Supporting Information for

Complexes of Manganese, Iron and Cobalt with Sterically Demanding Indenyl Ligands

Miyuki Maekawa,[a] Constantin G. Daniliuc,[a] Matthias Freytag,[a] Peter G. Jones[a] and Marc D. Walter[a,]*

Table of Contents:

1. Experimental Details for [(η^5-Cp')Fe(CO)$_2$I]

(1,2,4-Tri-*tert*-butylcyclopentadienyl)(dicarbonyl)iron(II)iodide, [Cp'Fe(CO)$_2$I]. $FeI_2(thf)_2$ (1.77 g, 3.9 mmol) and NaCp''' (1.00 g, 3.9 mmol) were dissolved in THF (50 mL) and stirred for 4 h at ambient temperature. Exposure of this solution to CO (1 atm) resulted in a colour change from dark red to dark brown. After stirring for 2 d the solvent was removed under dynamic vacuum and the residue was extracted with toluene (50 mL). The extracts were filtered and taken to dryness to give a dark purple solid. Yield: 1.32 g (2.8 mmol, 72%). Single crystals were grown from saturated pentane solutions at room temperature. ^{1}H NMR (300.0 MHz, C_6D_6, 24°C): δ 4.86 (s, 2H, ring-C*H*), 1.21 (s, 9H, *t*Bu-*H*), 1.18 (s, 18H, *t*Bu-*H*). $^{13}C\{^1H\}$ NMR (75.5 MHz, C_6D_6, 25°C): δ 216.1 (2C, *C*O), 108.4 (2C, ring-C_{ipso}), 107.9 (1C, ring-C_{ipso}), 88.6 (2C, ring-*C*H), 33.4 (6C, *t*Bu-*C*H$_3$), 32.6 (2C, *t*Bu-C_{ipso}), 32.0 (3C, *t*Bu-*C*H$_3$) 31.2 (1C, *t*Bu-C_{ipso}). The E.I. mass spectrum showed a molecular ion at m/e= 472 amu. The parent ion isotopic cluster was simulated: (calcd. %, observd. %): 470 (1, 7), 471 (1, 1), 472 (100, 100), 473 (24, 22), 474 (4, 4). IR (ATR; cm^{-1}): 3083(w), 2959(s), 2869 (m), 2013 (s), 1966 (m), 1936 (sh), 1481 (m), 1462 (m), 1391 (m), 1363 (s), 1245 (m), 1094 (m), 1021 (m), 798 (m), 611 (m). Mp: 115°C (dec.).

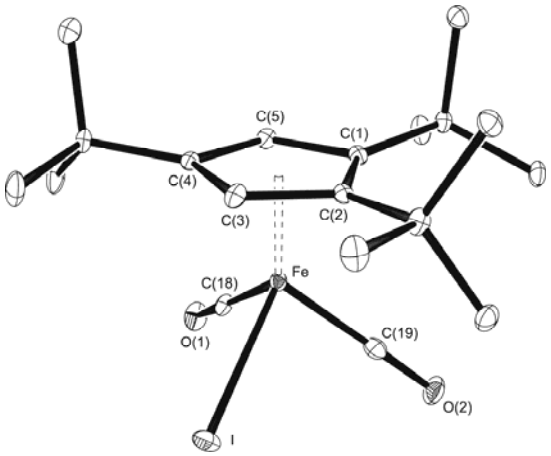


Figure S1. ORTEP diagram of **Cp'Fe(CO)$_2$I** with 30 % probability ellipsoids. Hydrogen atoms are omitted for clarity.

Empirical formula	$C_{19}H_{29}FeIO_2$	
Formula weight	472.17	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	orthorhombic	
Space group	*Pca*2$_1$	
Unit cell dimensions	a = 15.3534(3) Å	α = 90°
	b = 10.4548(2) Å	β = 90°
	c = 12.3471(3) Å	γ = 90°
Volume	1981.92(7) Å^3	

Z	4
Density (calculated)	1.582 Mg/m^3
Absorption coefficient	18.373 mm^{-1}
F(000)	952
Crystal size	0.12 x 0.03 x 0.02 mm^3
Theta range for data collection	4.23 to 75.87°
Index ranges	-19<=h<=19, -13<=k<=13, -13<=l<=15
Reflections collected	49188
Independent reflections	3932 [R(int) = 0.0983]
Completeness to theta = 75.00°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.05459
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3932 / 1 / 217
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0277, wR2 = 0.0704
R indices (all data)	R1 = 0.0286, wR2 = 0.0712
Absolute structure parameter	0.034(5)
Largest diff. peak and hole	0.978 and -0.664 $e.Å^{-3}$

2. ORTEP Diagrams for 1-Fe/Co and 2-Mn/Fe/Co

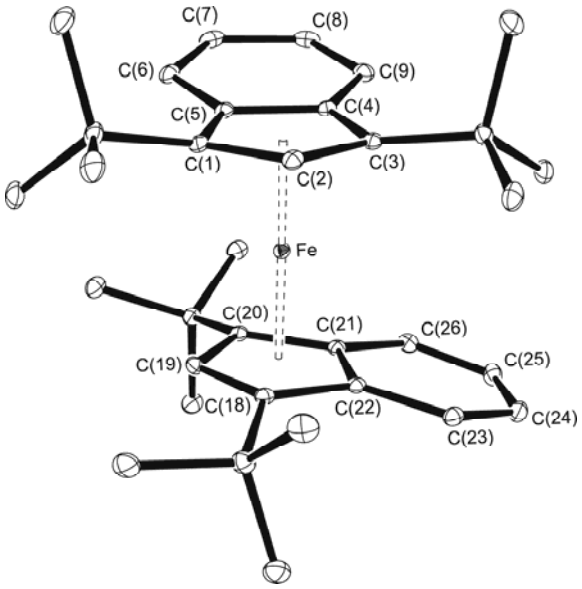


Figure S2. ORTEP diagram of **1-Fe** with 30 % probability ellipsoids. Hydrogen atoms are omitted for clarity.

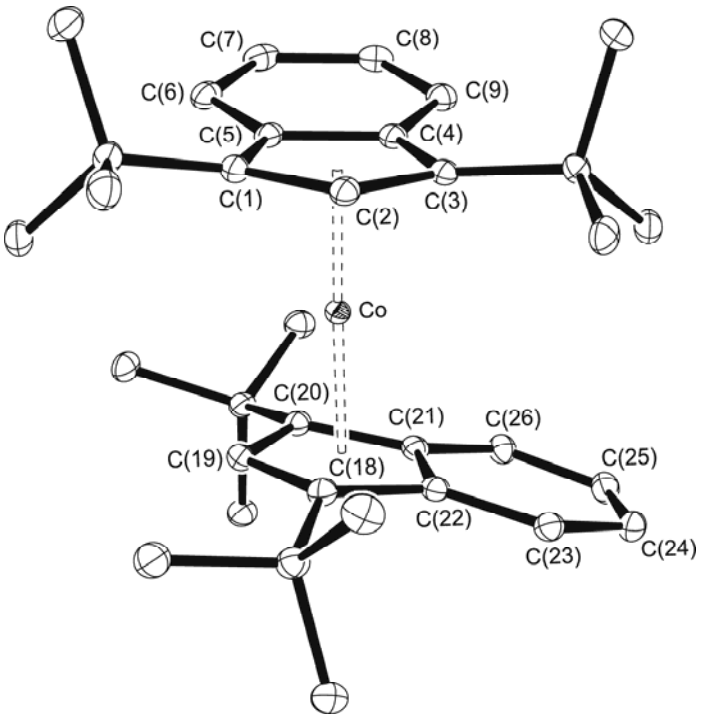


Figure S3. ORTEP diagram of **1-Co** with 30 % probability ellipsoids. Hydrogen atoms are omitted for clarity.

