2470), 551 (1220). Elemental analysis calcd (%) for $C_{38}H_{58}Fe_2O_4$: C 66.09, H 8.47; found: C 66.01, 8.83.

Crystallographic details:

Empirical formula	$C_{38}H_{58}Fe_2O_4$	
Formula weight	690.54	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 11.0245(7) Å	α= 93.174(5)°
	b = 12.0149(7) Å	β= 91.734(5)°

	c = 14.7311(8) Å γ = 113.619(6)°
Volume	1782.11(18) Å^3
Z	2
Density (calculated)	1.287 Mg/m^3
Absorption coefficient	6.809 mm^{-1}
F(000)	740
Crystal size	0.20 x 0.18 x 0.05 mm^3
Theta range for data collection	4.03 to 76.07°
Index ranges	-13<=h<=13, -15<=k<=15, -18<=l<=18
Reflections collected	49198
Independent reflections	7386 [R(int) = 0.0740]
Completeness to theta = 75.00°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.06431
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7386 / 0 / 415
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0329, wR2 = 0.0856
R indices (all data)	R1 = 0.0353, wR2 = 0.0873
Largest diff. peak and hole	1.018 and -0.585 e.Å^{-3}

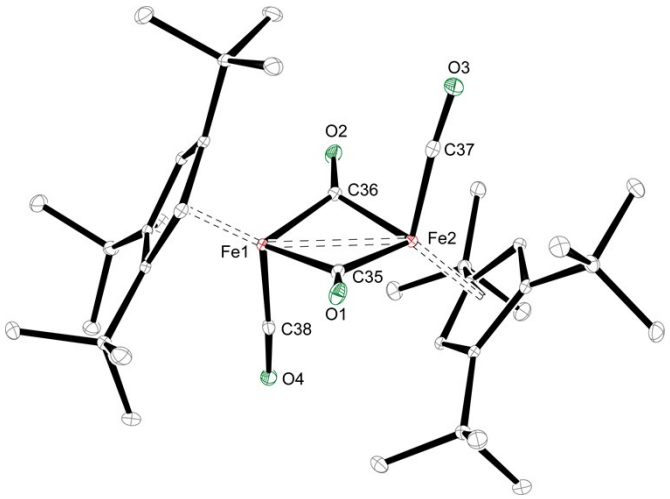

Figure S4. ORTEP diagram of **[Cp'Fe(CO)(μ-CO)]$_2$**. Thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms have been omitted for clarity. Selected bond distances (Å): Cp(cent)1-Fe1 1.77, Cp(cent)2-Fe2 1.79, Fe1-C38 1.7611(16), Fe1-C35 1.9566(16), Fe1-C36 1.9257(16), Fe2-C35 1.9317(16), Fe2-C36 1.9596(16), Fe2-C37 1.7544(17), Fe1···Fe2 2.5805(4)

Synthesis of [Cp'Fe(μ-S$_2$)]$_2$. A Schlenk tube was charged with [Cp'Fe(CO)(μ-CO)]$_2$ (0.020 g, 29 μmol) and freshly sublimed S$_8$ (0.004 g, 16 μmol), and toluene was added (0.7 mL). The reaction mixture was heated at 80 °C for six days. The solution was then allowed to cool to room temperature and the solvent was removed under dynamic vacuum. The residue was extracted with pentane (1 mL) and filtered. On cooling of the filtrate to –30 °C the product was

isolated as black blocks. Yield: 0.006 g (8 μmol, 28 %). ^{1}H NMR (200 MHz, C_7D_8, 300 K): δ = 5.64 (s, 4H, ring-C*H*), 1.31 (s, 36H, C*Me*$_3$), 0.88 (s, 18H, C*Me*$_3$) ppm. ^{13}C{^{1}H} NMR (50.3 MHz, C_7D_8, 300 K): δ = 105.2 (4C, ring-C_{ispo}), 103.7 (2C, ring-C_{ipso}), 84.7 (4C, ring-*C*H), 33.3 (12C, *C*H$_3$), 32.9 (4C, *C*Me$_3$), 31.4 (6C, *C*H$_3$), 29.5 (2C, *C*Me$_3$).

Crystallographic details:

Empirical formula	$C_{34}H_{58}Fe_2S_4$	
Formula weight	706.74	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 10.0731(3) Å	α= 80.822(3)°
	b = 12.2254(3) Å	β= 77.884(3)°
	c = 16.5630(5) Å	γ = 66.822(3)°
Volume	1826.57(9) Å^3	
Z	2	
Density (calculated)	1.285 Mg/m^3	
Absorption coefficient	1.044 mm^{-1}	
F(000)	756	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.23 to 30.91°	
Index ranges	-14<=h<=14, -17<=k<=17, -23<=l<=23	
Reflections collected	139454	
Independent reflections	10910 [R(int) = 0.0491]	
Completeness to theta = 30.00°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.97112	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10910 / 27 / 392	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.0862	
R indices (all data)	R1 = 0.0497, wR2 = 0.0925	
Largest diff. peak and hole	2.121 and -0.710 e.Å^{-3}	

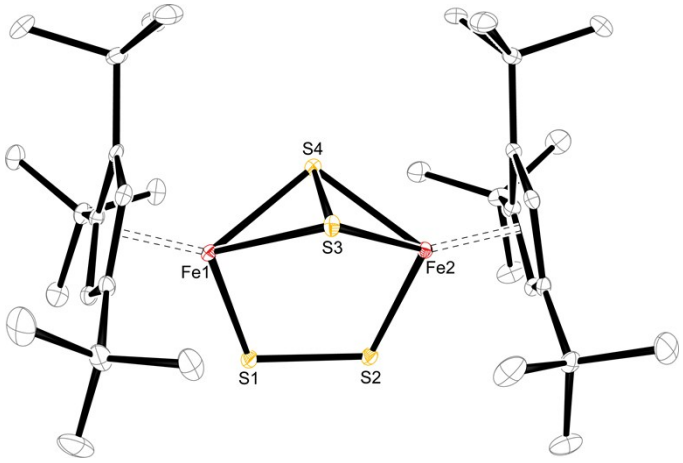

Figure S5. ORTEP diagram of **[Cp'Fe(μ-S$_2$)]$_2$**. Thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms have been omitted for clarity. Selected bond distances (Å): Cp(cent)1-Fe1 1.70, Cp(cent)2-Fe2 1.70, Fe1-S1 2.1171(5), Fe1-S3 2.2699(5), Fe1-S4 2.2615(5), Fe2-S2 2.1241(5), Fe2-S3 2.2786(5), Fe2-S4 2.2578(5), S1-S2 2.0121(6), S3-S4 2.0437(6), Fe1···Fe2 3.5075(3). The molecule displays approximate mirror symmetry (r.m.s. deviation 0.14 Å).

*3. Variable temperature ^{1}H NMR study of complex [Cp'Fe(μ-S)]$_2$ (**3**)*

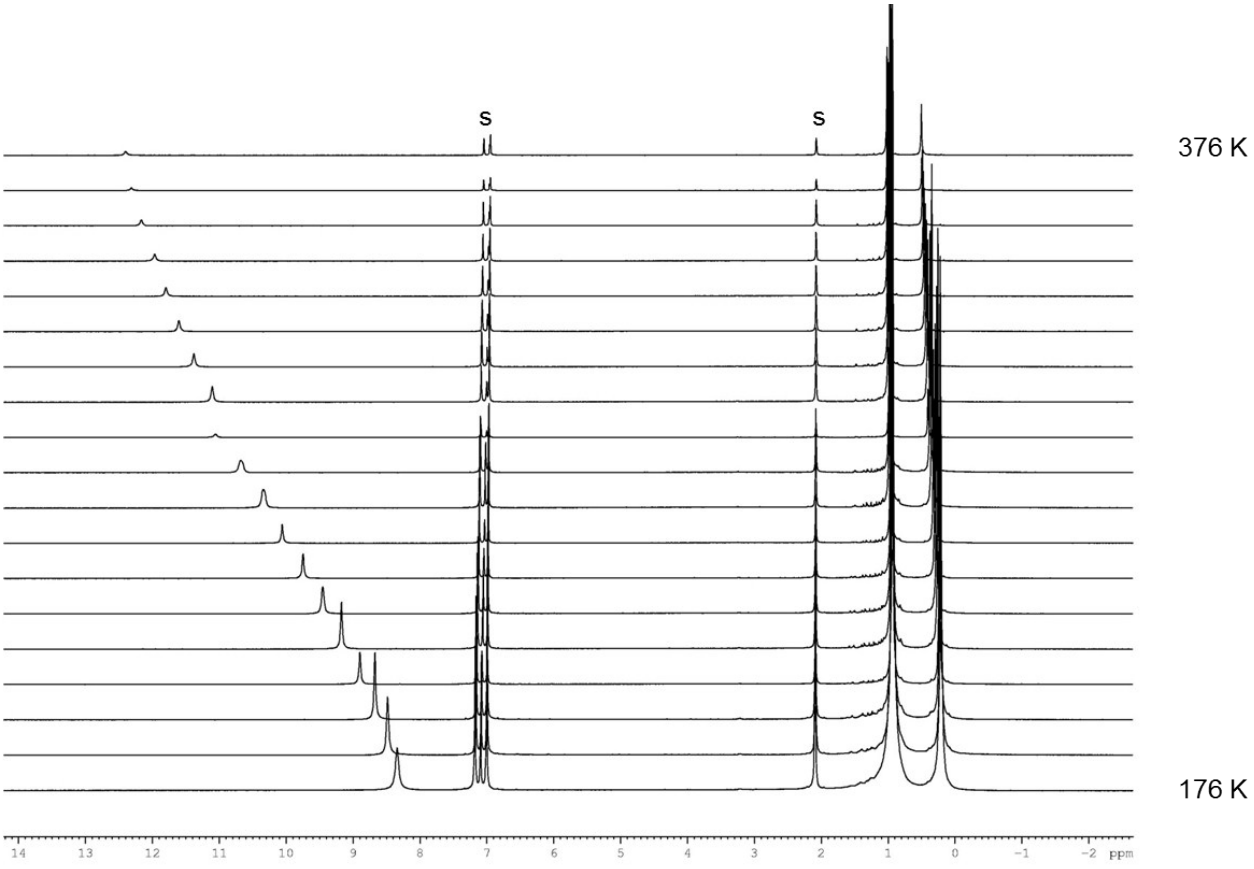

Figure S6. Variable temperature (VT) ^{1}H NMR study on [Cp'Fe(μ-S)]$_2$ (**3**) recorded in C_7D_8 between T = 176K and 376K. Resonances marked with "S" correspond to C_7D_7H.

*4. Chemical shift (δ) vs. T^{-1} plots for complexes **3**, **4** and **5***

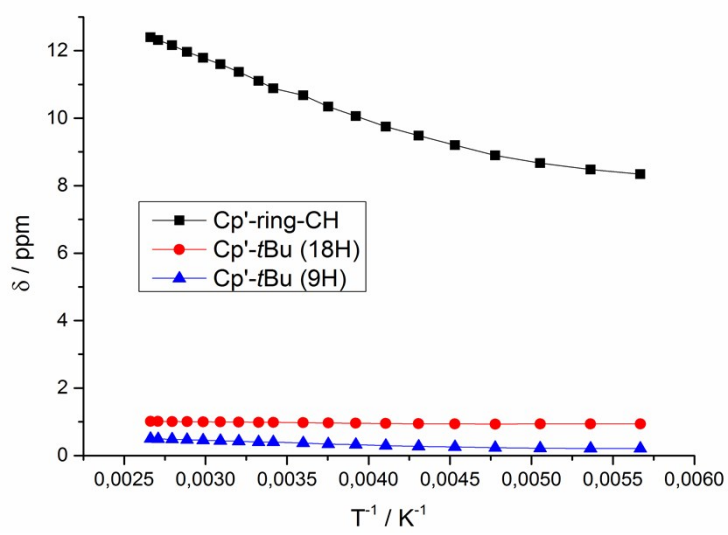

Figure S7. δ vs. T^{-1} plot for **[Cp'Fe(μ-S)]$_2$** (**3**) recorded in C_7D_8 at temperatures T = 176 K and 376 K.

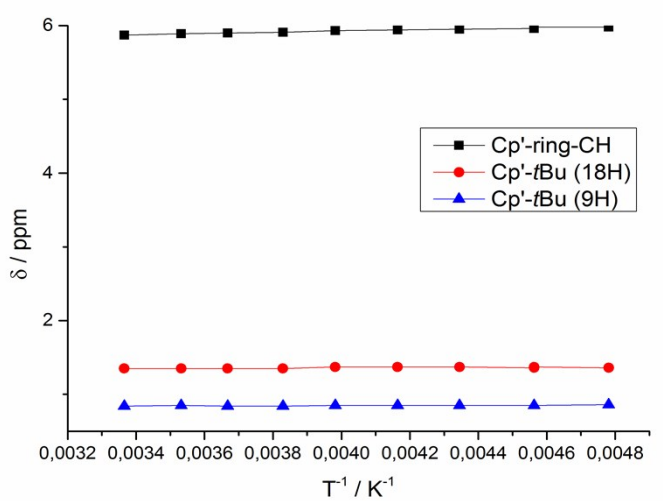

Figure S8. δ vs. T^{-1} plot for **[Cp'Fe(μ-Se$_2$)]$_2$** (**4**) recorded in C_7D_8 at temperatures T = 209K and 297K.

