A Oximato-Bridged Linear Trinuclear [$Mn^{IV}Mn^{III}Mn^{IV}$] Single Molecule Magnet

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Supporting Information

Table S1. Selected interatomic distances (Å) and bond angles (°) for **1**.

Mn(1)-O(5)	1.917(2)	Mn(2)-O(3)	1.870(2)
Mn(1)-O(6)	2.047(2)	Mn(2)-N(2)	1.992(2)
Mn(1)-O(4)	2.052(2)	Mn(2)-N(3)	1.993(2)
Mn(2)-O(2)	1.861(2)	Mn(2)-N(1)	1.995(2)
Mn(2)-O(1)	1.8649(19)		
O(5)-Mn(1)-O(5)#1	169.06(13)	O(6)-Mn(1)-O(4)#1	169.49(9)
O(5)-Mn(1)-O(6)#1	95.10(9)	O(4)-Mn(1)-O(4)#1	98.74(13)
O(5)#1-Mn(1)-O(6)#1	93.21(8)	O(2)-Mn(2)-O(1)	93.67(9)
O(5)-Mn(1)-O(6)	93.21(9)	O(2)-Mn(2)-O(3)	93.49(9)
O(5)#1-Mn(1)-O(6)	95.10(9)	O(1)-Mn(2)-O(3)	93.11(9)
O(6)#1-Mn(1)-O(6)	81.08(12)	O(2)-Mn(2)-N(2)	177.72(9)
O(5)-Mn(1)-O(4)	91.46(9)	O(1)-Mn(2)-N(2)	88.51(9)
O(5)#1-Mn(1)-O(4)	81.40(8)	O(3)-Mn(2)-N(2)	87.06(9)
O(6)#1-Mn(1)-O(4)	169.49(9)	O(2)-Mn(2)-N(3)	88.71(9)
O(6)-Mn(1)-O(4)	90.37(9)	O(1)-Mn(2)-N(3)	86.43(9)
O(5)-Mn(1)-O(4)#1	81.40(8)	O(3)-Mn(2)-N(3)	177.78(10)
O(5)#1-Mn(1)-O(4)#1	91.46(9)	N(2)-Mn(2)-N(3)	90.75(10)
O(6)#1-Mn(1)-O(4)#1	90.37(9)		

Symmetry transformations used to generate equivalent atoms:

#1 -x, y, -z+1/2

Table S2. Fitting data of Cole-Cole semicircles of **1** using extended Debye model at different temperatures.

T, K	χ_S, $cm^3 \cdot mol^{-1}$	χ_T, $cm^3 \cdot mol^{-1}$	τ, s	α	R
1.90	1.72	4.58	4×10^{-5}	0.256	8.3×10^{-4}
1.95	1.71	4.43	4×10^{-5}	0.247	7.5×10^{-5}
2.00	1.69	4.31	3×10^{-5}	0.243	8.5×10^{-5}
2.05	1.70	4.19	3×10^{-5}	0.234	9.9×10^{-5}
2.10	1.80	4.08	3×10^{-5}	0.197	7.0×10^{-5}

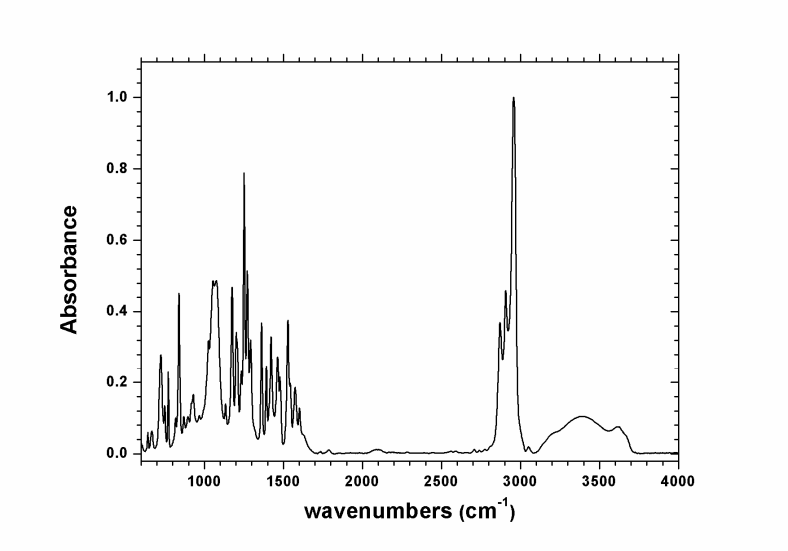

Figure S1. The IR spectra for **1**.

