

Electronic Supplementary Information for Structure modulation of manganese coordination polymers consisting of 1,4-naphthalene dicarboxylate and 1,10-phenanthroline

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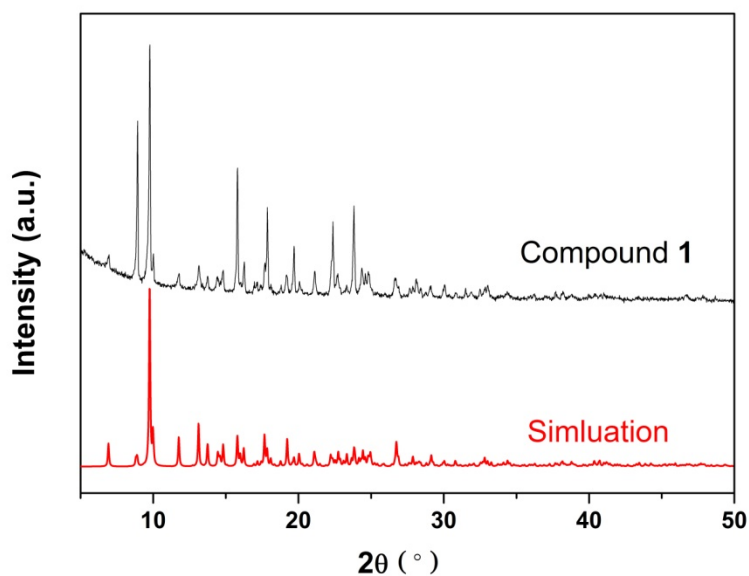


Fig. S1. PXRD pattern of compound 1 and simulated pattern from corresponding single crystal data.

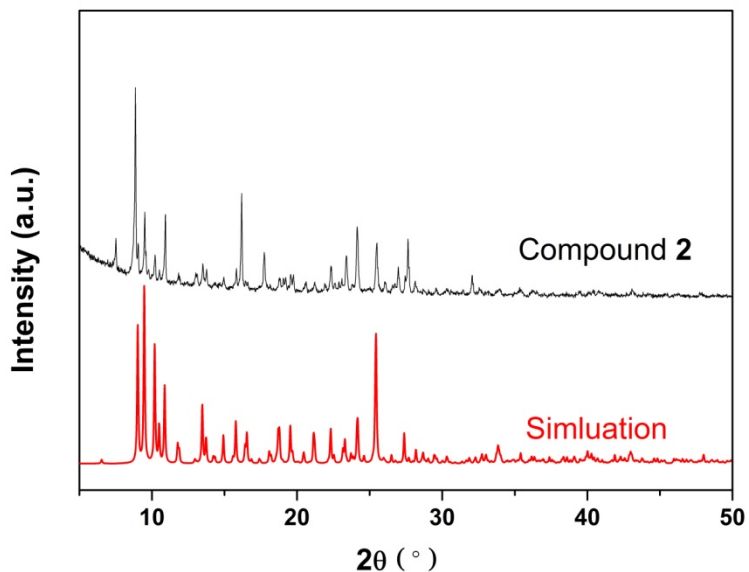


Fig. S2. PXRD pattern of compound 2 and simulated pattern from corresponding single crystal data.

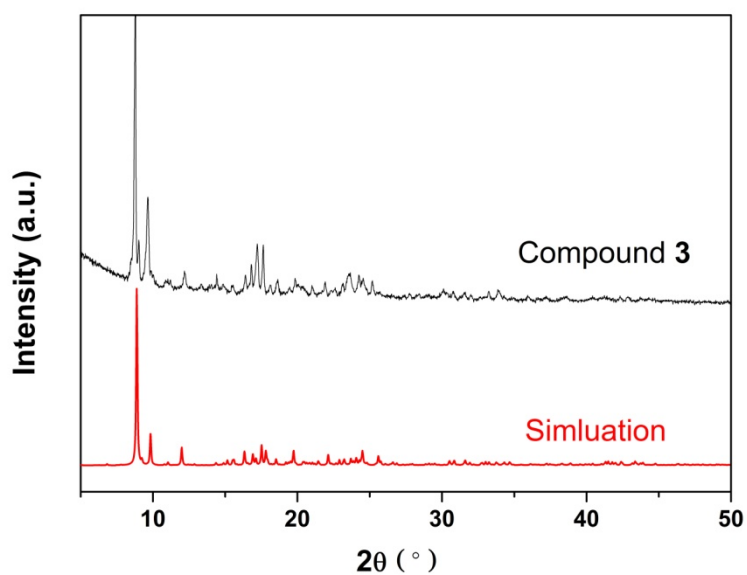


Fig. S3. PXRD pattern of compound 3 and simulated pattern from corresponding single crystal data.

