

Supplementary information.

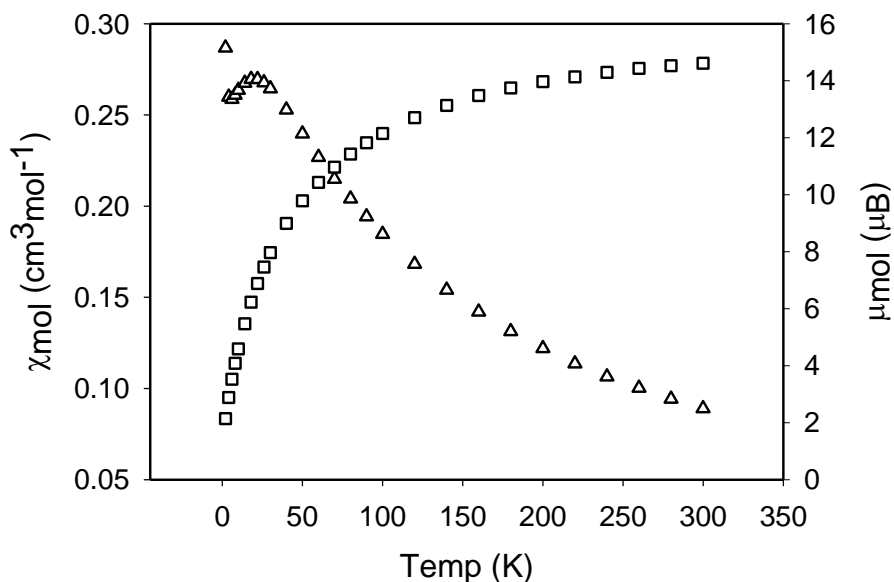


Fig. S1. Variable temperature magnetic data for **1**, expressed per mole.

X-Ray crystallographic details

For **1**, all measurements were made on a Rigaku Saturn CCD area detector with graphite monochromated Mo-K α radiation and equipped with a SHINE optic. Cell refinement and data reduction was performed using Rigaku's CrystalClear.¹ The structure was solved by direct methods² and expanded using Fourier techniques. Neutral atom scattering factors were taken from Cromer and Waber³. Anomalous dispersion effects were included in Fcalc⁴; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley⁵. The values for the mass attenuation coefficients are those of Creagh and Hubbell⁶. All calculations were performed using the CrystalStructure⁷ crystallographic software package except for refinement, which was performed using SHELXL-97². Protons were introduced in calculated positions and were refined on a riding model. Lattice solvent water and methanol molecules for which protons could not be located in difference map positions were omitted from the model, however, they were included in the formula for the calculation of intensive properties. All non-hydrogen atoms were refined anisotropically. Note that all Mn atoms are in the +3 oxidation state except Mn2, which is in the +2 oxidation state. Each ligand bears a charge of -3. The moieties represented by [O16 C36] and [O19 C39] are methoxides while [O20 C40] is a methanol molecule. O21 and O22 are disordered water molecules,

with an occupancy sum of one. With $Z = 2$, the formula, which includes protons omitted from the model, is: $\{[(C_{11}H_{10}O_4N_3)_3CsMn5(CH_3COO)_2(O)(CH_3O)_2(CH_3OH)] \bullet (H_2O)_1\}_2$

(1) CrystalClear: Rigaku Corporation, 1999. CrystalClear Software User's Guide, Molecular Structure Corporation, (c) 2000.J.W.Pflugrath (1999) Acta Cryst. D55, 1718-1725.

(2) SHELX97: Sheldrick, G.M. Acta Cryst. 2008, A64, 112-122.

(3) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(4) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(5) Creagh, D. C. & McAuley, W.J. ; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(6) Creagh, D. C. & Hubbell, J.H.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(7) CrystalStructure 4.0: Crystal Structure Analysis Package, Rigaku and Rigaku Americas (2000-2010). 9009 New Trails Dr. The Woodlands TX 77381 USA.