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, *

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1. Experimental Details for [(η⁵-Cp')Fe(CO)₂I]

(1,2,4-Tri-tert-butylcyclopentadienyl)(dicarbonyl)iron(II)iodide, [Cp'Fe(CO)₂I]. FeI₂(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. ¹H NMR (300.0 MHz, C₆D₆, 24°C): δ 4.86 (s, 2H, ring-C₆H), 1.21 (s, 9H, tBu-H), 1.18 (s, 18H, tBu-H). ¹³C{¹H} NMR (75.5 MHz, C₆D₆, 25°C): δ 216.1 (2C, CO), 108.4 (2C, ring-C₁₅), 107.9 (1C, ring-C₁₅), 88.6 (2C, ring-CH), 33.4 (6C, tBu-CH₃), 32.6 (2C, tBu-CH₂), 32.0 (3C, tBu-CH₃) 31.2 (1C, tBu-C₁₅). 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), 1391 (m), 1245 (m), 1094 (m), 1021 (m), 798 (m), 611 (m). Mp: 115°C (dec.).

Figure S1. ORTEP diagram of Cp'Fe(CO)₂I with 30% probability ellipsoids. Hydrogen atoms are omitted for clarity.

Empirical formula          C₁₉ H₂₉ Fe I O₂  
Formula weight            472.17   
Temperature              100(2) K  
Wavelength               1.54184 Å  
Crystal system           orthorhombic 
Space group             Pca₂₁  
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) Å³  

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

![ORTEP Diagram of 1-Fe with 30% probability ellipsoids. Hydrogen atoms are omitted for clarity.](image1)

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

![ORTEP Diagram of 1-Co with 30% probability ellipsoids. Hydrogen atoms are omitted for clarity.](image2)

**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 C₆D₆) 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) ¹H NMR spectra of 1-Fe recorded in C₇D₇.
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$_4$N][PF$_6$] supporting electrolyte. Scan rate: 500 mV/s. Referenced to SCE with internal Cp$_2$Fe/Cp$_2$Fe$^+$ 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$_4$N][PF$_6$] supporting electrolyte. Scan rate: 500 mV/s. Referenced to SCE with internal Cp$_2$Fe/Cp$_2$Fe$^+$ standard (at +560 mV).
Figure S16. Cyclic voltammogram (CV) and $E_{1/2}$ values for 1-Fe. CV recorded in CH$_2$Cl$_2$ with 0.1 M [n-Bu$_4$N][PF$_6$] supporting electrolyte. Scan rate: 100 mV/s. Referenced to SCE with internal Cp$_2$Fe/Cp$_2$Fe$^+$ standard (at +460 mV).

Figure S17. Cyclic voltammogram (CV) and $E_{1/2}$ values for 2-Fe. CV recorded in CH$_2$Cl$_2$ with 0.1 M [n-Bu$_4$N][PF$_6$] supporting electrolyte. Scan rate: 100 mV/s. Referenced to SCE with internal Cp$_2$Fe/Cp$_2$Fe$^+$ standard (at +460 mV).
Figure S18. Cyclic voltammogram (CV) and $E_{1/2}$ values for 1-Co. CV recorded in CH$_2$Cl$_2$ with 0.1 M [n-Bu$_4$N][PF$_6$] supporting electrolyte. Scan rate: 100 mV/s. Referenced to SCE with internal Cp$_2$Fe/Cp$_2$Fe$^+$ standard (at +460 mV).

Figure S19. Cyclic voltammogram (CV) and $E_{1/2}$ values for 2-Co. CV recorded in CH$_2$Cl$_2$ with 0.1 M [n-Bu$_4$N][PF$_6$] supporting electrolyte. Scan rate: 100 mV/s. Referenced to SCE with internal Cp$_2$Fe/Cp$_2$Fe$^+$ standard (at +460 mV).
Figure S20. Cyclic voltammogram (CV) and $E_{1/2}$ values for 1-FeCp'. CV recorded in CH$_2$Cl$_2$ with 0.1 M [$n$-Bu$_4$N][PF$_6$] supporting electrolyte. Scan rate: 100 mV/s. Referenced to SCE with internal Cp$_2$Fe/Cp$_2$Fe$^+$ 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. The all-electron triple-ζ basis set (6-311G**) 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 (C1) starting from available crystal structure data.

Energies for the optimized structure:

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aDFT energy incl. ZPE.

bStandard conditions T = 298.15 K and p = 1 atm.
(atom, x-, y-, z-positions in Å):

**Structure of 1-FeCp**

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**Electronic Supplementary Material (ESI)** for *Dalton Transactions* © The Royal Society of Chemistry 2012
(atom, x-, y-, z-positions in Å):

Structure of 1-Mn (low-spin)
(C₂ᵥ-Symm.) (atom, x-, y-, z-positions in Å):

**Structure of 1-Mn (high-spin)**

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Electronic Supplementary Material (ESI) for Dalton Transactions
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(atom, x-, y-, z-positions in Å):

Structure of 1-Co

atom, x-, y-, z-positions in Å:

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8. References
