

## Supporting information

### Syntheses, Structures, and Magnetic Properties of a Series of Mn-containing Coordination Polymers Based on 5-nitro-1,2,3-benzenetricarboxylic Acid and Different N-Donor Ligands

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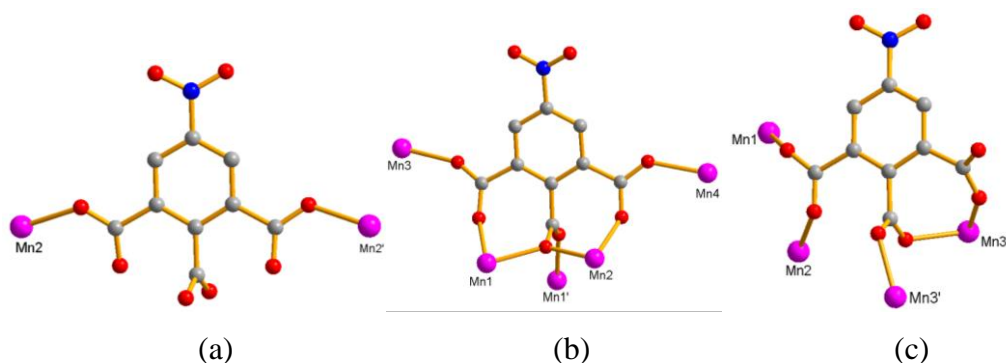


Fig. S1 Coordination modes of H<sub>3</sub>nbtta in complex **1** ((a)  $\mu_2: \eta^1: \eta^0: \eta^1$ , (b)  $\mu_5: \eta^2: \eta^3: \eta^2$ , (c)  $\mu_4: \eta^2: \eta^2: \eta^1$ )

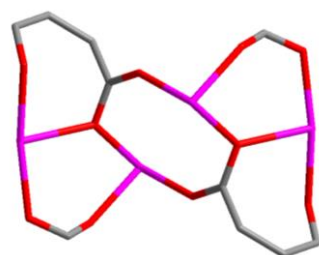


Fig. S2 Mn<sub>4</sub> core constructed by {Mn1}<sub>2</sub> dimer and two Mn2 atoms.

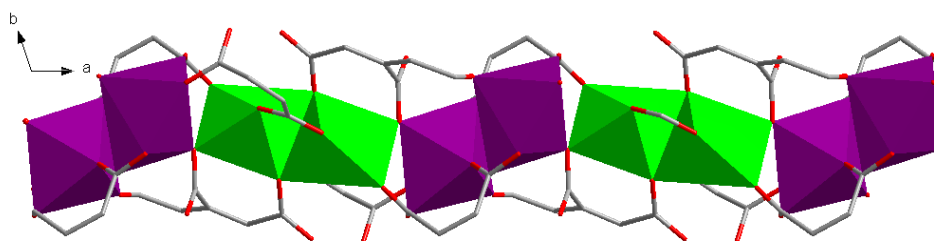


Fig. S3 One dimensional chains constructed by the octahedra of [Mn<sub>2</sub>O<sub>6</sub>] (green) and [Mn<sub>3</sub>O<sub>6</sub>] (purple).