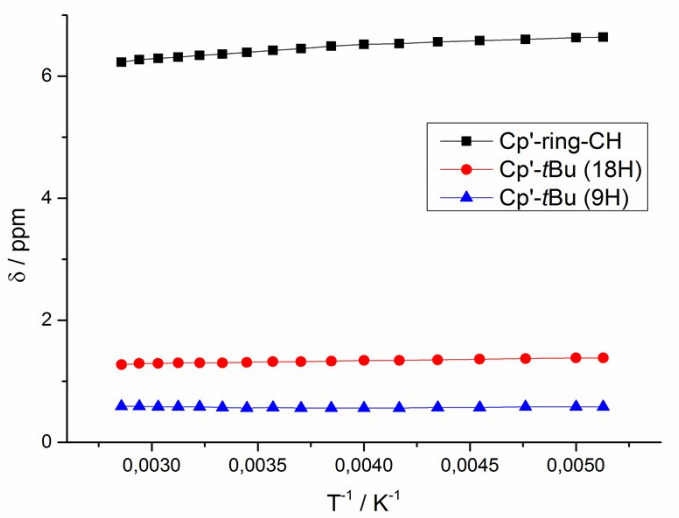

Figure S9. δ vs. T^{-1} plot for **[Cp'Fe(μ-N)]$_2$** (**5**) recorded in C_7D_8 at temperatures T = 181K and 358 K.

*5. Magnetic susceptibility studies on **3** and **5***

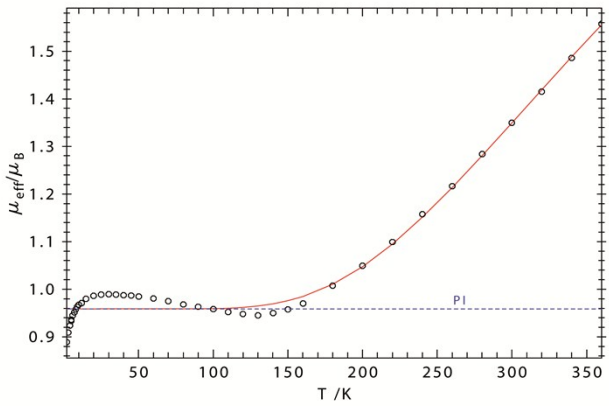

Figure S10. μ_{eff} vs. T plots for **[Cp'Fe(μ-S)]$_2$** (**3**) recorded with an applied magnetic field of 1 kG between T = 5 – 360 K. The magnetic trace may be simulated by assuming three different models:

	$S_1 = S_2 = 1/2$	$S_1 = S_2 = 3/2$	$S_1 = S_2 = 5/2$
J_{12} / cm^{-1}	-358	-354	-353
$g_1 = g_2$	2.286	2.244	2.238
Paramagnetic impurity (S = 5/2) / %	2.6	2.6	2.6
TIP / emu mol^{-1}	1088 x 10^{-6}	1087 x 10^{-6}	1086 x 10^{-6}

All three models can adequately describe the experimental data, and therefore we are unable to unambiguously establish electronic ground state at the individual Fe(III) centers in complex **3**. Nevertheless, the exchange coupling constant J_{12} is essentially identical regardless of the model employed.

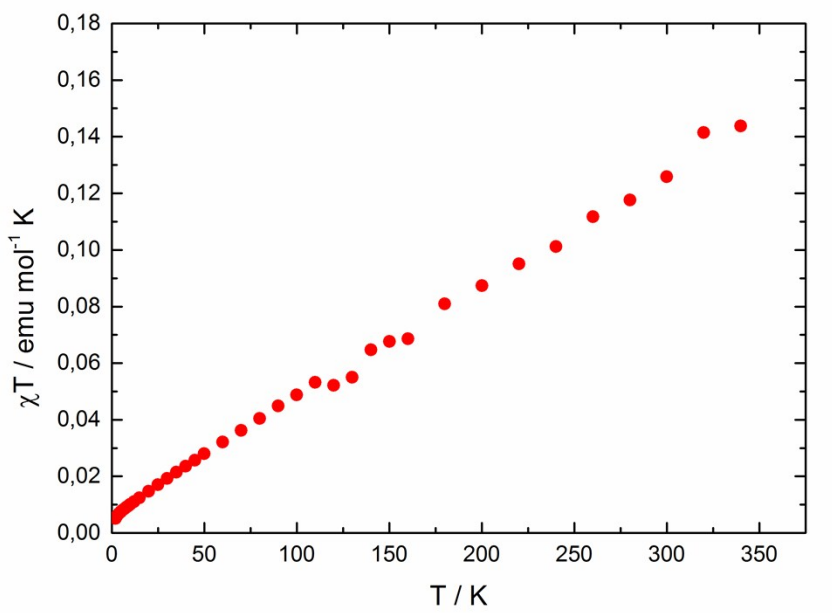

Figure S11. χT vs. T plots for **[Cp'Fe(μ-N)]$_2$** (**5**) recorded with an applied magnetic field of 1 kG between T = 5 – 340 K.

*6. ^{57}Fe Mössbauer spectrum of **5***

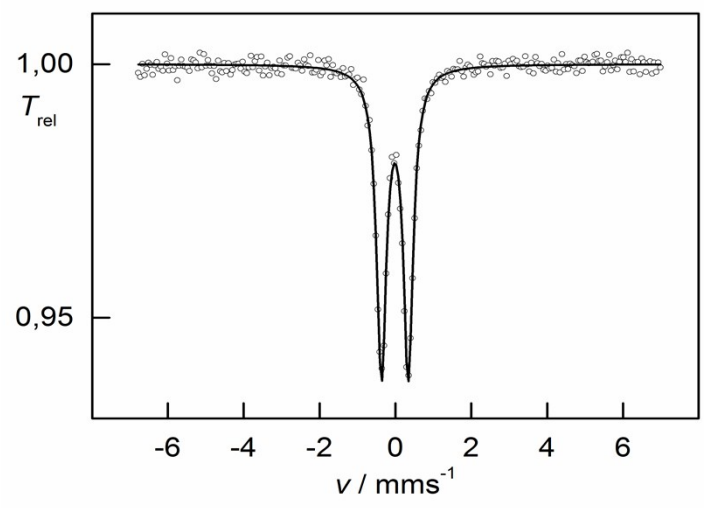

Figure S12. Zero-field Mössbauer spectra of **5** recorded at 77 K.

7. Computational studies

The different spin states for the different complexes are presented in the following figures as energy spectra. Then, the coordinates of the lowest energy complexes are listed.

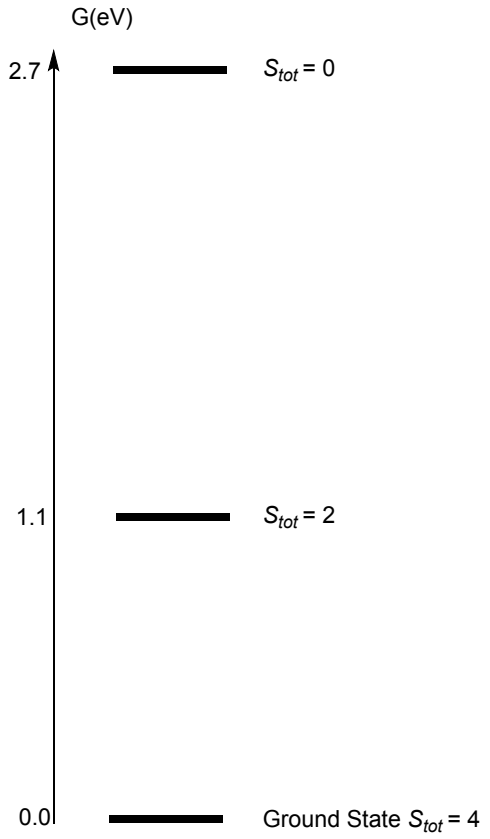

Figure S13. Computed spectrum of electronic spin states (at the B3PW91 level of theory) for **[Cp'Fe(μ-I)]$_2$** (**1**) with $S_{tot} = S_{Fe,1} + S_{Fe,2}$.

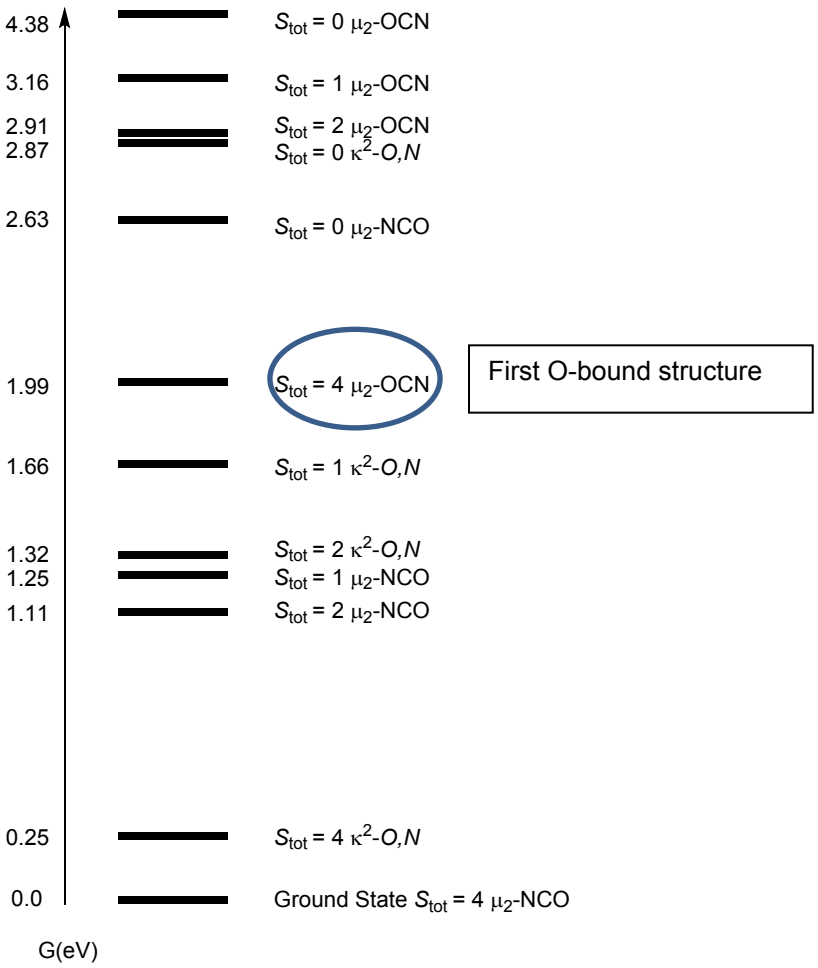

Figure S14. Computed spectrum of electronic spin states (at the B3PW91 level of theory) for **[Cp'Fe(μ-NCO)]$_2$** (**2**) with $S_{tot} = S_{Fe,1} + S_{Fe,2}$.

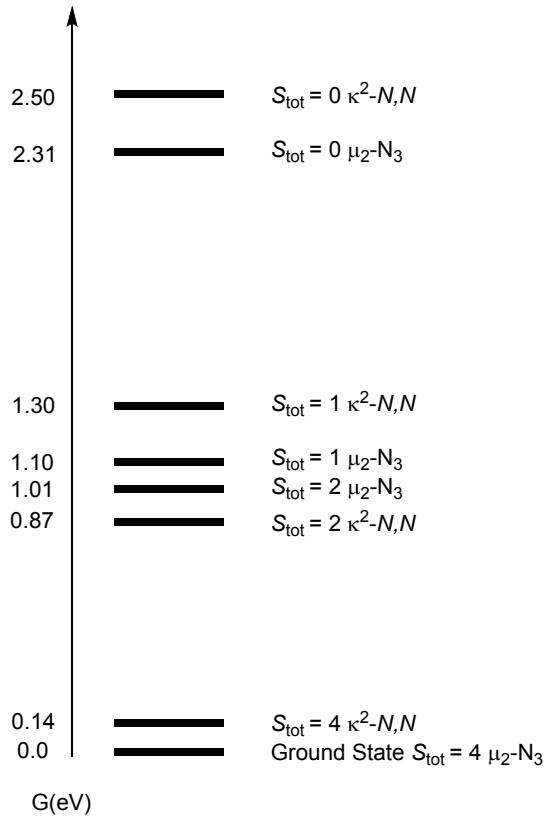

Figure S15. Computed spectrum of electronic spin states (at the B3PW91 level of theory) for **[Cp'Fe(N$_3$)]$_2$ (B)**, with $S_{tot} = S_{Fe,1} + S_{Fe,2}$.

