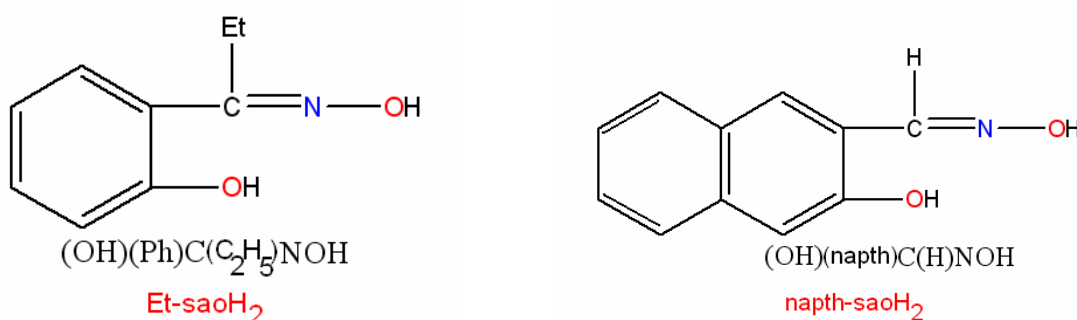


Turning up the spin, turning on single-molecule magnetism: from $S = 1$ to $S = 7$ in a $[\text{Mn}_8]$ cluster *via* ligand induced structural distortion

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Supplementary Information



Scheme S11. The ligands discussed in the text.

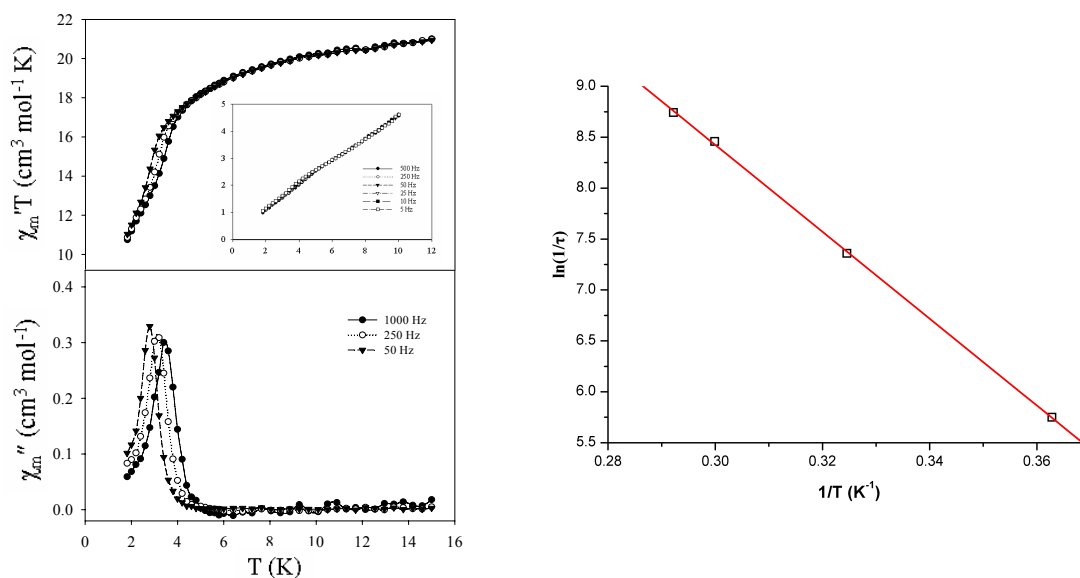
Complex 2

The complex analysed as (C, H, N) 2:3 MeOH, expected (found): C, 42.28 (42.36); H, 3.96 (3.85); N, 15.37 (15.29). Diffraction data were collected with Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$) on an Bruker Smart Apex CCD Diffractometer. Crystal Data¹⁰: C₈₄ H₁₁₄ Mn₈ N₂₄ O₃₂, M = 2411.5, dark brown block, Triclinic, P-1, a = 13.8273(3), b = 15.3275(3), c = 15.5166(4) \AA , $\alpha = 111.6580(10)$, $\beta = 109.8920(10)$, $\gamma = 102.6120(10)^\circ$, V = 2642.14(10) \AA^3 , 61412 reflections collected of which 14863 were independent (Rint = 0.0506), 694 parameters and 12 restraints, R1 = 0.0492 [based on $F > 4\sigma(F)$], wR2 = 0.1174 (based on F^2 and all data). CCDC 638207. See <http://www.rsc.org/suppdata/cc/b7/b703089d/> for crystallographic data in .cif or other electronic format

Complex 3

The complex analysed as (C, H, N) 3:2 MeOH, expected (found): C, 35.93 (36.02); H, 4.26 (4.20); N, 17.34 (17.27). Diffraction data were collected with Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$) on an Bruker Smart Apex CCD Diffractometer. Crystal Data¹⁰, C₆₆ H₁₁₄ Mn₈ N₂₄ O₃₂, M = 2195.3, black blocks, Triclinic, P-1, a = 11.698(2), b = 12.608(3), c = 17.019(3) \AA , $\alpha = 76.05(3)$, $\beta = 82.03(3)$, $\gamma = 75.41(3)^\circ$, V = 2349.4(9) \AA^3 , 67762 reflections collected of which 9606 were independent (Rint = 0.103), 496 parameters and 18 restraints, R1 = 0.0698 [based on $F > 4\sigma(F)$], wR2 = 0.0574 (based on F using the $I > 2\sigma(I)$ data). CCDC 638208. See <http://www.rsc.org/suppdata/cc/b7/b703089d/> for crystallographic data in .cif or other electronic format

Figure S11



In-phase (plotted as χ_M'/T) and out-of-phase ac susceptibility measurements for **3** at the indicated temperature and frequency ranges (left). The inset shows χ_M'/T vs T for complex **2**. Arrhenius plot for **3** using the ac (χ_M'') data. The solid line is a fit of the data yielding $U_{\text{eff}} = 44.6$ K and $\tau_0 = 6.05 \times 10^{-10}$ s.