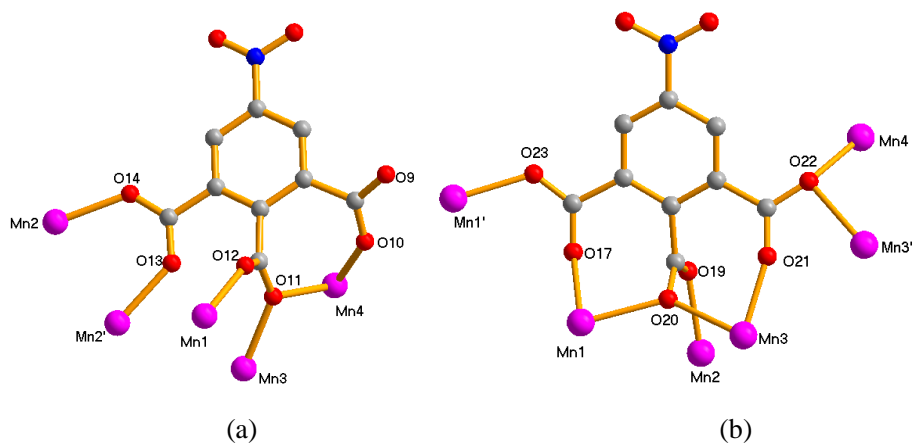


Fig. S4 Coordination modes of H<sub>3</sub>nbta in complex **2** ((a)  $\mu_5: \eta^2: \eta^3: \eta^1$ , (b)  $\mu_6: \eta^2: \eta^3: \eta^3$ ).

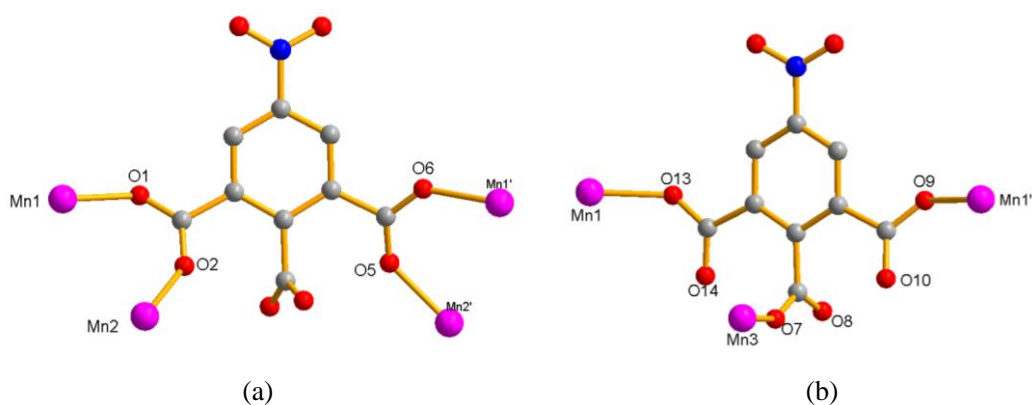


Fig. S5 Coordination modes of H<sub>3</sub>nbta in complex **3** ((a)  $\mu_4: \eta^2: \eta^0: \eta^2$ , (b)  $\mu_3: \eta^1: \eta^1: \eta^1$ ).

