Supplementary Information

Three Series of MOFs Featuring Various Metal(II)-Carboxylate Chains Cross-Linked by Dipyridyl-Typed Coligands: Synthesis, Structure, and Solvent-Dependent Luminescence

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

*Compound **1***			
Cd(1)-N(2)	2.331(4)	Cd(1)-O(4)#1	2.362(3)
Cd(1)-O(2)	2.383(5)	Cd(1)-O(3)#1	2.432(3)
Cd(1)-N(3)#2 [a]	2.439(3)	Cd(1)-N(1)	2.476(4)
Cd(1)-O(1)	2.557(5)		
N(2)-Cd(1)-O(4)#1	93.41(12)	N(2)-Cd(1)-O(2)	89.31(16)
O(4)#1-Cd(1)-O(2)	163.17(14)	N(2)-Cd(1)-O(3)#1	147.75(13)
O(4)#1-Cd(1)-O(3)#1	54.65(11)	O(2)-Cd(1)-O(3)#1	119.81(15)
N(2)-Cd(1)-N(3)#2	79.04(13)	O(4)#1-Cd(1)-N(3)#2	84.90(11)
O(2)-Cd(1)-N(3)#2	111.92(14)	O(3)#1-Cd(1)-N(3)#2	100.12(12)
N(2)-Cd(1)-N(1)	85.23(13)	O(4)#1-Cd(1)-N(1)	83.61(12)
O(2)-Cd(1)-N(1)	80.07(14)	O(3)#1-Cd(1)-N(1)	86.54(12)
N(3)#2-Cd(1)-N(1)	159.90(13)	N(2)-Cd(1)-O(1)	119.38(15)
O(4)#1-Cd(1)-O(1)	137.78(14)	O(2)-Cd(1)-O(1)	51.90(16)
O(3)#1-Cd(1)-O(1)	91.23(14)	N(3)#2-Cd(1)-O(1)	76.97(14)
N(1)-Cd(1)-O(1)	122.15(14)		
Compound **1a**			
Cd(1)-N(2)	2.338(4)	Cd(1)-N(3)#2	2.437(4)
Cd(1)-O(4)#1 [b]	2.364(3)	Cd(1)-O(1)	2.467(5)
Cd(1)-O(2)	2.401(5)	Cd(1)-N(1)	2.502(4)
Cd(1)-O(3)#1	2.417(3)	Cd(1)-C(23)#1	2.720(4)
N(2)-Cd(1)-O(4)#1	92.49(12)	O(4)#1-Cd(1)-O(1)	141.79(14)
N(2)-Cd(1)-O(2)	88.39(16)	O(2)-Cd(1)-O(1)	52.52(15)
O(4)#1-Cd(1)-O(2)	159.79(14)	O(3)#1-Cd(1)-O(1)	95.07(14)
N(2)-Cd(1)-O(3)#1	146.97(13)	N(3)#2-Cd(1)-O(1)	78.56(14)
O(4)#1-Cd(1)-O(3)#1	54.74(11)	N(2)-Cd(1)-N(1)	84.12(13)
O(2)-Cd(1)-O(3)#1	120.61(15)	O(4)#1-Cd(1)-N(1)	82.37(12)
N(2)-Cd(1)-N(3)#2	78.59(13)	O(2)-Cd(1)-N(1)	77.64(14)
O(4)#1-Cd(1)-N(3)#2	83.80(12)	O(3)#1-Cd(1)-N(1)	87.04(13)
O(2)-Cd(1)-N(3)#2	116.10(14)	N(3)#2-Cd(1)-N(1)	157.30(13)
O(3)#1-Cd(1)-N(3)#2	99.50(13)	O(1)-Cd(1)-N(1)	122.78(14)
N(2)-Cd(1)-O(1)	116.41(15)		
Compound **2**			
Co(1)-O(7)#1 [c]	2.052(3)	Co(2)-O(6)	1.999(3)
Co(1)-O(1)	2.055(3)	Co(2)-N(6)	2.141(4)
Co(1)-O(9)	2.168(3)	Co(2)-O(3)	2.159(3)
Co(1)-N(3)	2.174(4)	Co(2)-N(2)#2	2.173(4)
Co(1)-N(5)	2.182(4)	Co(2)-O(4)	2.174(3)
Co(1)-N(1)	2.209(4)	Co(2)-N(4)#3	2.268(4)
O(7)#1-Co(1)-O(1)	175.98(13)	O(6)-Co(2)-N(6)	91.93(15)
O(7)#1-Co(1)-O(9)	94.88(12)	O(6)-Co(2)-O(3)	168.24(14)
O(1)-Co(1)-O(9)	87.45(12)	N(6)-Co(2)-O(3)	99.04(14)
O(7)#1-Co(1)-N(3)	90.54(13)	O(6)-Co(2)-N(2)#2	93.67(15)
O(1)-Co(1)-N(3)	92.79(14)	N(6)-Co(2)-N(2)#2	89.75(15)
O(9)-Co(1)-N(3)	88.74(13)	O(3)-Co(2)-N(2)#2	90.60(14)
O(7)#1-Co(1)-N(5)	89.18(14)	O(6)-Co(2)-O(4)	107.21(13)
O(1)-Co(1)-N(5)	88.52(14)	N(6)-Co(2)-O(4)	159.08(14)
O(9)-Co(1)-N(5)	175.90(14)	O(3)-Co(2)-O(4)	61.33(12)
N(3)-Co(1)-N(5)	90.69(14)	N(2)#2-Co(2)-O(4)	97.20(13)

