Self-assembly of Metal-Organic Frameworks: From Packing Helical Channels to 2-Fold Interpenetration Helical Layers

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Supporting Information

Table 1. Structure Determination Summary for 1-2

Complex	**1**	**2**
Empirical formula	$C_{18}H_{23}CdN_5O_{10}$	$C_{18}H_{21}CdN_5O_9$
Formula weight	581.81	563.80
Temperature (K)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073
Crystal system, Space group	Monoclinic, *P*2(1)/*n*	Monoclinic, *P*2/*n*
a (Å)	9.1733(10)	10.5156(15)
b (Å)	10.6165(11)	9.3977(13)
c (Å)	24.064(3)	23.034(3)
α (°)	90	90
β (°)	90.7180(10)	99.967(2)
γ (°)	90	90
V (Å^3)	2343.3(4)	2241.9(5)
Z, D_{calc} (Mg·m^{-3})	4, 1.649	4, 1.670
F(000)	1176	1136
Absorption coefficient (mm^{-1})	0.994	1.033
θ range for data collection (°)	1.69 to 27.53	1.80 to 27.59
Reflections collected	19870	19006
Independent reflections	5358 [*R*(int) = 0.0471]	5158 [*R*(int) = 0.0323]
Data [I>2σ(I)]/parameters	5358 / 6 / 339	5158 / 0 / 306
Goodness-of-fit on F^2	1.122	1.107
R_1 indices (I > 2σ(I))	*R*1=0.0421, *wR*2=0.1032	*R*1 = 0.0370, *wR*2 = 0.1280
wR_2 indices (all data)	*R*1=0.0447, *wR*2= 0.1048	*R*1 = 0.0414, *wR*2 = 0.1350
Largest diff. peak and hole (e Å^{-3})	1.412 and -1.372	1.211 and -0.841

Table 2. Selected bond lengths (Å) and angles (°) for compounds **1** – **2**.

1					
Cd(1)-O(1)	2.249(3)	Cd(1)-N(5)#1	2.277(3)	Cd(1)-N(2)#2	2.285(3)
Cd(1)-N(4)	2.345(3)	Cd(1)-O(7)	2.500(3)		
O(1)-Cd(1)-N(5)#1	103.94(12)	O(1)-Cd(1)-N(2)#2	110.02(10)	N(4)-Cd(1)-O(7)	157.18(10)
O(1)-Cd(1)-N(4)	121.65(11)	N(5)#1-Cd(1)-N(4)	91.94(11)	N(2)#2-Cd(1)-N(4)	86.04(10)
O(1)-Cd(1)-O(7)	80.87(10)	N(5)#1-Cd(1)-O(7)	85.27(10)	N(2)#2-Cd(1)-O(7)	82.12(10)
Symmetry codes: #1 -x+3/2, y-1/2, -z+1/2; #2 -x+1, -y+1, -z+1; #3 -x+3/2, y+1/2, -z+1/2					
2					
Cd(1)-O(1)#1	2.229(3)	Cd(1)-N(1)	2.287(2)	Cd(1)-N(5)#2	2.312(2)
Cd(1)-N(4)	2.363(3)	Cd(1)-O(5)	2.430(2)		
O(1)#1-Cd(1)-N(1)	111.12(11)	N(4)-Cd(1)-O(5)	162.67(10)	N(1)-Cd(1)-N(5)#2	138.84(9)
O(1)#1-Cd(1)-N(4)	116.81(11)	N(1)-Cd(1)-N(4)	87.52(9)	N(5)#2-Cd(1)-N(4)	90.53(10)
O(1)#1-Cd(1)-O(5)	80.37(8)	N(1)-Cd(1)-O(5)	83.30(9)	N(5)#2-Cd(1)-O(5)	86.30(9)
Symmetry codes: #1 -x+1, -y+1, -z+1; #2 -x+3/2, y-1, -z+1/2; #3 -x+3/2, y+1, -z+1/2					

