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Slow magnetic relaxation in the O-Se-O bridged manganese(III) Schiff base complexes

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Supporting Information

Table of contents

Figure of contents

Table S1 Crystallographic data and structure refinement parameters for complexes **1**-**2**

Complex	1	2
Formula	$C_{38}H_{30}N_4O_{10}F_3ClMn_2Se$	$C_{51}H_{38}N_4O_{10}F_6Mn_2Se_2$
M	983.95	1248.65
Crystal system	triclinic	monoclinic
Space group	$P\bar{1}$	$P2_1/n$
a [Å]	10.0981(9)	12.3806(11)
b [Å]	14.1193(12)	15.7250(13)
c [Å]	14.3189(12)	25.915(2)
α [°]	103.946(2)	90
β [°]	93.8380(10)	98.002(2)
γ [°]	102.070(2)	90
V [Å3]	1922.7(3)	4996.2(8)
Z	2	4
ρ_{calcd}(g cm^{-3})	1.700	1.660
F(000)	988	2496
Crystal size (mm)	0.42×0.18×0.15	0.28×0.20×0.09
Reflections collected	9784	25108
Independent reflections	6658	8811
R_{int}	0.0250	0.1263
GOF	0.799	0.979
R_1[a], wR_2[b] (I>2σ(I))	0.0413, 0.1129	0.0892, 0.2136

[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 complex **1**.

Complex **1**			
Mn(1)-O(3)	1.879(3)	Mn(2)-O(6)	1.874(3)
Mn(1)-O(4)	1.897(3)	Mn(2)-O(5)	1.906(3)
Mn(1)-N(1)	1.980(4)	Mn(2)-N(4)	1.985(3)
Mn(1)-N(2)	1.986(4)	Mn(2)-N(3)	1.986(4)
Mn(1)-O(1)	2.103(3)	Mn(2)-O(2)	2.106(3)
Mn(1)-O(4)#1	2.707(2)	Mn(2)-O(5)#2	2.547(2)
Se(1)-O(1)	1.681(3)	Se(1)-O(2)	1.673(3)
O(3)-Mn(1)-O(4)	95.20(12)	O(6)-Mn(2)-O(5)	93.97(12)
O(3)-Mn(1)-N(1)	91.80(15)	O(6)-Mn(2)-N(4)	91.48(14)
O(4)-Mn(1)-N(1)	166.35(15)	O(5)-Mn(2)-N(4)	166.13(14)
O(3)-Mn(1)-N(2)	170.83(15)	O(6)-Mn(2)-N(3)	169.89(13)
O(4)-Mn(1)-N(2)	89.37(14)	O(5)-Mn(2)-N(3)	89.84(13)
N(1)-Mn(1)-N(2)	82.17(16)	N(4)-Mn(2)-N(3)	82.80(15)
O(3)-Mn(1)-O(1)	99.74(12)	O(6)-Mn(2)-O(2)	101.62(12)
O(4)-Mn(1)-O(1)	98.95(13)	O(5)-Mn(2)-O(2)	91.32(11)
N(1)-Mn(1)-O(1)	91.38(13)	N(4)-Mn(2)-O(2)	100.07(13)
N(2)-Mn(1)-O(1)	87.36(13)	N(3)-Mn(2)-O(2)	87.63(13)
O(1)-Mn(1)-O(4)#1	171.36(9)	O(2)-Mn(2)-O(5)#2	168.46(8)

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

Table S3. Selected bond lengths [Å] and angles [°] for complex **2**.

