Supporting Information

Syntheses, structures, magnetic and photoluminescence properties of metal-organic frameworks based on aromatic polycarboxylate acids

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Table S1 Selected Bond Distances (Å) and Angles (deg) for Compounds 1-3 (Co, Mn, and Cd).

Co compound			
Co1─ O1	2.0644(16)	Co1─ O3a	2.0762(15)
Co1─ O4b	2.1590(16)		
O1 ─ Co1 ─ O1d	92.30(9)	O1 ─ Co1 ─ O3c	176.83(6)
O1 ─ Co1 ─ O3a	87.87(6)	O3c ─ Co1 ─ O3a	92.15(8)
O1 ─ Co1 ─ O4e	83.17(6)	O3c ─ Co1 ─ O4e	93.66(6)
O3a ─ Co1 ─ O4e	85.52(6)	O1 ─ Co1 ─ O4f	97.65(6)
O4e ─ Co1 ─ O4f	178.82(9)		
Mn compound			
Mn1─ O1	2.210(2)	Mn1─ O3	2.144(2)
Mn1─ O4	2.181(2)		
O3 ─ Mn1 ─ O1	95.03(8)	O4 ─ Mn1 ─ O1	85.95(8)
O3 ─ Mn1 ─ O4	179.01(13)	O3a ─ Mn1 ─ O3	94.00(12)
O3a ─ Mn1 ─ O4	86.77(8)	O4a ─ Mn1 ─ O4	92.47(11)
O3a ─ Mn1 ─ O1	85.70(9)	O4a ─ Mn1 ─ O1	93.36(8)
O1a ─ Mn1 ─ O1	179.01(13)		
Cd compound			
Cd1 ─ N2	2.331(3)	Cd1a ─ O4	2.332(2)
Cd1 ─ O2	2.348(2)	Cd1 ─ N1	2.386(3)
Cd1 ─ O3	2.391(2)	Cd1b ─ O4	2.401(2)
Cd1a ─ O5	2.494(3)		
N2 ─ Cd1 ─ O4a	157.20(9)	N2 ─ Cd1 ─ O2	89.40(10)
O4a ─ Cd1 ─ O2	102.18(9)	N2 ─ Cd1 ─ N1	69.98(10)
O4a ─ Cd1 ─ N1	92.95(9)	O2 ─ Cd1 ─ N1	154.55(9)
N2 ─ Cd1 ─ O3	92.77(9)	O4a ─ Cd1 ─ O3	109.98(8)
O2 ─ Cd1 ─ O3	55.03(8)	N1 ─ Cd1 ─ O3	137.58(9)
N2 ─ Cd1 ─ O4b	89.84(9)	O4a ─ Cd1 ─ O4b	72.17(9)
O2 ─ Cd1 ─ O4b	84.12(8)	N1 ─ Cd1 ─ O4b	81.18(9)
O3 ─ Cd1 ─ O4b	139.00(8)	N2 ─ Cd1 ─ O5a	134.29(10)
O4a ─ Cd1 ─ O5a	53.72(8)	O2 ─ Cd1 ─ O5a	122.57(9)
N1 ─ Cd1 ─ O5a	82.88(9)	O3 ─ Cd1 ─ O5a	83.01(8)
O4b ─ Cd1 ─ O5a	122.26(8)	Cd1c ─ O4 ─ Cd1b	107.83(9)

Symmetry transformations used to generate equivalent atoms:
a = -*x*, -*y*, -*z*; b = -*x* + 1/2, -*y* + 1/2, *z* + 1/2. c = -*x*, -*y*, *z* - 1/2; d = -*x*, *y*, -*z* -1/2;
e = -*x* + 1/2, -*y* + 1/2, *z* - 1/2; f = *x* - 1/2, -*y* + 1/2, -*z*. (Co compound **1**)
a =-*x*, *y*, -*z* + 3/2. (Mn compound **2**)
a = *x* - 1/2, -*y* + 1, *z* - 1/2; b = -*x* + 3/2, *y*, -*z* + 3/2; c = *x* - 1/2, -*y* + 2, *z* - 1/2. (Cd compound **3**)

Table S2 Selected Bond Distances (Å) and Angles (deg) for compounds 4-6 (Eu, Nd, and Pr).

