Electronic Supplementary Material (ESI)

Aromatic selenite bridged Mn(III) chain compound showing the coexistence of single chain magnet and metamagnet behaviour

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Supporting Information

1.Experimental Section

Physical Measurements

Elemental analyses of carbon, hydrogen, and nitrogen were carried out on a Vario EL II Elementar. Infrared spectra of the samples were obtained on a Bruker Tensor 27 FT-IR spectrometer with the KBr pellets. Powder X-ray diffraction (PXRD) were recorded at 298 K on a Bruker D8 Advance diffractometer with Cu Kα X-ray source (operated at 40 kV and 40 mA). Magnetic properties of **1** were measured using a Quantum Design SQUID VSM magnetometer on polycrystalline samples. All magnetic data were corrected for the diamagnetism of the sample holder and of the constituent atoms according to Pascal's constants.

Materials and Synthesis

The starting materials $[Mn(salen)(H_2O)]_2(ClO_4)_2$[S1-S2], and 3-fluorobenzeneseleninic acid[S3] were synthesized according to the literature methods. All the other starting materials were purchased from commercial sources and used as received.

Preparations

Synthesis of Compound 1. A methanol solution (10 ml) of 3-fluorobenzeneseleninic acid (20.7 mg, 0.10 mmol) was added to a methanol solution (10 ml) of $[Mn(salen)(H_2O)]_2(ClO_4)_2$ (87.7 mg, 0.10 mmol). The resulting solution was stirred for 5 hours, and then filtered and left to stand at room temperature without disturbing. Dark-brown single crystals suitable for X-ray diffraction were obtained after several days. Yield: 60%. Elemental analysis (%) calculated for $C_{76}H_{64}N_8O_{20}F_2Cl_2Mn_4Se_2$: C, 48.15; H, 3.40; N, 5.91. Found: C, 48.27; H, 3.32; N, 5.84. IR (KBr, cm^{-1}): 3054(s), 2925(w), 1623(s), 1543(s), 1468(m), 1446(s), 1389(s), 1330(s), 1253(m), 1215(m),

1097(s), 1150(s), 975(m), 960(w), 904(s), 864(m), 827(m), 755(s), 649(m), 630(s), 594(s), 549(m), 533(s), 469(s)

2. X-ray Crystallography

Single-crystal X-ray diffraction data were collected on a Bruker SMART-1000 CCD diffractometer with graphite-monochromated Mo Kα (λ = 0.71073 Å) radiation at room temperature. The data were integrated and corrected for Lorentz and polarization effects using SAINT.[S4] Absorption corrections were applied with SADABS.[S5] The structures were solved by direct method and refined by full-matrix least-squares method on F^2 using the SHELXTL crystallographic software package.[S6] All the non-hydrogen atoms were refined anisotropically. Hydrogen atoms of the organic ligands were refined as riding on the corresponding non-hydrogen atoms. The fluorine atoms in compound **1** are disordered in two positions. And the occupancies of the two disordered parts are 0.51443 and 0.48557, respectively. Additional details of the data collections and structural refinement parameters were provided in Table S1. Selected bond lengths and bond angles of **1** were listed in Table S2. The phase purity of the compound was confirmed by their PXRD spectra (Fig. S2).

Table S1 Crystallographic data and structure refinement parameters for **1**.

Complex	1
Formula	$C_{76}H_{64}N_8O_{20}F_2Cl_2Mn_4Se_2$
M	1895.93
Crystal system	triclinic
Space group	$P\bar{1}$
a [Å]	10.3681(11)
b [Å]	13.6354(14)
c [Å]	14.6562(14)
α [°]	99.001
β [°]	109.776
γ [°]	100.880
V [Å^3]	1859.5(3)
Z	1
ρ_{calcd}(g cm^{-3})	1.693
F(000)	956
Crystal size (mm)	0.20×0.10×0.03
Reflections collected	9576
Independent reflections	6465
R_{int}	0.1247
GOF	1.051
R_1[a], wR_2[b] (I>2σ(I))	0.1084, 0.1907

[a]$R_1 = \sum||F_o| - |F_c||/\sum|F_o|$ [b]$wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$

Table S2. Selected bond lengths [Å] and angles [°] for compound **1**.

Complex **1**			
Mn(1)-O(3)	1.844(9)	Mn(2)-O(6)	1.904(9)
Mn(1)-O(4)	1.895(9)	Mn(2)-O(5)	1.867(10)
Mn(1)-N(1)	1.992(12)	Mn(2)-N(4)	1.923(14)
Mn(1)-N(2)	1.981(12)	Mn(2)-N(3)	1.926(12)
Mn(1)-O(1)	2.141(11)	Mn(2)-O(2)	2.079(10)
Mn(1)-O(4)#1	2.527(1)	Mn(2)-O(6)#2	2.824(9)
Se(1)-O(1)	1.677(9)	Se(1)-O(2)	1.694(9)
O(3)-Mn(1)-O(4)	95.3(4)	O(6)-Mn(2)-O(5)	93.1(4)
O(3)-Mn(1)-N(1)	90.9(5)	O(6)-Mn(2)-N(4)	88.5(5)
O(4)-Mn(1)-N(1)	166.3(4)	O(5)-Mn(2)-N(4)	165.5(5)
O(3)-Mn(1)-N(2)	173.6(5)	O(6)-Mn(2)-N(3)	166.8(5)
O(4)-Mn(1)-N(2)	89.3(5)	O(5)-Mn(2)-N(3)	91.8(5)
N(1)-Mn(1)-N(2)	83.7(5)	N(4)-Mn(2)-N(3)	83.8(6)
O(3)-Mn(1)-O(1)	97.1(4)	O(6)-Mn(2)-O(2)	95.4(4)
O(4)-Mn(1)-O(1)	94.0(4)	O(5)-Mn(2)-O(2)	94.3(4)
N(1)-Mn(1)-O(1)	97.4(4)	N(4)-Mn(2)-O(2)	100.0(5)
N(2)-Mn(1)-O(1)	87.0(4)	N(3)-Mn(2)-O(2)	96.5(5)
O(1)-Mn(1)-O(4)#1	171.71(4)	O(2)-Mn(2)-O(6)#2	177.99(3)