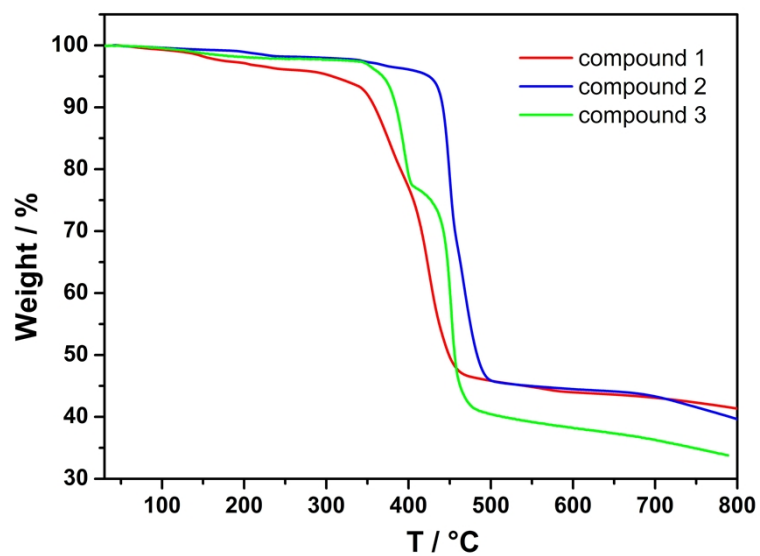


Fig. S4. TGA curves of compounds 1–3.

