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Supporting Information for

Synthesis, structures and properties of Mn(II) coordination frameworks based on R-isophthalate (R = $–CH_3$ or $–C(CH_3)_3$) and various dipyridyl-type co-ligands

Lu-Fang Ma[a,b], Li-Ya Wang[a,*], Yao-Yu Wang [b,*], Miao Du[c], Jian-Ge Wang[a]

[a] College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, P. R. China

[b] Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, Department of Chemistry, Northwest University, Xi'an 710069, P. R. China

[c] College of Chemistry and Life Science, Tianjin Normal University, Tainjin 300387, P. R. China

Table S1. Selected bond lengths (Å) and angles (º) for **1**

Mn(1)-O(2)#1	2.0930(15)	O(1)-Mn(1)-N(2)#3	88.84(6)
Mn(1)-O(1)	2.0989(15)	O(3)#2-Mn(1)-N(2)#3	96.84(7)
Mn(1)-O(3)#2	2.1662(16)	O(2)#1-Mn(1)-N(1)	90.52(7)
Mn(1)-N(2)#3	2.2980(17)	O(1)-Mn(1)-N(1)	91.58(6)
Mn(1)-N(1)	2.3304(18)	O(3)#2-Mn(1)-N(1)	83.91(7)
Mn(1)-O(4)#2	2.480(2)	N(2)#3-Mn(1)-N(1)	177.70(7)
O(2)#1-Mn(1)-O(1)	112.72(6)	O(2)#1-Mn(1)-O(4)#2	148.55(7)
O(2)#1-Mn(1)-O(3)#2	96.82(7)	O(1)-Mn(1)-O(4)#2	96.46(6)
O(1)-Mn(1)-O(3)#2	150.19(7)	O(3)#2-Mn(1)-O(4)#2	55.87(6)
O(2)#1-Mn(1)-N(2)#3	87.23(7)	N(2)#3-Mn(1)-O(4)#2	81.69(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y+3/2,-z ; #2 -x+1/2,y-1/2,-z+1/2; #3 x-1/2,y+1/2,z

Table S2. Selected bond lengths (Å) and angles (º) for **2**

Mn(1)-O(3)#1	2.078(6)	O(4)#2-Mn(1)-O(1)	146.2(3)
Mn(1)-O(4)#2	2.094(6)	N(2)#3-Mn(1)-O(1)	97.2(3)
Mn(1)-N(2)#3	2.246(9)	O(3)#1-Mn(1)-N(1)	86.0(3)
Mn(1)-O(1)	2.257(7)	O(4)#2-Mn(1)-N(1)	91.4(3)
Mn(1)-N(1)	2.292(9)	N(2)#3-Mn(1)-N(1)	172.9(3)
Mn(1)-O(2)	2.323(7)	O(1)-Mn(1)-N(1)	84.3(3)
O(3)#1-Mn(1)-O(4)#2	122.6(3)	O(3)#1-Mn(1)-O(2)	147.2(3)
O(3)#1-Mn(1)-N(2)#3	87.0(3)	O(4)#2-Mn(1)-O(2)	90.2(3)

To whom correspondence should be addressed. E-mail: wlya@lynu.edu.cn

O(4)#2-Mn(1)-N(2)#3	91.2(3)	N(2)#3-Mn(1)-O(2)	91.6(3)
O(3)#1-Mn(1)-O(1)	90.6(3)	O(1)-Mn(1)-O(2)	57.1(2)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1,z-1/2; #2 -x+1/2,y-1/2,-z+1/2; #3 x+1/2,y-1/2,z