Eu compound			
Eu1 ─ O3	2.359(7)	Eu1 ─ O5	2.443(6)
Eu1a ─ O2	2.446(6)	Eu1b ─ O6	2.490(6)
Eu1 ─ O7	2.524(7)	Eu1c ─ O1	2.548(6)
Eu1c ─ O2	2.587(6)	O4d ─ Eu1	2.334(7)
O4d ─ Eu1 ─ O3	85.9(2)	O4d ─ Eu1 ─ O5	121.9(3)
O3 ─ Eu1 ─ O5	74.8(2)	O4d ─ Eu1 ─ O2a	81.0(2)
O3 ─ Eu1 ─ O2a	132.3(2)	O5 ─ Eu1 ─ O2a	74.2(2)
O4d ─ Eu1 ─ O6b	81.1(2)	O5 ─ Eu1 ─ O6b	135.8(2)
O3 ─ Eu1 ─ O6b	148.8(2)	O4d ─ Eu1 ─ O7	78.5(3)
O2a ─ Eu1 ─ O6b	73.4(2)	O3 ─ Eu1 ─ O7	77.6(2)
O5 ─ Eu1 ─ O7	143.7(2)	O2a ─ Eu1 ─ O7	142.0(2)
O6b ─ Eu1 ─ O7	72.1(2)	O4d ─ Eu1 ─ O1c	155.3(2)
O3 ─ Eu1 ─ O1c	85.0(2)	O5 ─ Eu1 ─ O1c	77.4(2)
O2a ─ Eu1 ─ O1c	121.6(2)	O6b ─ Eu1 ─ O1d	95.2(2)
O7 ─ Eu1 ─ O1d	77.1(2)	O4d ─ Eu1 ─ O2c	145.8(2)
O3 ─ Eu1 ─ O2c	128.0(2)	O5 ─ Eu1 ─ O2c	70.7(2)
O2a ─ Eu1 ─ O2c	72.1(2)	O6b ─ Eu1 ─ O2c	71.3(2)
O7 ─ Eu1 ─ O2c	110.5(2)	O1c ─ Eu1 ─ O2c	50.5(2)
O4d ─ Eu1 ─ Eu1b	115.57(19)	O5 ─ Eu1 ─ Eu1b	68.04(17)
O3 ─ Eu1 ─ Eu1b	142.74(16)	O6b ─ Eu1 ─ Eu1b	67.95(15)
O2a ─ Eu1 ─ Eu1b	37.23(14)	O7 ─ Eu1 ─ Eu1b	134.1(2)
O1c ─ Eu1 ─ Eu1b	84.90(15)	O2c ─ Eu1 ─ Eu1b	34.89(13)
Eu1e ─ O2 ─ Eu1c	107.9(2)		
Nd compound			
Nd1a─O4	2.333(5)	Nd1b─O3	2.335(5)
Nd1c─O2	2.418(4)	Nd1─O5	2.420(4)
Nd1c─O6	2.472(4)	Nd1─O7	2.496(6)
Nd1─O1	2.534(4)	Nd1─O2	2.589(4)
O4d─Nd1	2.333(5)	O4a─Nd1─O3b	85.47(17)
O3b─Nd1─O2c	131.75(17)	O4a─Nd1─O2c	80.40(16)
O4a─Nd1─O5	121.40(18)	O3b─Nd1─O5	74.49(17)
O2c─Nd1─O5	74.37(16)	O5─Nd1─O6c	136.25(16)
O4a─Nd1─O6c	81.28(17)	O4a─Nd1─O7	78.65(19)
O3b─Nd1─O6c	148.71(16)	O3b─Nd1─O7	77.82(19)
O2c─Nd1─O6c	73.63(15)	O2c─Nd1─O7	141.77(17)
O5─Nd1─O7	143.71(18)	O3b─Nd1─O1	85.13(16)
O6c─Nd1─O7	71.85(18)	O2c─Nd1─O1	122.41(14)
O4a─Nd1─O1	155.16(17)	O5─Nd1─O1	77.79(17)
O6c─Nd1─O1	95.20(17)	O5─Nd1─O2	70.77(16)