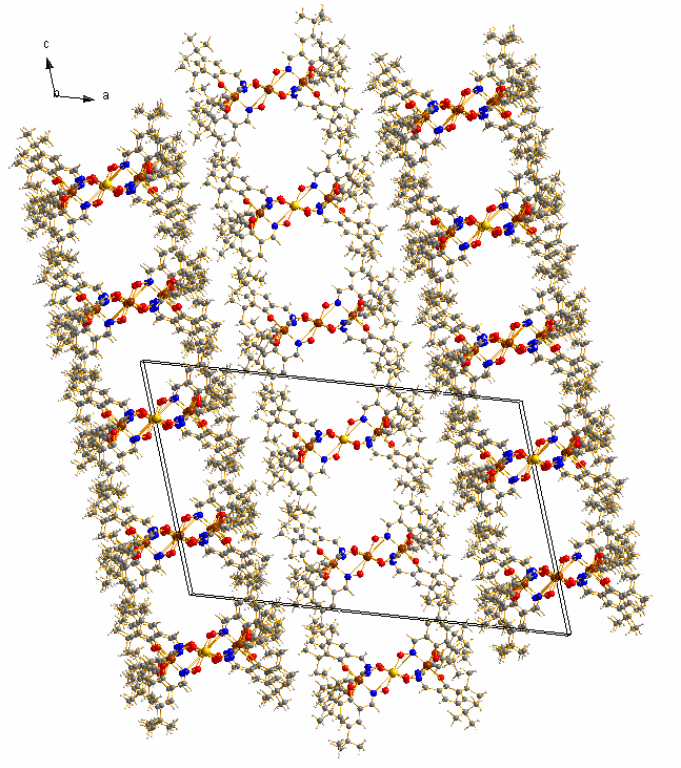

Figure S2. The packing diagram for **1**. (Brown = Mn, yellow = Na, red = oxygen, blue = nitrogen, grey = carbon)

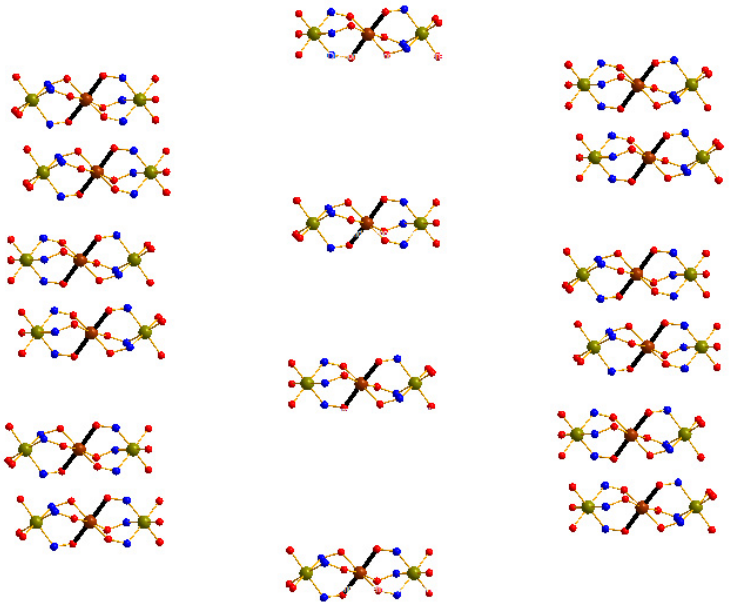

Figure S3. The Jahn-Teller axes in **1**. (Thick black line; carbon, hydrogen and sodium atoms are omitted for clearance)

