Supporting Information

Fe and Mn complexes of 2-carbonyl pyrrolyls; scorpionate sandwich anions and extended structures

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Magnetism of $[Na(THF)_6][(FeL^2_3)Na(L^2_3Fe)]$

The isotropic Heisenberg magnetic model (HDVV) was used to describe the magnetism of the material.

$$H = -J \, S_A \bullet S_B$$

$$S = S_A + S_B$$

S_A, S_B are the local spin operators

$$\chi_M = \frac{2Ng^2\beta^2}{kT} \frac{e^x + 5e^{3x} + 14e^{6x} + 30e^{10x} + 55e^{15x}}{1 + 3e^x + 5e^{3x} + 7e^{6x} + 9e^{10x} + 11e^{15x}}$$

With $x = J/kT$ for local spins $S_A = S_B = 5/2$.

A least squares fit to the equation gives $J = -1.34$ cm^{-1} and $g = 1.80$, confirming that the material is antiferromagnetic. However, possibly due to that the magnetic model does not count magnetic anisotropy of Fe(II) ion a small *g-factor* was obtained.
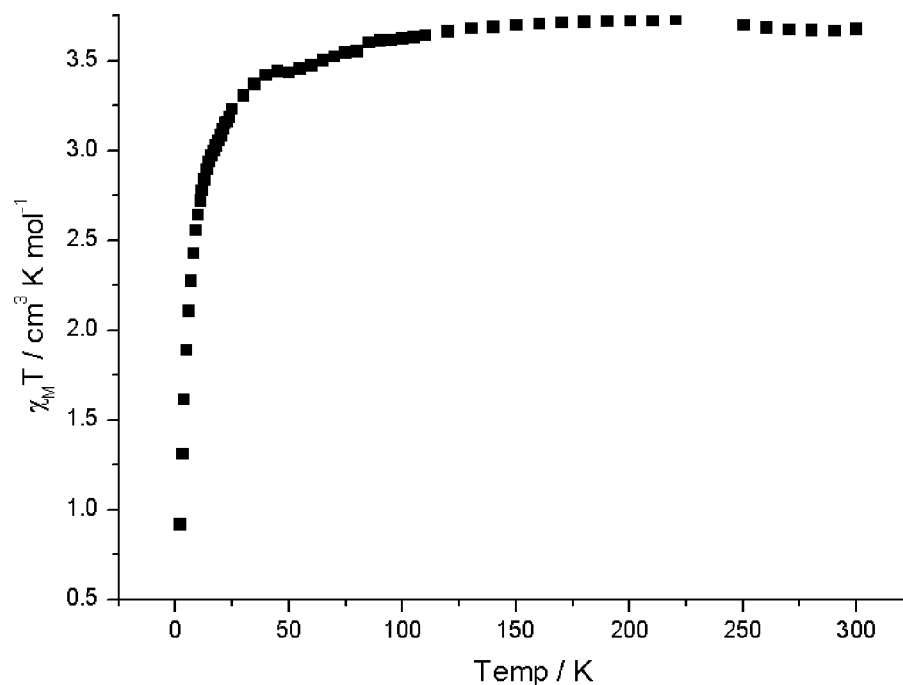