Complex **2**			
Mn(1)-O(5)	1.872(7)	Mn(2)-O(7)	1.868(9)
Mn(1)-O(6)	1.888(8)	Mn(2)-O(8)	1.863(9)
Mn(1)-N(1)	1.971(9)	Mn(2)-N(3)	1.987(10)
Mn(1)-N(2)	1.991(10)	Mn(2)-N(4)	2.004(10)
Mn(1)-O(3)	2.180(7)	Mn(2)-O(4)	2.198(7)
Mn(1)-O(2)	2.197(7)	Mn(2)-O(1)#1	2.236(9)
Se(1)-O(1)	1.663(7)	Se(1)-O(2)	1.690(7)
Se(2)-O(3)	1.674(7)	Se(2)-O(4)	1.667(7)
O(5)-Mn(1)-O(6)	93.8(3)	O(7)-Mn(2)-O(8)	93.2(4)
O(5)-Mn(1)-N(1)	93.1(3)	O(7)-Mn(2)-N(3)	93.2(4)
O(6)-Mn(1)-N(1)	173.1(4)	O(8)-Mn(2)-N(3)	173.6(4)
O(5)-Mn(1)-N(2)	174.8(4)	O(7)-Mn(2)-N(4)	174.8(4)
O(6)-Mn(1)-N(2)	90.9(4)	O(8)-Mn(2)-N(4)	91.5(4)
N(1)-Mn(1)-N(2)	82.3(4)	N(3)-Mn(2)-N(4)	82.1(4)
O(5)-Mn(1)-O(3)	91.3(3)	O(7)-Mn(2)-O(4)	91.3(3)
O(6)-Mn(1)-O(3)	95.3(3)	O(8)-Mn(2)-O(4)	92.2(3)
N(1)-Mn(1)-O(3)	84.3(3)	N(3)-Mn(2)-O(4)	88.2(3)
N(2)-Mn(1)-O(3)	90.5(3)	N(4)-Mn(2)-O(4)	86.3(3)
O(5)-Mn(1)-O(2)	90.1(3)	O(7)-Mn(2)-O(1)#1	92.5(4)
O(6)-Mn(1)-O(2)	92.8(3)	O(8)-Mn(2)-O(1)#1	94.9(5)
N(1)-Mn(1)-O(2)	87.4(3)	N(3)-Mn(2)-O(1)#1	84.5(4)
N(2)-Mn(1)-O(2)	87.4(3)	N(4)-Mn(2)-O(1)#1	88.7(5)
O(3)-Mn(1)-O(2)	171.6(3)	O(4)-Mn(2)-O(1)#1	171.6(4)

Symmetry code for complex **2**: #1: x+1, y, z

Table S4 The parameters obtained by fitting Cole-Cole plot for **1**.

T / K	χ_S	χ_T	τ	a
2.0	0.562	2.488	0.002916	0.13
2.2	0.629	2.330	0.000857	0.09
2.4	0.674	2.170	0.000297	0.05
2.6	0.652	2.027	0.000113	0.03
2.8	0.144	1.904	0.000033	0.04
3.0	0.276	1.797	0.000017	~0

Table S5 The parameters obtained by fitting Cole-Cole plot for **2**.

T / K	χ_S	χ_T	τ	a
2.0	0.244	0.913	0.003041	0.12
2.2	0.262	0.859	0.000894	0.09
2.4	0.274	0.802	0.000307	0.05
2.6	0.250	0.753	0.000110	0.06
2.8	~0	0.711	0.000026	0.011
3.0	~0	0.677	0.000008	0.21

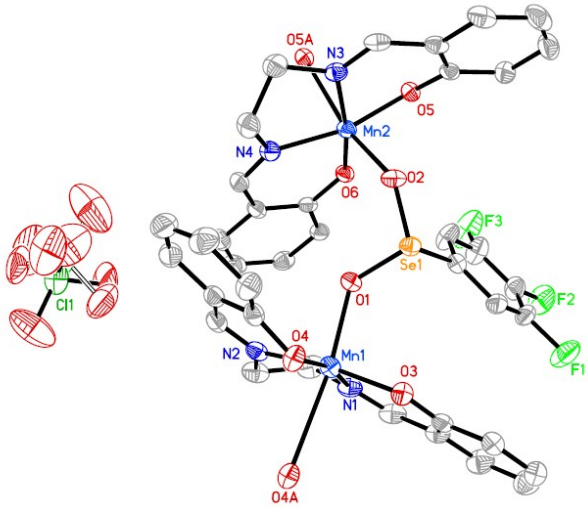

Figure S1 The asymmetric unit of complex **1**, rendered with 30% probability ellipsoids. Hydrogen atoms are omitted for clarity.