O7─Nd1─O1	76.91(18)	O6c─Nd1─O2	71.62(15)
O4a─Nd1─O2	145.83(15)	O7─Nd1─O2	110.86(18)
O3b─Nd1─O2	128.19(15)	O1─Nd1─O2	50.99(14)
O2c─Nd1─O2	72.39(16)	O5─Nd1─O2	70.77(16)
O4a─Nd1─Nd1c	115.48(13)	O3b─Nd1─Nd1c	142.60(13)
O2c─Nd1─Nd1c	37.62(10)	O6c─Nd1─Nd1c	68.25(11)
O5─Nd1─Nd1c	68.16(11)	O7c─Nd1─Nd1	134.27(15)
O1c─Nd1─Nd1	85.27(10)	O2c─Nd1─Nd1	34.76(10)
Nd1c─O2─Nd1	107.61(16)		
Pr compound			
O1─Pr1	2.292(5)	O3─Pr1	2.421(5)
O2─Pr1	2.445(6)	O4─Pr1	2.371(5)
O5a─Pr1	2.493(5)	O8b─Pr1	2.282(5)
O7a─Pr1	2.546(5)	Pr1c─O7	2.375(5)
Pr1d─O7─Pr1a	107.66(18)	O1─Pr1─O4	74.07(19)
O8b─Pr1─O1	85.34(19)	O8b─Pr1─O7	80.52(18)
O8b─Pr1─O4	120.7(2)	O1─Pr1─O7	131.69(19)
O4─Pr1─O7c	74.33(18)	O4─Pr1─O3	136.95(18)
O8b─Pr1─O3	81.62(19)	O7c─Pr1─O3	74.16(17)
O1─Pr1─O3	148.40(18)	O8b─Pr1─O2	79.3(2)
O1─Pr1─O2	77.2(2)	O8b─Pr1─O5a	155.04(19)
O4─Pr1─O2	142.8(2)	O1─Pr1─O5a	84.14(18)
O7c─Pr1─O2	142.75(19)	O4─Pr1─O5a	77.69(19)
O3─Pr1─O2	72.2(2)	O7c─Pr1─O5a	122.89(16)
O3─Pr1─O5a	95.84(18)	O4─Pr1─O7a	71.37(18)
O2─Pr1─O5a	76.4(2)	O7c─Pr1─O7a	72.34(18)
O8b─Pr1─O7a	145.96(17)	O3─Pr1─O7a	71.60(17)
O1─Pr1─O7a	128.18(17)	O2─Pr1─O7a	110.77(19)
O5a─Pr1─O7a	51.71(15)	O4─Pr1─Pr1e	68.52(13)
O8b─Pr1─Pr1e	115.63(14)	O7c─Pr1─Pr1e	37.63(11)
O1─Pr1─Pr1e	142.52(14)	O3─Pr1─Pr1e	68.57(12)
O2─Pr1─Pr1e	134.66(16)	O7a─Pr1─Pr1e	34.72(11)
O5a─Pr1─Pr1e	85.84(11)		

Symmetry transformations used to generate equivalent atoms:

a = *x* + 1/2, -*y* + 1/2, *z*-1/2; b = -*x* + 5/2, -*y* + 1/2, -*z* + 1; c = -*x* + 2, *y*, -*z* + 3/2;
d = -*x* + 2, *y*, -*z* + 1/2; e = *x* -1/2, -*y* + 1/2, *z* + 1/2. (Eu compound **4**)

a = *x*, *y*, *z* – 1; b= -*x*, *y*, -*z* + 3/2; c = -*x* + 1/2, -*y* + 1/2, -*z* + 1; d = *x*, *y*, *z* + 1. (Nd compound **5**)

a = -*x*, *y*, -*z* + 1/2; b = -*x*, *y*, -*z* - 1/2; c = *x* + 1/2, -*y* + 1/2, *z* -1/2; d = *x* - 1/2, -*y* + 1/2, *z* + 1/2; e = -*x* + 1/2, -*y* + 1/2, -*z*. (Pr compound **6**)

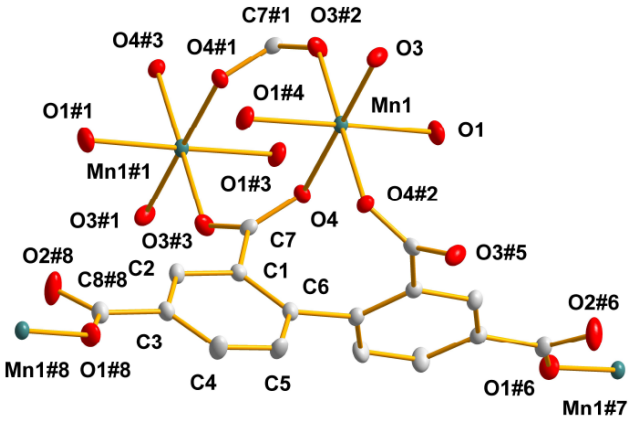

Figure S1. An ORTEP drawing of Mn compound **2** showing 30% ellipsoid probability (hydrogen atoms are omitted for clarity). Symmetry codes: #1= -x, 2-y, 2-z; #2= -x, y, 1.5-z; #3= x, 2-y, 0.5+z; #4= -x, y, 1.5-z; #5= -x, 2-y, 1-z; #6= -0.5-x, -0.5+y, z; #7= -0.5+x, -0.5+y, 1.5-z; #8= 0.5+x, -0.5+y, 1.5-z.