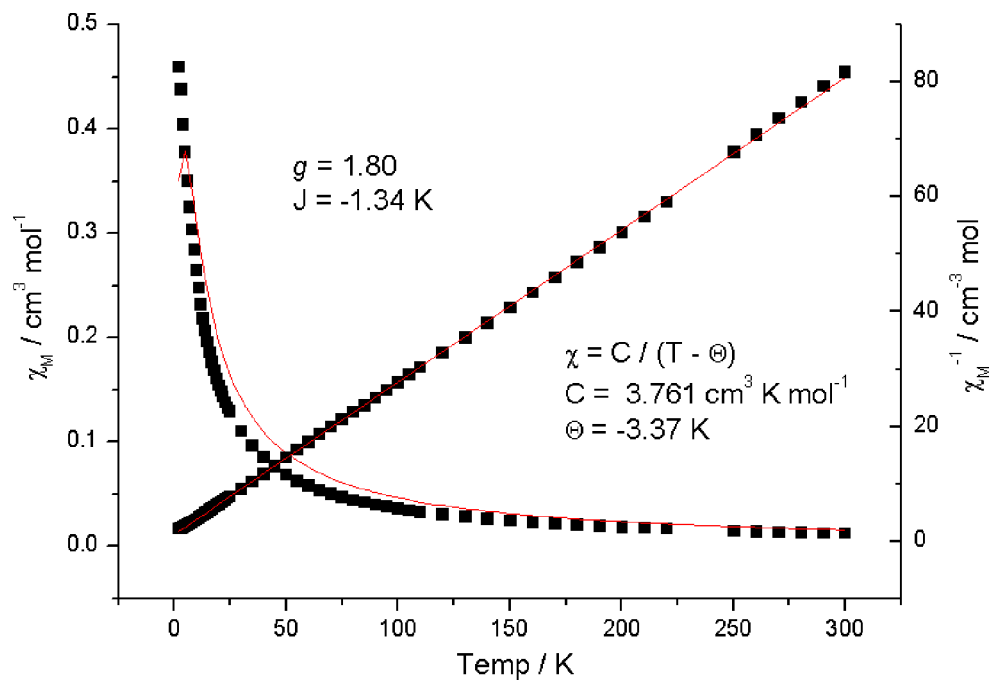**Figure S1.** $\chi_M T$ *vs* T for complex $[Na(THF)_6][(FeL^2_3)Na(L^2_3Fe)]$ measured at 1000 Oe

Figure S2. χ_M^{-1} *vs* T for complex [Na(THF)$_6$][(FeL^2$_3$)Na(L^2$_3$Fe)] measured at 1000 Oe

Magnetism of [Na(THF)₆][(MnL²₃)Na(L²₃Mn)]
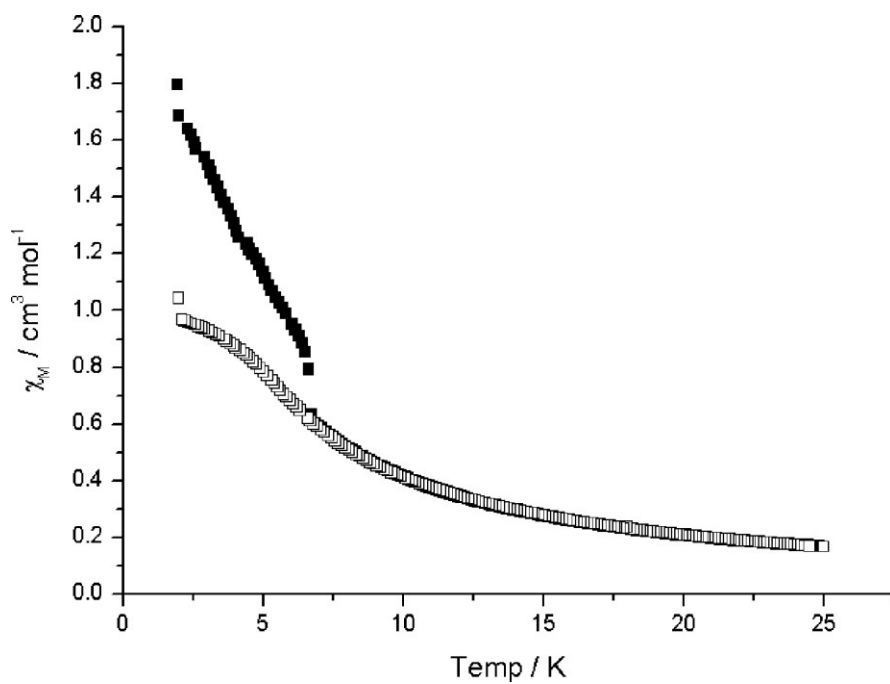
Figure S3. ZFCW and FCC M *vs.* *T* curves for [Na(THF)₆][(MnL²₃)Na(L²₃Mn)] measured at 1000 Oe.