Table S3. Selected bond lengths (Å) and angles (º) for **3**

Mn(1)-O(4)#1	2.090(2)	O(3)#2-Mn(1)-N(2)#3	86.95(10)
Mn(1)-O(3)#2	2.124(2)	O(2)-Mn(1)-N(2)#3	89.89(11)
Mn(1)-O(2)	2.205(2)	O(4)#1-Mn(1)-N(1)	93.53(11)
Mn(1)-N(2)#3	2.289(3)	O(3)#2-Mn(1)-N(1)	83.77(9)
Mn(1)-N(1)	2.299(3)	O(2)-Mn(1)-N(1)	95.01(10)
Mn(1)-O(1)	2.377(2)	N(2)#3-Mn(1)-N(1)	167.68(10)
O(4)#1-Mn(1)-O(3)#2	116.16(9)	O(4)#1-Mn(1)-O(1)	145.78(9)
O(4)#1-Mn(1)-O(2)	89.27(9)	O(3)#2-Mn(1)-O(1)	97.70(8)
O(3)#2-Mn(1)-O(2)	154.57(9)	O(2)-Mn(1)-O(1)	56.96(7)
O(4)#1-Mn(1)-N(2)#3	97.84(11)	N(2)#3-Mn(1)-O(1)	88.27(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+2; #2 x-1,y,z; #3 x,y-1,z+1

Table S4. Selected bond lengths (Å) and angles (º) for **4**

Mn(1)-O(3)#1	2.099(3)	O(2)-Mn(1)-N(1)	88.35(9)
Mn(1)-O(4)#2	2.119(3)	O(3)#1-Mn(1)-N(2)#3	89.56(12)
Mn(1)-O(2)	2.216(3)	O(4)#2-Mn(1)-N(2)#3	86.48(9)
Mn(1)-N(1)	2.292(3)	O(2)-Mn(1)-N(2)#3	90.32(8)
Mn(1)-N(2)#3	2.308(3)	N(1)-Mn(1)-N(2)#3	178.01(9)
Mn(1)-O(1)	2.343(3)	O(3)#1-Mn(1)-O(1)	155.42(9)
O(3)#1-Mn(1)-O(4)#2	108.22(8)	O(4)#2-Mn(1)-O(1)	95.89(9)
O(3)#1-Mn(1)-O(2)	97.95(8)	O(2)-Mn(1)-O(1)	57.74(7)
O(4)#2-Mn(1)-O(2)	153.58(9)	N(1)-Mn(1)-O(1)	90.91(12)
O(3)#1-Mn(1)-N(1)	92.08(13)	N(2)#3-Mn(1)-O(1)	87.14(12)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1; #2 x,y+1,z; #3 x+1,y,z-1

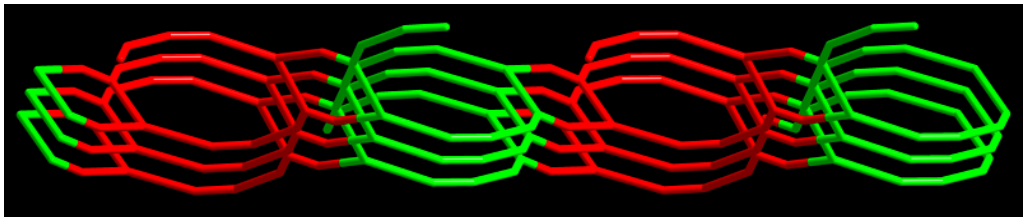
Table S5. Selected bond lengths (Å) and angles (º) for **5**

Mn(1)-O(1)	2.1423(15)	O(9)-Mn(1)-O(5)	82.87(6)
Mn(1)-O(9)	2.1566(16)	O(6)-Mn(1)-O(5)	54.78(5)
Mn(1)-O(6)	2.1905(13)	O(7)#1-Mn(1)-O(5)	169.90(6)
Mn(1)-O(7)#1	2.1952(14)	N(1)-Mn(1)-O(5)	91.74(6)
Mn(1)-N(1)	2.2315(18)	O(2)#2-Mn(2)-O(2)	180.0
Mn(1)-O(5)	2.5295(14)	O(2)#2-Mn(2)-O(8)#1	89.38(6)
Mn(2)-O(2)#2	2.1211(15)	O(2)-Mn(2)-O(8)#1	90.62(6)
Mn(2)-O(2)	2.1212(15)	O(2)#2-Mn(2)-O(8)#3	90.62(6)
Mn(2)-O(8)#1	2.1550(14)	O(2)-Mn(2)-O(8)#3	89.38(6)