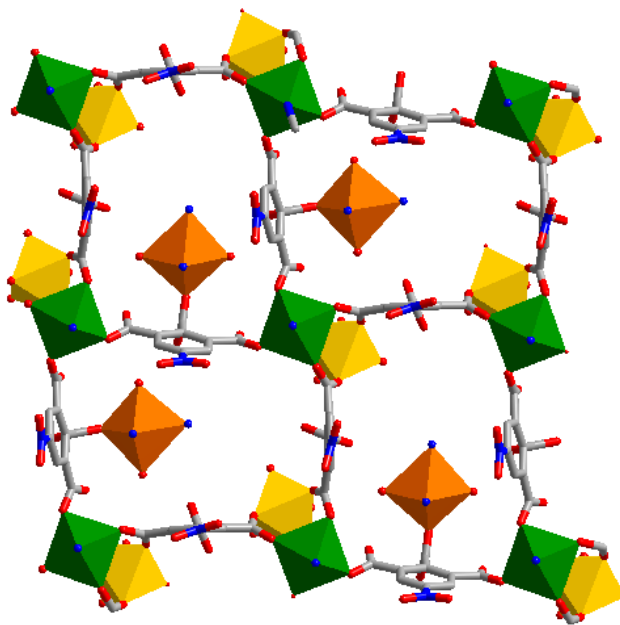
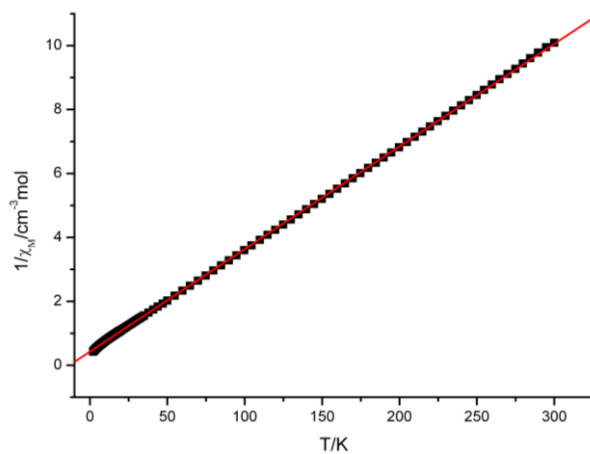
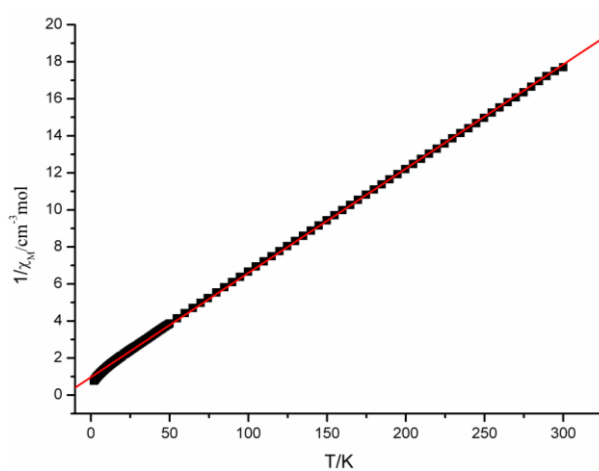


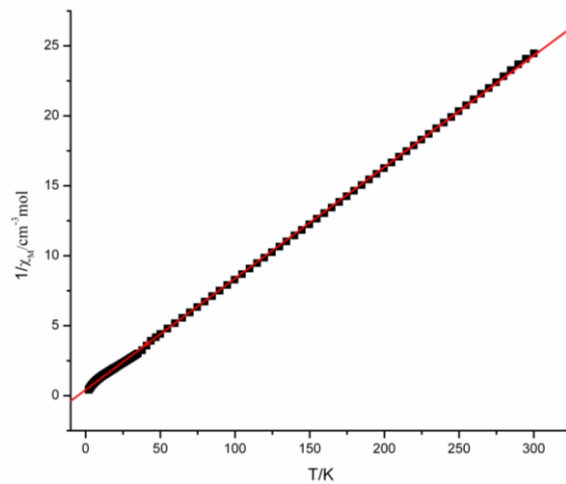
Fig. S6 2D Mn<sub>2</sub>(nbta)<sub>3</sub> sheet of complex **3**.



(a)



(b)



(c)

Fig. S7 Temperature dependence of  $1/\chi_M$  vs.  $T$  for complexes **1** - **3**: (a) for **1**, (b) for **2**, (c) for **3**. The red lines show the Curie – Weiss fitting.