g = 1.8
J = -0.37 K

$\chi = C / (T - \Theta)$
C = 4.496 cm³ K mol⁻¹
Θ = -4.70 K
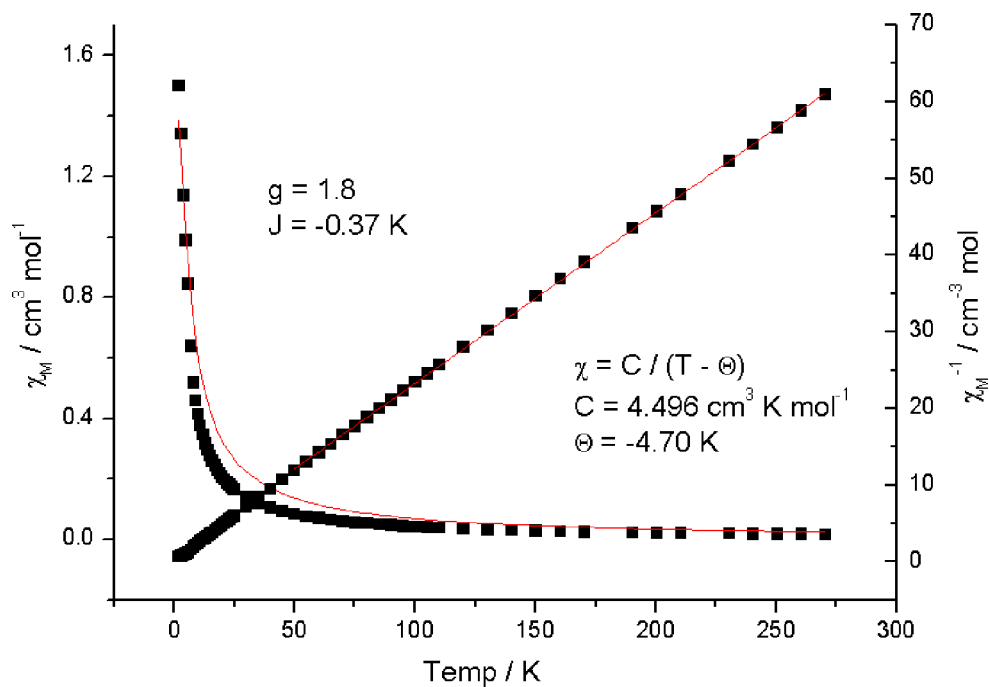
Figure S4. χ_M, χ_{M⁻¹} *vs.* *T* curves for [Na(THF)₆][(MnL²₃)Na(L²₃Mn)]
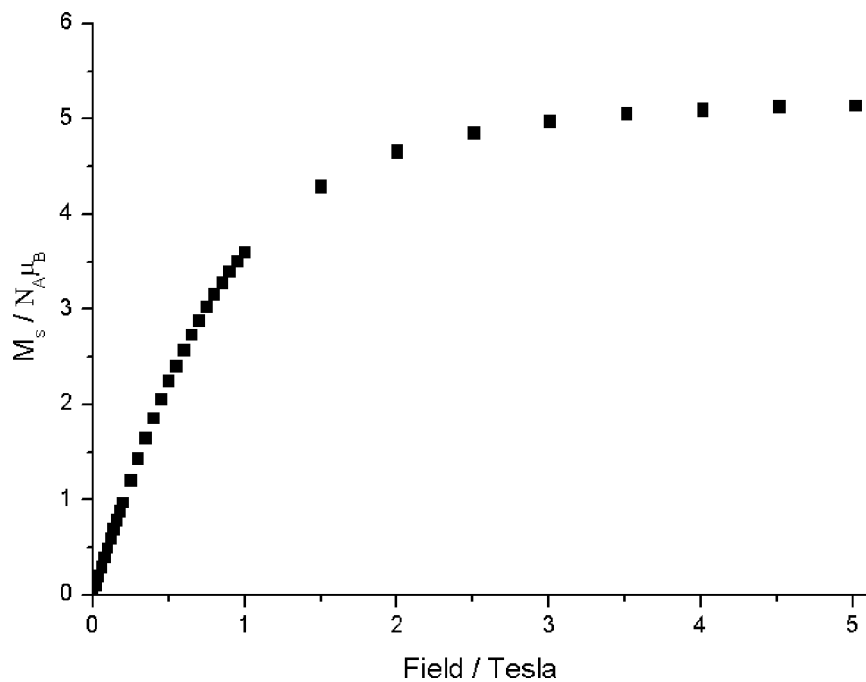
Figure S5. *M vs. H* curve for [Na(THF)$_6$][(Mn**L²**$_3$)Na(**L²**$_3$Mn)] measured at 2 K.