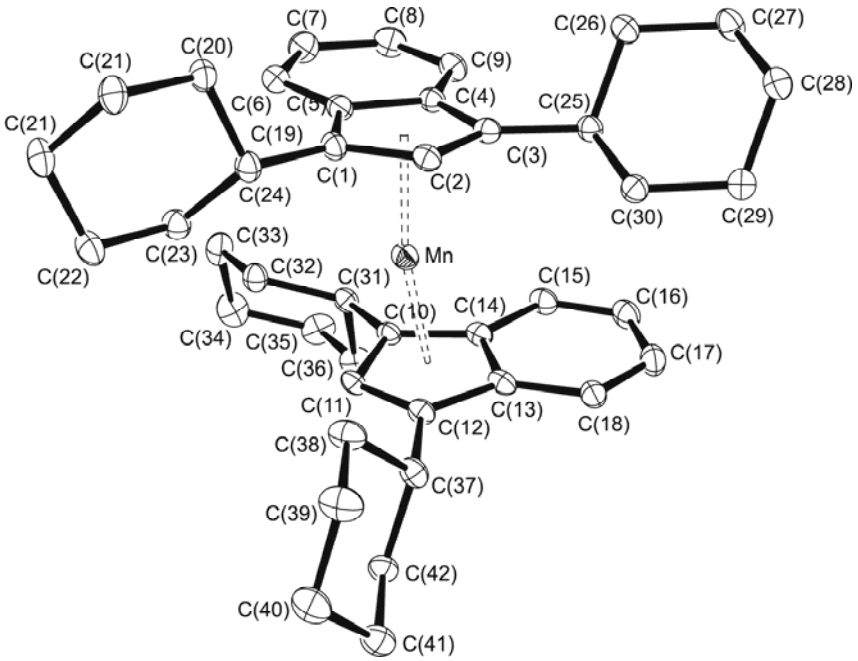


Figure S4. ORTEP diagram of **2-Mn** with 30 % probability ellipsoids. Hydrogen atoms are omitted for clarity.

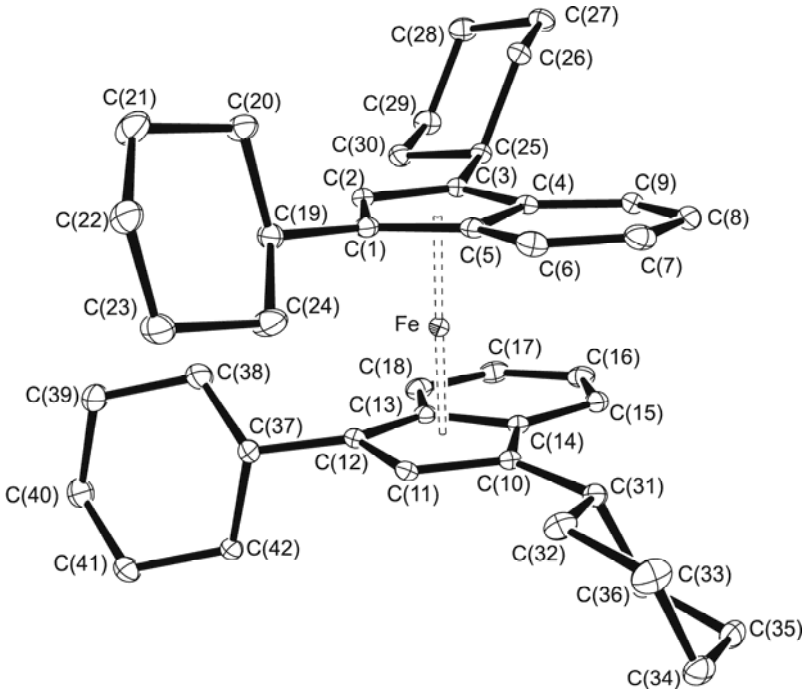


Figure S5. ORTEP diagram of **2-Fe** with 30 % probability ellipsoids. Hydrogen atoms are omitted for clarity.

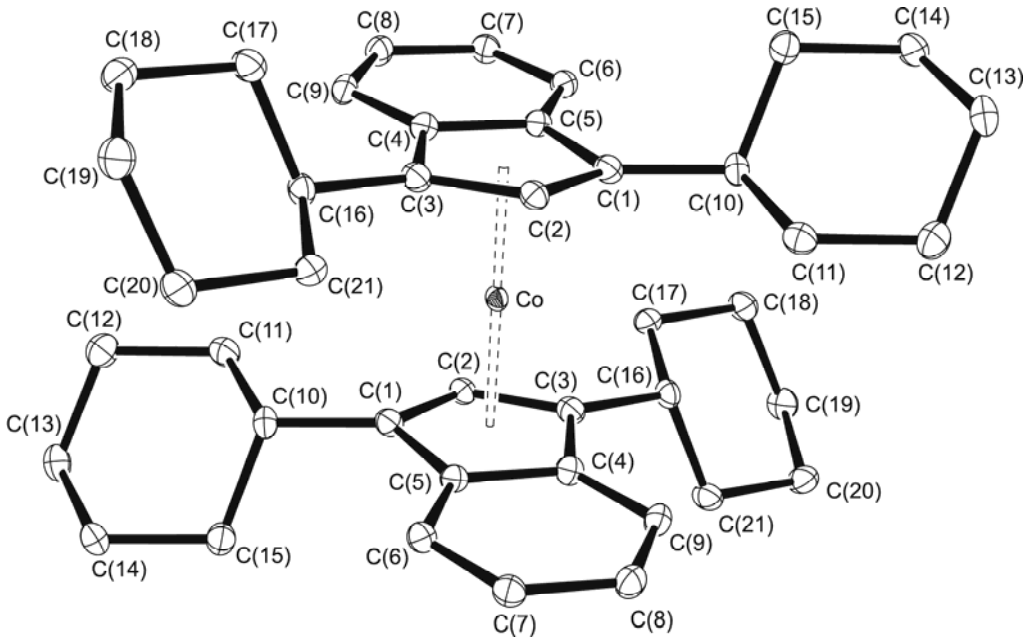


Figure S6. ORTEP diagram of **2-Co*(3 C_6D_6)** with 30 % probability ellipsoids. Hydrogen atoms and benzene solvates are omitted for clarity.

3. Variable temperature NMR studies on 1-Fe

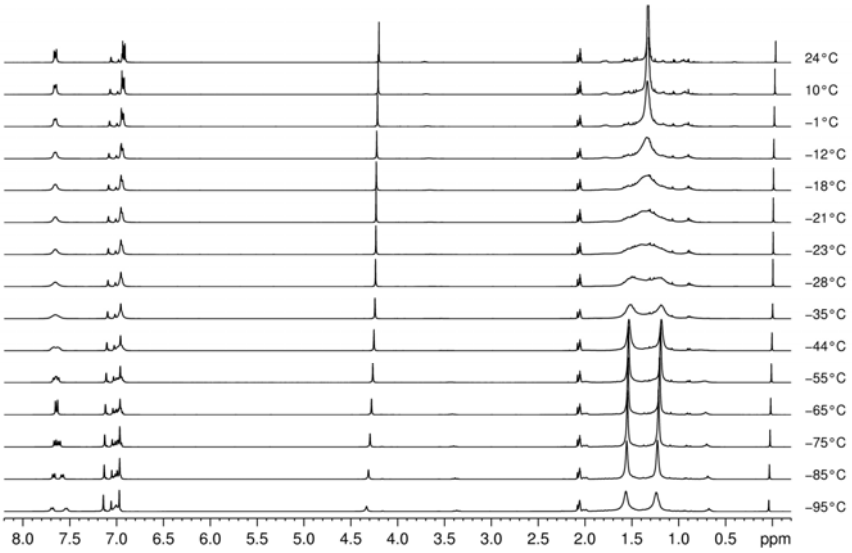


Figure S6. Variable temperature (VT) ^{1}H NMR spectra of **1-Fe** recorded in C_7D_8.

4. UV-Vis Spectra of Bis(indenyl)metal Complexes

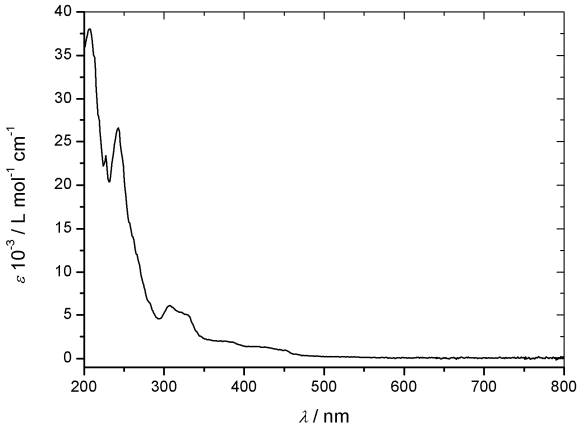


Figure S7. UV-vis spectrum of **1-Mn**.