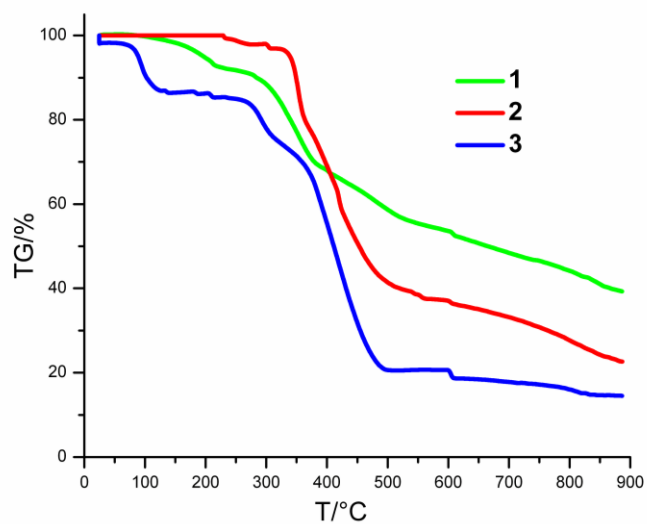
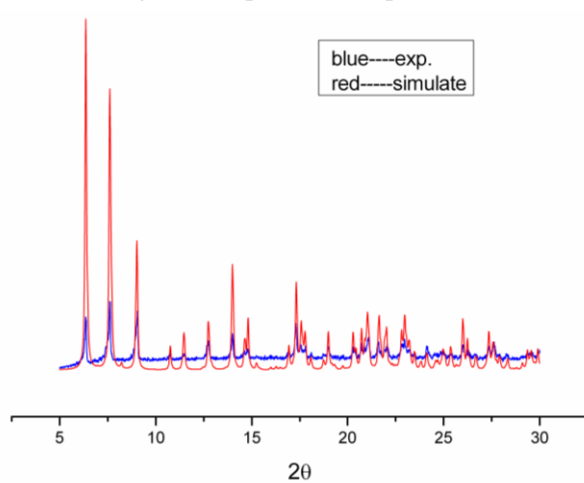
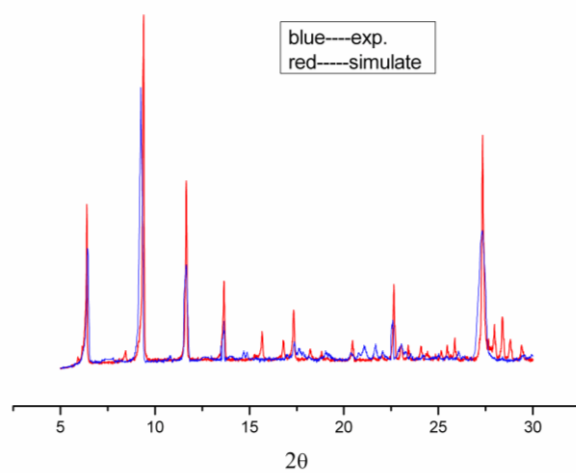


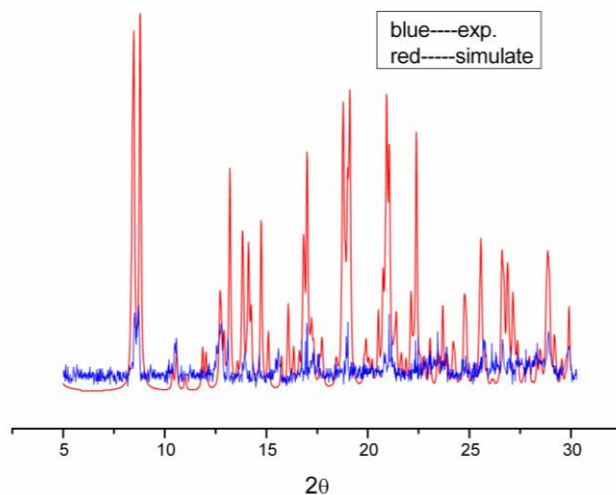
Fig. S8 TG plots of complexes **1-3**.



(a)



(b)



(c)

Fig. S9 The exp. and simulated PXRD patterns of **1** (a), **2** (b) and **3** (c).

