Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Three Mn(II) metal organic frameworks with the same chemical compositions, but different topological structures and properties

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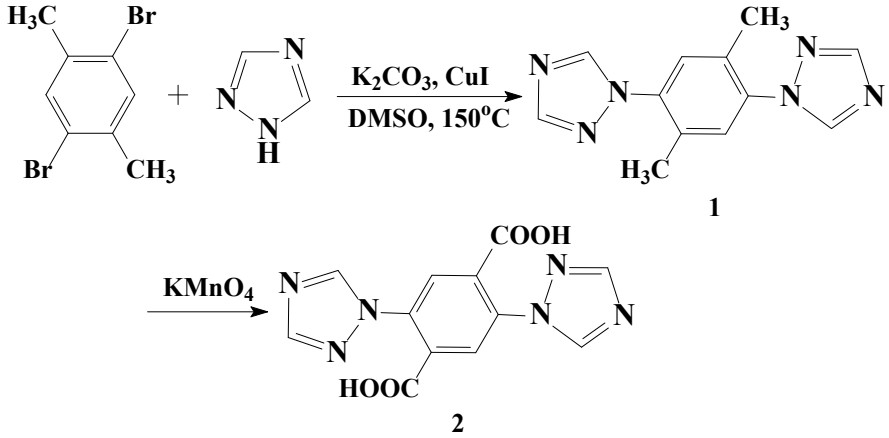
Syhthesis of H_2TTPA



Synthesis of 1: 1,4-Dimethyl-2,5-dibromobenzene (0.96 g, 3.2 mmol), triazole (2.18 g, 12.8 mmol), K_2CO_3 (2.96 g, 21.0 mmol), CuI (0.03 g, 0.13 mmol) and 7 drops of N, N'-dimethyl ethane amine were mixed in 15 ml dry DMSO solution and heated at 150 °C for 36 h under a nitrogen atmosphere. The mixture was cooled to room temperature, filtered and the solid was washed with DMSO. The filtrate was distilled under reduced pressure to remove the solvent and the residue was extracted with CH_2Cl_2 (6 × 30 mL). The organic layer was separated, dried over magnesium sulfate, and evaporated to dryness to give the crude product, which was further separated under column chromatography to give 0.45 g of **1**. Yield: 63%.

Synthesis of 2: The product (1.5 g, 6 mmol) of the first step is dissolved in 180 mL of pyridine: water (80:20) solution. And 10.96 g $KMnO_4$ is added to the solution. During solution is refluxed, add another portion of $KMnO_4$ twice in 1 hr interval. The dark solution was filtered and the filtrate was evaporated under reduced pressure. 20 ml water was added and 6 N HCl was dropped until pH = 2. The precipitates were filtered out and washed with water several times. Dry the precipitates to afford **2** (0.83 g, 58%). 1 H NMR (400 MHz, DMSO-d_6, δ): 8.95 (s, 2H; triazole), 8.44 (s, 2H; triazole), 7.56 (s, 2H; ArH).