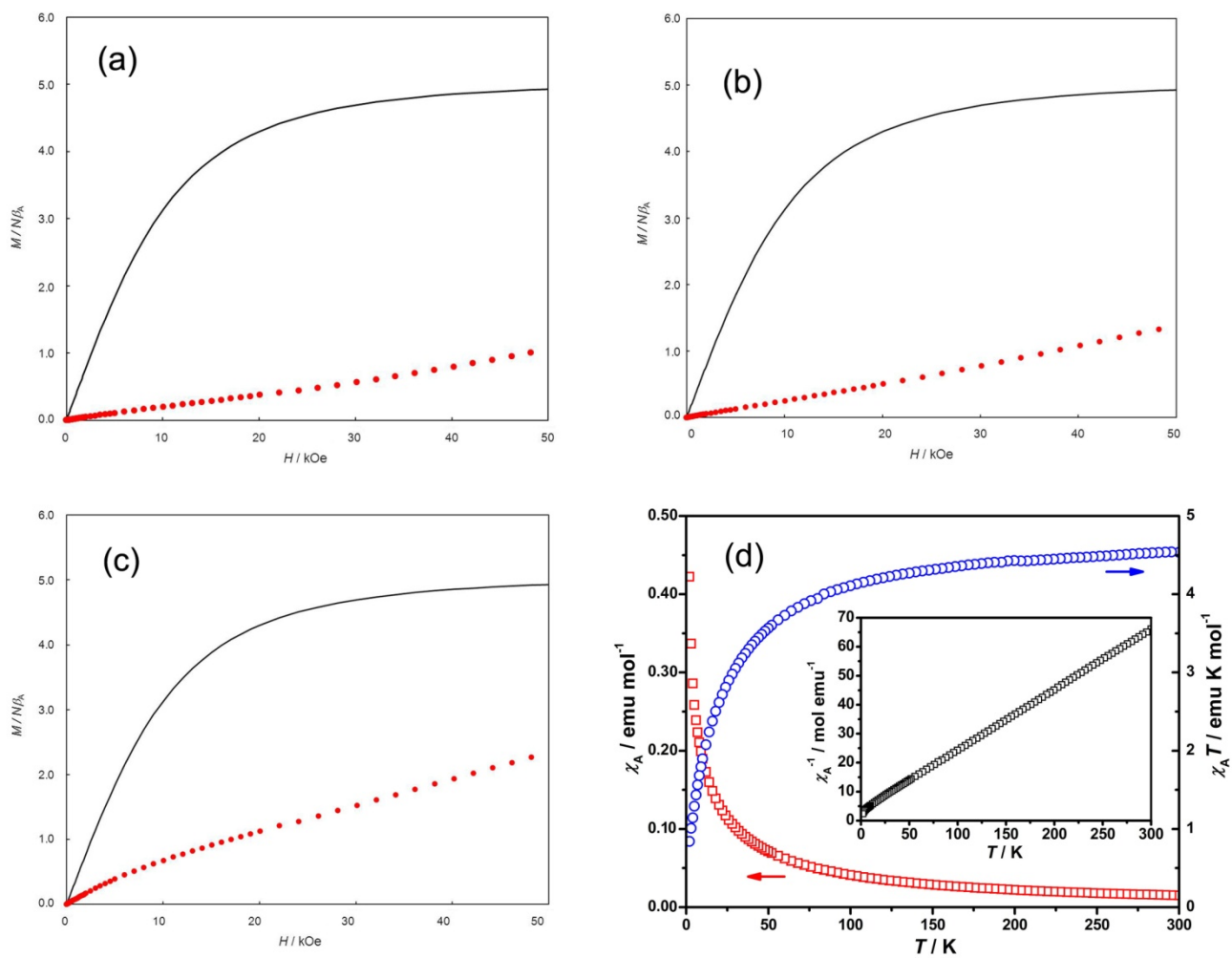


Fig. S5. M vs H plot at 2 K for **1** (a), **2** (b), and **3** (c) (black solid line: theoretical data for $S = 5/2$, red dot line: experimental data), and temperature dependences of χ_A (\square) and $\chi_A T$ (\circ) (Inset: χ_A^{-1} vs. T plot) for **3** (d).

Table S1 Selected Bond Lengths (Å) and Bond Angles (°) for compound **1**, **2** and **3**