O(7)#1-Co(1)-N(1)	91.75(14)	O(6)-Co(2)-N(4)#3	91.85(14)
O(1)-Co(1)-N(1)	85.03(13)	N(6)-Co(2)-N(4)#3	89.54(15)
O(9)-Co(1)-N(1)	88.60(13)	O(3)-Co(2)-N(4)#3	84.08(13)
N(3)-Co(1)-N(1)	176.63(15)	N(2)#2-Co(2)-N(4)#3	174.45(16)
N(5)-Co(1)-N(1)	91.81(14)	O(4)-Co(2)-N(4)#3	81.64(13)
Compound **2a**			
Ni(1)-O(1)	2.035(5)	Ni(2)-N(6)	2.092(6)
Ni(1)-O(7)#1[d]	2.061(5)	Ni(2)-N(2)#2	2.121(6)
Ni(1)-O(9)	2.120(5)	Ni(2)-O(3)	2.123(5)
Ni(1)-N(3)	2.125(6)	Ni(2)-O(4)	2.147(5)
Ni(1)-N(5)	2.130(6)	Ni(2)-N(4)#3	2.182(6)
Ni(1)-N(1)	2.144(6)	Ni(2)-C(8)	2.436(7)
Ni(2)-O(6)	2.001(5)		
O(1)-Ni(1)-O(7)#1	175.68(19)	O(6)-Ni(2)-N(6)	90.9(2)
O(1)-Ni(1)-O(9)	88.54(18)	O(6)-Ni(2)-N(2)#2	93.4(2)
O(7)#1-Ni(1)-O(9)	94.32(19)	N(6)-Ni(2)-N(2)#2	90.1(2)
O(1)-Ni(1)-N(3)	93.1(2)	O(6)-Ni(2)-O(3)	168.2(2)
O(7)#1-Ni(1)-N(3)	90.2(2)	N(6)-Ni(2)-O(3)	100.0(2)
O(9)-Ni(1)-N(3)	88.2(2)	N(2)#2-Ni(2)-O(3)	91.0(2)
O(1)-Ni(1)-N(5)	88.2(2)	O(6)-Ni(2)-O(4)	106.9(2)
O(7)#1-Ni(1)-N(5)	89.0(2)	N(6)-Ni(2)-O(4)	161.0(2)
O(9)-Ni(1)-N(5)	176.6(2)	N(2)#2-Ni(2)-O(4)	95.3(2)
N(3)-Ni(1)-N(5)	90.9(2)	O(3)-Ni(2)-O(4)	61.82(18)
O(1)-Ni(1)-N(1)	85.3(2)	O(6)-Ni(2)-N(4)#3	91.1(2)
O(7)#1-Ni(1)-N(1)	91.6(2)	N(6)-Ni(2)-N(4)#3	91.0(2)
O(9)-Ni(1)-N(1)	88.7(2)	N(2)#2-Ni(2)-N(4)#3	175.3(2)
N(3)-Ni(1)-N(1)	176.5(2)	O(3)-Ni(2)-N(4)#3	84.3(2)
N(5)-Ni(1)-N(1)	92.2(2)	O(4)-Ni(2)-N(4)#3	82.2(2)
Compound **3**			
Cu(1)-O(1)	1.932(5)	Cu(1)-N(2)	2.003(7)
Cu(1)-O(3)#1[e]	1.979(5)	Cu(1)-C(8)#1	2.546(8)
Cu(1)-N(1)	1.995(6)	O(3)-Cu(1)#2	1.979(5)
O(1)-Cu(1)-O(3)#1	161.1(3)	O(1)-Cu(1)-N(2)	94.6(3)
O(1)-Cu(1)-N(1)	95.2(2)	O(3)#1-Cu(1)-N(2)	88.2(3)
O(3)#1-Cu(1)-N(1)	90.0(3)	N(1)-Cu(1)-N(2)	154.3(3)
Compound **3a**			
Cu(1)-O(3)#1[f]	1.950(2)	Cu(1)-N(2)	2.024(3)
Cu(1)-O(1)	1.965(2)	Cu(1)-N(1)#2	2.025(2)
O(3)#1-Cu(1)-O(1)	172.39(11)	O(3)#1-Cu(1)-N(1)#2	95.29(11)
O(3)#1-Cu(1)-N(2)	89.27(10)	O(1)-Cu(1)-N(1)#2	90.24(11)
O(1)-Cu(1)-N(2)	87.59(11)	N(2)-Cu(1)-N(1)#2	157.45(12)
Compound **3b**			
Cu(1)-O(1)	1.9532(19)	Cu(1)-N(2)	2.029(2)
Cu(1)-O(3)#1[g]	1.9629(18)	Cu(1)-N(1)#2	2.032(2)
O(1)-Cu(1)-O(3)#1	167.15(8)	O(1)-Cu(1)-N(1)#2	89.19(9)
O(1)-Cu(1)-N(2)	94.21(9)	O(3)#1-Cu(1)-N(1)#2	93.27(9)
O(3)#1-Cu(1)-N(2)	89.99(9)	N(2)-Cu(1)-N(1)#2	149.93(10)