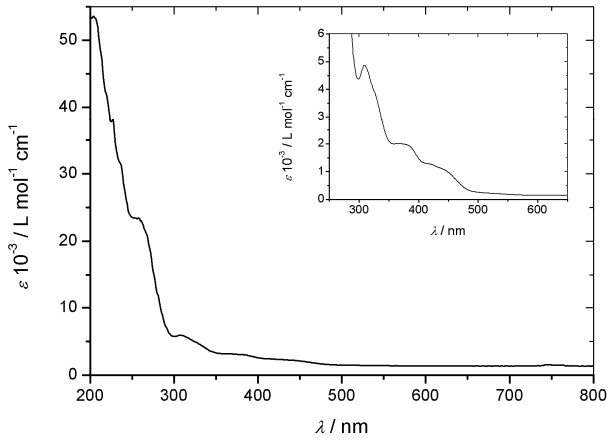


Figure S8. UV-vis spectrum of **2-Mn**.

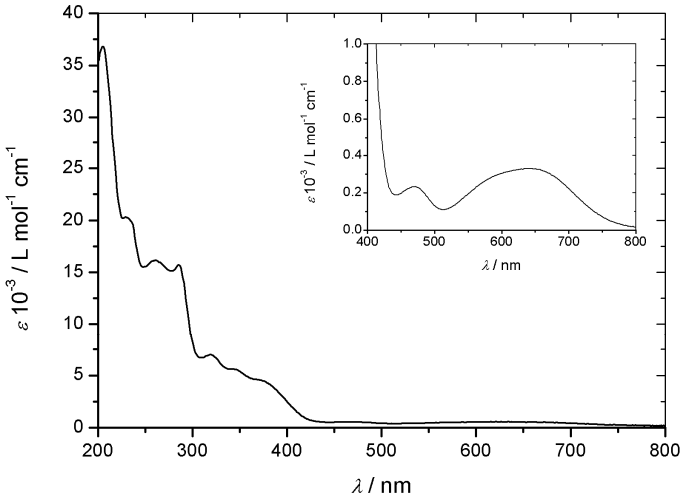


Figure S9. UV-vis spectrum of **1-Fe**.

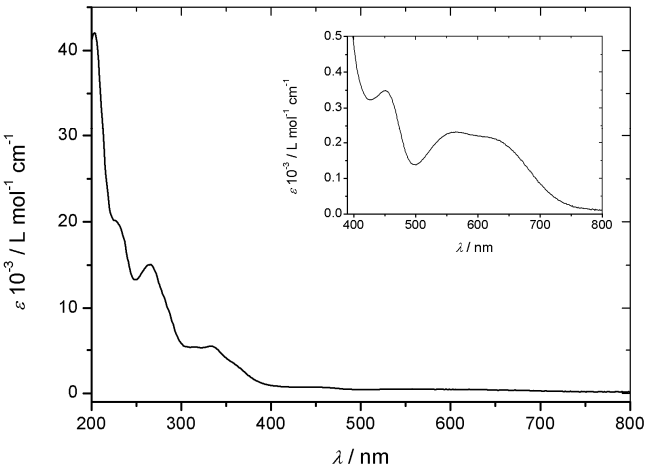


Figure S10. UV-vis spectrum of **2-Fe**.

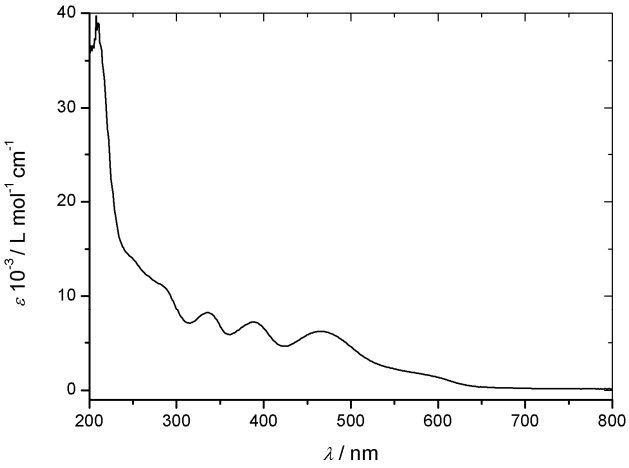


Figure S11. UV-vis spectrum of **1-Co**.

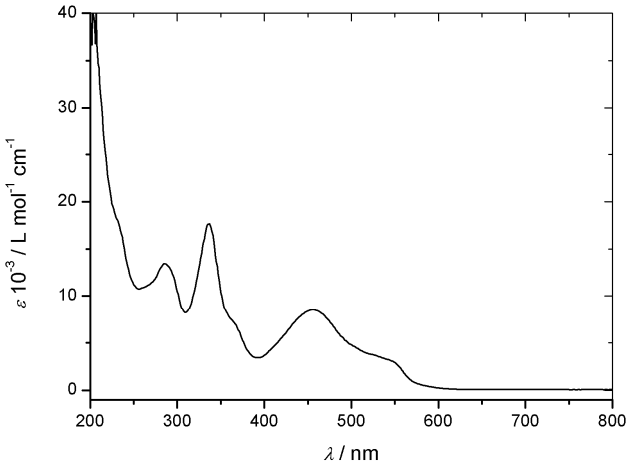


Figure S12. UV-vis spectrum of **2-Co**.

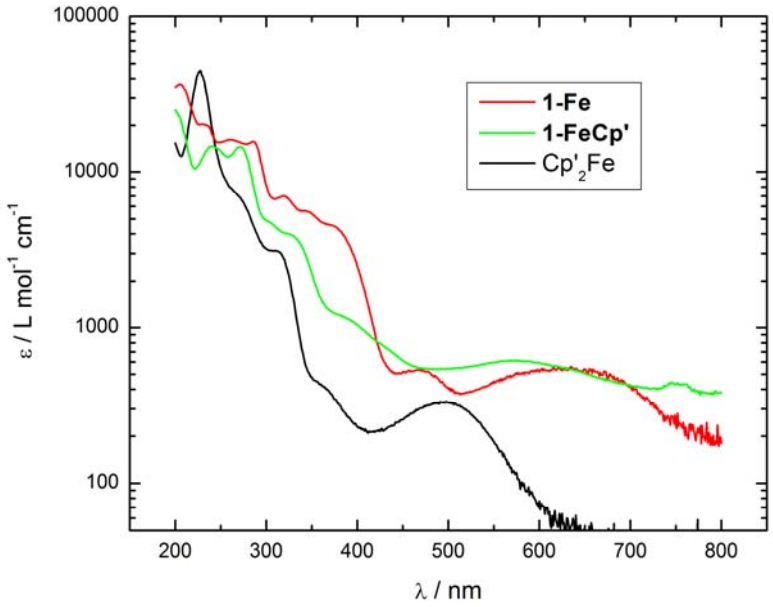


Figure S13. UV-vis spectra for **1-Fe**, **1-FeCp'** and Cp'_2Fe.

5. Electrochemical Studies

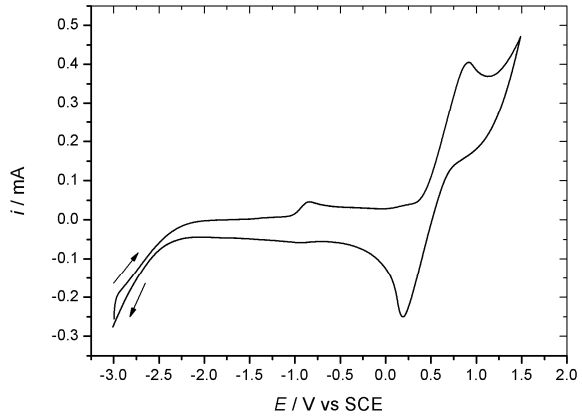


Figure S14. Cyclic voltammogram (CV) and $E_{1/2}$ values for **1-Mn**. CV recorded in THF with 0.4 M [*n*-Bu_4N][PF_6] supporting electrolyte. Scan rate: 500 mV/s. Referenced to SCE with internal Cp_2Fe/Cp_2Fe^+ standard (at +560 mV).