1					
Mn(1)-O(5)	2.0640(16)	Mn(1)-N(2)	2.2591(18)	Mn(2)-O(8) ^a	2.1772(16)
Mn(1)-O(7) ^a	2.1026(16)	Mn(1)-O(2)	2.3328(15)	Mn(2)-N(4)	2.2491(18)
Mn(1)-O(1)	2.2286(16)	Mn(2)-O(4) ^b	2.0567(17)	Mn(2)-N(3)	2.2619(18)
Mn(1)-N(1)	2.2413(19)	Mn(2)-O(6)	2.1598(16)	Mn(2)-O(2)	2.3593(15)
O(5)-Mn(1)-O(7) ^a	94.36(7)	O(5)-Mn(1)-O(2)	101.83(6)	O(8) ^a -Mn(2)-N(4)	98.98(6)
O(5)-Mn(1)-O(1)	159.37(6)	O(7) ^a -Mn(1)-O(2)	97.02(6)	O(4) ^b -Mn(2)-N(3)	109.48(6)
O(7) ^a -Mn(1)-O(1)	87.49(7)	O(1)-Mn(1)-O(2)	57.59(5)	O(6)-Mn(2)-N(3)	87.13(7)
O(5)-Mn(1)-N(1)	95.09(7)	N(1)-Mn(1)-O(2)	161.32(6)	O(8) ^a -Mn(2)-N(3)	86.54(6)
O(7) ^a -Mn(1)-N(1)	89.43(7)	N(2)-Mn(1)-O(2)	96.82(6)	N(4)-Mn(2)-N(3)	73.14(7)
O(1)-Mn(1)-N(1)	105.48(6)	O(4) ^b -Mn(2)-O(6)	89.14(7)	O(4) ^b -Mn(2)-O(2)	85.04(6)
O(5)-Mn(1)-N(2)	94.71(7)	O(4) ^b -Mn(2)-O(8) ^a	163.21(6)	O(6)-Mn(2)-O(2)	105.77(6)
O(7) ^a -Mn(1)-N(2)	161.53(6)	O(6)-Mn(2)-O(8) ^a	86.60(6)	O(8) ^a -Mn(2)-O(2)	80.52(5)
O(1)-Mn(1)-N(2)	89.66(6)	O(4) ^b -Mn(2)-N(4)	90.77(7)	N(4)-Mn(2)-O(2)	95.12(6)
N(1)-Mn(1)-N(2)	73.76(7)	O(6)-Mn(2)-N(4)	159.02(6)	N(3)-Mn(2)-O(2)	161.01(6)
2					
Mn(1)-O(6)	2.1060(18)	Mn(1)-O(4) ^b	2.202(2)	Mn(2)-O(1)	2.2195(18)
Mn(1)-O(8) ^a	2.1375(19)	Mn(2)-O(3) ^b	2.1185(19)	Mn(2)-N(2)	2.255(2)
Mn(1)-O(9)	2.165(2)	Mn(2)-O(5)	2.1403(18)	Mn(2)-N(1)	2.257(2)
Mn(1)-O(1)	2.1882(17)	Mn(2)-O(7) ^c	2.1851(18)		
O(6)-Mn(1)-O(8) ^a	175.96(8)	O(1)-Mn(1)-O(4) ^b	119.19(8)	O(5)-Mn(2)-N(2)	94.06(8)
O(6)-Mn(1)-O(9)	94.77(9)	O(3) ^b -Mn(2)-O(5)	98.64(8)	O(7) ^c -Mn(2)-N(2)	89.66(8)
O(8) ^a -Mn(1)-O(9)	88.04(9)	O(3) ^b -Mn(2)-O(7) ^c	93.67(8)	O(1)-Mn(2)-N(2)	95.03(7)
O(6)-Mn(1)-O(1)	90.61(7)	O(5)-Mn(2)-O(7) ^c	84.13(7)	O(3) ^b -Mn(2)-N(1)	93.55(9)
O(8) ^a -Mn(1)-O(1)	89.14(7)	O(3) ^b -Mn(2)-O(1)	82.51(7)	O(5)-Mn(2)-N(1)	167.14(8)
O(9)-Mn(1)-O(1)	139.05(10)	O(5)-Mn(2)-O(1)	92.00(7)	O(7) ^c -Mn(2)-N(1)	99.22(7)
O(6)-Mn(1)-O(4) ^b	89.50(8)	O(7) ^c -Mn(2)-O(1)	174.13(7)	O(1)-Mn(2)-N(1)	85.51(8)
O(8) ^a -Mn(1)-O(4) ^b	87.11(8)	O(3) ^b -Mn(2)-N(2)	167.13(8)	N(2)-Mn(2)-N(1)	73.64(9)
O(9)-Mn(1)-O(4) ^b	101.45(11)				
3					
Mn(1)-O(15) ^a	2.125(5)	Mn(2)-O(3)	2.195(5)	Mn(3)-N(1)	2.284(6)
Mn(1)-O(10)	2.146(4)	Mn(2)-O(4)	2.238(5)	Mn(3)-N(3)	2.331(6)
Mn(1)-O(16) ^c	2.178(5)	Mn(2)-N(7)	2.317(6)	Mn(4)-O(11) ^e	2.126(5)