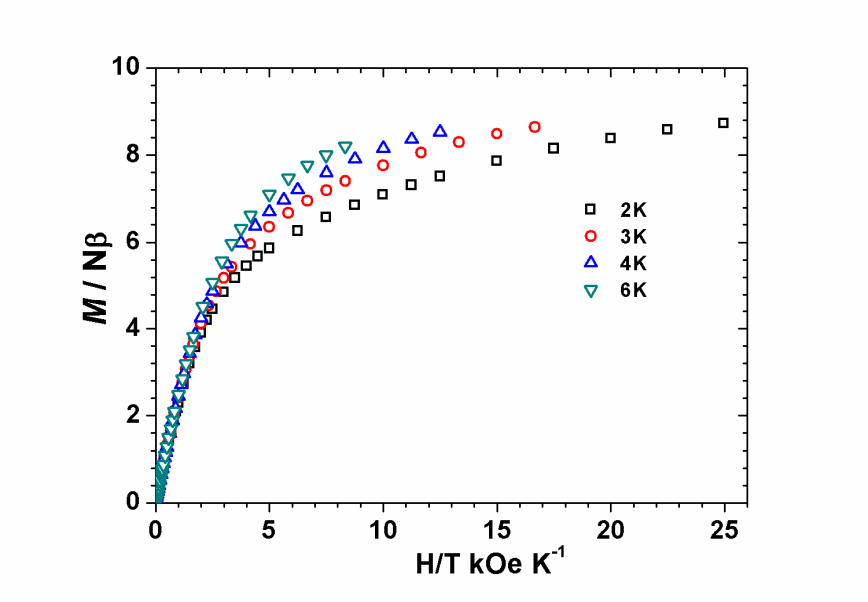

Figure S4. The reduced magnetization of **1** plotted as M *vs.* H/T at indicated temperatures.

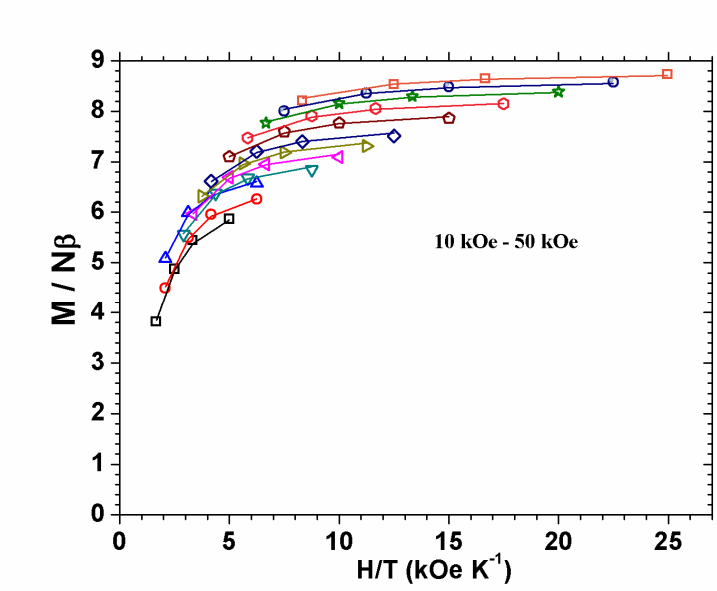

Figure S5. The fitting curve of reduced magnetization of **1**.