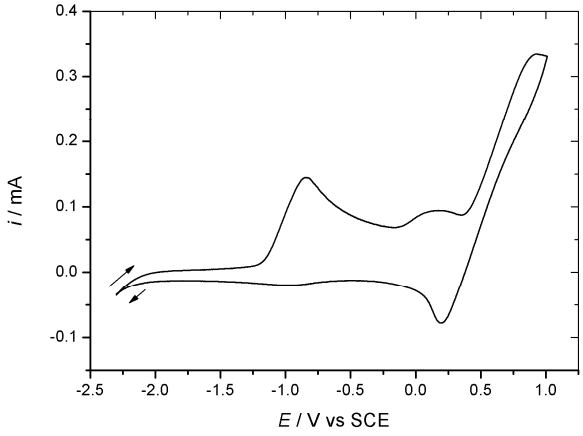


Figure S15. Cyclic voltammogram (CV) and $E_{1/2}$ values for **2-Mn**. CV recorded in THF with 0.4 M [*n*-Bu_4N][PF_6] supporting electrolyte. Scan rate: 500 mV/s. Referenced to SCE with internal Cp_2Fe/Cp_2Fe^+ standard (at +560 mV).

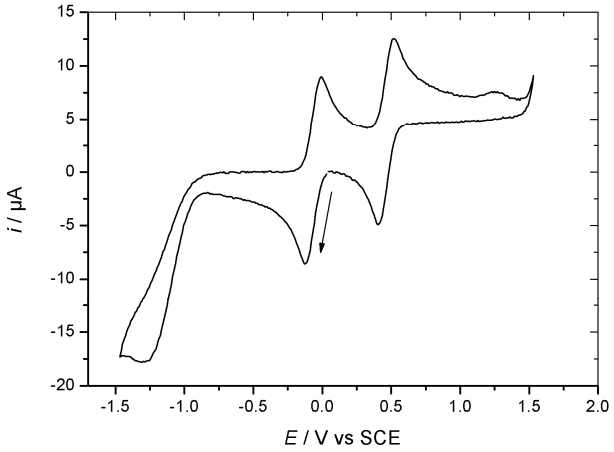


Figure S16. Cyclic voltammogram (CV) and $E_{1/2}$ values for **1-Fe**. CV recorded in CH_2Cl_2 with 0.1 M [*n*-Bu_4N][PF_6] supporting electrolyte. Scan rate: 100 mV/s. Referenced to SCE with internal Cp_2Fe/Cp_2Fe^+ standard (at +460 mV).

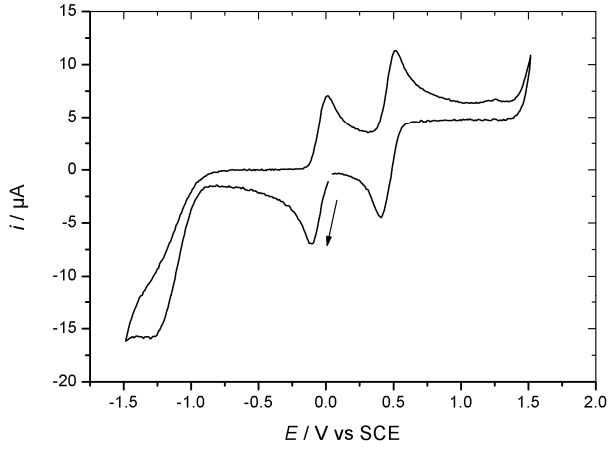


Figure S17. Cyclic voltammogram (CV) and $E_{1/2}$ values for **2-Fe**. CV recorded in CH_2Cl_2 with 0.1 M [*n*-Bu_4N][PF_6] supporting electrolyte. Scan rate: 100 mV/s. Referenced to SCE with internal Cp_2Fe/Cp_2Fe^+ standard (at +460 mV).

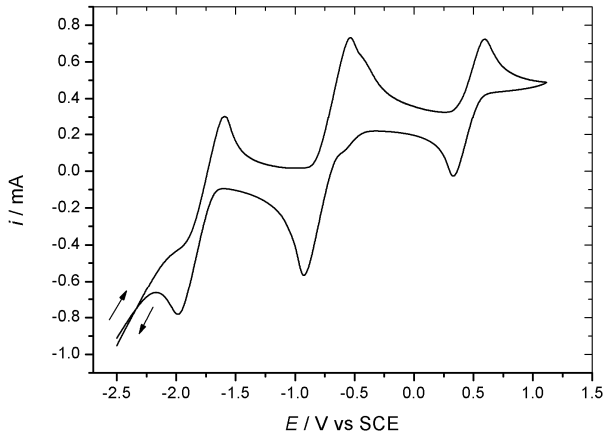


Figure S18. Cyclic voltammogram (CV) and $E_{1/2}$ values for **1-Co**. CV recorded in CH_2Cl_2 with 0.1 M [*n*-Bu_4N][PF_6] supporting electrolyte. Scan rate: 100 mV/s. Referenced to SCE with internal Cp_2Fe/Cp_2Fe^+ standard (at +460 mV).

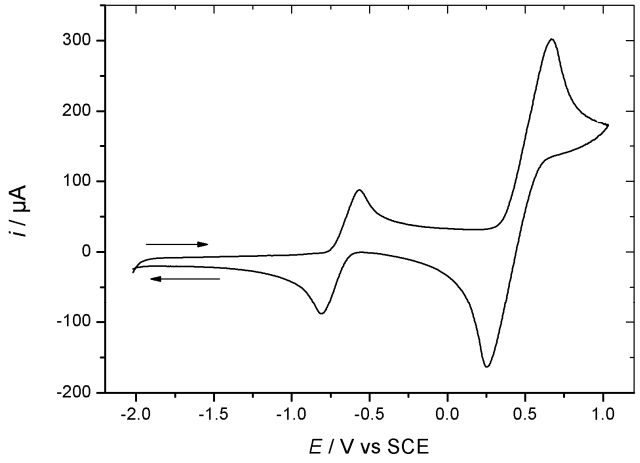


Figure S19. Cyclic voltammogram (CV) and $E_{1/2}$ values for **2-Co**. CV recorded in CH_2Cl_2 with 0.1 M [*n*-Bu_4N][PF_6] supporting electrolyte. Scan rate: 100 mV/s. Referenced to SCE with internal Cp_2Fe/Cp_2Fe^+ standard (at +460 mV).

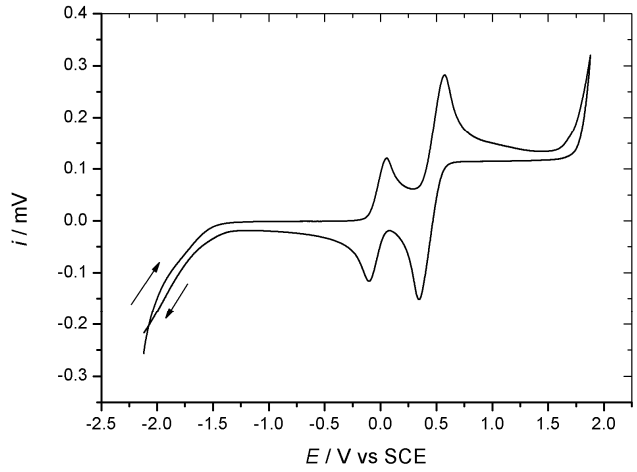


Figure S20. Cyclic voltammogram (CV) and $E_{1/2}$ values for **1-FeCp'**. CV recorded in CH_2Cl_2 with 0.1 M [*n*-Bu_4N][PF_6] supporting electrolyte. Scan rate: 100 mV/s. Referenced to SCE with internal Cp_2Fe/Cp_2Fe^+ standard (at +460 mV).