**Table S1 Selected bond lengths (Å) and angles (°) for 1-3.**

<b>1</b>			
Mn(1)-O(10)	2.110(2)	Mn(1)-O(2)	2.148(2)
Mn(1)-O(4)#2	2.198(2)	Mn(1)-O(3)	2.223(2)
Mn(1)-N(4)	2.270(3)	Mn(1)-N(3)	2.278(3)
Mn(2)-O(21)	2.141(2)	Mn(2)-O(18)	2.145(2)
Mn(2)-O(9)	2.143(2)	Mn(2)-O(22)	2.183(2)
Mn(2)-O(8)	2.209(2)	Mn(2)-O(3)	2.221(2)
Mn(3)-O(13)#2	2.125(2)	Mn(3)-O(15)#2	2.159(2)
Mn(3)-O(14)#3	2.206(2)	Mn(3)-N(2)	2.239(3)
Mn(3)-O(1)	2.238(2)	Mn(3)-N(1)	2.230(11)
Mn(4)-O(23)	2.180(3)	Mn(4)-O(23)#4	2.180(3)
Mn(4)-O(24)	2.188(3)	Mn(4)-O(24)#4	2.188(3)
Mn(4)-O(7)#4	2.223(2)	Mn(4)-O(7)	2.223(2)
O(4)-Mn(1)#2	2.198(2)	O(13)-Mn(3)#2	2.125(2)
O(14)-Mn(3)#5	2.206(2)	O(15)-Mn(3)#2	2.159(2)
O(10)-Mn(1)-O(2)	162.87(9)	O(10)-Mn(1)-O(4)#2	89.72(9)
O(2)-Mn(1)-O(4)#2	96.73(9)	O(10)-Mn(1)-O(3)	82.09(8)
O(2)-Mn(1)-O(3)	81.31(8)	O(4)#2-Mn(1)-O(3)	97.97(8)
O(10)-Mn(1)-N(4)	92.25(10)	O(2)-Mn(1)-N(4)	104.01(10)
O(4)#2-Mn(1)-N(4)	85.79(9)	O(3)-Mn(1)-N(4)	173.15(10)
O(10)-Mn(1)-N(3)	88.09(9)	O(2)-Mn(1)-N(3)	91.81(9)
O(4)#2-Mn(1)-N(3)	157.51(9)	O(3)-Mn(1)-N(3)	103.88(9)
N(4)-Mn(1)-N(3)	71.95(10)	O(21)-Mn(2)-O(18)	91.81(10)
O(21)-Mn(2)-O(9)	88.67(10)	O(18)-Mn(2)-O(9)	105.89(10)
O(21)-Mn(2)-O(22)	86.73(9)	O(18)-Mn(2)-O(22)	168.18(10)