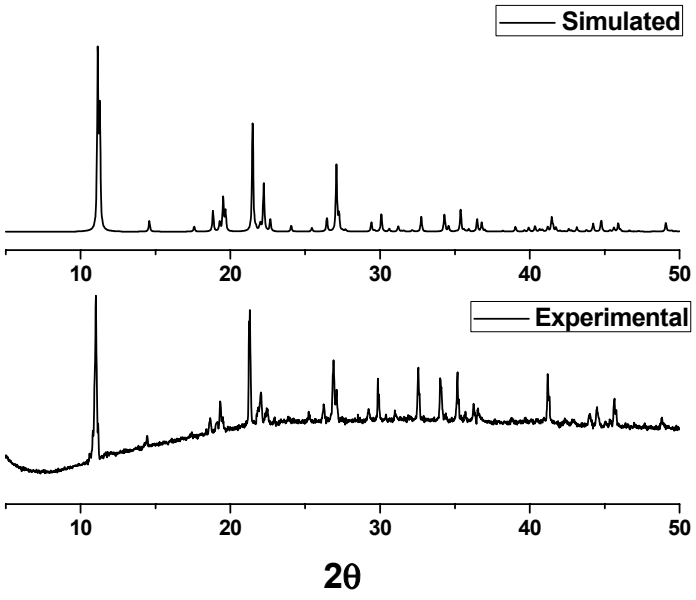

Figure S2. Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of Co compound **1** at 293K.

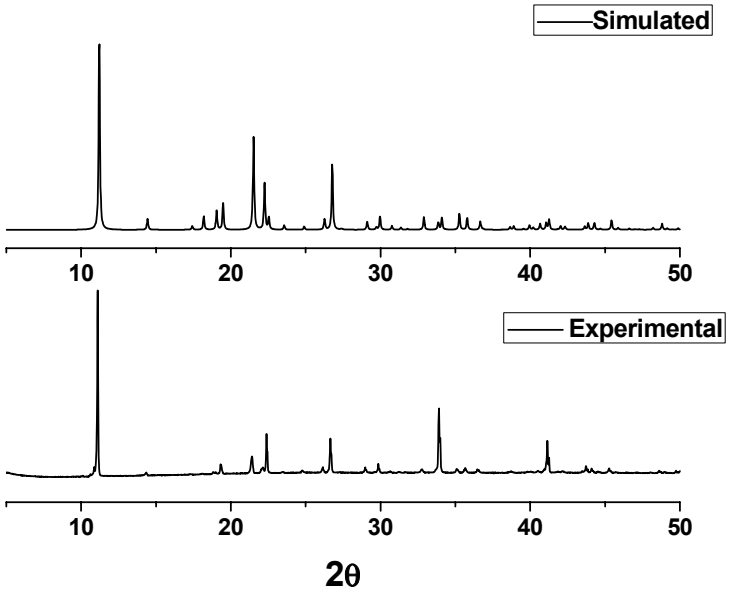

Figure S3. Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of Mn compound **2** at 293K.

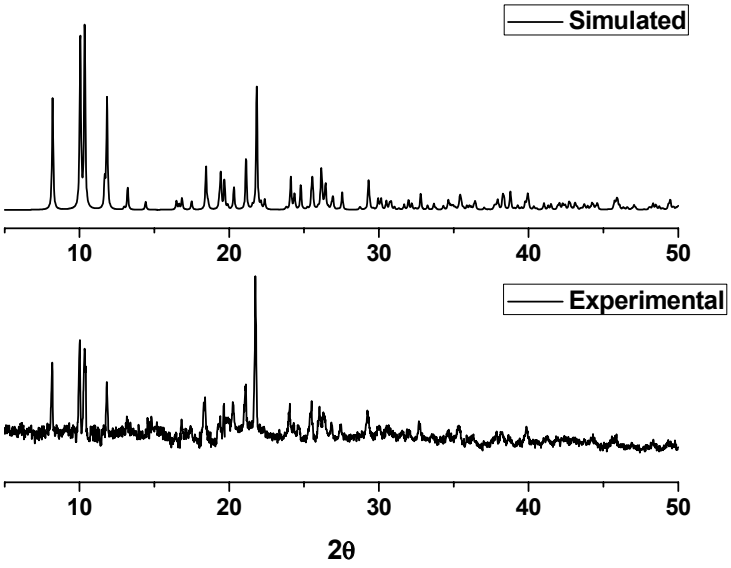

Figure S4. Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of Cd compound **3** at 293K.