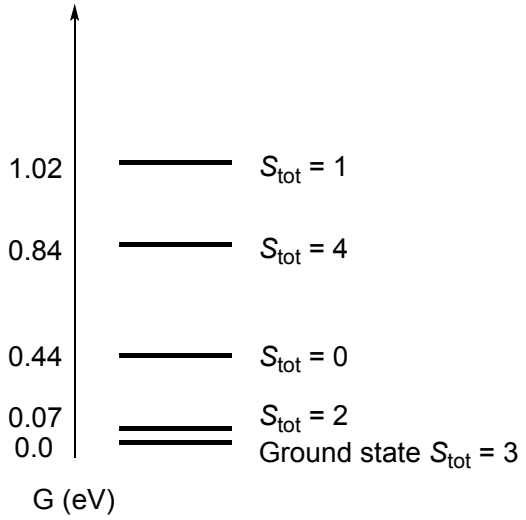

Figure S16. Computed spectrum of electronic spin states (at the B3PW91 level of theory) for **[Cp'Fe(μ-N)]$_2$ (5)**, with $S_{tot} = S_{Fe,1} + S_{Fe,2}$.

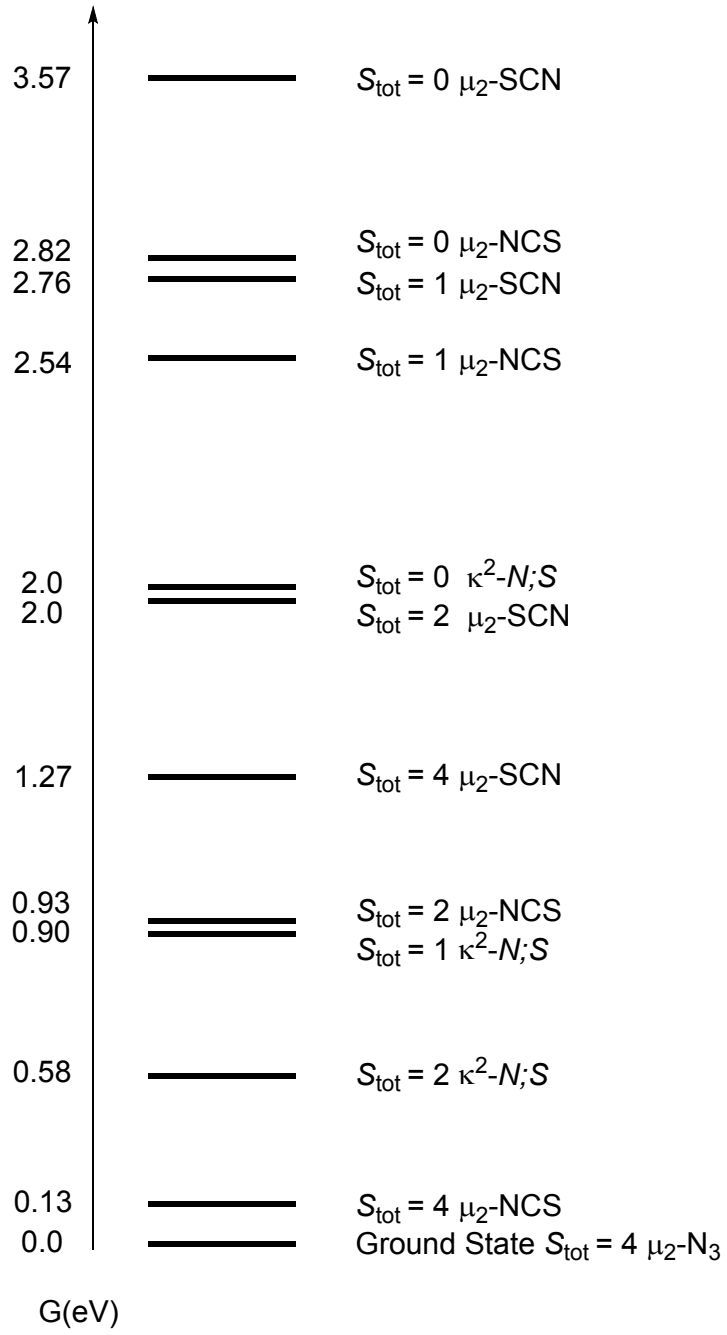

Figure S17. Computed spectrum of electronic spin states (at the B3PW91 level of theory) for **[Cp'Fe(SCN)]$_2$**, with $S_{tot} = S_{Fe,1} + S_{Fe,2}$.

Cartesian coordinates of the optimized structures

[Cp'FeI]$_2$ complex

96

C	-1.113681	12.805466	15.173252
C	-0.204145	13.096852	14.058070

C	-0.584036	14.381742	13.549653
H	-0.139324	14.860470	12.690834
C	-1.713331	14.888447	14.251594
C	-2.016424	13.914768	15.245479
H	-2.859819	13.976740	15.917519
C	-5.286351	11.484025	8.978015
C	-6.310056	11.346189	10.019879
C	-5.984891	10.157368	10.755238
H	-6.521627	9.804545	11.622598
C	-4.782776	9.577325	10.266692
C	-4.370971	10.401131	9.180148
H	-3.456400	10.263207	8.621891
C	-1.136326	11.728511	16.272340
C	-0.069622	12.105597	17.325299
H	0.940877	12.113190	16.913695
H	-0.092551	11.388107	18.153941
H	-0.269854	13.100906	17.735828
C	-0.904385	10.291974	15.782260
H	-1.639787	10.015270	15.020110
H	-1.016665	9.598932	16.623409
H	0.094638	10.137976	15.373512
C	-2.492442	11.722556	17.007541
H	-2.681732	12.661544	17.536108
H	-2.485415	10.928556	17.761440
H	-3.325715	11.530155	16.326343
C	0.964856	12.315820	13.424913
C	0.496717	11.028069	12.720229
H	-0.039325	10.350285	13.383438
H	1.363851	10.489249	12.319454
H	-0.164943	11.269307	11.882998
C	2.047798	11.989052	14.470446
H	2.366603	12.891566	15.002993
H	2.926974	11.568091	13.969860
H	1.715423	11.258626	15.209025
C	1.653551	13.174361	12.344649
H	0.974969	13.416668	11.520844
H	2.491240	12.610496	11.921295
H	2.055268	14.106301	12.756346
C	-2.407837	16.226958	14.069624
C	-3.935542	16.054213	14.078073
H	-4.264432	15.429546	13.242081
H	-4.425223	17.030954	13.992864
H	-4.287495	15.587191	15.003544
C	-1.986798	16.899068	12.755668
H	-0.910731	17.103050	12.733355
H	-2.504616	17.857839	12.644425
H	-2.238356	16.276821	11.890955
C	-1.991928	17.130998	15.248844

H	-2.303577	16.702400	16.207116
H	-2.455816	18.119359	15.153026
H	-0.905570	17.266931	15.277803
C	-5.152412	12.371089	7.727171
C	-3.724150	12.288354	7.149039
H	-3.479654	11.282199	6.795131
H	-2.968125	12.594504	7.877390
H	-3.648328	12.956940	6.285230
C	-6.095902	11.798674	6.644802
H	-5.981256	12.365335	5.713373
H	-7.145782	11.842780	6.939502
H	-5.851341	10.752034	6.435300
C	-5.450838	13.861583	7.942163
H	-5.256974	14.407374	7.012151
H	-4.806209	14.283070	8.719783
H	-6.490040	14.053132	8.211780
C	-7.536816	12.196708	10.403379
C	-8.511701	12.332589	9.218659
H	-8.779110	11.350166	8.814718
H	-8.106639	12.935424	8.404945
H	-9.434071	12.819172	9.555395
C	-8.327316	11.510472	11.535642
H	-8.693614	10.521752	11.239344
H	-9.198458	12.124621	11.786917
H	-7.730231	11.406142	12.446961
C	-7.139512	13.588678	10.933219
H	-8.042074	14.176053	11.140981
H	-6.526696	14.152950	10.231340
H	-6.575619	13.496556	11.866472
C	-4.105724	8.297133	10.724392
C	-2.589490	8.504532	10.869168
H	-2.368015	9.259769	11.629666
H	-2.130903	8.826967	9.928913
H	-2.108446	7.565901	11.166928
C	-4.674874	7.815932	12.065581
H	-4.534162	8.567878	12.848327
H	-4.164703	6.898910	12.379312
H	-5.743860	7.588531	11.992551
C	-4.370589	7.219993	9.652163
H	-3.914709	6.268193	9.948240
H	-3.948982	7.510689	8.684260
H	-5.444533	7.054353	9.516039
Fe	-4.469013	11.498958	10.873316
Fe	-2.141355	13.088088	13.406216
I	-2.464408	13.216981	10.779322
I	-4.380240	11.695342	13.513605

[Cp'Fe(N_3)]$_2$ complex

100

C	5.735076	7.303787	6.763449
C	7.086516	6.893979	6.985231
C	7.249900	5.619287	6.300794
C	5.980570	5.325464	5.694457
C	5.035984	6.354314	5.973246
Fe	5.584535	5.273523	7.870222
N	4.715678	5.846256	9.697267
N	4.510039	6.970980	10.116801
N	4.321423	8.033091	10.502489
C	8.039880	7.766822	7.825786
C	9.344218	8.083190	7.070530
C	8.462310	4.720918	5.993269
C	9.401860	4.480880	7.185661
C	3.632366	6.482331	5.401362
C	2.743842	7.346121	6.308784
Fe	4.328108	3.987147	10.512845
C	4.174918	1.958936	11.621476
C	2.823830	2.369330	11.398365
C	2.660622	3.644547	12.081807
C	3.929616	3.938182	12.688806
C	4.873911	2.908670	12.411525
C	1.870723	1.496382	10.557616
C	0.565426	1.181416	11.311787
C	1.448443	4.543784	12.387641
C	0.510293	4.783772	11.194140
C	6.277014	2.780279	12.984603
C	7.166035	1.916170	12.077961
N	5.198278	3.414591	8.686691
N	5.403332	2.289919	8.266638
N	5.591531	1.227910	7.880504
C	2.522221	0.130789	10.255639
C	1.554567	2.139882	9.191590
C	1.911000	5.942662	12.847406
C	0.659971	3.932250	13.566767
C	6.173741	2.110113	14.370592
C	6.930451	4.161817	13.145806
C	7.387851	9.131783	8.129475
C	8.357766	7.122445	9.190992
C	8.000099	3.321968	5.533348
C	9.249186	5.333511	4.813644
C	3.734282	7.152607	4.015327
C	2.979231	5.100594	5.240640
H	4.132907	4.810285	13.294016
H	4.616308	1.060791	11.214836
H	2.785598	-0.404774	11.173492
H	3.419741	0.224498	9.637006
H	1.812078	-0.490319	9.699800

H	0.877584	1.496319	8.617034
H	2.470885	2.260583	8.603092
H	1.085861	3.119974	9.283344
H	0.779039	0.721711	12.282423
H	-0.036049	0.473325	10.730535
H	-0.051228	2.063576	11.484411
H	2.537934	6.438884	12.100193
H	2.461289	5.910709	13.791902
H	1.032795	6.575292	13.013014
H	-0.179807	4.581906	13.841183
H	1.307372	3.828742	14.443738
H	0.260054	2.944389	13.332591
H	-0.276259	5.489957	11.482250
H	0.014379	3.876914	10.847648
H	1.054976	5.220511	10.349691
H	5.557473	2.708033	15.049988
H	7.166536	1.996438	14.821703
H	5.719821	1.116894	14.291961
H	7.012114	4.677371	12.182008
H	7.939667	4.059246	13.559754
H	6.362417	4.804777	13.825809
H	6.772890	0.900167	11.971557
H	8.172329	1.833766	12.503108
H	7.256431	2.352076	11.077177
H	5.777309	4.453846	5.088531
H	5.293484	8.201311	7.171232
H	7.123170	9.667884	7.212314
H	6.491058	9.037044	8.749002
H	8.098208	9.752913	8.685023
H	9.034908	7.765991	9.765379
H	7.442096	7.000701	9.780274
H	8.827019	6.142738	9.098008
H	9.129316	8.543828	6.100616
H	9.945982	8.790958	7.651879
H	9.961120	7.201526	6.896267
H	7.374184	2.825094	6.280992
H	7.448854	3.353989	4.589414
H	8.878493	2.689896	5.366622
H	10.089153	4.684584	4.538081
H	8.600850	5.436985	3.937361
H	9.648634	6.321548	5.047901
H	10.188522	3.775312	6.896348
H	9.897603	5.387854	7.532091
H	8.858332	4.043375	8.030457
H	4.350164	6.554926	3.335370
H	2.741074	7.266005	3.565057
H	4.187962	8.145960	4.093642
H	2.898428	4.585051	6.204519