O(9)-Mn(2)-O(22)	85.81(9)	O(21)-Mn(2)-O(8)	93.25(10)
O(18)-Mn(2)-O(8)	88.31(9)	O(9)-Mn(2)-O(8)	165.60(9)
O(22)-Mn(2)-O(8)	80.06(9)	O(21)-Mn(2)-O(3)	173.12(9)
O(18)-Mn(2)-O(3)	93.87(9)	O(9)-Mn(2)-O(3)	93.48(8)
O(22)-Mn(2)-O(3)	86.92(8)	O(8)-Mn(2)-O(3)	83.06(8)
O(13)#2-Mn(3)-O(15)#2	86.76(9)	O(13)#2-Mn(3)-O(14)#3	91.42(8)
O(15)#2-Mn(3)-O(14)#3	99.13(9)	O(13)#2-Mn(3)-N(2)	106.61(11)
O(15)#2-Mn(3)-N(2)	166.47(11)	O(14)#3-Mn(3)-N(2)	78.87(10)
O(13)#2-Mn(3)-O(1)	86.31(9)	O(15)#2-Mn(3)-O(1)	93.39(9)
O(14)#3-Mn(3)-O(1)	167.13(9)	N(2)-Mn(3)-O(1)	89.63(10)
O(13)#2-Mn(3)-N(1)	167.0(3)	O(15)#2-Mn(3)-N(1)	91.4(2)
O(14)#3-Mn(3)-N(1)	101.6(3)	N(2)-Mn(3)-N(1)	76.0(2)
O(1)-Mn(3)-N(1)	81.0(3)	O(23)-Mn(4)-O(23)#4	180.00(16)
O(23)-Mn(4)-O(24)	87.84(12)	O(23)#4-Mn(4)-O(24)	92.16(12)
O(23)-Mn(4)-O(24)#4	92.16(12)	O(23)#4-Mn(4)-O(24)#4	87.84(12)
O(24)-Mn(4)-O(24)#4	180.00(11)	O(23)-Mn(4)-O(7)#4	86.13(12)
O(23)#4-Mn(4)-O(7)#4	93.87(12)	O(24)-Mn(4)-O(7)#4	89.43(9)
O(24)#4-Mn(4)-O(7)#4	90.57(9)	O(23)-Mn(4)-O(7)	93.87(12)
O(23)#4-Mn(4)-O(7)	86.13(12)	O(24)-Mn(4)-O(7)	90.57(9)
O(24)#4-Mn(4)-O(7)	89.43(9)	O(7)#4-Mn(4)-O(7)	180.0
Mn(1)-O(3)-Mn(2)	129.65(10)		
2			
Mn(1)-O(1)	2.205(4)	Mn(1)-N(1)	2.219(5)
Mn(1)-O(17)	2.146(5)	Mn(1)-O(25)	2.178(4)
Mn(1)-O(11)#2	2.278(4)	Mn(1)-O(13)#2	2.142(4)
Mn(2)-O(2)	2.154(4)	Mn(2)-O(18)#3	2.188(5)
Mn(2)-O(11)#4	2.193(4)	Mn(2)-O(19)	2.229(4)
Mn(2)-O(1)#3	2.268(4)	Mn(2)-O(4)	2.308(4)
Mn(3)-O(9)	2.147(4)	Mn(3)-O(10)#4	2.175(4)
Mn(3)-O(3)	2.193(4)	Mn(3)-O(19)	2.202(4)
Mn(3)-O(21)#4	2.284(5)	Mn(3)-O(21)	2.307(4)
Mn(4)-O(5)#5	2.146(4)	Mn(4)-O(6)	2.153(4)
Mn(4)-O(12)#6	2.167(4)	Mn(4)-N(5)	2.190(6)
Mn(4)-O(22)#6	2.201(5)	Mn(4)-O(4)#5	2.309(4)
O(1)-Mn(2)#3	2.268(4)	O(4)-Mn(4)#5	2.309(4)
O(5)-Mn(4)#5	2.146(4)	O(10)-Mn(3)#4	2.175(4)
O(11)-Mn(2)#4	2.193(4)	O(11)-Mn(1)#7	2.278(4)
O(12)-Mn(4)#8	2.167(4)	O(13)-Mn(1)#7	2.142(4)
O(18)-Mn(2)#3	2.188(5)	O(21)-Mn(3)#4	2.284(5)
O(22)-Mn(4)#8	2.201(5)		
O(13)#2-Mn(1)-O(17)	90.39(17)	O(13)#2-Mn(1)-O(25)	98.98(17)
O(17)-Mn(1)-O(25)	170.49(16)	O(13)#2-Mn(1)-O(1)	155.58(16)
O(17)-Mn(1)-O(1)	87.47(17)	O(25)-Mn(1)-O(1)	84.67(16)
O(13)#2-Mn(1)-N(1)	104.53(18)	O(17)-Mn(1)-N(1)	89.7(2)