7. IR Spectra

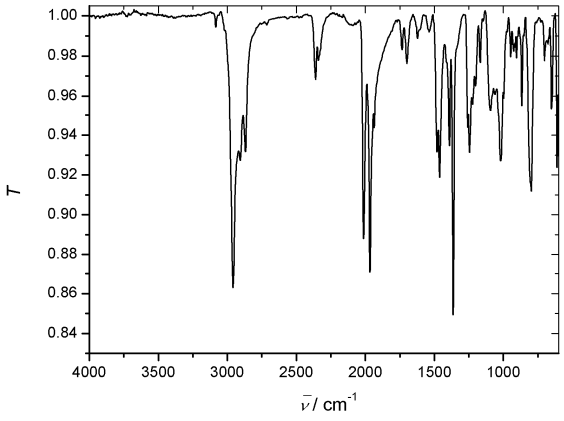


Figure S21. IR spectrum of **Cp'Fe(CO)$_2$I**

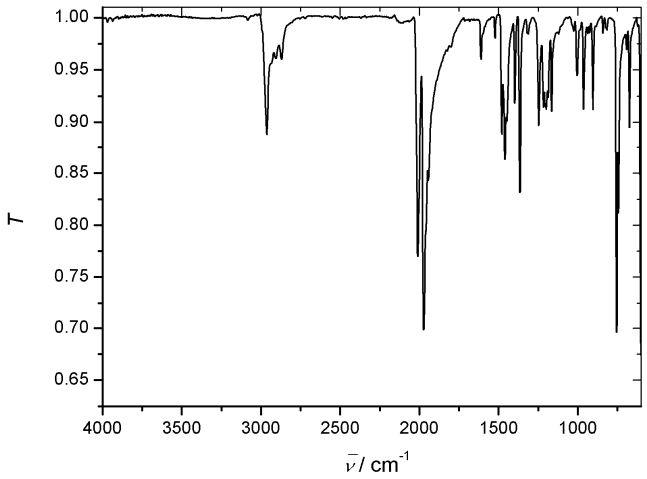


Figure S22. IR spectrum of **1-Fe(CO)$_2$I**

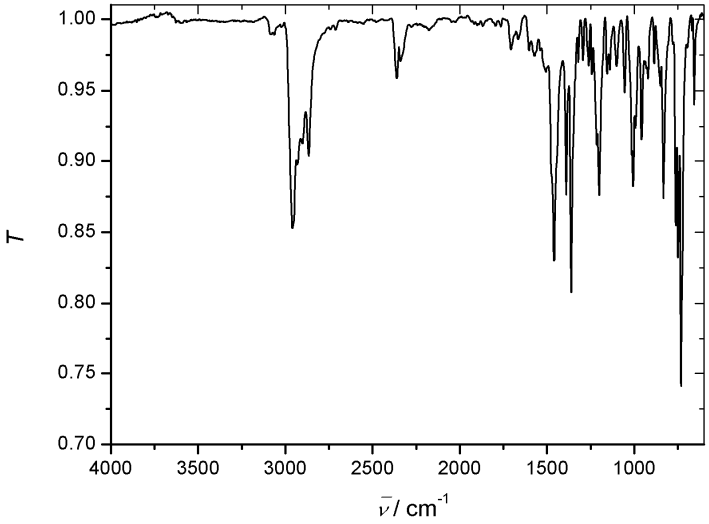


Figure S23. IR spectrum of **1-Mn**

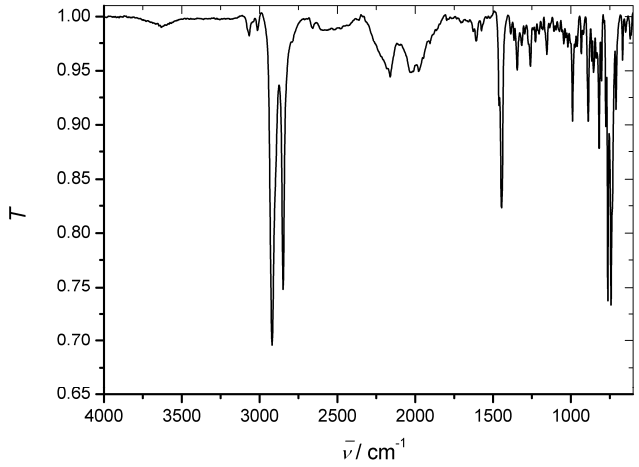


Figure S24. IR spectrum of **2-Mn**

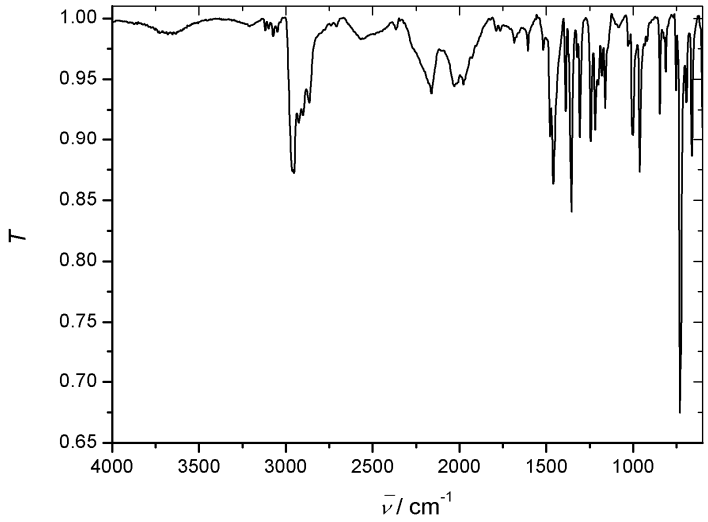


Figure S25. IR spectrum of **1-Fe**

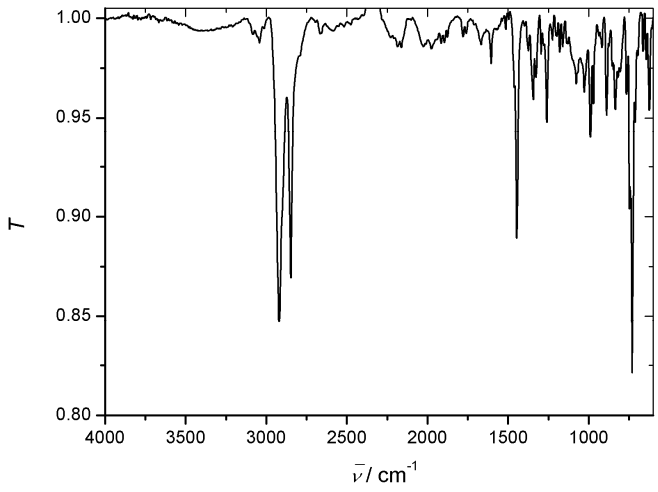


Figure S26. IR spectrum of **2-Fe**

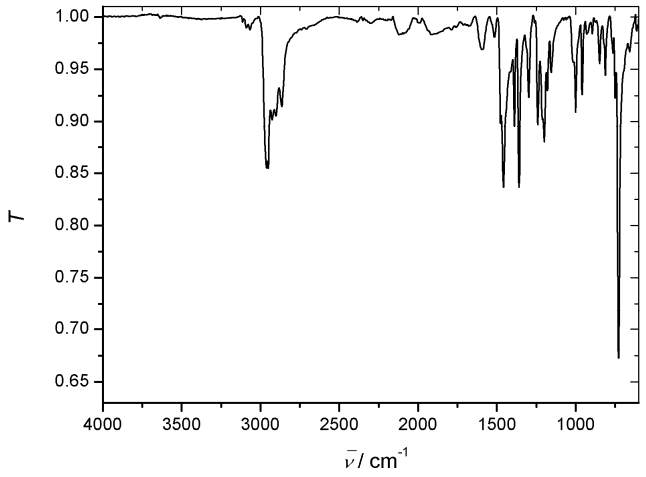


Figure S27. IR spectrum of **1-Co**

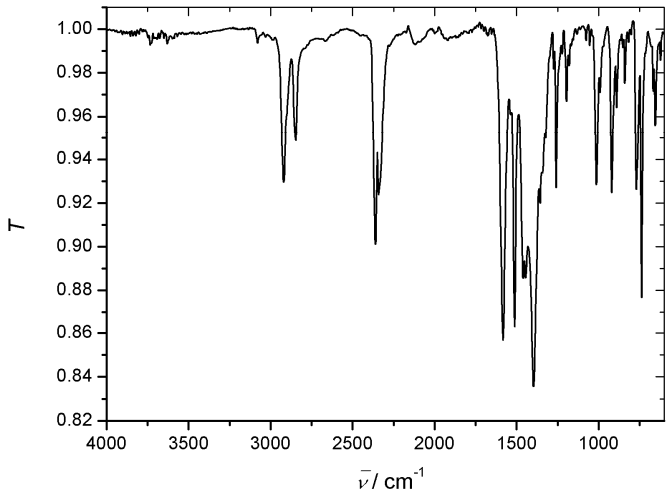


Figure S28. IR spectrum of **2-Co**

7. Computational Details

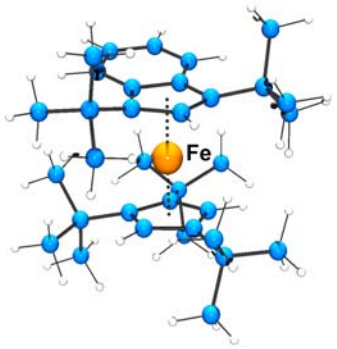
All computations were performed using the DFT functional method B97D as implemented in the Gaussian09 program.[1] The all-electron triple-ζ basis set (6-311G**)[2] was applied for all elements (Mn, Fe, Co, C and H). Unrestricted calculations were performed for all the paramagnetic species studied. Full geometry optimizations were performed without any symmetry constraints (C_1) starting from available crystal structure data.

Energies for the optimized structure:

Compound	E(0 K)[a] [Ha]	H(298 K)[b] [Ha]	G(298 K)[b] [Ha]
$[(Cp')_2Fe]$	-2593.366968	-2593.325104	-2593.430417
$[(Cp')Fe(Ind^{tBu})]$ (**1-FeCp'**)	-2589.813632	-2589.773971	-2589.875565
$[(1,3\text{-}(Me_3C)_2C_9H_6)_2Mn]$ (**1-Mn, low-spin**) (S=1/2)	-2473.439739	-2473.401537	-2473.502172
$[(1,3\text{-}(Me_3C)_2C_9H_6)_2Mn]$ (**1-Mn, high-spin**) (S=5/2)	-2473.446399	-2473.407473	-2473.513696
$[(1,3\text{-}(Me_3C)_2C_9H_6)_2Fe]$ (**1-Fe**)	-2586.250969	-2586.213389	-2586.311265
$[(1,3\text{-}(Me_3C)_2C_9H_6)_2Co]$ (**1-Co**)	-2705.380227	-2705.341669	-2705.443768
Mn^{2+} (S=1/2)	-1150.321281	-1150.318920	-1150.337598
Mn^{2+} (S=5/2)	-1150.467726	-1150.465365	-1150.485080
Fe^{2+} (S=0)	-1263.018363	-1263.016002	-1263.034041
Co^{2+} (S=1/2)	-1382.205507	-1382.203147	-1382.221924
$[Ind^{tBu}]^-$	-661.040066	-661.021354	-661.082948
$[Cp']^-$	-664.578791	-664.557361	-664.625176

[a]DFT energy incl. ZPE.

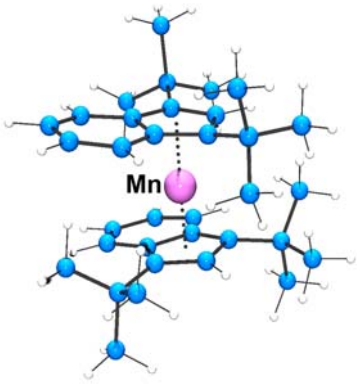
[b]standard conditions T = 298.15 K and p = 1 atm.



(atom, x-, y-, z-positions in Å):

Structure of 1-FeCp'			
Fe	0.139400	0.049300	-0.072900
C	1.975800	-0.398700	0.831000
C	1.969200	-0.716800	-0.561600
H	2.659400	-0.309100	-1.285800
C	0.951500	-1.677600	-0.875400
C	0.336600	-2.032800	0.390100
C	0.962200	-1.228100	1.436500