H	1.969682	5.202834	4.827417
H	3.546980	4.457781	4.560258
H	3.136731	8.362258	6.414837
H	1.737150	7.428174	5.884511
H	2.654468	6.910199	7.309649

TS for N-N_2 bond breaking from [Cp'Fe(N_3)]$_2$

100

C	4.958250	3.056363	12.359382
C	4.294015	2.177165	11.447807
C	2.911085	2.564640	11.256988
C	2.738948	3.773911	12.007327
C	4.009589	4.050205	12.649836
Fe	4.468083	4.063463	10.427378
N	5.344721	3.550534	8.921180
N	5.956678	2.053595	8.362584
N	5.941025	1.032565	8.852434
C	1.978302	1.702052	10.380420
C	1.745528	2.341045	8.995999
C	1.526985	4.670902	12.312463
C	0.663127	3.994457	13.401064
C	6.340715	2.882223	12.965463
C	6.900255	4.228120	13.448729
N	4.542054	5.893289	9.818262
N	4.216765	7.018604	10.140335
N	3.935629	8.099507	10.397552
Fe	5.559849	5.181302	8.024177
C	4.953498	6.172528	6.041132
C	5.634562	7.113830	6.859119
C	6.999750	6.719832	7.044767
C	7.178441	5.478831	6.291054
C	5.916779	5.185899	5.700415
C	7.955534	7.593252	7.884874
C	8.288690	6.936819	9.241124
C	8.396486	4.595900	5.965845
C	9.197667	5.239715	4.813028
C	3.532313	6.294787	5.510548
C	3.022663	4.944776	4.985216
C	9.251676	7.927430	7.124652
C	7.294427	8.949344	8.207787
C	9.319823	4.323266	7.164368
C	7.934852	3.210843	5.464786
C	2.575854	6.793466	6.606396
C	3.538151	7.311639	4.350197
C	0.628402	1.416689	11.063139
C	2.618151	0.319748	10.133309
C	0.673312	5.005117	11.078858
C	1.976809	6.023025	12.905178

C	7.318078	2.270338	11.950504
C	6.210880	1.930505	14.173708
H	4.196641	4.911434	13.275275
H	4.743204	1.294036	11.017756
H	2.829939	-0.201648	11.073063
H	3.543773	0.384341	9.556378
H	1.921704	-0.299640	9.558756
H	1.100596	1.695766	8.387406
H	2.697797	2.467547	8.471350
H	1.270478	3.321668	9.063671
H	0.774026	0.975522	12.054710
H	0.060872	0.699583	10.459774
H	0.006327	2.305232	11.172349
H	2.656030	6.565760	12.242843
H	2.460850	5.908342	13.879474
H	1.096382	6.655033	13.059400
H	-0.167611	4.653057	13.680831
H	1.259700	3.807074	14.300121
H	0.243041	3.042542	13.076182
H	-0.127984	5.696401	11.362100
H	0.202037	4.128856	10.634363
H	1.277935	5.492595	10.306734
H	5.531407	2.341223	14.927954
H	7.188205	1.772457	14.644531
H	5.821930	0.954580	13.865143
H	6.989643	4.941867	12.622824
H	7.896135	4.086512	13.881960
H	6.269262	4.677443	14.222771
H	6.991947	1.280114	11.618564
H	8.308232	2.155487	12.405390
H	7.415098	2.905867	11.064954
H	5.710214	4.313586	5.098346
H	5.190879	8.012449	7.262545
H	7.021320	9.493741	7.298093
H	6.399996	8.840832	8.828662
H	8.001560	9.569698	8.768430
H	8.968779	7.576053	9.817081
H	7.377665	6.807461	9.837634
H	8.759878	5.958951	9.134558
H	9.026905	8.390742	6.158333
H	9.848853	8.638294	7.707073
H	9.876267	7.052810	6.943357
H	7.284661	2.714841	6.191573
H	7.406470	3.271554	4.508722
H	8.812039	2.575175	5.303905
H	10.038191	4.594966	4.528930
H	8.559100	5.368785	3.932958
H	9.599468	6.219409	5.076710

H	10.111801	3.627257	6.866233
H	9.809953	5.221046	7.542285
H	8.763476	3.860803	7.986757
H	4.213636	6.988171	3.551568
H	2.533239	7.419070	3.924755
H	3.869967	8.297191	4.692314
H	3.034547	4.178760	5.768242
H	1.992550	5.044851	4.626375
H	3.627480	4.583284	4.147310
H	2.886269	7.763165	7.007999
H	1.563932	6.912613	6.203043
H	2.523642	6.083907	7.440010

N_2-adduct to [Cp'Fe(N_3)-Cp'FeN]

100

Fe	4.435998	4.786081	10.358869
Fe	6.409607	6.492826	5.945853
N	6.072973	4.591813	6.715754
N	5.934318	4.309637	7.852254
N	5.807182	3.996944	8.978875
C	6.834317	8.430717	4.686858
C	8.079256	7.775346	4.930635
C	7.976614	6.449467	4.323906
C	6.657322	6.375026	3.757584
C	5.944826	7.587072	3.981513
C	9.198178	8.487571	5.716403
C	9.419251	7.849677	7.104104
C	8.982915	5.316016	4.049174
C	9.826628	5.690192	2.811281
C	4.553229	7.921973	3.466882
C	3.572078	6.778957	3.779932
N	5.646243	7.442923	7.655152
N	4.922473	6.975003	8.455734
C	4.346231	2.905511	11.765118
C	3.016603	3.224843	11.350418
C	2.744466	4.576500	11.833823
C	3.944333	5.009329	12.497454
C	4.935320	3.987128	12.458150
C	2.185629	2.212811	10.537636
C	1.990538	2.680856	9.080489
C	1.479091	5.451755	11.908709
C	0.611533	4.968724	13.091330
C	6.306659	4.039184	13.114217
C	7.025622	5.351666	12.755561
C	10.518163	8.525514	4.924310
C	8.814510	9.958309	5.976602
C	9.907338	4.976007	5.228330
C	8.237548	4.007375	3.709574

C	4.027854	9.214735	4.105984
C	4.630394	8.114067	1.938762
C	0.824648	1.923605	11.197107
C	2.917602	0.857841	10.461944
C	0.638819	5.484434	10.621960
C	1.857544	6.920394	12.197853
C	7.176299	2.858682	12.660640
C	6.120892	3.967543	14.643203
H	4.064129	5.963409	12.991085
H	4.861494	1.990462	11.515035
H	3.105457	0.440542	11.456481
H	3.871321	0.934365	9.930624
H	2.295823	0.143390	9.912065
H	1.391883	1.951432	8.521570
H	2.960720	2.764372	8.576397
H	1.488800	3.646344	9.009874
H	0.959413	1.578142	12.227533
H	0.303416	1.133980	10.643776
H	0.166835	2.792851	11.218529
H	2.540264	7.318987	11.440760
H	2.315383	7.045430	13.183470
H	0.949962	7.533291	12.189462
H	-0.269330	5.612271	13.202603
H	1.181345	5.010139	14.025492
H	0.264701	3.941856	12.959948
H	-0.205915	6.169279	10.757280
H	0.221031	4.513407	10.355249
H	1.231434	5.851769	9.777489
H	5.524166	4.809202	15.009515
H	7.091549	3.992712	15.152480
H	5.609305	3.043285	14.931003
H	7.201381	5.419936	11.675280
H	7.999424	5.405534	13.255594
H	6.447334	6.229213	13.062500
H	6.732493	1.899985	12.949137
H	8.164912	2.917766	13.128723
H	7.314700	2.859262	11.574426
H	6.269198	5.523197	3.217072
H	6.575966	9.411401	5.057271
H	8.635609	10.504103	5.044489
H	7.924746	10.044832	6.607803
H	9.635905	10.456214	6.502607
H	10.217348	8.376949	7.640812
H	8.507869	7.928069	7.708068
H	9.699159	6.797299	7.047558
H	10.367537	8.986824	3.942572
H	11.260298	9.123063	5.466147
H	10.950077	7.536658	4.767590

H	7.548931	3.715313	4.508735
H	7.675017	4.080078	2.774114
H	8.966776	3.200815	3.578824
H	10.516782	4.875503	2.561192
H	9.178274	5.862395	1.945891
H	10.416525	6.595430	2.968618
H	10.546632	4.127909	4.958300
H	10.568073	5.796862	5.507036
H	9.326259	4.684929	6.110100
H	4.979979	7.202577	1.443313
H	3.644778	8.366127	1.529883
H	5.322947	8.922181	1.681870
H	3.467476	6.635281	4.862036
H	2.578296	7.003900	3.375908
H	3.900183	5.830137	3.343553
H	4.659801	10.072803	3.854160
H	3.017786	9.431173	3.741683
H	3.983591	9.132571	5.197269
N	4.185535	6.537354	9.265096

TS for the second N-N_2 bond breaking

100

C	4.958250	3.056363	12.359382
C	4.294015	2.177165	11.447807
C	2.911085	2.564640	11.256988
C	2.738948	3.773911	12.007327
C	4.009589	4.050205	12.649836
Fe	4.468083	4.063463	10.427378
N	5.344721	3.550534	8.921180
N	5.956678	2.053595	8.362584
N	5.941025	1.032565	8.852434
C	1.978302	1.702052	10.380420
C	1.745528	2.341045	8.995999
C	1.526985	4.670902	12.312463
C	0.663127	3.994457	13.401064
C	6.340715	2.882223	12.965463
C	6.900255	4.228120	13.448729
N	4.542054	5.893289	9.818262
N	4.216765	7.018604	10.140335
N	3.935629	8.099507	10.397552
Fe	5.559849	5.181302	8.024177
C	4.953498	6.172528	6.041132
C	5.634562	7.113830	6.859119
C	6.999750	6.719832	7.044767
C	7.178441	5.478831	6.291054
C	5.916779	5.185899	5.700415
C	7.955534	7.593252	7.884874
C	8.288690	6.936819	9.241124

C	8.396486	4.595900	5.965845
C	9.197667	5.239715	4.813028
C	3.532313	6.294787	5.510548
C	3.022663	4.944776	4.985216
C	9.251676	7.927430	7.124652
C	7.294427	8.949344	8.207787
C	9.319823	4.323266	7.164368
C	7.934852	3.210843	5.464786
C	2.575854	6.793466	6.606396
C	3.538151	7.311639	4.350197
C	0.628402	1.416689	11.063139
C	2.618151	0.319748	10.133309
C	0.673312	5.005117	11.078858
C	1.976809	6.023025	12.905178
C	7.318078	2.270338	11.950504
C	6.210880	1.930505	14.173708
H	4.196641	4.911434	13.275275
H	4.743204	1.294036	11.017756
H	2.829939	-0.201648	11.073063
H	3.543773	0.384341	9.556378
H	1.921704	-0.299640	9.558756
H	1.100596	1.695766	8.387406
H	2.697797	2.467547	8.471350
H	1.270478	3.321668	9.063671
H	0.774026	0.975522	12.054710
H	0.060872	0.699583	10.459774
H	0.006327	2.305232	11.172349
H	2.656030	6.565760	12.242843
H	2.460850	5.908342	13.879474
H	1.096382	6.655033	13.059400
H	-0.167611	4.653057	13.680831
H	1.259700	3.807074	14.300121
H	0.243041	3.042542	13.076182
H	-0.127984	5.696401	11.362100
H	0.202037	4.128856	10.634363
H	1.277935	5.492595	10.306734
H	5.531407	2.341223	14.927954
H	7.188205	1.772457	14.644531
H	5.821930	0.954580	13.865143
H	6.989643	4.941867	12.622824
H	7.896135	4.086512	13.881960
H	6.269262	4.677443	14.222771
H	6.991947	1.280114	11.618564
H	8.308232	2.155487	12.405390
H	7.415098	2.905867	11.064954
H	5.710214	4.313586	5.098346
H	5.190879	8.012449	7.262545
H	7.021320	9.493741	7.298093

H	6.399996	8.840832	8.828662
H	8.001560	9.569698	8.768430
H	8.968779	7.576053	9.817081
H	7.377665	6.807461	9.837634
H	8.759878	5.958951	9.134558
H	9.026905	8.390742	6.158333
H	9.848853	8.638294	7.707073
H	9.876267	7.052810	6.943357
H	7.284661	2.714841	6.191573
H	7.406470	3.271554	4.508722
H	8.812039	2.575175	5.303905
H	10.038191	4.594966	4.528930
H	8.559100	5.368785	3.932958
H	9.599468	6.219409	5.076710
H	10.111801	3.627257	6.866233
H	9.809953	5.221046	7.542285
H	8.763476	3.860803	7.986757
H	4.213636	6.988171	3.551568
H	2.533239	7.419070	3.924755
H	3.869967	8.297191	4.692314
H	3.034547	4.178760	5.768242
H	1.992550	5.044851	4.626375
H	3.627480	4.583284	4.147310
H	2.886269	7.763165	7.007999
H	1.563932	6.912613	6.203043
H	2.523642	6.083907	7.440010