O(25)-Mn(1)-N(1)	86.39(19)	O(1)-Mn(1)-N(1)	99.78(18)
O(13)#2-Mn(1)-O(11)#2	81.19(16)	O(17)-Mn(1)-O(11)#2	91.42(16)
O(25)-Mn(1)-O(11)#2	91.64(16)	O(1)-Mn(1)-O(11)#2	74.55(15)
N(1)-Mn(1)-O(11)#2	174.17(17)	O(5)#5-Mn(4)-O(4)#5	81.46(14)
O(2)-Mn(2)-O(18)#3	81.61(17)	O(2)-Mn(2)-O(11)#4	158.22(15)
O(18)#3-Mn(2)-O(11)#4	88.44(16)	O(2)-Mn(2)-O(19)	81.85(16)
O(18)#3-Mn(2)-O(19)	159.98(16)	O(11)#4-Mn(2)-O(19)	110.85(17)
O(2)-Mn(2)-O(1)#3	123.71(16)	O(18)#3-Mn(2)-O(1)#3	88.40(16)
O(11)#4-Mn(2)-O(1)#3	74.99(15)	O(19)-Mn(2)-O(1)#3	91.46(15)
O(2)-Mn(2)-O(4)	77.96(15)	O(18)#3-Mn(2)-O(4)	100.96(16)
O(11)#4-Mn(2)-O(4)	85.04(15)	O(19)-Mn(2)-O(4)	86.50(15)
O(1)#3-Mn(2)-O(4)	157.75(16)	O(9)-Mn(3)-O(10)#4	152.60(18)
O(9)-Mn(3)-O(3)	80.28(17)	O(10)#4-Mn(3)-O(3)	124.13(16)
O(9)-Mn(3)-O(19)	112.36(16)	O(10)#4-Mn(3)-O(19)	85.10(16)
O(3)-Mn(3)-O(19)	83.39(16)	O(9)-Mn(3)-O(21)#4	81.78(16)
O(10)#4-Mn(3)-O(21)#4	77.76(15)	O(3)-Mn(3)-O(21)#4	110.99(15)
O(19)-Mn(3)-O(21)#4	161.92(14)	O(9)-Mn(3)-O(21)	82.45(15)
O(10)#4-Mn(3)-O(21)	79.25(14)	O(3)-Mn(3)-O(21)	151.02(15)
O(19)-Mn(3)-O(21)	81.90(15)	O(21)#4-Mn(3)-O(21)	89.21(13)
O(5)#5-Mn(4)-O(6)	101.57(16)	O(5)#5-Mn(4)-O(12)#6	162.94(15)
O(6)-Mn(4)-O(12)#6	91.79(15)	O(5)#5-Mn(4)-N(5)	96.62(18)
O(6)-Mn(4)-N(5)	94.24(19)	O(12)#6-Mn(4)-N(5)	92.88(19)
O(5)#5-Mn(4)-O(22)#6	79.95(16)	O(6)-Mn(4)-O(22)#6	89.34(17)
O(12)#6-Mn(4)-O(22)#6	89.75(16)	N(5)-Mn(4)-O(22)#6	175.49(18)
O(6)-Mn(4)-O(4)#5	176.83(16)	O(12)#6-Mn(4)-O(4)#5	85.41(14)
N(5)-Mn(4)-O(4)#5	84.42(18)	O(22)#6-Mn(4)-O(4)#5	92.14(16)
Mn(1)-O(1)-Mn(2)#3	100.46(16)	Mn(2)-O(4)-Mn(4)#5	133.77(17)
Mn(2)#4-O(11)-Mn(1)#7	100.52(17)	Mn(3)-O(19)-Mn(2)	110.47(16)
Mn(3)#4-O(21)-Mn(3)	90.79(13)		
3			
Mn(1)-O(6)	2.110(2)	Mn(1)-O(13)	2.123(2)
Mn(1)-O(9)	2.1246(19)	Mn(1)-O(15)	2.3951(19)
Mn(1)-O(1)	2.1657(19)	Mn(1)-N(1)	2.202(2)
Mn(2)-O(5)	2.113(2)	Mn(2)-O(45)	2.159(2)
Mn(2)-O(2)	2.136(2)	Mn(2)-O(20)	2.169(2)
Mn(2)-O(18)	2.1951(19)	Mn(2)-O(15)	2.3095(19)
Mn(3)-O(19)	2.164(2)	Mn(3)-O(22)	2.199(2)
Mn(3)-O(7)	2.2084(19)	Mn(3)-N(5)	2.211(2)
Mn(3)-N(2)	2.248(3)	Mn(3)-O(23)	2.249(2)
O(6)-Mn(1)-O(13)	91.99(9)	O(6)-Mn(1)-O(9)	179.02(9)
O(13)-Mn(1)-O(9)	88.47(8)	O(6)-Mn(1)-O(1)	90.37(9)
O(13)-Mn(1)-O(1)	173.89(8)	O(9)-Mn(1)-O(1)	89.26(8)
O(6)-Mn(1)-N(1)	87.41(9)	O(13)-Mn(1)-N(1)	96.62(9)
O(9)-Mn(1)-N(1)	91.68(9)	O(1)-Mn(1)-N(1)	89.12(9)