Symmetry transformations used to generate equivalent atoms: (a) #1 –x + 1/2, y - 1/2, -z + 1/2; #2 x - 1/2, y + 1/2, z for **1**. (b) #1 –x + 1/2, y - 1/2, -z + 1/2; #2 x - 1/2, y + 1/2, z for **1a**. (c) #1 –x + 1/2,-y + 3/2, z + 1/2; #2 y - 1/2, -x + 1/2, -z + 3/2; #3 y - 1/2, -x + 3/2, -z + 3/2 for **2**. (d) #1 –x + 1/2, -y + 3/2, z + 1/2; #2 y - 1/2, -x + 1/2, -z + 3/2; #3 y - 1/2, -x + 3/2, -z + 3/2 for **2a**. (e) #1 –x + 3/2, y + 1/2, -z + 1/2; #2 –x + 3/2, y - 1/2, -z + 1/2 for **3**. (f) #1 -x, -y + 1, z + 1/2; #2 x - 1/2, -y + 1/2, z + 1 for **3a**; (g) #1 -x, -y + 2, z + 1/2; #2 x - 1/2, -y + 3/2, z + 1 for **3b**.

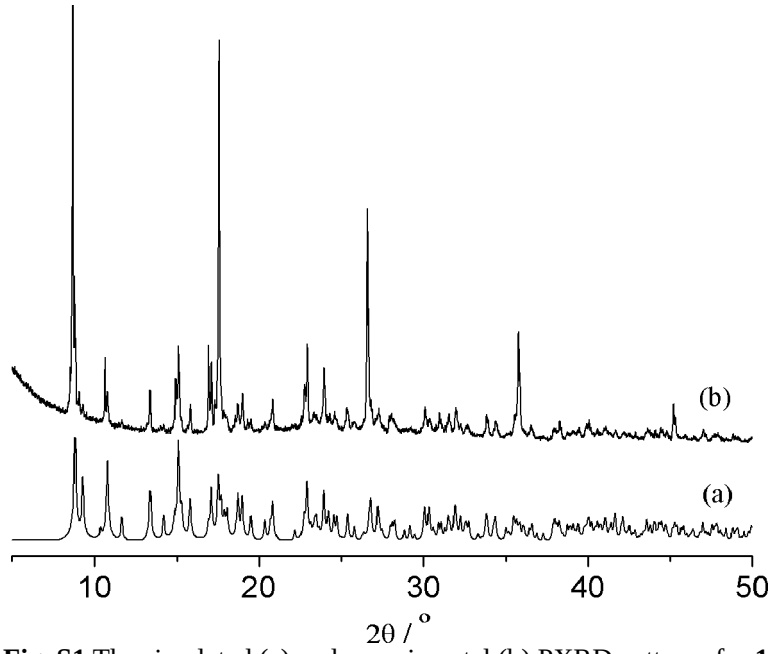

Fig. S1 The simulated (a) and experimental (b) PXRD patterns for **1**.