N_2 adducts to [Cp'FeN]$_2$ complex

100

C	4.938033	3.332376	12.365303
C	4.458193	2.362663	11.439100
C	3.038917	2.552673	11.165244
C	2.653561	3.718931	11.903536
C	3.839192	4.186262	12.584511
Fe	4.398951	4.165702	10.371631
N	5.162233	3.669964	8.827914
N	7.764488	-0.474862	8.318263
N	7.349645	-0.480238	9.341400
C	2.286077	1.555557	10.261501
C	1.885772	2.174692	8.907035
C	1.313299	4.433275	12.151422
C	0.577267	3.697656	13.293535
C	6.307598	3.389894	13.020747
C	6.695740	4.839124	13.350102
N	4.418375	6.054784	9.786197
N	4.321744	7.159797	10.287528
N	4.236835	8.218149	10.717542
Fe	5.395759	5.262098	8.055508

C	4.884795	6.509843	6.135927
C	5.743640	7.285375	6.958586
C	7.026777	6.660956	7.084034
C	6.957786	5.422138	6.318935
C	5.641987	5.373618	5.755809
C	8.146934	7.338387	7.899075
C	8.400515	6.614617	9.237659
C	7.973442	4.318016	5.970330
C	8.827831	4.780396	4.769683
C	3.493248	6.892848	5.656619
C	2.726658	5.661850	5.151486
C	9.452196	7.447280	7.090271
C	7.748039	8.785122	8.256483
C	8.883236	3.901617	7.136580
C	7.234771	3.033618	5.537030
C	2.681204	7.553458	6.782550
C	3.648797	7.897803	4.495650
C	1.052835	0.973994	10.977763
C	3.197458	0.357436	9.926078
C	0.399477	4.532411	10.921110
C	1.542556	5.883197	12.628405
C	7.378760	2.782038	12.102904
C	6.246785	2.577267	14.331132
H	3.873704	5.078721	13.193142
H	5.050953	1.561600	11.025212
H	3.531351	-0.171168	10.825424
H	4.073620	0.669853	9.350760
H	2.637439	-0.355323	9.311680
H	1.372374	1.424260	8.293552
H	2.781432	2.508826	8.374190
H	1.219245	3.029966	9.014721
H	1.330625	0.525906	11.937986
H	0.605209	0.188613	10.358473
H	0.278103	1.718855	11.165125
H	2.120387	6.467282	11.905987
H	2.049111	5.932964	13.596443
H	0.573048	6.376361	12.753038
H	-0.361182	4.212634	13.530903
H	1.191585	3.681441	14.199861
H	0.340472	2.664085	13.033817
H	-0.490210	5.119761	11.174324
H	0.051976	3.561384	10.568805
H	0.907514	5.036998	10.092690
H	5.502290	2.992941	15.018250
H	7.219855	2.587467	14.835959
H	5.977797	1.534313	14.133918
H	6.739804	5.452536	12.444113
H	7.681895	4.866639	13.826347

H	5.986522	5.304059	14.042886
H	7.188294	1.722489	11.904903
H	8.364402	2.854742	12.575742
H	7.415485	3.301985	11.140211
H	5.270000	4.563903	5.145805
H	5.473564	8.230761	7.407227
H	7.539549	9.382310	7.362815
H	6.874505	8.826157	8.914299
H	8.575076	9.262778	8.792088
H	9.202318	7.114491	9.794290
H	7.500240	6.642572	9.862710
H	8.682079	5.569580	9.107972
H	9.277446	7.964068	6.140888
H	10.191649	8.024977	7.656406
H	9.898083	6.477622	6.868760
H	6.540981	2.693147	6.312357
H	6.680617	3.166642	4.602924
H	7.967061	2.238862	5.360443
H	9.518417	3.983584	4.468939
H	8.188251	5.014493	3.912165
H	9.419049	5.670257	4.996012
H	9.523453	3.070494	6.819927
H	9.543645	4.701339	7.472080
H	8.286751	3.559986	7.989230
H	4.220239	7.459256	3.671148
H	2.666639	8.195896	4.110244
H	4.172859	8.800873	4.825065
H	2.624253	4.903742	5.935654
H	1.720993	5.952294	4.828797
H	3.223922	5.197901	4.293497
H	3.175088	8.449964	7.170161
H	1.696409	7.856730	6.410106
H	2.528377	6.862917	7.618856

$[Cp'FeS]_2$ complex $M_s=5$

96

C	-0.029012	0.399915	-0.065009
C	0.040461	0.497218	1.361287
C	1.457442	0.534832	1.698408
C	2.166923	0.438448	0.457144
C	1.266622	0.347579	-0.634992
C	-1.249660	0.390600	2.192664
C	-1.310601	1.326375	3.409530
Fe	1.034562	2.406407	0.388724
S	2.807999	3.687430	-0.036587
Fe	1.156394	5.164065	0.012010
S	-0.617063	3.883017	0.437262
C	2.227181	0.659967	3.028321

C	2.075314	2.069273	3.637280
C	1.599465	0.151180	-2.104942
C	1.242632	-1.299641	-2.489030
C	-2.479297	0.732723	1.324466
C	-1.416476	-1.077569	2.644809
C	1.800533	-0.414536	4.044755
C	3.736396	0.452178	2.789388
C	0.780084	1.119656	-2.975309
C	3.093043	0.386808	-2.367415
C	2.150502	7.073306	-0.960701
C	0.733525	7.035666	-1.297855
C	0.024023	7.131986	-0.056626
C	0.924315	7.222855	1.035546
C	2.219964	7.170596	0.465588
C	3.440626	7.179897	-1.792059
C	4.670220	6.837788	-0.923802
C	-0.036198	6.910478	-2.627761
C	-1.545453	7.117832	-2.388738
C	0.591436	7.419348	2.505476
C	0.948145	8.870234	2.889441
C	3.607447	8.648056	-2.244239
C	3.501596	6.244077	-3.008892
C	0.116023	5.501266	-3.236846
C	0.390127	7.985218	-3.644095
C	1.410891	6.451013	3.375927
C	-0.902126	7.183625	2.767959
H	-1.049985	7.108235	0.040350
H	3.140949	7.189332	1.030186
H	3.240928	0.462199	0.360136
H	-0.950002	0.381238	-0.629600
H	2.796623	8.981355	-2.894324
H	4.550391	8.764760	-2.791632
H	3.635950	9.316172	-1.377022
H	3.384325	5.200228	-2.701447
H	4.478687	6.344736	-3.494305
H	2.747011	6.472779	-3.761975
H	4.824587	7.564655	-0.120377
H	5.568220	6.860532	-1.549971
H	4.587770	5.839575	-0.483800
H	1.154157	5.241096	-3.445123
H	-0.443287	5.434876	-4.177789
H	-0.292288	4.748478	-2.552404
H	0.284371	8.989207	-3.219441
H	-0.250539	7.927191	-4.531314
H	1.420242	7.867467	-3.981422
H	-1.967322	6.347031	-1.736597
H	-2.070607	7.055458	-3.347540
H	-1.758863	8.100848	-1.955759

H	1.164244	5.409594	3.141631
H	1.196951	6.619523	4.437432
H	2.487440	6.584158	3.229030
H	-1.524487	7.901152	2.222416
H	-1.118209	7.306817	3.834696
H	-1.202305	6.172661	2.473420
H	2.013981	9.070608	2.739113
H	0.713959	9.054449	3.944311
H	0.381921	9.586547	2.284972
H	-2.633777	0.005799	0.521116
H	-2.396814	1.730894	0.884378
H	-3.377250	0.710086	1.950707
H	-2.359403	-1.194285	3.192229
H	-0.605635	-1.410901	3.294858
H	-1.445014	-1.745659	1.777572
H	-2.287660	1.225658	3.894994
H	-1.193403	2.370239	3.102103
H	-0.555962	1.097682	4.162566
H	1.905857	-1.418597	3.620162
H	0.770493	-0.296357	4.382159
H	2.441300	-0.356690	4.931914
H	3.949577	-0.531008	2.356687
H	4.261542	0.514687	3.748186
H	4.158469	1.222700	2.137048
H	2.634758	2.135646	4.578145
H	1.037261	2.329663	3.845678
H	2.483677	2.821917	2.952714
H	1.026835	2.161035	-2.740947
H	-0.296475	0.986604	-2.828401
H	0.993990	0.951200	-4.036829
H	3.393292	1.397732	-2.072811
H	3.309115	0.263677	-3.434161
H	3.715353	-0.330802	-1.821921
H	1.476797	-1.483784	-3.543917
H	0.176779	-1.499938	-2.338717
H	1.808795	-2.016056	-1.884626

$[Cp'FeS]_2$ complex M_s=7

96

C	-0.010999	0.533849	-0.106092
C	0.064553	0.636578	1.344909
C	1.468198	0.601313	1.686316
C	2.171772	0.545157	0.442246
C	1.271518	0.440455	-0.665195
C	-1.229428	0.513816	2.168094
C	-1.289437	1.407877	3.414651
Fe	1.021333	2.414822	0.353745
S	2.727372	3.657680	-0.217087

Fe	1.169651	5.155682	0.046803
S	-0.536392	3.912830	0.617645
C	2.241471	0.716401	3.014571
C	2.106651	2.126426	3.624176
C	1.619689	0.214021	-2.127726
C	1.281495	-1.251143	-2.473668
C	-2.460448	0.879119	1.311551
C	-1.391028	-0.970763	2.568703
C	1.806419	-0.356240	4.029731
C	3.747557	0.490248	2.771863
C	0.797893	1.149951	-3.028996
C	3.112953	0.455832	-2.386148
C	2.126364	6.933905	-0.944426
C	0.722684	6.969212	-1.285726
C	0.019221	7.025362	-0.041586
C	0.919563	7.130047	1.065779
C	2.202031	7.036619	0.506572
C	3.420317	7.056662	-1.767660
C	4.651328	6.691311	-0.911137
C	-0.050746	6.854122	-2.613909
C	-1.556826	7.080145	-2.371032
C	0.571520	7.356456	2.528344
C	0.909713	8.821622	2.874277
C	3.581977	8.541242	-2.168238
C	3.480320	6.162583	-3.014204
C	0.084083	5.444146	-3.223618
C	0.384049	7.926847	-3.629090
C	1.393418	6.420535	3.429530
C	-0.921717	7.114610	2.786895
H	-1.055520	7.020918	0.055363
H	3.127747	7.045546	1.062921
H	3.246523	0.549612	0.345393
H	-0.936671	0.524896	-0.662515
H	2.773474	8.891745	-2.811986
H	4.527962	8.679122	-2.704805
H	3.603264	9.180854	-1.279412
H	3.368640	5.110013	-2.737403
H	4.454665	6.284870	-3.500148
H	2.720402	6.409849	-3.755676
H	4.811008	7.399939	-0.092736
H	5.546458	6.726970	-1.540726
H	4.567560	5.683768	-0.494451
H	1.119443	5.169339	-3.425311
H	-0.472657	5.387378	-4.166770
H	-0.334447	4.697393	-2.539971
H	0.282600	8.931500	-3.204686
H	-0.255399	7.872549	-4.517390
H	1.414002	7.804497	-3.965200

H	-1.988558	6.309232	-1.725575
H	-2.083822	7.032762	-3.329644
H	-1.757553	8.062548	-1.930112
H	1.158622	5.372556	3.216809
H	1.168696	6.615029	4.484330
H	2.469754	6.563230	3.288894
H	-1.547668	7.812518	2.220130
H	-1.144969	7.264362	3.848766
H	-1.209573	6.093694	2.517142
H	1.975132	9.027886	2.728742
H	0.662560	9.033264	3.920992
H	0.342896	9.515806	2.244708
H	-2.620007	0.170556	0.493067
H	-2.376784	1.886715	0.894974
H	-3.355606	0.843290	1.941089
H	-2.337040	-1.108683	3.105211
H	-0.582544	-1.321202	3.212514
H	-1.412219	-1.610396	1.679890
H	-2.263738	1.285494	3.900657
H	-1.177871	2.460461	3.137858
H	-0.529442	1.160676	4.156068
H	1.907938	-1.360924	3.605418
H	0.776388	-0.233843	4.365595
H	2.445668	-0.301896	4.918171
H	3.948239	-0.492140	2.330886
H	4.274440	0.537504	3.730543
H	4.179447	1.261167	2.126518
H	2.663209	2.183204	4.567434
H	1.071273	2.401342	3.825640
H	2.525382	2.873099	2.940563
H	1.032713	2.197924	-2.816271
H	-0.278459	1.007297	-2.888442
H	1.022692	0.955432	-4.083774
H	3.400800	1.476751	-2.116400
H	3.336299	0.306044	-3.447994
H	3.738840	-0.242070	-1.819305
H	1.528738	-1.462806	-3.520357
H	0.216059	-1.457383	-2.328226
H	1.848240	-1.945329	-1.844038