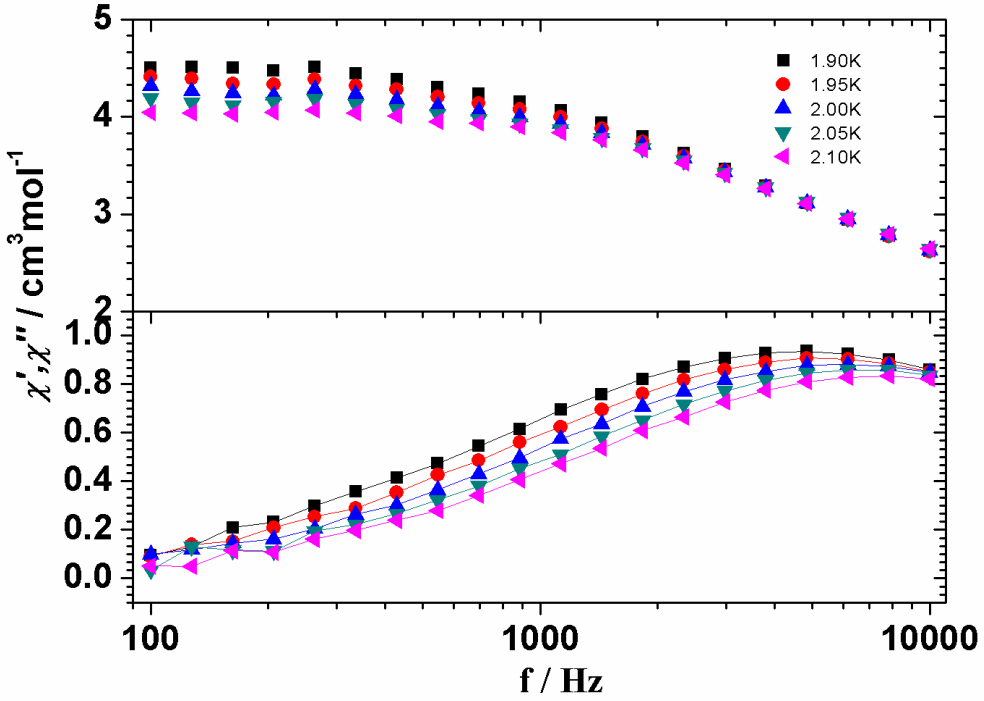

Figure S6. Frequency dependence of ac susceptibilities of **1** under a zero-applied dc field with an oscillating ac field of 3 Oe in frequencies of 100−10000 Hz. The data were collected at the indicated temperatures.

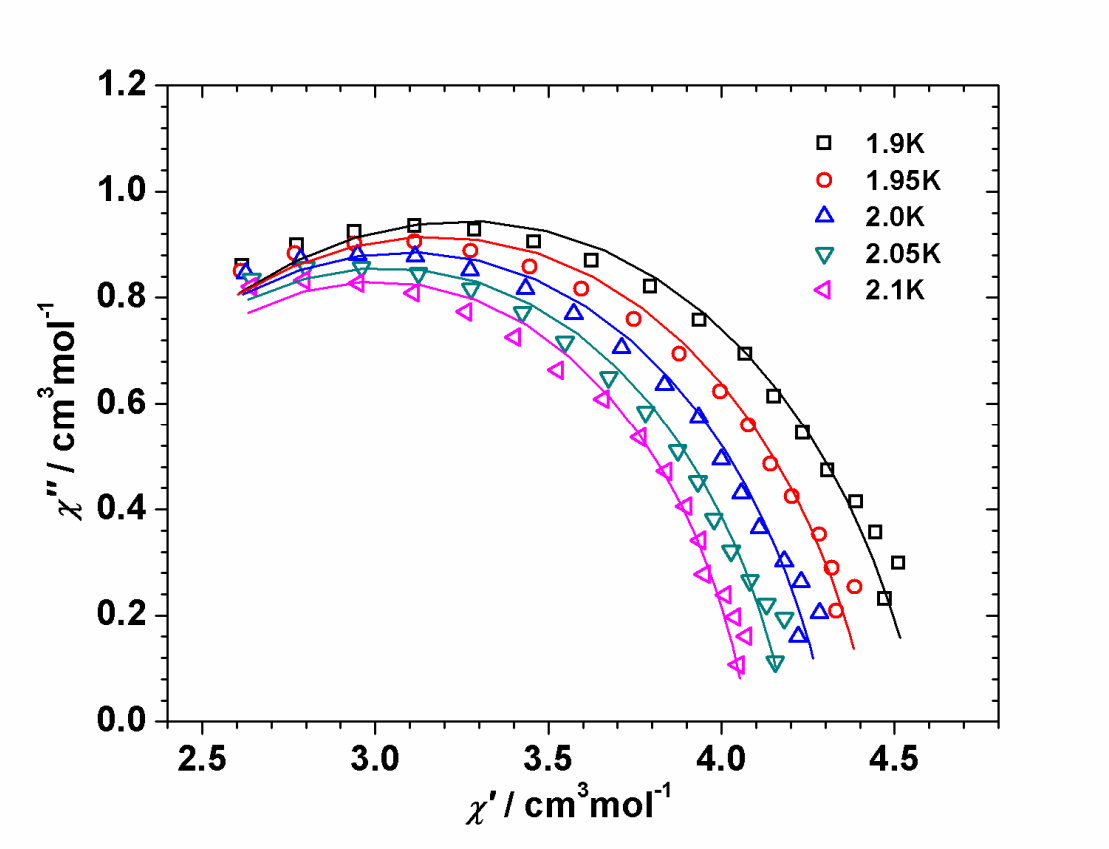

Figure S7. The cole-cole diagram for **1.** Solid lines are the fit curves using extended Debye model.

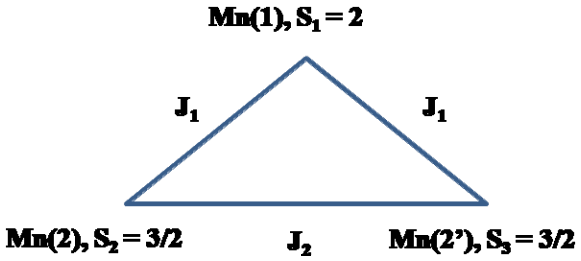

Figure S7. The 2-J coupling scheme in **1**.