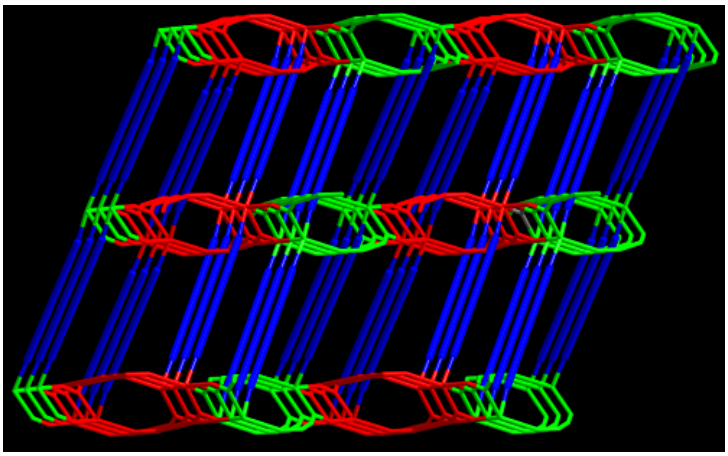
Mn(2)-O(8)#3	2.1551(14)	O(8)#1-Mn(2)-O(8)#3	180.00(5)
Mn(2)-O(6)	2.2459(13)	O(2)#2-Mn(2)-O(6)	89.13(5)
Mn(2)-O(6)#2	2.2459(13)	O(2)-Mn(2)-O(6)	90.86(5)
O(1)-Mn(1)-O(9)	177.12(6)	O(8)#1-Mn(2)-O(6)	80.86(5)
O(1)-Mn(1)-O(6)	93.75(6)	O(8)#3-Mn(2)-O(6)	99.13(5)
O(9)-Mn(1)-O(6)	88.22(6)	O(2)#2-Mn(2)-O(6)#2	90.86(5)
O(1)-Mn(1)-O(7)#1	93.25(6)	O(2)-Mn(2)-O(6)#2	89.14(5)
O(9)-Mn(1)-O(7)#1	87.46(6)	O(8)#1-Mn(2)-O(6)#2	99.14(5)
O(6)-Mn(1)-O(7)#1	122.19(5)	O(8)#3-Mn(2)-O(6)#2	80.87(5)
O(1)-Mn(1)-N(1)	84.91(7)	O(6)-Mn(2)-O(6)#2	180.0
O(9)-Mn(1)-N(1)	92.28(7)	O(7)#1-Mn(1)-N(1)	91.57(6)
O(6)-Mn(1)-N(1)	146.21(6)	O(1)-Mn(1)-O(5)	96.55(6)

Symmetry transformations used to generate equivalent atoms:

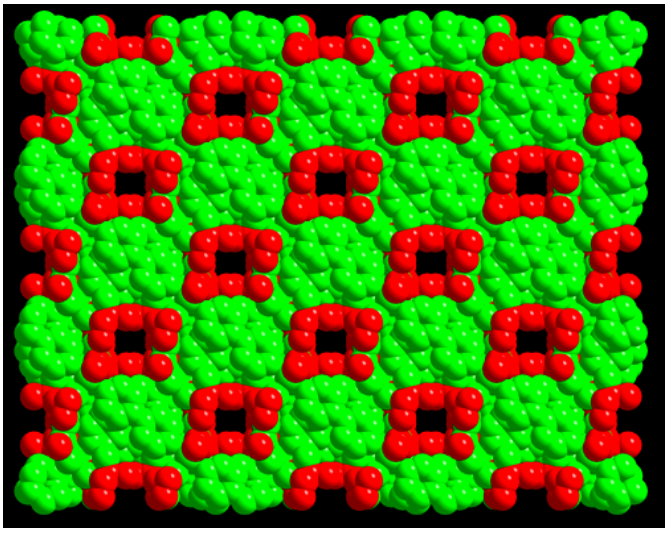
#1 x+1,y,z; #2 -x+1,-y,-z+1; #3 -x,-y,-z+1



(a)



(b)



(c)

Fig. S1. (a) 2D helical layer in **1**. (b) Schematic illustration of the pillared helical-layer structure of **1**. Left-helical chains are marked as green and right-helical chains are marked as red. Blue sticks represent bipy molecules. (c) Space-filling model to show the channels along the *c*-axis direction.