[Cp'FeS]$_2$ complex M_s=3

96

C	0.041997	0.776404	-0.182637
C	0.022131	0.869113	1.250179
C	1.420781	0.899702	1.673908
C	2.205062	0.764581	0.480416
C	1.375100	0.711875	-0.670335
C	-1.311135	0.726215	2.004237

C	-1.458287	1.627613	3.236984
Fe	1.034712	2.479645	0.365852
S	2.813369	3.675762	0.183941
Fe	1.210246	5.068755	0.041179
S	-0.564826	3.874599	0.237875
C	2.106386	1.007360	3.050956
C	1.880147	2.381309	3.708058
C	1.797536	0.502509	-2.113322
C	1.537027	-0.978874	-2.459194
C	-2.504266	1.048216	1.080959
C	-1.458178	-0.759218	2.407612
C	1.649656	-0.122394	3.993143
C	3.632472	0.851251	2.893588
C	0.976970	1.397208	-3.053563
C	3.288331	0.809708	-2.305029
C	2.124257	6.671841	-0.950869
C	0.683847	6.666009	-1.198585
C	0.055783	6.794789	0.085208
C	1.023885	6.834571	1.124185
C	2.284021	6.763392	0.472957
C	3.359430	6.795278	-1.859877
C	4.647501	6.428291	-1.094670
C	-0.167325	6.602088	-2.483622
C	-1.660848	6.773970	-2.138403
C	0.773690	7.061980	2.604079
C	0.626202	8.585478	2.808479
C	3.496555	8.282947	-2.258823
C	3.332105	5.912194	-3.114371
C	-0.047197	5.251105	-3.212122
C	0.192341	7.756545	-3.438680
C	1.954660	6.557808	3.445693
C	-0.512232	6.365258	3.070546
H	-1.010978	6.792895	0.246080
H	3.233695	6.730905	0.984318
H	3.283031	0.777115	0.451617
H	-0.837752	0.791155	-0.808524
H	2.642023	8.646864	-2.831095
H	4.396547	8.420459	-2.869236
H	3.595494	8.913474	-1.368707
H	3.210383	4.859738	-2.840578
H	4.281937	6.016554	-3.650189
H	2.540209	6.188054	-3.811290
H	4.851319	7.118619	-0.270546
H	5.497789	6.495007	-1.781338
H	4.608374	5.409546	-0.700327
H	0.980333	4.999679	-3.470843
H	-0.630230	5.282749	-4.140508
H	-0.439828	4.448319	-2.582315

H	0.145147	8.724320	-2.927508
H	-0.524020	7.781405	-4.267419
H	1.186350	7.649070	-3.874981
H	-2.022566	5.970290	-1.489892
H	-2.244703	6.734798	-3.063874
H	-1.865444	7.738332	-1.660539
H	2.137906	5.493697	3.272813
H	1.740982	6.701115	4.510297
H	2.876681	7.104841	3.222222
H	-1.392391	6.731489	2.532124
H	-0.674972	6.560052	4.136442
H	-0.451481	5.285003	2.913901
H	1.528967	9.117263	2.489644
H	0.455484	8.810070	3.867488
H	-0.219749	8.982014	2.237232
H	-2.587102	0.343176	0.248028
H	-2.445517	2.063116	0.678803
H	-3.430640	0.965911	1.658935
H	-2.423686	-0.913622	2.902922
H	-0.672848	-1.090027	3.088867
H	-1.427429	-1.404536	1.523121
H	-2.463099	1.506340	3.656517
H	-1.329708	2.677886	2.958526
H	-0.750223	1.384974	4.029930
H	1.780144	-1.104873	3.526529
H	0.606542	-0.025123	4.296477
H	2.256008	-0.103363	4.905540
H	3.905570	-0.120593	2.467994
H	4.101099	0.921202	3.880678
H	4.058253	1.644657	2.271912
H	2.355223	2.399307	4.696221
H	0.826165	2.625167	3.834776
H	2.331238	3.162549	3.090568
H	1.143448	2.452607	-2.822705
H	-0.096726	1.199530	-2.972981
H	1.269317	1.216341	-4.093963
H	3.513961	1.841922	-2.020070
H	3.564830	0.670232	-3.355775
H	3.919818	0.140756	-1.710157
H	1.839102	-1.184783	-3.492268
H	0.475866	-1.230657	-2.360303
H	2.105261	-1.644606	-1.800699

$[Cp'FeS]_2$ complex M_s=11

96

C	0.168207	0.646066	-0.275566
C	0.010348	0.698158	1.146426
C	1.362314	0.736463	1.706145

C	2.255675	0.665022	0.580877
C	1.533509	0.603674	-0.638099
C	-1.394837	0.519560	1.747543
C	-1.650548	1.245690	3.074624
Fe	1.131346	2.445230	0.500804
S	2.837906	3.783950	0.348144
Fe	1.292707	5.308137	0.254481
S	-0.298262	4.001751	0.990738
C	1.912740	0.753012	3.144701
C	1.561680	2.048911	3.899601
C	2.092000	0.451907	-2.041572
C	1.866078	-1.011018	-2.478323
C	-2.473176	1.018607	0.761941
C	-1.613831	-0.999045	1.939902
C	1.428289	-0.484959	3.923877
C	3.453234	0.677769	3.121002
C	1.365527	1.389700	-3.018365
C	3.595367	0.759504	-2.073754
C	2.064747	6.836683	-1.006073
C	0.604624	6.825816	-1.115949
C	0.101637	7.075438	0.195615
C	1.157011	7.213690	1.133278
C	2.356377	7.066516	0.380979
C	3.206346	6.844368	-2.037361
C	4.557917	6.554906	-1.352650
C	-0.364957	6.598594	-2.292084
C	-1.818173	6.835942	-1.833574
C	1.052005	7.536547	2.612527
C	1.413219	9.026760	2.789219
C	3.301891	8.268742	-2.629382
C	3.060195	5.810833	-3.162266
C	-0.309697	5.150393	-2.814112
C	-0.101316	7.596103	-3.435481
C	2.031480	6.673941	3.424738
C	-0.373151	7.298764	3.129596
H	-0.943685	7.064297	0.462096
H	3.349626	7.093805	0.803472
H	3.331626	0.700398	0.650812
H	-0.650658	0.667424	-0.979746
H	2.396363	8.564014	-3.162345
H	4.141528	8.323264	-3.331894
H	3.478697	9.004187	-1.837234
H	2.969375	4.802743	-2.746287
H	3.952807	5.837016	-3.797062
H	2.203555	6.003574	-3.808687
H	4.839144	7.339267	-0.643099
H	5.342418	6.522722	-2.115834
H	4.547916	5.593238	-0.832129

H	0.683766	4.862007	-3.154526
H	-1.001680	5.037073	-3.657234
H	-0.608316	4.454720	-2.024327
H	-0.121342	8.628993	-3.071311
H	-0.884100	7.494454	-4.195224
H	0.855282	7.429489	-3.931971
H	-2.121593	6.123140	-1.060913
H	-2.487427	6.694537	-2.688437
H	-1.971494	7.853827	-1.459001
H	1.799706	5.611070	3.309463
H	1.964542	6.932954	4.487276
H	3.068630	6.828347	3.110603
H	-1.098657	7.952060	2.632386
H	-0.419799	7.516157	4.202006
H	-0.678888	6.259318	2.975636
H	2.435726	9.231130	2.455082
H	1.338573	9.310444	3.845086
H	0.735199	9.669226	2.217167
H	-2.517269	0.416101	-0.150524
H	-2.307993	2.064803	0.488593
H	-3.455730	0.939753	1.238565
H	-2.627285	-1.183706	2.314567
H	-0.906685	-1.433028	2.650817
H	-1.503113	-1.532228	0.989698
H	-2.693324	1.088204	3.371416
H	-1.485243	2.321237	2.967239
H	-1.028221	0.873918	3.889059
H	1.690662	-1.408206	3.395531
H	0.350121	-0.486360	4.089450
H	1.910553	-0.513248	4.907323
H	3.815150	-0.243750	2.652371
H	3.824493	0.690378	4.150945
H	3.891676	1.536259	2.602593
H	1.981833	2.007992	4.911672
H	0.490048	2.217536	3.984394
H	1.989419	2.911195	3.379834
H	1.498338	2.434453	-2.722836
H	0.291132	1.182707	-3.059069
H	1.765047	1.261567	-4.030606
H	3.798340	1.774052	-1.716597
H	3.970737	0.671876	-3.098878
H	4.164467	0.056142	-1.456192
H	2.269740	-1.172625	-3.484439
H	0.800106	-1.260816	-2.496361
H	2.365048	-1.707967	-1.796713

[Cp'FeS]$_2$ complex M_s=9

96

C	-0.039073	0.622559	0.021307
C	0.038985	0.615578	1.461589
C	1.438551	0.624973	1.793568
C	2.151107	0.633346	0.538663
C	1.254983	0.576072	-0.567497
C	-1.256731	0.490468	2.281406
C	-1.286123	1.324053	3.570331
Fe	1.023857	2.423217	0.432176
S	2.746782	3.746921	0.474600
Fe	1.166769	5.147373	-0.031749
S	-0.556192	3.823768	-0.073851
C	2.215194	0.631453	3.124259
C	2.077769	1.969267	3.878417
C	1.593386	0.376404	-2.033204
C	1.436509	-1.127059	-2.348768
C	-2.474542	0.945031	1.449099
C	-1.470244	-1.004547	2.611587
C	1.784229	-0.542110	4.024406
C	3.722999	0.442393	2.859081
C	0.642113	1.183497	-2.929737
C	3.038545	0.803322	-2.325549
C	2.152002	6.954973	-1.060900
C	0.752475	6.945698	-1.393073
C	0.039746	6.937360	-0.138252
C	0.935735	6.994501	0.968021
C	2.229865	6.947920	0.379387
C	3.447814	7.079953	-1.880587
C	4.665551	6.625603	-1.048064
C	-0.024016	6.939182	-2.723862
C	-1.531825	7.128482	-2.458889
C	0.597215	7.194048	2.433723
C	0.755842	8.697201	2.749890
C	3.661351	8.574913	-2.211027
C	3.477344	6.246122	-3.169349
C	0.113307	5.601222	-3.477795
C	0.407207	8.112529	-3.624150
C	1.547266	6.385460	3.330214
C	-0.848521	6.768756	2.725543
H	-1.035394	6.925788	-0.049020
H	3.154427	6.940842	0.937027
H	3.226236	0.645133	0.449299
H	-0.963712	0.629486	-0.536202
H	2.861492	8.985236	-2.830300
H	4.607751	8.704214	-2.748934
H	3.712552	9.169708	-1.292912
H	3.309241	5.187080	-2.950469
H	4.463128	6.340841	-3.637895
H	2.742054	6.570445	-3.905867

H	4.845916	7.275052	-0.186220
H	5.562537	6.674819	-1.674034
H	4.549586	5.597073	-0.694384
H	1.146328	5.354106	-3.718403
H	-0.450283	5.649083	-4.417415
H	-0.292757	4.785937	-2.872102
H	0.316923	9.067934	-3.096053
H	-0.241587	8.155121	-4.506087
H	1.433091	8.018466	-3.981653
H	-1.949881	6.297233	-1.883268
H	-2.059818	7.158683	-3.417547
H	-1.743582	8.066525	-1.934424
H	1.456653	5.314481	3.126245
H	1.309359	6.562990	4.384937
H	2.593504	6.668526	3.176232
H	-1.570601	7.380412	2.173978
H	-1.064877	6.891497	3.792284
H	-1.010944	5.720107	2.456661
H	1.783955	9.031829	2.576200
H	0.507645	8.893620	3.799172
H	0.092625	9.304354	2.124612
H	-2.655077	0.295727	0.587183
H	-2.358527	1.973599	1.095545
H	-3.371451	0.895798	2.075178
H	-2.416588	-1.133952	3.149568
H	-0.670320	-1.414982	3.230708
H	-1.521536	-1.599178	1.693371
H	-2.271838	1.229194	4.038994
H	-1.118116	2.383145	3.351622
H	-0.550713	0.999640	4.306690
H	1.874615	-1.497412	3.496140
H	0.758359	-0.448261	4.382009
H	2.433109	-0.584741	4.906277
H	3.934836	-0.495635	2.334622
H	4.251140	0.412317	3.817662
H	4.140834	1.273686	2.283360
H	2.641466	1.921329	4.817968
H	1.044742	2.216199	4.119186
H	2.483655	2.784722	3.272831
H	0.731088	2.254633	-2.725850
H	-0.403691	0.898802	-2.775769
H	0.880280	1.006268	-3.984450
H	3.199793	1.852265	-2.057134
H	3.254802	0.680363	-3.392286
H	3.761504	0.192795	-1.773886
H	1.684627	-1.323568	-3.398052
H	0.408859	-1.462866	-2.174624
H	2.100667	-1.733151	-1.723463