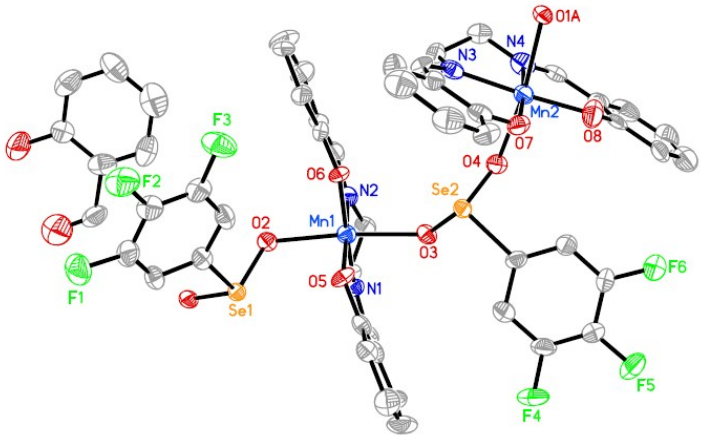

Figure S2 The asymmetric unit of complex **2**, rendered with 30% probability ellipsoids. Hydrogen atoms are omitted for clarity.

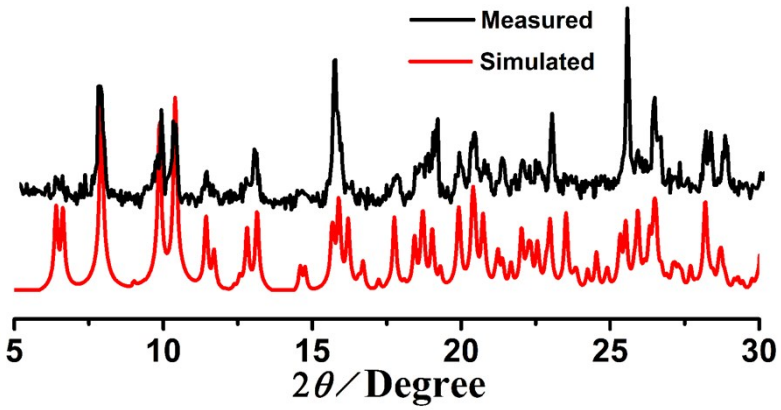

Figure S3. The powder XRD pattern of **1** in black and its simulation in red.

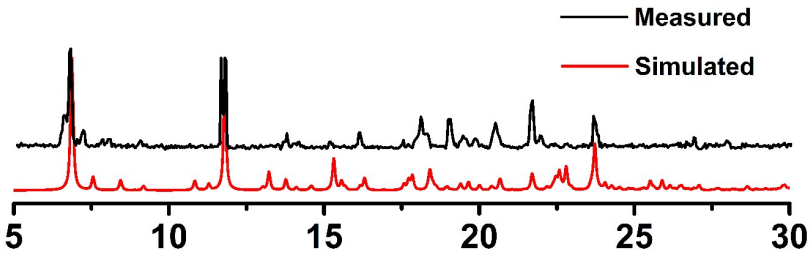

Figure S4. The powder XRD pattern of **2** in black and its simulation in red.

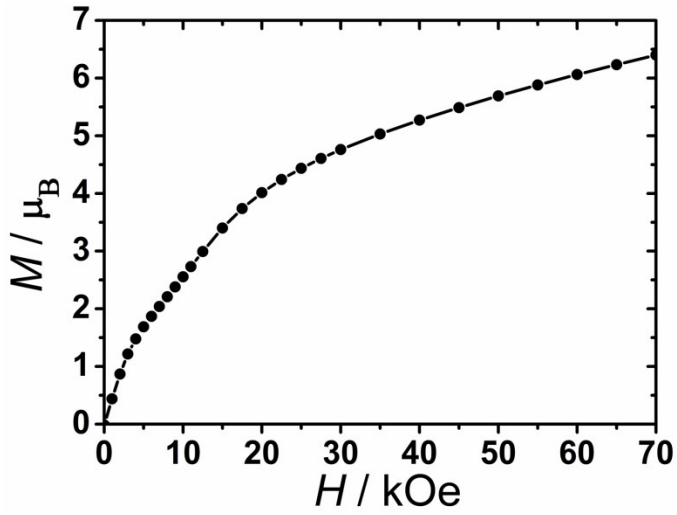

Figure S5. Field dependent magnetization of **1** measured at 2 K.