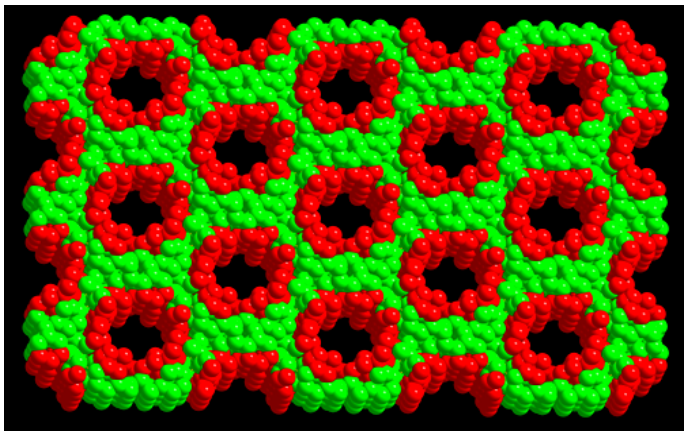
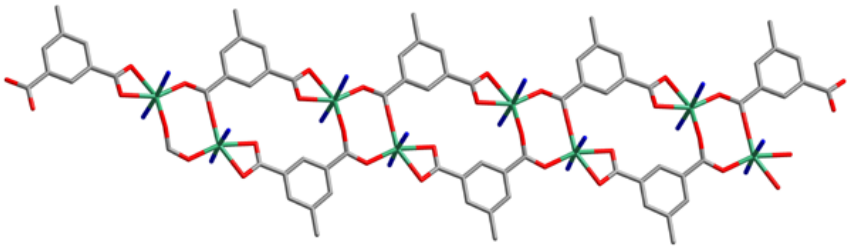
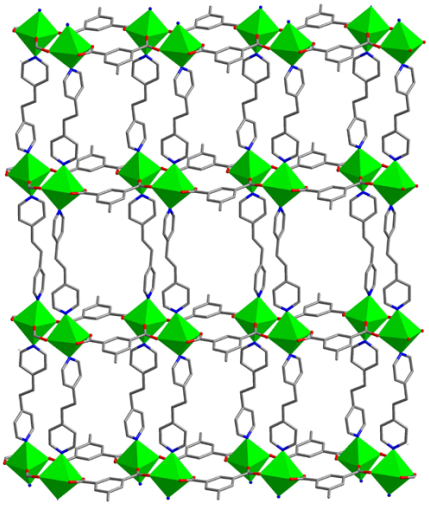


Fig. S2. Space-filling model to show the channels along the *c*-axis. Guest water molecules are ommitted for clarity.



(a)



(b)

Fig. S3. (a) View of a 1D ribbonlike chain of Mn atoms bridged by mip ligand in **4**. (b) Ribbon like chains pillared by flexible bpa ligands into a 2D layer.