[Cp'FeN]$_2$ complex

96

C	0.250100	0.680947	-0.314914
C	0.046359	0.694522	1.102519
C	1.371419	0.666022	1.710267
C	2.302393	0.653188	0.620499
C	1.629911	0.651633	-0.629188
C	-1.387257	0.634142	1.658691
C	-1.605021	1.429647	2.953875
Fe	1.177217	2.551142	0.492260
N	2.401200	3.799281	0.240311
Fe	1.213203	5.106033	0.269474
N	0.000001	3.866998	0.589285
C	1.870758	0.582166	3.165898
C	1.661136	1.898282	3.940630
C	2.250598	0.549482	-2.011305
C	2.246935	-0.937353	-2.425703
C	-2.381963	1.218729	0.632635
C	-1.766686	-0.846783	1.876937
C	1.213323	-0.595889	3.910043
C	3.388478	0.306884	3.189538
C	1.438514	1.356527	-3.035960
C	3.697066	1.065324	-2.002814
C	1.999884	6.812932	-1.012470
C	0.545471	6.800844	-1.072990
C	0.091692	7.001752	0.271699
C	1.184818	7.151182	1.165834
C	2.344156	7.026670	0.360341
C	3.117337	6.752914	-2.068243
C	4.446602	6.320596	-1.412282
C	-0.467989	6.653252	-2.224200
C	-1.893383	6.947516	-1.713474
C	1.127395	7.512372	2.639775
C	1.210983	9.049717	2.753181
C	3.324394	8.171681	-2.642351
C	2.869630	5.760063	-3.212624
C	-0.506748	5.222619	-2.797773
C	-0.191859	7.674946	-3.343188
C	2.304303	6.887975	3.404570
C	-0.188170	7.034639	3.271935
H	-0.945028	7.006665	0.571783
H	3.355535	7.049050	0.737731
H	3.375605	0.673542	0.733175
H	-0.542699	0.726794	-1.046777
H	2.436244	8.544833	-3.157179
H	4.154684	8.168733	-3.358420
H	3.569360	8.879237	-1.843440

H	2.714809	4.749589	-2.822704
H	3.748043	5.736242	-3.867051
H	2.015546	6.026280	-3.835917
H	4.824301	7.065713	-0.705455
H	5.210568	6.207232	-2.188703
H	4.338694	5.364510	-0.890367
H	0.453553	4.902373	-3.199842
H	-1.246136	5.165992	-3.605928
H	-0.794674	4.511352	-2.017470
H	-0.178920	8.695696	-2.946353
H	-0.983980	7.617984	-4.098176
H	0.756172	7.499936	-3.852955
H	-2.214371	6.220321	-0.961435
H	-2.594776	6.879836	-2.551580
H	-1.977634	7.953558	-1.289308
H	2.284935	5.795864	3.332963
H	2.254012	7.163947	4.463638
H	3.269015	7.235894	3.021478
H	-1.057793	7.514534	2.810946
H	-0.204580	7.285178	4.338194
H	-0.304830	5.950831	3.171400
H	2.147347	9.425701	2.327931
H	1.164620	9.360740	3.803400
H	0.383110	9.528626	2.219944
H	-2.445679	0.616409	-0.278704
H	-2.110118	2.243823	0.363682
H	-3.384600	1.231753	1.072976
H	-2.805089	-0.921634	2.220663
H	-1.129817	-1.335127	2.617758
H	-1.679870	-1.408492	0.940816
H	-2.663783	1.384216	3.232483
H	-1.338539	2.481059	2.809332
H	-1.036270	1.037704	3.797279
H	1.366151	-1.534014	3.365746
H	0.140925	-0.461918	4.055204
H	1.665224	-0.705944	4.902340
H	3.644643	-0.623608	2.672031
H	3.718470	0.210713	4.229185
H	3.960836	1.125473	2.742233
H	2.007112	1.782759	4.975045
H	0.618937	2.213915	3.966536
H	2.239634	2.703771	3.477189
H	1.406473	2.415750	-2.763107
H	0.407525	0.996505	-3.114042
H	1.892326	1.269881	-4.029398
H	3.744336	2.103237	-1.658366
H	4.118839	1.014857	-3.012619
H	4.337854	0.460922	-1.352036

H	2.693610	-1.058558	-3.419468
H	1.227422	-1.335377	-2.460687
H	2.821839	-1.544193	-1.718486

[Cp'Fe(OCN)]$_2$ complex

100

Fe	4.353779	3.982426	10.484835
O	5.642250	1.150170	7.884743
N	5.207357	3.380851	8.646594
C	2.836244	2.375642	11.379696
C	2.676896	3.649387	12.065714
C	3.947483	3.940574	12.668436
H	4.154971	4.814375	13.269761
C	4.889744	2.909806	12.390226
C	4.186890	1.961701	11.601572
H	4.624976	1.061215	11.196569
C	1.879967	1.504642	10.539907
C	2.531470	0.140655	10.230214
H	2.798166	-0.398693	11.144894
H	3.426908	0.236802	9.609036
H	1.819701	-0.478584	9.674315
C	1.556485	2.151397	9.177112
H	0.876630	1.508707	8.604951
H	2.469581	2.274388	8.584486
H	1.087615	3.130943	9.273675
C	0.577811	1.186122	11.298014
H	0.795131	0.725357	12.267329
H	-0.024293	0.477915	10.717518
H	-0.039818	2.067111	11.473457
C	1.465272	4.546582	12.379522
C	1.926791	5.942388	12.849278
H	2.549115	6.446782	12.104158
H	2.480816	5.903256	13.791336
H	1.047719	6.571427	13.023786
C	0.679652	3.926917	13.556507
H	-0.160636	4.573823	13.835926
H	1.328707	3.819714	14.431804
H	0.280870	2.939803	13.317784
C	0.524425	4.793507	11.189610
H	-0.260860	5.498894	11.483094
H	0.026911	3.888578	10.840208
H	1.067548	5.233741	10.346071
C	6.290991	2.775620	12.966697
C	6.181271	2.106599	14.352759
H	5.566176	2.707801	15.030313
H	7.172390	1.988357	14.806404
H	5.722747	1.115544	14.273466
C	6.950262	4.154227	13.129103

H	7.037928	4.668748	12.165362
H	7.957432	4.047333	13.546918
H	6.382622	4.800344	13.806449
C	7.178543	1.907031	12.062960
H	6.781338	0.892588	11.956384
H	8.183461	1.820650	12.490573
H	7.273360	2.341568	11.062001
C	5.431094	2.250536	8.255985
Fe	5.561386	5.276395	7.898231
O	4.272531	8.109115	10.497771
N	4.706732	5.878048	9.736687
C	7.073264	6.888478	7.003895
C	7.234301	5.615080	6.317380
C	5.963687	5.322196	5.715210
H	5.757299	4.448618	5.113174
C	5.020050	6.351386	5.994609
C	5.721861	7.300250	6.783124
H	5.282476	8.199597	7.189237
C	8.028911	7.760656	7.843135
C	7.375068	9.122985	8.155140
H	7.105875	9.662707	7.241413
H	6.480800	9.024365	8.777593
H	8.086436	9.743144	8.710534
C	8.355889	7.113275	9.204799
H	9.035553	7.756685	9.776375
H	7.444028	6.988145	9.798879
H	8.826386	6.134698	9.106550
C	9.329122	8.082590	7.083105
H	9.109135	8.544274	6.114822
H	9.930957	8.791137	7.663469
H	9.948086	7.203020	6.905237
C	8.447324	4.720426	6.001537
C	7.987950	3.323527	5.532894
H	7.367884	2.818114	6.279221
H	7.432297	3.361180	4.591743
H	8.868013	2.696224	5.357134
C	9.229436	5.341755	4.823145
H	10.070793	4.696845	4.542329
H	8.578636	5.447365	3.948953
H	9.626257	6.329850	5.061157
C	9.390955	4.475659	7.189693
H	10.177236	3.771993	6.894750
H	9.887151	5.381708	7.538060
H	8.850435	4.034263	8.034299
C	3.617948	6.483166	5.419690
C	3.725136	7.150855	4.032791
H	4.340050	6.549669	3.355054
H	2.733291	7.267459	3.580317

H	4.182602	8.142526	4.110469
C	2.960301	5.103510	5.259602
H	2.874390	4.590045	6.224062
H	1.952533	5.208584	4.842756
H	3.528057	4.457325	4.582414
C	2.730393	7.351558	6.323599
H	3.126366	8.366658	6.428494
H	1.724806	7.436089	5.897191
H	2.637480	6.918026	7.325162
C	4.483292	7.008514	10.126906

[Cp'Fe(κ2-OCN)]$_2$ complex

100

C	7.002975	6.199860	3.646699
C	6.021884	7.223837	3.784186
C	6.644401	8.251120	4.532443
C	7.983068	7.894011	4.880965
C	8.223193	6.573343	4.306302
Fe	6.541098	6.308458	5.804071
N	6.448471	4.706427	6.943190
C	6.039311	4.128015	7.896966
O	5.625935	3.532224	8.869462
Fe	4.385827	4.685308	10.369687
N	4.446013	6.273840	9.211623
C	4.847056	6.847769	8.251741
O	5.251730	7.440536	7.273746
C	4.641731	7.242364	3.144809
C	3.783917	8.375194	3.724918
C	8.852400	8.848241	5.723235
C	10.202533	9.141773	5.044075
C	9.465085	5.671799	4.172185
C	10.321311	5.563730	5.443805
C	4.913741	3.696948	12.308121
C	4.063446	2.804490	11.606680
C	2.759702	3.369494	11.431360
C	2.789543	4.681396	12.061805
C	4.116027	4.847141	12.578380
C	6.326331	3.438410	12.811636
C	6.933130	2.203828	12.130895
C	1.671053	2.585712	10.671442
C	0.354048	2.507350	11.464588
C	1.728279	5.764132	12.327244
C	0.807241	6.059914	11.132396
C	8.150073	10.212021	5.880298
C	9.071597	8.308545	7.152215
C	9.042792	4.227201	3.828599
C	10.329269	6.181704	2.998664

C	4.809784	7.466295	1.628292
C	3.919726	5.904035	3.377070
C	2.119771	1.126189	10.452221
C	1.419668	3.177854	9.268514
C	2.405578	7.107871	12.672525
C	0.889038	5.355484	13.557286
C	6.263784	3.192157	14.332628
C	7.230802	4.651726	12.535752
H	4.460886	5.718617	13.117018
H	4.371266	1.841554	11.228133
H	2.339301	0.622622	11.399226
H	3.002962	1.056920	9.809791
H	1.315145	0.572448	9.957021
H	0.647019	2.601939	8.744703
H	2.332976	3.124763	8.663479
H	1.096593	4.218985	9.299031
H	0.524222	2.075320	12.456338
H	-0.359292	1.864469	10.936296
H	-0.122980	3.478415	11.598304
H	3.080129	7.436557	11.875181
H	2.968303	7.063017	13.609618
H	1.636094	7.876497	12.800449
H	0.160318	6.139098	13.796998
H	1.535224	5.215453	14.430112
H	0.342054	4.424353	13.397885
H	0.128344	6.880938	11.389202
H	0.186321	5.210862	10.846688
H	1.390496	6.369978	10.258912
H	5.857215	4.062310	14.858227
H	7.264108	2.990093	14.733583
H	5.624790	2.333244	14.562434
H	7.326623	4.831960	11.458611
H	8.236318	4.480883	12.937033
H	6.841166	5.564085	12.998893
H	6.359702	1.298984	12.358193
H	7.956176	2.042728	12.487973
H	6.966633	2.323741	11.043338
H	6.855718	5.276663	3.104206
H	6.149425	9.155673	4.852914
H	7.947240	10.678726	4.910890
H	7.208096	10.128146	6.430649
H	8.799276	10.887717	6.447249
H	9.697096	9.000491	7.729169
H	8.112270	8.219766	7.675202
H	9.555808	7.331658	7.167238
H	10.050295	9.532906	4.032611
H	10.751109	9.897722	5.617600
H	10.843087	8.262655	4.970502

H	8.361643	3.815018	4.580476
H	8.563261	4.155485	2.848032
H	9.932482	3.589504	3.794075
H	11.192633	5.522546	2.848594
H	9.746552	6.193608	2.071706
H	10.702839	7.193586	3.168287
H	11.143511	4.859894	5.271358
H	10.771440	6.510947	5.741281
H	9.729798	5.183592	6.283700
H	5.398589	6.663348	1.172937
H	3.833173	7.495172	1.130608
H	5.322582	8.412799	1.428506
H	3.753833	5.726749	4.446372
H	2.941461	5.904875	2.882951
H	4.490561	5.059001	2.978811
H	4.226165	9.356388	3.523317
H	2.787488	8.364076	3.269925
H	3.663901	8.271374	4.808360