C	0.614700	-1.449900	2.806400
H	1.103400	-0.878700	3.590800
C	-0.296200	-2.429200	3.130200
H	-0.546500	-2.614400	4.173900
C	-0.921300	-3.211100	2.109500
H	-1.639000	-3.979600	2.393400
C	-0.627200	-3.018200	0.777200
H	-1.105400	-3.644300	0.033900
C	3.087600	0.346500	1.562200
C	3.860400	-0.686800	2.427300
H	3.222300	-1.125100	3.203000
H	4.715000	-0.195000	2.915600
H	4.239700	-1.502600	1.796400
C	2.557800	1.473500	2.471900
H	2.109700	2.270300	1.869900
H	3.388000	1.900800	3.053600
H	1.796800	1.111700	3.171200
C	4.099200	0.943600	0.561100
H	4.606300	0.145800	0.001300
H	4.860700	1.520900	1.103600
H	3.610600	1.607300	-0.159400
C	0.959500	-2.424900	-2.208300
C	-0.291700	-3.282700	-2.475300
H	-0.356000	-4.129300	-1.781800
H	-0.231800	-3.696600	-3.492300
H	-1.207800	-2.689200	-2.404300
C	2.186700	-3.376700	-2.166500
H	3.116600	-2.803200	-2.053700
H	2.244000	-3.962600	-3.096400
H	2.104500	-4.070400	-1.318200
C	1.132400	-1.452800	-3.394400
H	0.259300	-0.797100	-3.485100
H	1.237300	-2.027300	-4.326100
H	2.023100	-0.824400	-3.279800
C	-1.466700	1.154400	0.662100
C	-1.823800	0.531400	-0.618000
C	-0.853000	1.000700	-1.570500
H	-0.827300	0.735200	-2.617300
C	0.051900	1.921000	-0.962300
C	-0.329800	1.993700	0.407000
H	0.169800	2.599300	1.147800
C	-2.163600	1.240000	2.027900
C	-2.917400	-0.037200	2.442200
H	-3.812000	-0.205700	1.837900
H	-3.242800	0.056600	3.488400
H	-2.261800	-0.909400	2.359600
C	-1.135700	1.536000	3.149800
H	-1.654200	1.534700	4.118600
H	-0.667600	2.520400	3.027900
H	-0.355200	0.772500	3.166000
C	-3.137200	2.450000	1.993000
H	-3.904000	2.344500	1.219500
H	-2.578100	3.375100	1.794300
H	-3.636600	2.548900	2.968800
C	-3.083600	-0.223900	-1.093300
C	-3.054400	-0.387700	-2.635800
H	-2.170600	-0.945900	-2.966500
H	-3.056600	0.588800	-3.139000
H	-3.948400	-0.942000	-2.952800
C	-3.269900	-1.640600	-0.510900
H	-4.262900	-2.019600	-0.797300
H	-3.180000	-1.678900	0.573500
H	-2.517400	-2.316200	-0.923100
C	-4.338700	0.635900	-0.791400
H	-4.194900	1.665800	-1.146000
H	-4.574400	0.667100	0.274900
H	-5.206500	0.204800	-1.312500
C	0.964200	2.876700	-1.715000
C	1.924600	2.144800	-2.671200
H	2.687900	1.593600	-2.112900
H	2.430800	2.872900	-3.322200
H	1.379500	1.432900	-3.302900
C	1.756700	3.780200	-0.751000
H	1.072500	4.394200	-0.149400
H	2.410700	4.453500	-1.323000
H	2.378300	3.193900	-0.066500

C	0.032000	3.786800	-2.561800
H	-0.520000	3.194600	-3.304100
H	0.628400	4.545200	-3.090900
H	-0.696500	4.296900	-1.916500

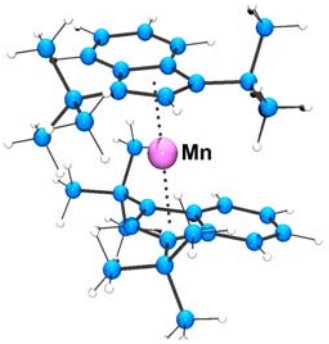


(atom, x-, y-, z-positions in Å):