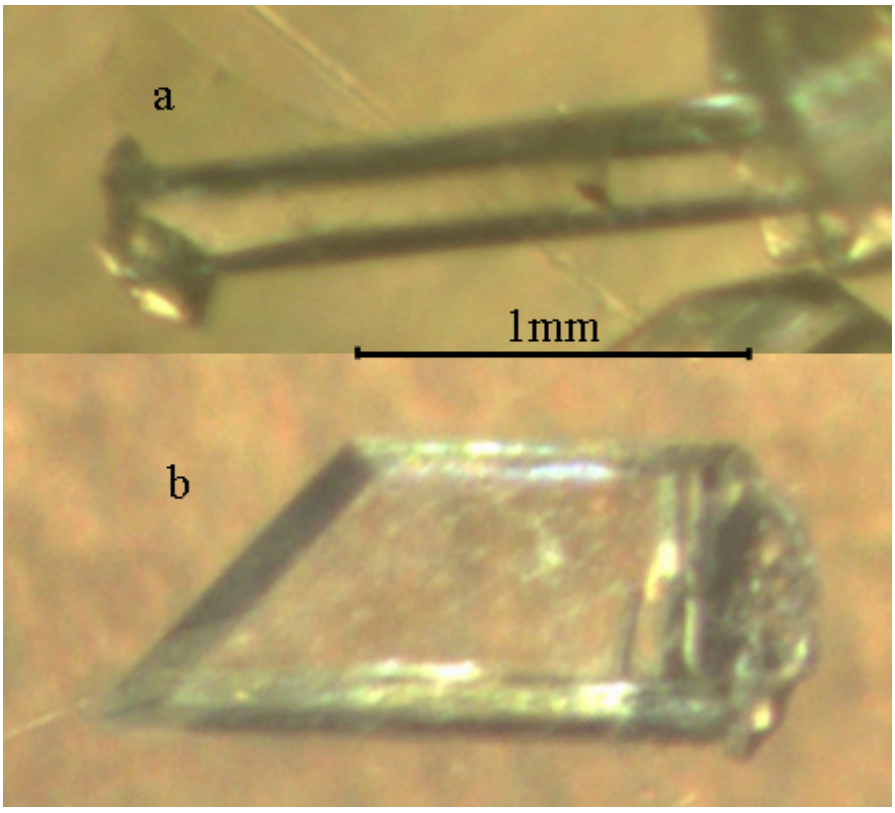

Figure S1. (a) for complex **1**; (b) for **2**.

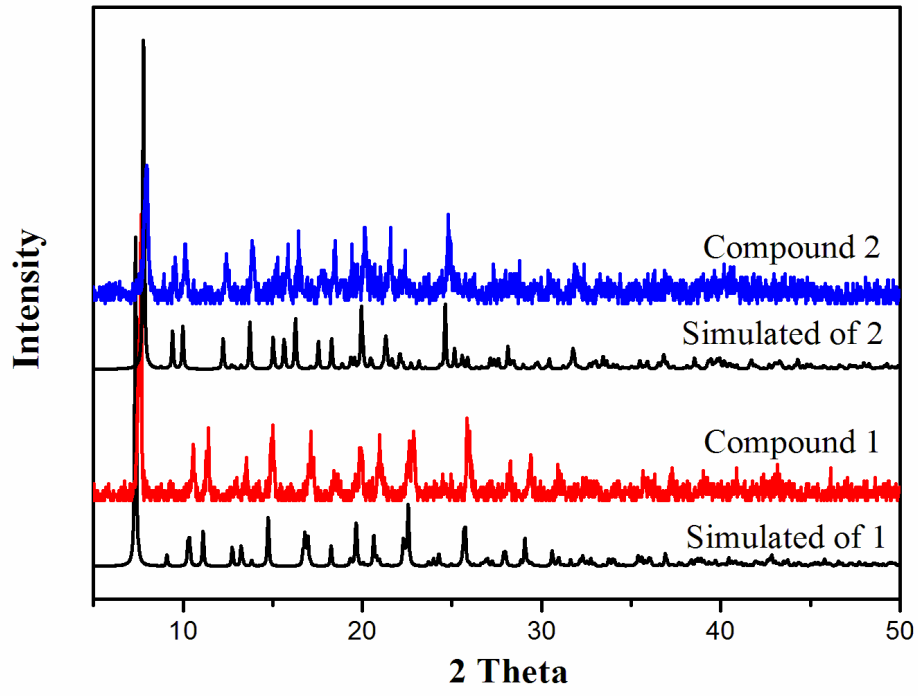

Figure S2. Experimental and simulated powder XRD patterns of **1** and **2**.