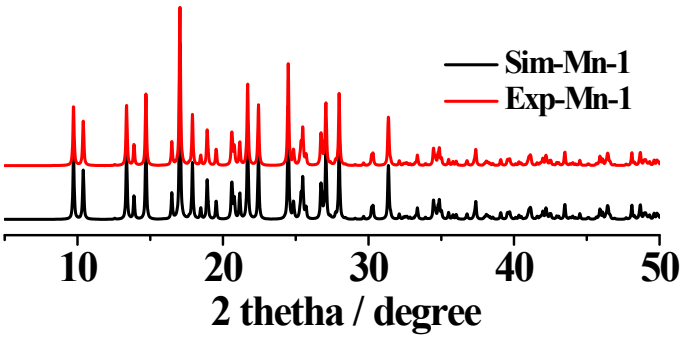


Figure S1. Powder X-ray diffractions of **Mn-1.**

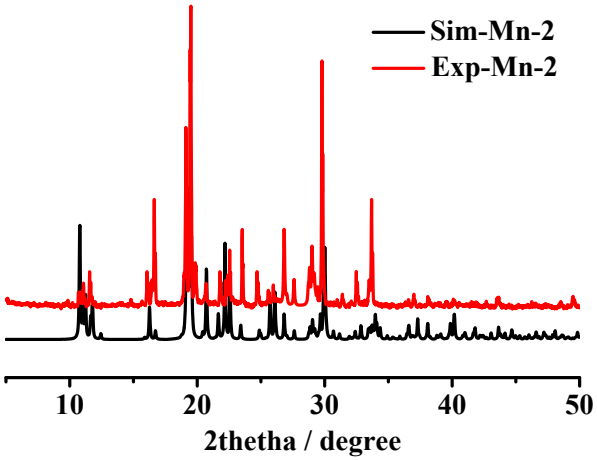


Figure S2. Powder X-ray diffractions of **Mn-2.**

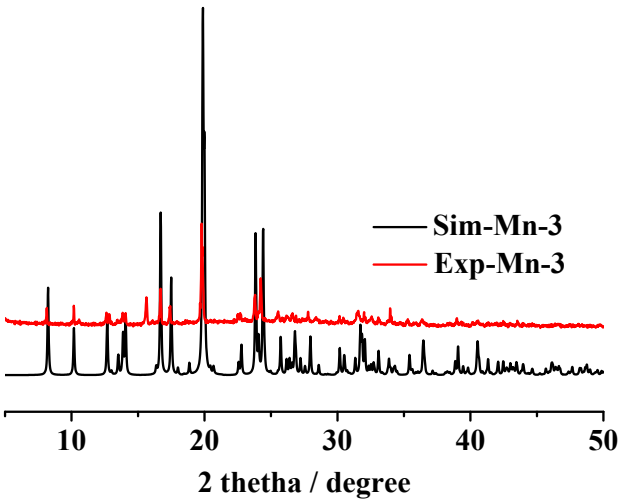


Figure S3. Powder X-ray diffractions of **Mn-3.**

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

Mn1–O1	2.1225(18)	O1–Mn1–O4#1	101.52(7)
Mn1–O3#1	2.4033(16)	O1–Mn1–O5	170.29(6)
Mn1–O4#1	2.1301(16)	O1–Mn1–N3#2	84.09(7)
Mn1–O5	2.2748(18)	O4#1–Mn1–O3#1	57.73(6)
Mn1–N3#2	2.1875(19)	O4#1–Mn1–O5	86.14(6)
Mn1–N6#3	2.1675(19)	O5–Mn1–O3#1	99.15(6)
O1–Mn1–O3#1	90.05(6)	N3#2–Mn1–O5	88.03(7)

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

Table S2. Selected bond lengths (Å) and bond angles (°) for complex **Mn-2**.

Mn1–O1	2.1810(15)	O1–Mn1–N3#3	96.50(6)
Mn1–O2#1	2.1458(14)	O1–Mn1–N6#3	82.37(6)
Mn1–O3	2.1148(15)	O2#1–Mn1–O1	93.54(6)
Mn1–O5	2.2996(16)	O2#1–Mn1–O5	93.54(6)
Mn1–N3#2	2.2869(19)	O2#1–Mn1–N3#2	86.25(6)
Mn1–N6#3	2.2922(18)	O3–Mn1–O1	94.75(6)
O1–Mn1–O5	168.94(6)	N3#2–Mn1–N6#3	88.13(7)

#1: 1-*x*, 1-*y*, 1-*z*; #2: -*x*, 1-*y*, 1-*z*; #3: -1+*x*, *y*, *z*.

Table S3. Selected bond lengths (Å) and bond angles (°) for complex **Mn-3**.

Mn1–O1	2.1572(13)	O1–Mn1–O4#1	168.33(5)
Mn1–O3	2.1606(14)	O1–Mn1–N6#3	82.37(6)
Mn1–O4#1	2.1578(13)	O3–Mn1–O5	170.62(6)
Mn1–O5	2.1845(15)	O3–Mn1–N6#3	86.62(6)
Mn1–N3#2	2.2591(16)	O4#1–Mn1–N3#2	102.89(6)
Mn1–N6#3	2.2922(18)	O5–Mn1–N6#3	88.00(7)
O1–Mn1–O3	97.53(5)	N3#2–Mn1–N6#3	169.58(6)

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