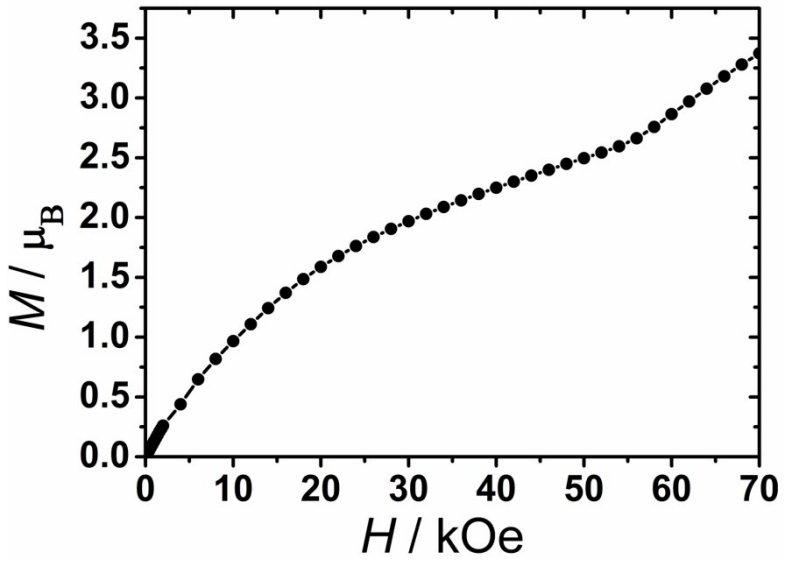

Figure S6. Field dependent magnetization of **1** measured at 2 K.

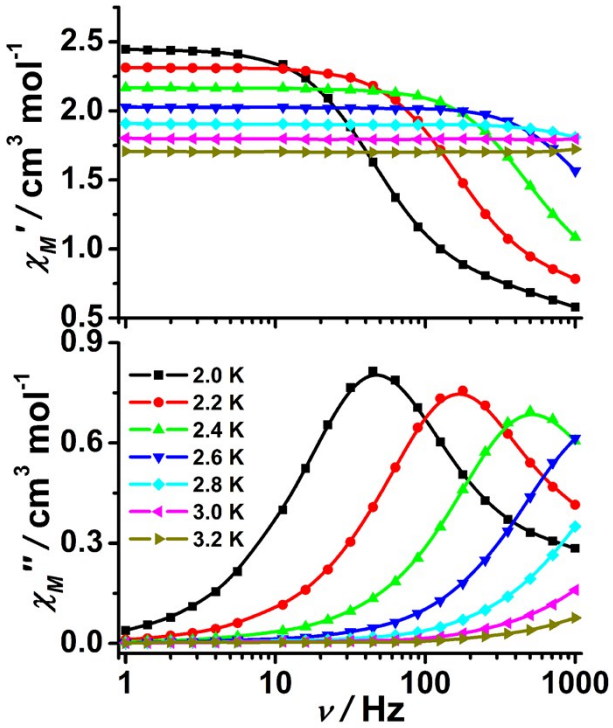

Figure S7. Frequency dependent ac susceptibilities of **1** at different temperatures under H_{ac} = 2 Oe and H_{dc} = 0 Oe. The solid lines are guides for the eye.

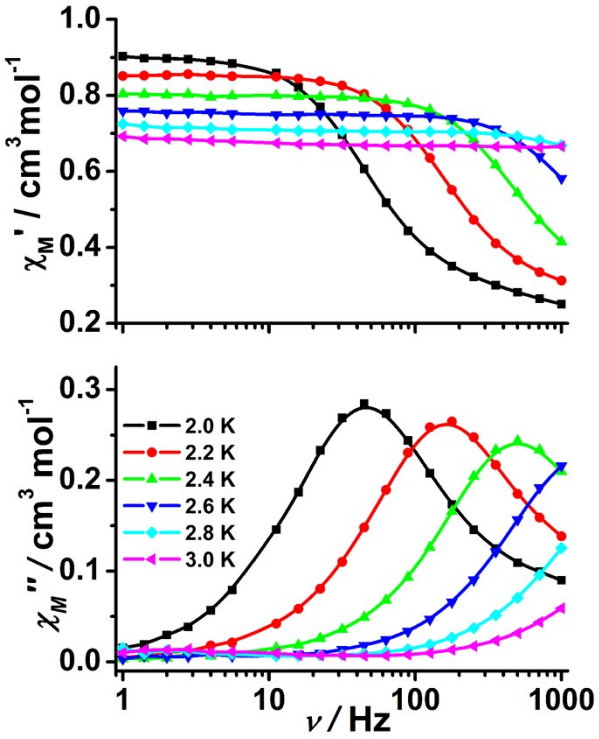

Figure S8. Frequency dependent ac susceptibilities of **2** at different temperatures under H_{ac} = 2 Oe and H_{dc} = 0 Oe. The solid lines are guides for the eye.