Structure of 1-Mn (low-spin)

Mn	0.001700	-0.004900	0.009000
C	1.683400	-1.117200	0.681300
C	0.727900	-1.954400	0.011700
H	0.231700	-2.802700	0.461200
C	0.549200	-1.533600	-1.346300
C	1.505700	-0.468900	-1.572100
C	2.200600	-0.215300	-0.326100
C	3.216500	0.780900	-0.274900
H	3.750200	0.971500	0.651400
C	3.558600	1.468800	-1.425900
H	4.353800	2.212000	-1.396200
C	2.860300	1.240800	-2.642300
H	3.127000	1.818600	-3.526200
C	1.829500	0.318000	-2.715800
H	1.301600	0.177900	-3.651900
C	2.346300	-1.421400	2.023700
C	2.341000	-0.206700	2.975200
H	2.762200	0.686600	2.500400
H	2.935500	-0.435500	3.872600
H	1.319200	0.031100	3.288900
C	1.653100	-2.609100	2.722800
H	0.585100	-2.422900	2.876500
H	2.118700	-2.781400	3.703300
H	1.760500	-3.525200	2.126100
C	3.813600	-1.847500	1.746000
H	3.834300	-2.703300	1.057000
H	4.299000	-2.143900	2.687900
H	4.394900	-1.034100	1.295900
C	-0.228600	-2.326800	-2.390800
C	0.768200	-3.310100	-3.057100
H	1.594900	-2.760200	-3.528000
H	0.255800	-3.902800	-3.830300
H	1.191100	-3.996800	-2.310300
C	-1.350300	-3.146800	-1.718400
H	-0.944700	-3.867400	-0.995900
H	-1.900700	-3.709100	-2.485800
H	-2.047800	-2.481400	-1.199400
C	-0.859700	-1.425600	-3.476200
H	-1.316600	-0.537700	-3.030900
H	-1.637500	-1.983700	-4.017700
H	-0.116800	-1.110200	-4.219000
C	-1.664000	0.087800	1.317500
C	-0.713900	1.128000	1.597100
H	-0.205700	1.257500	2.540900
C	-0.552900	1.985400	0.461300
C	-1.520600	1.543200	-0.521900
C	-2.201600	0.379600	0.005500
C	-3.228300	-0.245300	-0.758300
H	-3.754300	-1.109200	-0.362600
C	-3.591300	0.289300	-1.981700
H	-4.395300	-0.168600	-2.555800
C	-2.904900	1.414100	-2.514400
H	-3.189900	1.797000	-3.493300
C	-1.866200	2.014700	-1.821900
H	-1.349100	2.862200	-2.256800
C	-2.315200	-0.825800	2.354800
C	-1.603800	-0.701100	3.718200
H	-0.540800	-0.951600	3.642600
H	-2.069500	-1.383000	4.443500
H	-1.687100	0.323700	4.105800
C	-2.322500	-2.308600	1.926400
H	-2.769800	-2.445100	0.935700
H	-2.900700	-2.900900	2.651300
H	-1.303200	-2.706000	1.889900
C	-3.779000	-0.349100	2.560700
H	-3.795800	0.711800	2.847000
H	-4.250500	-0.936900	3.362500
H	-4.377000	-0.464900	1.649100
C	0.218500	3.300900	0.480500

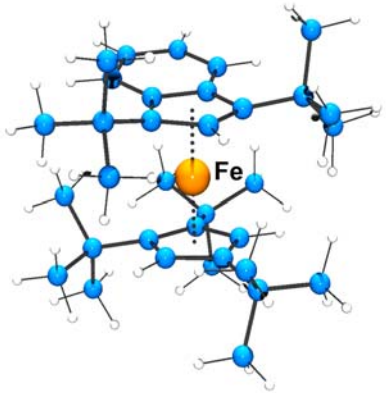
C	-0.776000	4.413200	0.902100
H	-1.611900	4.471200	0.191400
H	-0.266100	5.388500	0.924300
H	-1.183900	4.207500	1.901800
C	1.356900	3.238500	1.521400
H	0.966300	3.075000	2.534600
H	1.908000	4.189700	1.520300
H	2.053900	2.429000	1.279000
C	0.827700	3.658600	-0.894900
H	1.272300	2.779900	-1.369800
H	1.610400	4.420500	-0.766600
H	0.075200	4.083600	-1.570600



(C_{2v}-Symm.) (atom, x-, y-, z-positions in Å):

Structure of 1-Mn (high-spin)			
Mn	0.228200	-0.037500	-0.180800
C	-2.168600	1.176200	-0.448800
C	-1.322700	0.863200	-1.543300
H	-0.876200	1.595800	-2.205600
C	-1.203200	-0.567600	-1.722800
C	-2.092200	-1.153100	-0.736500
C	-2.661200	-0.076600	0.062900
C	-3.546100	-0.392400	1.123100
H	-3.961000	0.394000	1.749000
C	-3.908700	-1.715800	1.347400
H	-4.601900	-1.956400	2.152400
C	-3.390300	-2.758200	0.538600
H	-3.702600	-3.785200	0.723900
C	-2.484600	-2.489500	-0.481900
H	-2.101200	-3.305100	-1.089800
C	-2.537800	2.567800	0.036600
C	-2.106000	2.763400	1.510200
H	-2.567600	2.015800	2.166300
H	-2.397400	3.763900	1.863900
H	-1.016300	2.666200	1.600000
C	-1.854300	3.653300	-0.820600
H	-0.761200	3.558600	-0.789500
H	-2.123100	4.649000	-0.441000
H	-2.177000	3.584400	-1.868800
C	-4.071200	2.765200	-0.082300
H	-4.386900	2.648600	-1.128000
H	-4.346700	3.774900	0.258100
H	-4.619800	2.032700	0.520600
C	-0.584300	-1.273400	-2.929300
C	-1.708700	-1.839500	-3.826500
H	-2.325900	-2.559100	-3.274000
H	-1.278600	-2.347000	-4.703700
H	-2.361600	-1.027000	-4.174500
C	0.266300	-0.282600	-3.750700
H	-0.351200	0.525600	-4.165900
H	0.753200	-0.809500	-4.582800
H	1.051600	0.165100	-3.123800
C	0.350800	-2.413900	-2.463400
H	1.198600	-2.010800	-1.891600
H	0.762500	-2.950300	-3.331500
H	-0.169700	-3.136800	-1.826200
C	2.181800	1.153200	0.445400
C	1.354100	0.913800	1.581200
H	0.863200	1.688400	2.157200
C	1.224700	-0.485100	1.844900
C	2.065300	-1.156200	0.880000
C	2.645700	-0.138300	0.000200
C	3.494900	-0.543300	-1.065600
H	3.922100	0.195500	-1.739000
C	3.797700	-1.887500	-1.229100
H	4.459400	-2.195500	-2.037300
C	3.260500	-2.871400	-0.355500
H	3.526500	-3.917100	-0.502500
C	2.401000	-2.521800	0.676000
H	2.004800	-3.288800	1.335900

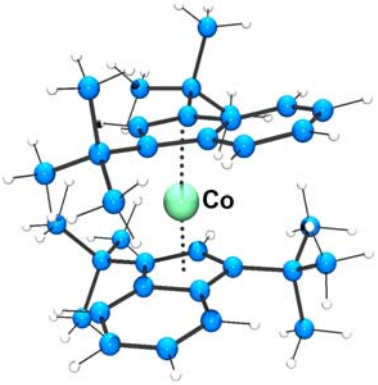
C	2.584600	2.507000	-0.119900
C	1.927300	3.650300	0.679600
H	0.832700	3.572600	0.660200
H	2.211100	4.618400	0.244200
H	2.256200	3.632200	1.727800
C	2.149100	2.628800	-1.600200
H	2.574500	1.824700	-2.213100
H	2.477200	3.592400	-2.017400
H	1.055000	2.574300	-1.678900
C	4.122100	2.669900	-0.016700
H	4.439100	2.602500	1.032900
H	4.423300	3.651300	-0.413000
H	4.648300	1.890800	-0.580700
C	0.471300	-1.123700	3.002500
C	1.490400	-1.759500	3.979300
H	2.088900	-2.531300	3.478700
H	0.962600	-2.222400	4.826600
H	2.176600	-0.994400	4.368400
C	-0.356300	-0.065000	3.758800
H	0.289100	0.714800	4.187300
H	-0.907700	-0.545400	4.578600
H	-1.082600	0.408700	3.085200
C	-0.505600	-2.200500	2.480300
H	-1.263500	-1.746000	1.833200
H	-1.025600	-2.682000	3.321200
H	0.009600	-2.977900	1.905200