O(6)-Mn(1)-O(15)	98.24(8)	O(13)-Mn(1)-O(15)	83.05(8)
O(9)-Mn(1)-O(15)	82.67(7)	O(1)-Mn(1)-O(15)	91.04(7)
N(1)-Mn(1)-O(15)	174.34(8)	O(5)-Mn(2)-O(2)	93.21(8)
O(5)-Mn(2)-O(45)	169.62(10)	O(2)-Mn(2)-O(45)	96.73(10)
O(5)-Mn(2)-O(20)	90.45(9)	O(5)-Mn(2)-O(18)	80.97(8)
O(2)-Mn(2)-O(20)	84.27(8)	O(2)-Mn(2)-O(18)	173.83(8)
O(45)-Mn(2)-O(20)	87.56(10)	O(45)-Mn(2)-O(18)	89.20(9)
O(20)-Mn(2)-O(18)	97.73(8)	O(5)-Mn(2)-O(15)	97.95(8)
O(2)-Mn(2)-O(15)	85.80(7)	O(45)-Mn(2)-O(15)	85.80(9)
O(20)-Mn(2)-O(15)	167.33(8)	O(18)-Mn(2)-O(15)	92.96(7)
O(19)-Mn(3)-O(22)	167.25(9)	O(19)-Mn(3)-O(7)	82.80(8)
O(22)-Mn(3)-O(7)	87.58(8)	O(19)-Mn(3)-N(5)	92.20(9)
O(22)-Mn(3)-N(5)	96.81(10)	O(7)-Mn(3)-N(5)	173.83(9)
O(19)-Mn(3)-N(2)	103.46(9)	O(22)-Mn(3)-N(2)	85.68(9)
O(7)-Mn(3)-N(2)	95.19(8)	N(5)-Mn(3)-N(2)	89.48(9)
O(19)-Mn(3)-O(23)	87.18(9)	O(22)-Mn(3)-O(23)	84.95(9)
O(7)-Mn(3)-O(23)	92.85(8)	N(5)-Mn(3)-O(23)	83.25(9)
N(2)-Mn(3)-O(23)	167.38(9)	Mn(2)-O(15)-Mn(1)	106.33(7)

Symmetry transformations used to generate equivalent atoms for **1**: #1 -x, y, -z+1/2; #2 -x, -y+1, -z; #3 x, y-1, z; #4 -x-1/2, -y+3/2, -z; #5 x, y+1, z.

Symmetry transformations used to generate equivalent atoms for **2**: #1 -x+2, -y+1, -z+1; #2 x-1, y, z; #3 -x, -y, -z+1; #4 -x+1, -y, -z+1; #5 -x+1, -y+1, -z+1; #6 x, y+1, z; #7 x+1, y, z; #8 x, y-1, z.

Symmetry transformations used to generate equivalent atoms for **3**: #1 x, -y-1/2, z+1/2; #2 x, -y-1/2, z-1/2; #3 -x, -y, -z+2; #4 x, -y+1/2, z+1/2; #5 x, -y+1/2, z-1/2.

**Table S2 Selected Mn···Mn Distances (Å) and Mn-O-Mn Angles (°) in 1-3.**

<b>1</b>			
Mn1···Mn1	4.672	Mn1···Mn2	4.022
Mn1···Mn3	5.854	Mn2···Mn4	5.133
Mn3···Mn3	4.609	Mn1-O3-Mn2	129.66
<b>2</b>			
Mn1···Mn2	3.438	Mn2···Mn3	3.640
Mn2···Mn4	4.426	Mn3···Mn4	4.133
Mn2···Mn2	3.872	Mn4···Mn4	4.645
Mn1-O1-Mn2	100.47	Mn1-O11-Mn2	100.53
Mn2-O19-Mn3	110.47	Mn2-O4-Mn4	133.79
<b>3</b>			
Mn1···Mn2	3.766	Mn1-O15-Mn2	106.33