TS for N-CO bond breakings

100

C	1.720609	0.482394	-0.467225
C	0.335267	0.620848	-0.171392
C	0.125273	0.661004	1.261244
C	1.402083	0.515233	1.871838
C	2.367636	0.531077	0.809216
Fe	1.279839	2.439132	0.498913
C	0.879485	4.129806	-1.254543
O	0.731911	3.655160	-2.309971
C	-1.285610	0.595320	1.856965
C	-2.319661	1.335113	0.974529
C	1.792505	0.205711	3.323876
C	1.053183	-1.082483	3.756753
C	2.346700	0.168073	-1.810306
C	1.533273	0.799749	-2.948815
Fe	1.202067	5.260480	0.027474
C	2.158510	3.720162	1.891017
O	2.657685	3.892193	3.032391
C	2.265301	7.124899	0.168759
C	1.930057	6.988351	-1.224336
C	0.478325	7.062452	-1.300692
C	0.013663	7.151575	0.051153
C	1.100015	7.247417	0.968841
C	3.064561	7.032077	-2.256559
C	3.307510	8.505959	-2.661529
C	-0.506167	7.198038	-2.482930
C	-0.752367	5.885212	-3.243999
C	1.046173	7.531558	2.458289

C	2.288880	6.948520	3.165281
N	0.062114	3.810556	0.350613
N	2.529065	3.901436	0.454521
C	2.818218	6.162394	-3.500209
C	4.385711	6.535075	-1.629821
C	-0.054600	8.289593	-3.473465
C	-1.872834	7.690416	-1.953061
C	-0.225559	6.933140	3.079452
C	1.020740	9.063314	2.642933
C	-1.715977	-0.886896	1.917062
C	-1.391284	1.219033	3.256877
C	3.302854	-0.111853	3.416606
C	1.519199	1.336233	4.344998
C	3.798883	0.667297	-1.870222
C	2.352016	-1.368016	-1.981189
H	-1.035098	7.152958	0.308999
H	3.271773	7.109285	0.557712
H	3.438783	0.485861	0.953904
H	-0.464187	0.650583	-0.895138
H	2.445584	8.962014	-3.146965
H	4.153183	8.562019	-3.356524
H	3.554977	9.109563	-1.782185
H	2.688235	5.108450	-3.225296
H	3.689825	6.227029	-4.160428
H	1.949865	6.463707	-4.085725
H	4.755534	7.204132	-0.848364
H	5.156866	6.499872	-2.406019
H	4.281994	5.531130	-1.205161
H	0.179490	5.406171	-3.518834
H	-1.373438	6.070797	-4.124617
H	-1.293427	5.169830	-2.615615
H	0.106790	9.243833	-2.960877
H	-0.841038	8.440987	-4.219745
H	0.854672	8.034954	-4.014908
H	-2.350581	6.964324	-1.287818
H	-2.548817	7.837544	-2.801630
H	-1.785051	8.645266	-1.425090
H	2.394990	5.871866	3.023951
H	2.238799	7.166740	4.236777
H	3.204989	7.418250	2.791357
H	-1.132584	7.378251	2.656779
H	-0.237949	7.125684	4.157472
H	-0.273437	5.849756	2.930867
H	1.919424	9.527868	2.222929
H	0.978843	9.311290	3.709001
H	0.148849	9.510628	2.153948
H	-2.489690	0.851353	0.009328
H	-2.021503	2.373380	0.799930

H	-3.284766	1.335728	1.492823
H	-2.736955	-0.963990	2.309153
H	-1.058456	-1.479078	2.561351
H	-1.704788	-1.339624	0.919978
H	-2.435106	1.199688	3.587795
H	-1.055182	2.260177	3.254293
H	-0.814334	0.666348	4.004379
H	1.235200	-1.904477	3.056631
H	-0.026956	-0.929041	3.828861
H	1.402649	-1.398799	4.746600
H	3.599332	-0.941649	2.764286
H	3.531572	-0.402797	4.445647
H	3.923638	0.759597	3.181115
H	1.808029	1.003532	5.345975
H	0.462053	1.617588	4.389047
H	2.075585	2.217515	4.071038
H	1.479147	1.870380	-2.810829
H	0.511890	0.407388	-2.974527
H	1.986558	0.564234	-3.917604
H	3.857538	1.747511	-1.699765
H	4.231191	0.453247	-2.854032
H	4.426397	0.171281	-1.122852
H	2.805369	-1.642586	-2.941052
H	1.332918	-1.768701	-1.960482
H	2.922999	-1.854121	-1.183645

[Cp'Fe(SCN)]$_2$ complex

100

Fe	4.246769	3.935800	10.424975
S	5.486970	0.862595	7.425930
N	5.163681	3.401260	8.554583
C	2.746548	2.387052	11.325492
C	2.845029	3.578308	12.164573
C	4.213130	3.642343	12.605003
H	4.609031	4.394645	13.272823
C	4.955410	2.537215	12.097640
C	4.042367	1.782779	11.324262
H	4.306796	0.902256	10.757566
C	1.590882	1.764598	10.515338
C	2.007619	0.386760	9.962347
H	2.286454	-0.304812	10.764055
H	2.841212	0.455262	9.257195
H	1.162993	-0.052996	9.421694
C	1.226475	2.634436	9.294232
H	0.403568	2.176127	8.732836
H	2.082305	2.713123	8.613277
H	0.917969	3.643656	9.571114
C	0.341264	1.512369	11.379181

H	0.586830	0.892604	12.247922
H	-0.412048	0.978044	10.789272
H	-0.123399	2.430488	11.739321
C	1.808222	4.545798	12.765208
C	2.506695	5.787965	13.357540
H	3.109842	6.317599	12.613832
H	3.145349	5.536475	14.209375
H	1.747322	6.486959	13.722599
C	1.095276	3.841243	13.940653
H	0.394647	4.531772	14.424800
H	1.824710	3.518726	14.690946
H	0.535262	2.960773	13.622189
C	0.771362	5.078299	11.763431
H	0.113729	5.796453	12.265375
H	0.134879	4.297011	11.348023
H	1.258209	5.602975	10.934547
C	6.401007	2.203514	12.434574
C	6.475941	1.822013	13.927233
H	6.155580	2.651340	14.566149
H	7.502637	1.557051	14.205599
H	5.832024	0.963310	14.143222
C	7.308345	3.420329	12.182278
H	7.312856	3.691711	11.120006
H	8.341277	3.198180	12.473783
H	6.982609	4.294942	12.754754
C	6.906449	1.022750	11.595400
H	6.324261	0.115509	11.787670
H	7.950137	0.804302	11.845747
H	6.856522	1.236690	10.522924
C	5.304365	2.306851	8.060386
Fe	5.435009	5.333797	7.857031
S	3.217394	8.359758	10.151884
N	4.333038	5.852094	9.613596
C	6.925558	7.035657	7.134084
C	7.301983	5.777100	6.509438
C	6.163681	5.349158	5.747806
H	6.126301	4.444766	5.157730
C	5.092068	6.278547	5.868423
C	5.579749	7.303043	6.726695
H	5.003861	8.161247	7.042237
C	7.669905	8.017466	8.062238
C	6.868567	9.327886	8.204408
H	6.699530	9.806274	7.234067
H	5.901173	9.175485	8.691542
H	7.434729	10.028319	8.827342
C	7.833758	7.447769	9.486522
H	8.360944	8.168050	10.123496
H	6.853729	7.262690	9.939108

H	8.394117	6.512178	9.506398
C	9.041678	8.425554	7.493522
H	8.939164	8.832063	6.481885
H	9.483831	9.205070	8.124116
H	9.752555	7.600002	7.455694
C	8.624747	4.996524	6.404498
C	8.370463	3.556596	5.911691
H	7.688341	3.008736	6.568679
H	7.966897	3.528146	4.895532
H	9.319907	3.011529	5.891658
C	9.520039	5.672505	5.342191
H	10.448961	5.104168	5.213967
H	9.006247	5.702378	4.375766
H	9.785028	6.696719	5.608398
C	9.390646	4.856207	7.729652
H	10.280806	4.236520	7.573930
H	9.730626	5.809055	8.134907
H	8.772813	4.363205	8.488187
C	3.781133	6.277140	5.096618
C	3.981531	7.104459	3.809861
H	4.775981	6.676764	3.189562
H	3.060102	7.127185	3.216069
H	4.258871	8.136571	4.047210
C	3.371127	4.848158	4.710314
H	3.237221	4.216227	5.595339
H	2.422687	4.862775	4.162435
H	4.114571	4.371472	4.063404
C	2.653323	6.909336	5.926590
H	2.877294	7.945494	6.198446
H	1.719336	6.915341	5.353813
H	2.477893	6.349595	6.851948
C	3.846457	6.933766	9.852503

[Cp'Fe(κ2-SCN)]$_2$ complex

100

C	6.735530	6.414175	3.618735
C	6.003377	7.624720	3.765953
C	6.869940	8.519211	4.435174
C	8.127629	7.899359	4.720663
C	8.051546	6.544272	4.181973
Fe	6.493059	6.659288	5.811951
N	6.413546	5.007492	6.939634
C	6.241042	4.249836	7.824282
S	5.997077	3.198751	9.059633
Fe	4.477838	4.606532	10.558790
N	4.574215	6.266426	9.445725
C	4.845106	7.055186	8.614593
S	5.219136	8.148638	7.450568

C	4.613116	7.902291	3.213951
C	4.086061	9.258207	3.701902
C	9.236735	8.679102	5.454290
C	10.548983	8.695204	4.648417
C	9.073322	5.409328	3.982199
C	10.009228	5.163317	5.175975
C	4.844305	3.807941	12.681625
C	4.210420	2.760210	11.972620
C	2.914425	3.157922	11.517653
C	2.714538	4.526479	11.984268
C	3.916708	4.887040	12.684073
C	6.184972	3.775093	13.400011
C	6.988801	2.527407	13.010446
C	2.036500	2.186250	10.704442
C	0.655897	1.987857	11.356759
C	1.511002	5.487745	12.005615
C	0.703085	5.540150	10.699590
C	8.825508	10.155155	5.627928
C	9.482659	8.130488	6.875355
C	8.345760	4.069359	3.737570
C	9.905467	5.709970	2.716841
C	4.697935	7.924750	1.674303
C	3.629771	6.801145	3.648587
C	2.689639	0.790042	10.655237
C	1.881987	2.639329	9.237831
C	1.984565	6.934247	12.264412
C	0.586035	5.097139	13.178769
C	5.922579	3.746645	14.919364
C	7.012465	5.025814	13.055511
H	4.082838	5.838588	13.169320
H	4.666467	1.804151	11.762040
H	2.840714	0.373820	11.656536
H	3.651762	0.804806	10.133632
H	2.034119	0.106414	10.105551
H	1.249860	1.931806	8.687741
H	2.859565	2.661292	8.742413
H	1.432655	3.627911	9.143708
H	0.761835	1.651315	12.393575
H	0.093080	1.222094	10.810802
H	0.051474	2.895418	11.358572
H	2.716286	7.259530	11.517886
H	2.423311	7.057862	13.258728
H	1.125074	7.610683	12.210597
H	-0.252502	5.800013	13.252637
H	1.135780	5.125792	14.125265
H	0.174562	4.092154	13.064600
H	-0.089146	6.291504	10.791113
H	0.218249	4.594524	10.456192

H	1.339228	5.830616	9.856698
H	5.369131	4.634213	15.242571
H	6.868294	3.716277	15.473095
H	5.335849	2.865323	15.198445
H	7.239328	5.063149	11.983382
H	7.964435	5.017646	13.598664
H	6.486485	5.947571	13.324513
H	6.462510	1.607537	13.286098
H	7.952160	2.524316	13.531655
H	7.189714	2.500264	11.934272
H	6.364281	5.529680	3.120455
H	6.599257	9.520900	4.734510
H	8.631515	10.640232	4.665783
H	7.937487	10.263315	6.258605
H	9.639266	10.699966	6.117861
H	10.275293	8.704030	7.370962
H	8.575681	8.228867	7.483323
H	9.780362	7.081725	6.880553
H	10.382800	9.101598	3.645106
H	11.285969	9.331979	5.151095
H	10.994957	7.706172	4.540237
H	7.663035	3.824448	4.557529
H	7.780802	4.065712	2.801005
H	9.085940	3.265671	3.664515
H	10.604888	4.889199	2.517693
H	9.251575	5.816938	1.845170
H	10.484216	6.631040	2.811730
H	10.652489	4.302427	4.962499
H	10.666707	6.006701	5.387786
H	9.437858	4.933820	6.081527
H	5.042294	6.962554	1.281676
H	3.715051	8.136890	1.237366
H	5.396135	8.695820	1.332465
H	3.523031	6.780127	4.739535
H	2.637501	6.980823	3.219020
H	3.959208	5.810436	3.318810
H	4.732367	10.080645	3.377538
H	3.087362	9.441695	3.291238
H	4.009852	9.289152	4.793804