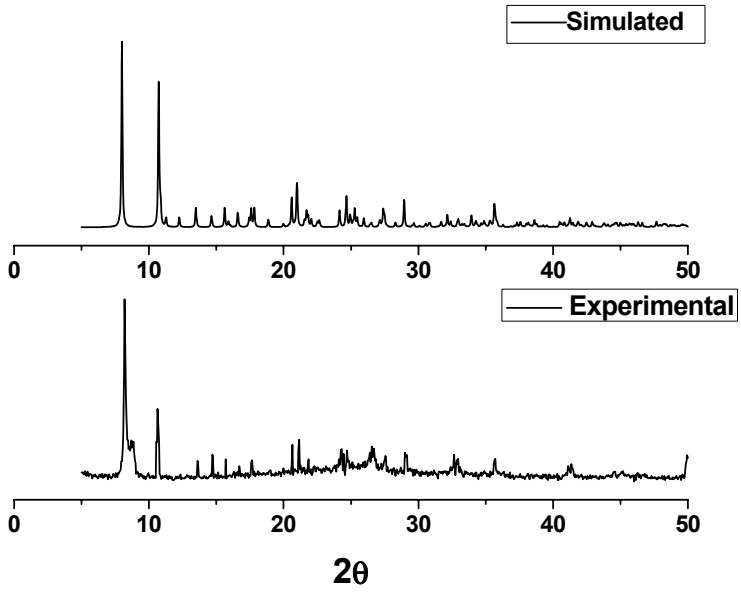

Figure S5. Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of Eu compound **4** at 293K.

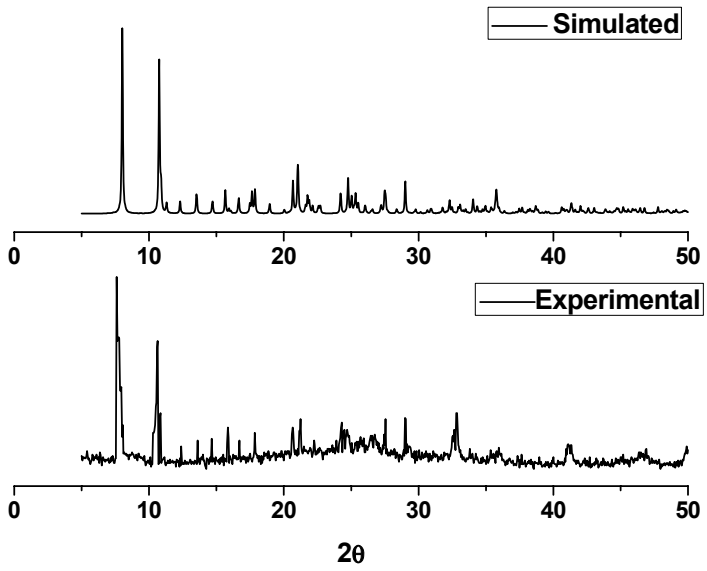

Figure S6. Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of Nd compound **5** at 293K.

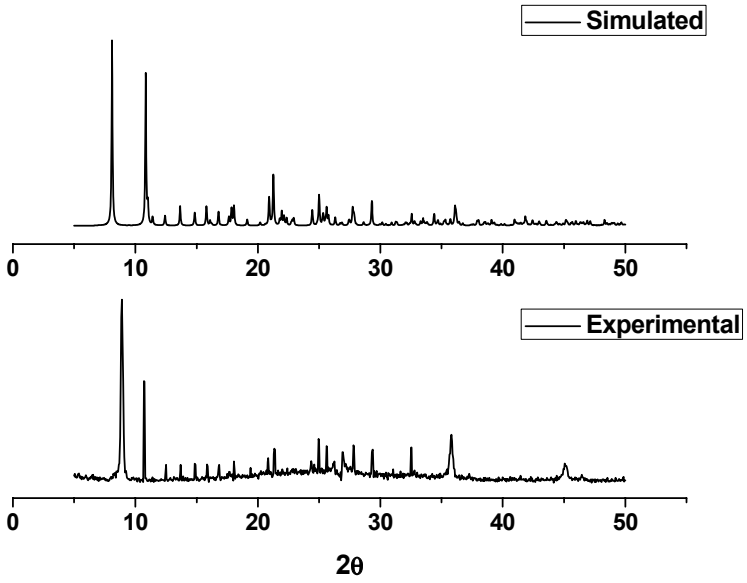

Figure S7. Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of Pr compound **6** at 293K.