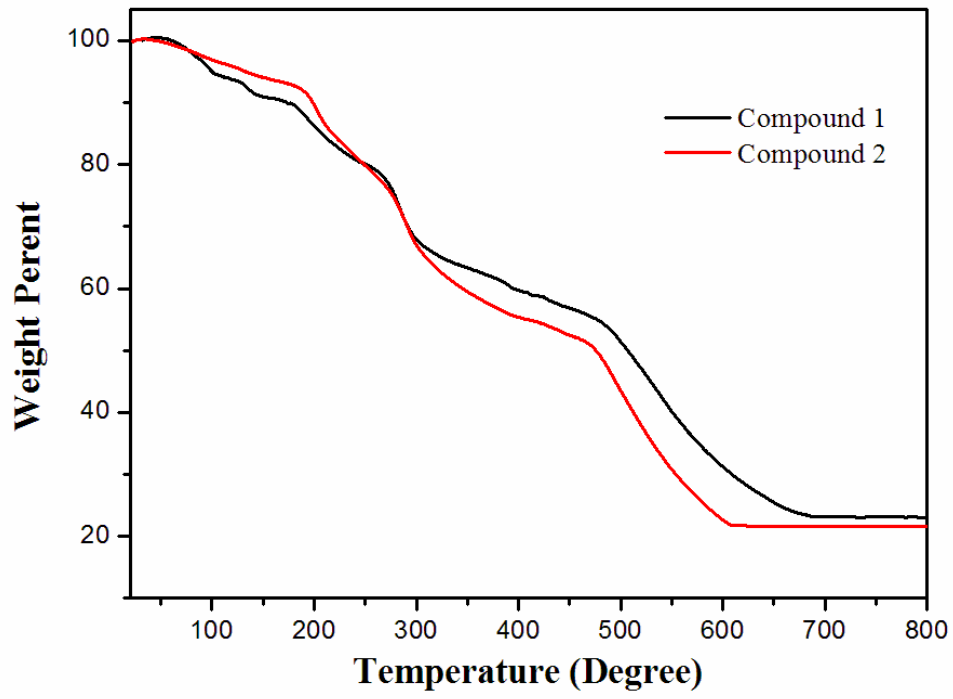

Figure S3. The thermogravimetric analyses patterns of **1** and **2**.

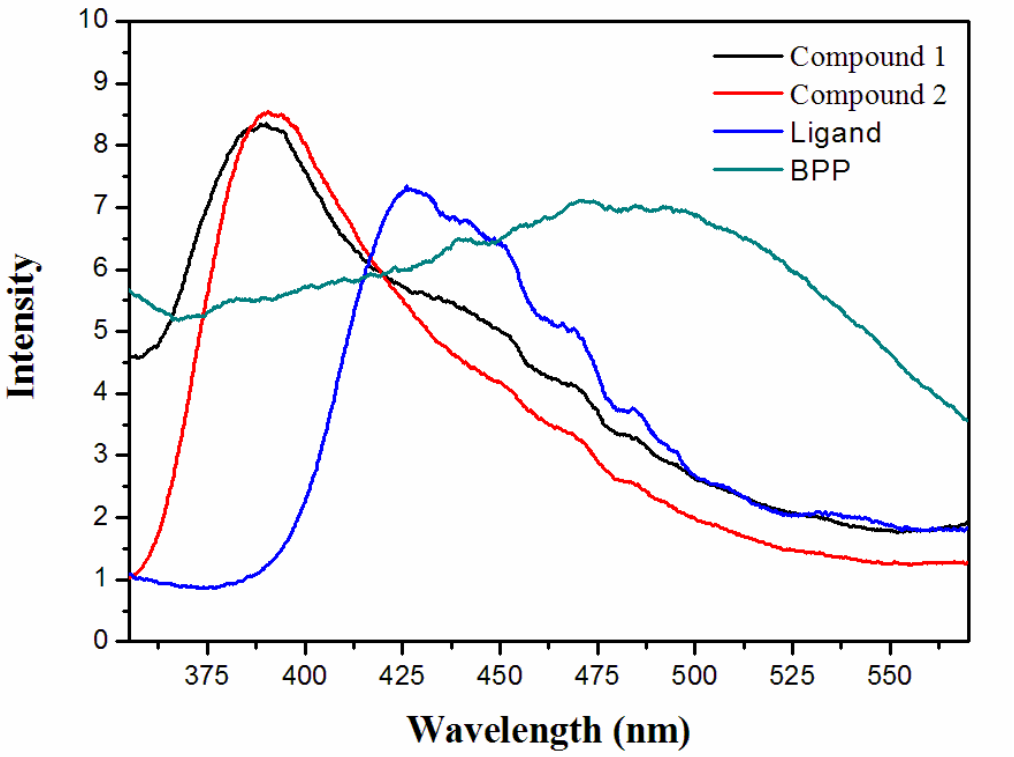

Figure S4. The solid-state emission spectra of organic ligands, **1** and **2** at room temperature.