Symmetry code for compound **1**: 1-x, 2-y, 1-z; #2: 1-x, 1-y, -z

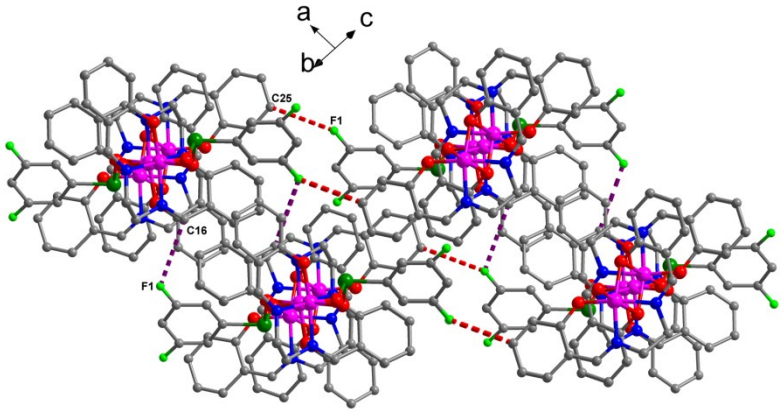

Figure S1 The 3D structure constructed from the C-H···F hydrogen bond interactions of compound **1**.

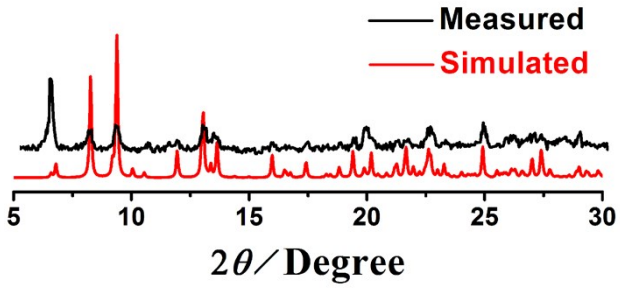

Figure S2. The powder XRD pattern of compound **1** in black and its simulation in red.

3. Magnetic Properties

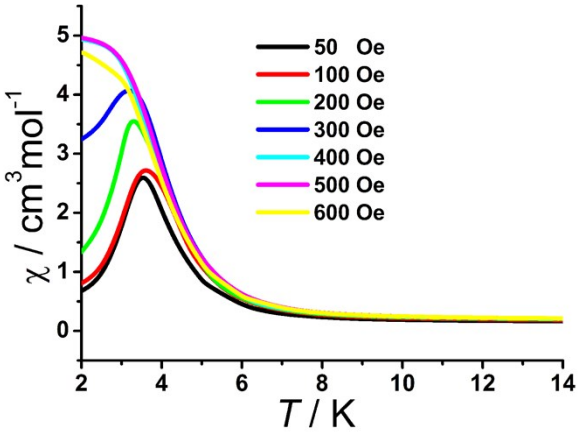

Figure S3 The χ_M *versus T* plots measured at different external fields of compound **1**.

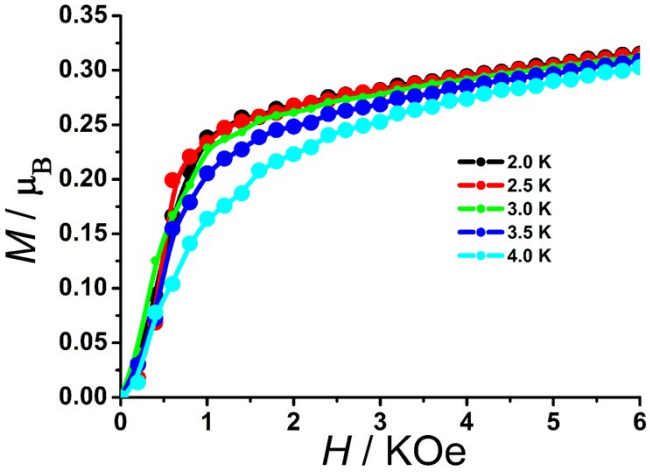

Figure S4 The *M versus H* plots measured at different temperature of compound **1**.

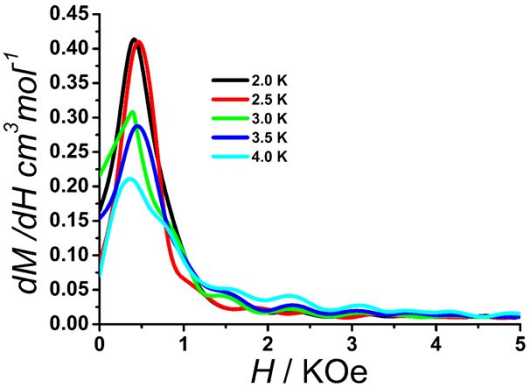

Figure S5. The derivative of field-dependent magnetization of compound **1** measured at different temperatures.

Table S3 The parameters obtained by fitting Cole-Cole plot for compound **1**.

T / K	χ_S	χ_T	τ	a
2.0	0.157	1.077	0.11887	0.29
2.2	0.159	1.088	0.01978	0.24
2.4	0.158	1.202	0.00438	0.21
2.6	0.161	1.407	0.00118	0.17
2.8	0.187	1.769	0.00041	0.11
3.0	0.231	2.397	0.00016	0.07

4. Reference

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