By Kambe's method, The general expression for magnetic susceptibilities χ_M of **1** is:

$$\chi_M = \frac{N\beta^2}{3kT} \times \frac{A}{B};$$

$$A = 30e^{(12u+12v)} + 6e^{(18u+10v)} + 30e^{(14u+10v)} + 84e^{(8u+10v)} + 6e^{(22u+6v)} + 30e^{(18u+6v)}$$
$$+ 84e^{(12u+6v)} + 180e^{(4u+6v)} + 6e^{28u} + 30e^{24u} + 84e^{18u} + 180e^{10u} + 330,$$

$$B = 5e^{(12u+12v)} + 3e^{(18u+10v)} + 5e^{(14u+10v)} + 7e^{(8u+10v)} + e^{(24u+6v)} + 3e^{(22u+6v)} + 5e^{(18u+6v)}$$
$$+ 7e^{(12u+6v)} + 9e^{(4u+6v)} + 3e^{28u} + 5e^{24u} + 7e^{18u} + 9e^{10u} + 11.$$

$$u = -\frac{J_1}{kT}, v = -\frac{J_2}{kT};$$

The ZFS and the intermolecular interactions are neglected, and the Lande factor g is assumed to be isotropic.

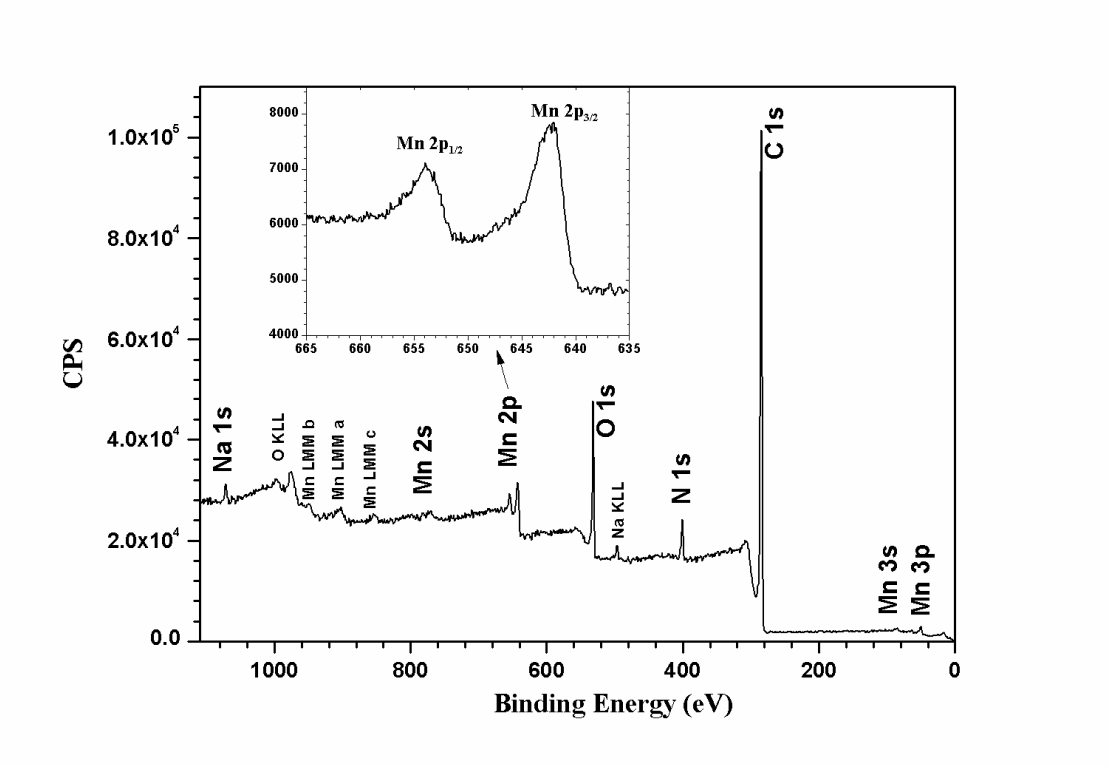

Figure S8. X-Ray photoelectron spectrum of **1**.