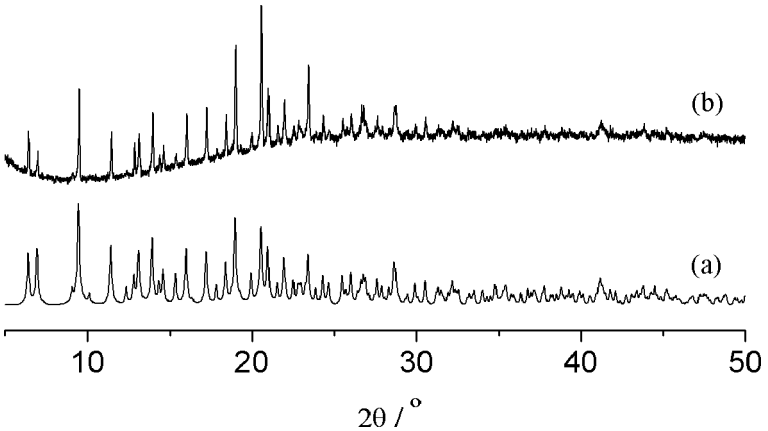

Fig. S2 The simulated (a) and experimental (b) PXRD patterns for **2**.

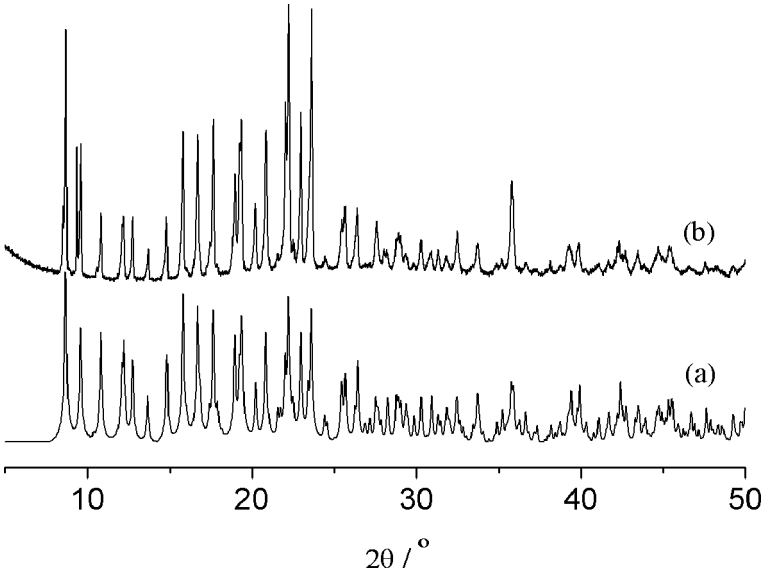

Fig. S3 The simulated (a) and experimental (b) PXRD patterns for **3**.

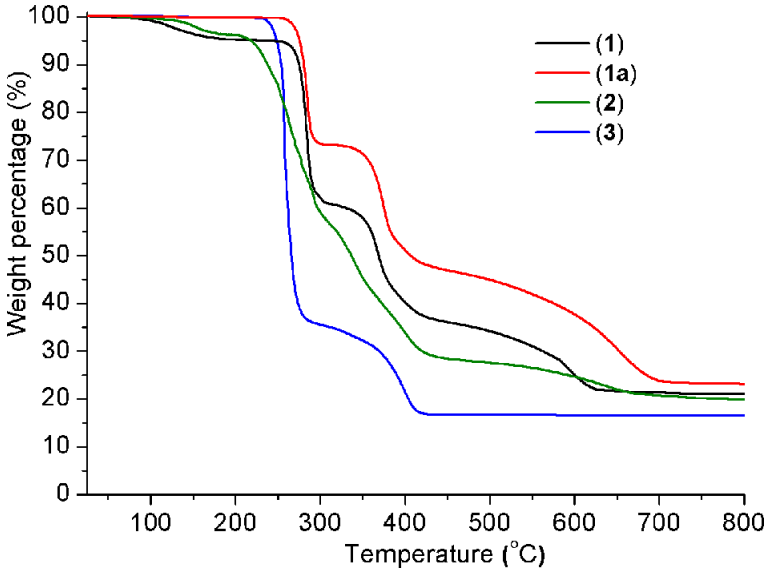

Fig. S4 TGA plots of **1**-**3.**