(atom, x-, y-, z-positions in Å):

Structure of 1-Fe			
Fe	0.000000	-0.000100	0.027600
C	1.405500	-1.064600	1.117100
C	0.213500	-1.833100	0.916900
H	-0.407300	-2.219400	1.711600
C	-0.059300	-2.005600	-0.475700
C	1.046000	-1.389200	-1.187200
C	1.950700	-0.814900	-0.200300
C	3.198000	-0.260200	-0.627300
H	3.901000	0.128400	0.104200
C	3.532300	-0.283800	-1.962700
H	4.493700	0.111900	-2.287000
C	2.626400	-0.806900	-2.937500
H	2.909600	-0.788100	-3.989100
C	1.402600	-1.326700	-2.571500
H	0.734800	-1.718400	-3.330500
C	2.153000	-0.926400	2.438800
C	2.580000	0.525200	2.739000
H	3.120900	0.972300	1.898300
H	3.234700	0.541900	3.623000
H	1.705900	1.150700	2.947500
C	1.302900	-1.457300	3.611900
H	0.337900	-0.944100	3.675900
H	1.841300	-1.305400	4.557800
H	1.110500	-2.532600	3.494400
C	3.419400	-1.822500	2.350200
H	3.134700	-2.859200	2.123100
H	3.951200	-1.807500	3.313100
H	4.105400	-1.479000	1.567400
C	-1.092900	-2.980200	-1.024100
C	-0.399000	-4.367600	-1.089600
H	0.488600	-4.322700	-1.735700
H	-1.094600	-5.116000	-1.498800
H	-0.084300	-4.690900	-0.087600
C	-2.308000	-3.092200	-0.079500
H	-2.009500	-3.417500	0.925500
H	-3.010700	-3.836400	-0.480600
H	-2.824700	-2.131500	0.000800
C	-1.587200	-2.598800	-2.438600
H	-1.733500	-1.520000	-2.527000
H	-2.542600	-3.100500	-2.648700
H	-0.876200	-2.924500	-3.208300

C	-1.405300	1.064500	1.117200
C	-0.213300	1.833000	0.917000
H	0.407500	2.219100	1.711700
C	0.059300	2.005600	-0.475600
C	-1.046000	1.389100	-1.187000
C	-1.950600	0.814800	-0.200000
C	-3.197900	0.260000	-0.627000
H	-3.900900	-0.128600	0.104600
C	-3.532300	0.283600	-1.962300
H	-4.493700	-0.112100	-2.286600
C	-2.626500	0.806800	-2.937300
H	-2.909800	0.787900	-3.988800
C	-1.402700	1.326600	-2.571300
H	-0.735000	1.718200	-3.330300
C	-2.152600	0.926100	2.439100
C	-1.302600	1.457700	3.612100
H	-0.337100	0.945400	3.675600
H	-1.840500	1.305100	4.558200
H	-1.111300	2.533100	3.494600
C	-2.579200	-0.525500	2.739500
H	-3.119700	-0.973000	1.898800
H	-3.234000	-0.542300	3.623300
H	-1.704900	-1.150800	2.948400
C	-3.419400	1.821800	2.350600
H	-3.135200	2.858500	2.123200
H	-3.951000	1.806800	3.313600
H	-4.105400	1.477700	1.568000
C	1.092700	2.980500	-1.024100
C	0.398300	4.367700	-1.089000
H	-0.489400	4.322800	-1.734800
H	1.093600	5.116400	-1.498100
H	0.083800	4.690700	-0.086800
C	2.307900	3.092700	-0.079700
H	2.009600	3.417700	0.925400
H	3.010200	3.837300	-0.480800
H	2.825000	2.132200	0.000300
C	1.586700	2.599800	-2.438800
H	1.733700	1.521100	-2.527600
H	2.541700	3.102200	-2.649000
H	0.875200	2.925400	-3.208200



(atom, x-, y-, z-positions in Å):

Structure of 1-Co			
Co	-0.034900	-0.023000	-0.047300
C	1.452200	-0.505500	-1.441800
C	0.556200	0.492900	-1.927400
H	-0.082000	0.382300	-2.792300
C	0.596100	1.646700	-1.085700
C	1.703800	1.444500	-0.145400
C	2.230600	0.116400	-0.369500
C	3.358200	-0.325400	0.355900
H	3.782600	-1.308800	0.175800
C	3.952900	0.532000	1.283200
H	4.836900	0.203700	1.828200
C	3.419400	1.812900	1.528900
H	3.891800	2.459600	2.266800
C	2.294400	2.269100	0.834900
H	1.899000	3.256400	1.044000
C	1.835600	-1.762900	-2.211100
C	0.839100	-2.022900	-3.359200
H	-0.184800	-2.087100	-2.975800
H	1.087000	-2.967800	-3.861800
H	0.878500	-1.216800	-4.104300
C	1.896800	-3.023400	-1.324500
H	2.572600	-2.895900	-0.473400
H	2.256100	-3.872800	-1.923600
H	0.902900	-3.269900	-0.936300
C	3.233900	-1.512700	-2.838500
H	3.206300	-0.624800	-3.485300
H	3.527400	-2.381100	-3.446700
H	3.996200	-1.350500	-2.067500
C	-0.066000	2.969100	-1.447300
C	0.934200	3.728100	-2.360500
H	1.886800	3.887900	-1.837400
H	0.516800	4.707800	-2.637700

H	1.131300	3.157000	-3.278400
C	-1.368200	2.729900	-2.240400
H	-1.176700	2.188100	-3.175600
H	-1.820400	3.698100	-2.497200
H	-2.081500	2.156300	-1.640700
C	-0.382900	3.841000	-0.210700
H	-0.779800	3.236000	0.607500
H	-1.129400	4.602300	-0.477700
H	0.508700	4.373300	0.142200
C	-1.976000	-1.072100	-0.020700
C	-0.934300	-1.771200	0.655700
H	-0.610600	-2.770900	0.402900
C	-0.411500	-1.011300	1.761900
C	-1.152000	0.223400	1.774300
C	-2.097700	0.191700	0.650100
C	-3.041000	1.259700	0.500600
H	-3.759000	1.242900	-0.314800
C	-3.072600	2.276500	1.426400
H	-3.807800	3.074100	1.327300
C	-2.139400	2.319200	2.512200
H	-2.178300	3.152000	3.212800
C	-1.186400	1.336400	2.673200
H	-0.486900	1.397800	3.499100
C	-2.900400	-1.639400	-1.086200
C	-2.900400	-0.776900	-2.368200
H	-3.161700	0.264900	-2.151200
H	-3.630300	-1.175300	-3.088700
H	-1.909200	-0.783500	-2.835400
C	-2.495000	-3.084000	-1.449800
H	-1.458900	-3.139200	-1.804000
H	-3.152500	-3.462900	-2.244600
H	-2.593600	-3.744900	-0.577500
C	-4.340200	-1.696700	-0.508600
H	-4.357800	-2.307500	0.404600
H	-5.020700	-2.148200	-1.246200
H	-4.715400	-0.698300	-0.256000
C	0.496400	-1.579700	2.842100
C	-0.417800	-2.225100	3.916300
H	-1.101600	-1.476200	4.339700
H	0.193400	-2.642800	4.731000
H	-1.017800	-3.034500	3.477200
C	1.419100	-2.668200	2.257000
H	0.843700	-3.495400	1.821700
H	2.051800	-3.078800	3.056400
H	2.061100	-2.237000	1.484000
C	1.379900	-0.500300	3.509800
H	1.804200	0.180900	2.767000
H	2.206900	-0.982900	4.050300
H	0.812900	0.081400	4.246700

8. References

[1] Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[2] X. Cao and M. Dolg, *J. Chem. Phys.* 2001, **115**, 7348.