Magnetism of [Na(THF)$_4$][(Mn**L^3**$_3$)Na(**L^3**$_3$Mn)]
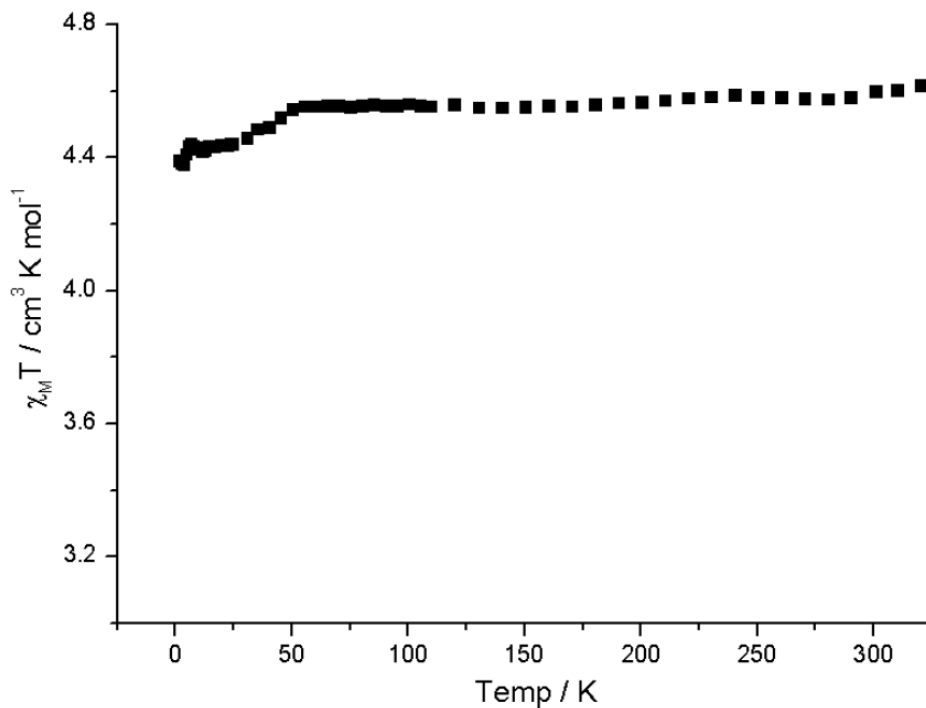
Figure S6. $\chi_M T$ *vs. T* for [Na(THF)$_4$][(Mn**L^3**$_3$)Na(**L^3**$_3$Mn)] measured at 1000 Oe

g = 1.8
J = -0.23 K

$\chi = C / (T - \Theta)$
C = 4.765 cm^3 K mol^{-1}
Θ = - 0.25 K

Figure S7. χ_M and χ_M^{-1} *vs. T* for [Na(THF)$_4$][(Mn**L^3**$_3$)Na(**L^3**$_3$Mn)] measured at 1000 Oe