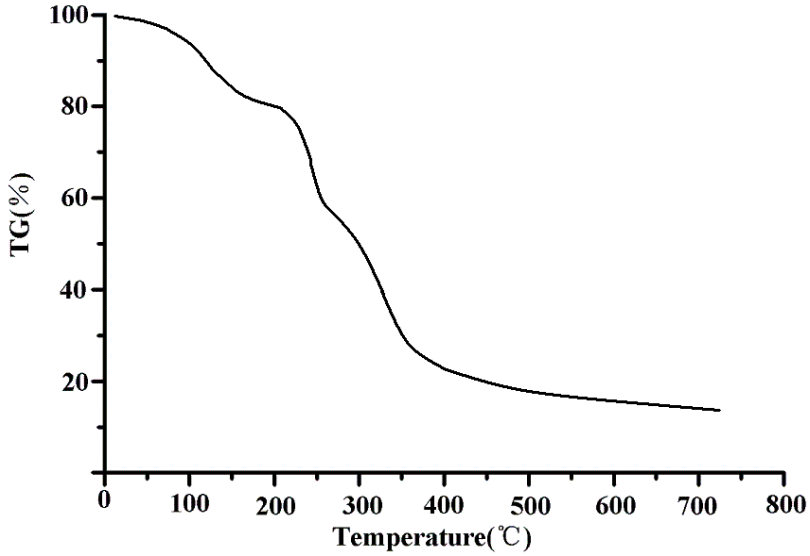


Figure S4a. TGA plot of complex **2**.

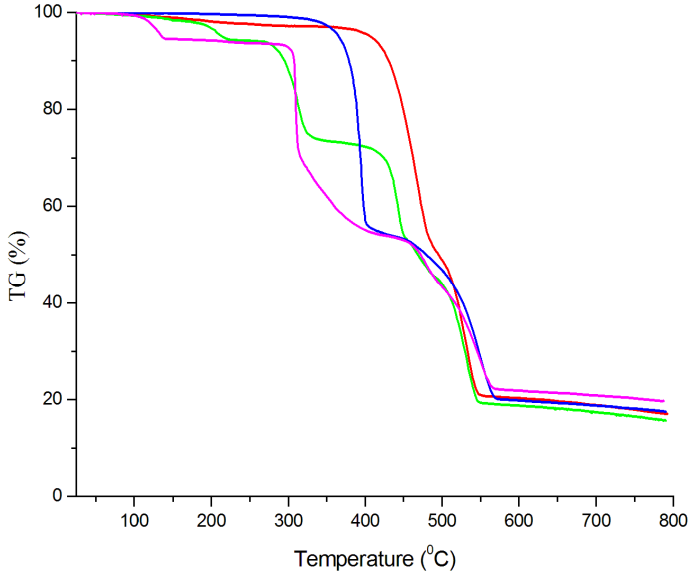


Figure S4b. TGA plot of complexes **1**, **3**, **4**, **5**. (Red for 1, Green for **3**, Blue for **4** and Magenta for **5**).

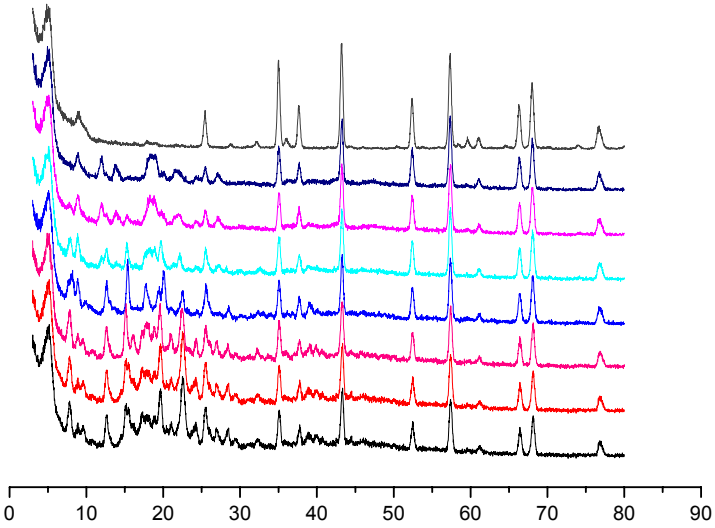


Figure S5. Temperature progressive of X-ray power diffraction patterns for **2**. 25 °C (black); 100 °C (red); 150 °C (pink); 200 °C (blue); 230 °C (cyan); 260 °C (magenta); 300 °C (navy); 350 °C (dark gray).