Mn(1)-O(14) ^b	2.248(5)	Mn(2)-N(8)	2.369(7)	Mn(4)-O(13) ^d	2.189(5)
Mn(1)-N(6)	2.332(6)	Mn(3)-O(6)	2.094(5)	Mn(4)-O(12) ^f	2.212(5)
Mn(1)-N(5)	2.358(6)	Mn(3)-O(1)	2.117(5)	O(8)-Mn(4)	2.125(5)
Mn(2)-O(2)	2.130(5)	Mn(3)-O(9)	2.220(5)	N(2)-Mn(4)	2.311(6)
Mn(2)-O(5)	2.147(5)	Mn(3)-O(7)	2.225(5)	N(4)-Mn(4)	2.345(6)
O(15) ^a -Mn(1)-O(10)	161.87(19)	O(3)-Mn(2)-O(4)	128.11(19)	O(6)-Mn(3)-N(3)	88.3(2)
O(15) ^a -Mn(1)-O(16) ^c	88.7(2)	O(2)-Mn(2)-N(7)	99.1(2)	O(1)-Mn(3)-N(3)	107.1(2)
O(10)-Mn(1)-O(16) ^c	85.5(2)	O(5)-Mn(2)-N(7)	89.9(2)	O(9)-Mn(3)-N(3)	82.10(19)
O(15) ^a -Mn(1)-O(14) ^b	85.0(2)	O(3)-Mn(2)-N(7)	149.8(2)	O(7)-Mn(3)-N(3)	153.53(15)
O(10)-Mn(1)-O(14) ^b	84.7(2)	O(4)-Mn(2)-N(7)	81.8(2)	N(1)-Mn(3)-N(3)	71.7(2)
O(16) ^c -Mn(1)-O(14) ^b	126.51(19)	O(2)-Mn(2)-N(8)	91.6(2)	O(8)-Mn(4)-O(11) ^e	166.4(2)
O(15) ^a -Mn(1)-N(6)	98.3(2)	O(5)-Mn(2)-N(8)	100.5(2)	O(8)-Mn(4)-O(13) ^d	89.5(2)
O(10)-Mn(1)-N(6)	95.12(19)	O(3)-Mn(2)-N(8)	80.2(2)	O(11) ^e -Mn(4)-O(13) ^d	85.4(2)
O(16) ^c -Mn(1)-N(6)	150.4(2)	O(4)-Mn(2)-N(8)	151.5(2)	O(8)-Mn(4)-O(12) ^f	84.3(2)
O(14) ^b -Mn(1)-N(6)	82.9(2)	N(7)-Mn(2)-N(8)	70.4(2)	O(11) ^e -Mn(4)-O(12) ^f	88.5(2)
O(15) ^a -Mn(1)-N(5)	87.1(2)	O(6)-Mn(3)-O(1)	161.4(2)	O(13) ^d -Mn(4)-O(12) ^f	125.8(2)
O(10)-Mn(1)-N(5)	109.0(2)	O(6)-Mn(3)-O(9)	84.22(19)	O(8)-Mn(4)-N(2)	92.9(2)
O(16) ^c -Mn(1)-N(5)	81.7(2)	O(1)-Mn(3)-O(9)	87.52(19)	O(11) ^e -Mn(4)-N(2)	97.6(2)
O(14) ^b -Mn(1)-N(5)	150.3(2)	O(6)-Mn(3)-O(7)	84.5(2)	O(13) ^d -Mn(4)-N(2)	151.6(2)
N(6)-Mn(1)-N(5)	70.0(2)	O(1)-Mn(3)-O(7)	85.93(19)	O(12) ^f -Mn(4)-N(2)	82.7(2)
O(2)-Mn(2)-O(5)	166.89(19)	O(9)-Mn(3)-O(7)	122.23(18)	O(8)-Mn(4)-N(4)	85.5(2)
O(2)-Mn(2)-O(3)	87.9(2)	O(6)-Mn(3)-N(1)	96.07(19)	O(11) ^e -Mn(4)-N(4)	106.1(2)
O(5)-Mn(2)-O(3)	89.1(2)	O(1)-Mn(3)-N(1)	98.7(2)	O(13) ^d -Mn(4)-N(4)	81.3(2)
O(2)-Mn(2)-O(4)	86.62(19)	O(9)-Mn(3)-N(1)	153.77(19)	O(12) ^f -Mn(4)-N(4)	150.9(2)
O(5)-Mn(2)-O(4)	85.24(19)	O(7)-Mn(3)-N(1)	83.78(19)	N(2)-Mn(4)-N(4)	70.7(2)

Symmetry codes for **1**: ^a $x + 1/2, -y + 3/2, z + 1/2$; ^b $-x + 1, y, -z + 3/2$; ^c $-x + 1/2, -y + 3/2, -z + 1$; ^d $-x, y, -z + 1/2$; ^e $x - 1/2, -y + 1/2, z - 1/2$; ^f $-x + 1/2, -y + 1/2, -z + 1$. For **2**: ^a $x - 1, -y + 3/2, z - 1/2$; ^b $-x + 1, y + 1/2, -z + 3/2$; ^c $x, -y + 3/2, z - 1/2$. For **3**: ^a $x, -y + 1, z + 1/2$; ^b $x, -y, z - 1/2$

