Anion-dependent assembly and solvent-mediated structural transformations of three Cd(II) coordination polymers based on 1H-imidazole-4-carboxylic acid

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Supporting information

Table S1 Selected bond lengths [Å] and angles[°] for the compounds.[a]

Compound **1**

Cd(1)-N(1)	2.250(2)	Cd(1)-N(3)	2.272(2)
Cd(1)-O(4)#1	2.272(2)	Cd(1)-O(1W)	2.300(2)
Cd(1)-O(3)	2.385(2)	Cd(1)-O(1)	2.397(2)
N(1)-Cd(1)-N(3)	117.93(9)	N(1)-Cd(1)-O(4)#1	146.06(9)
N(3)-Cd(1)-O(4)#1	89.72(8)	N(1)-Cd(1)-O(1W)	105.11(9)
N(3)-Cd(1)-O(1W)	88.78(8)	O(4)#1-Cd(1)-O(1W)	94.04(8)
N(1)-Cd(1)-O(3)	82.32(8)	N(3)-Cd(1)-O(3)	71.77(8)
O(4)#1-Cd(1)-O(3)	88.93(8)	O(1W)-Cd(1)-O(3)	160.32(8)
N(1)-Cd(1)-O(1)	72.07(8)	N(3)-Cd(1)-O(1)	169.96(8)
O(4)#1-Cd(1)-O(1)	81.27(7)	O(1W)-Cd(1)-O(1)	87.46(8)
O(3)-Cd(1)-O(1)	112.22(8)		

Compound **2**

Cd(1)-O(1)	2.290(4)	Cd(1)-N(1)	2.293(5)
Cd(1)-O(2)#2	2.355(4)		
O(1)-Cd(1)-O(1)#1	171.9(2)	O(1)-Cd(1)-N(1)#1	111.87(16)
O(1)-Cd(1)-N(1)	73.37(15)	N(1)#1-Cd(1)-N(1)	104.4(2)
O(1)-Cd(1)-O(2)#2	88.32(15)	O(1)#1-Cd(1)-O(2)#2	85.55(13)
N(1)#1-Cd(1)-O(2)#2	157.56(14)	N(1)-Cd(1)-O(2)#2	90.35(14)

Compound **3**

Cd(1)-O(3)	2.227(7)	Cd(1)-N(1)	2.240(9)
Cd(1)-O(2)#1	2.268(8)	Cd(1)-O(1W)	2.300(9)
Cd(1)-O(5)	2.326(8)	Cd(1)-O(1)	2.398(8)
Cd(2)-O(1)#2	2.223(8)	Cd(2)-N(3)#3	2.264(10)
Cd(2)-O(7)	2.276(9)	Cd(2)-O(4)#2	2.278(8)
Cd(2)-O(2W)	2.369(9)	Cd(2)-O(3)#3	2.374(8)
O(3)-Cd(1)-N(1)	173.8(3)	O(3)-Cd(1)-O(2)#1	93.3(3)
N(1)-Cd(1)-O(2)#1	87.8(3)	O(3)-Cd(1)-O(1W)	91.4(3)
N(1)-Cd(1)-O(1W)	94.7(3)	O(2)#1-Cd(1)-O(1W)	88.5(3)
O(3)-Cd(1)-O(5)	80.5(3)	N(1)-Cd(1)-O(5)	93.3(3)
O(2)#1-Cd(1)-O(5)	105.4(3)	O(1W)-Cd(1)-O(5)	164.2(3)
O(3)-Cd(1)-O(1)	106.6(3)	N(1)-Cd(1)-O(1)	72.7(3)
O(2)#1-Cd(1)-O(1)	159.9(3)	O(1W)-Cd(1)-O(1)	88.2(3)
O(5)-Cd(1)-O(1)	81.2(3)	O(1)#2-Cd(2)-N(3)#3	175.9(3)
O(1)#2-Cd(2)-O(7)	95.2(3)	N(3)#3-Cd(2)-O(7)	87.7(3)
O(1)#2-Cd(2)-O(4)#2	93.7(3)	N(3)#3-Cd(2)-O(4)#2	89.0(3)
O(7)-Cd(2)-O(4)#2	90.5(4)	O(1)#2-Cd(2)-O(2W)	82.1(3)
N(3)#3-Cd(2)-O(2W)	94.9(3)	O(7)-Cd(2)-O(2W)	177.2(3)

[a]Symmetry transformations used to generate equivalentatoms: #1 x, -y + 3/2, z + 1/2 for compound **1**; #1 –x + 1/2, -y + 1/2, z, #2 x - 1/4, -y + 3/4, z + 1/4 for compound **2**; #1 x - 1, y, z, #2 x-1, y+1, z, #3 x, y + 1, z for compound 3.

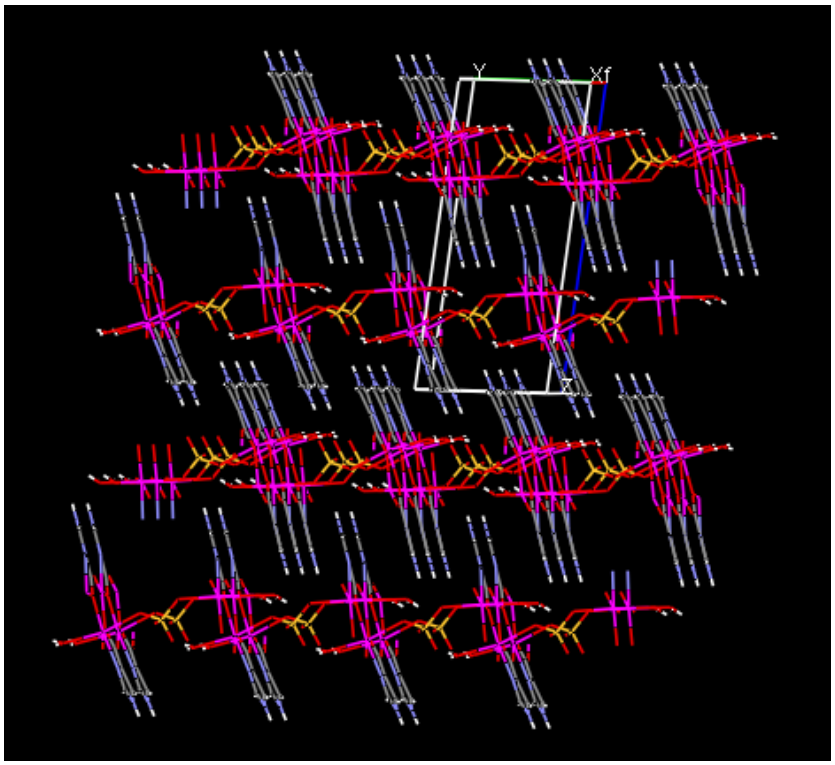

Fig. S1 The 3D supramolecular framework in compound **3**.

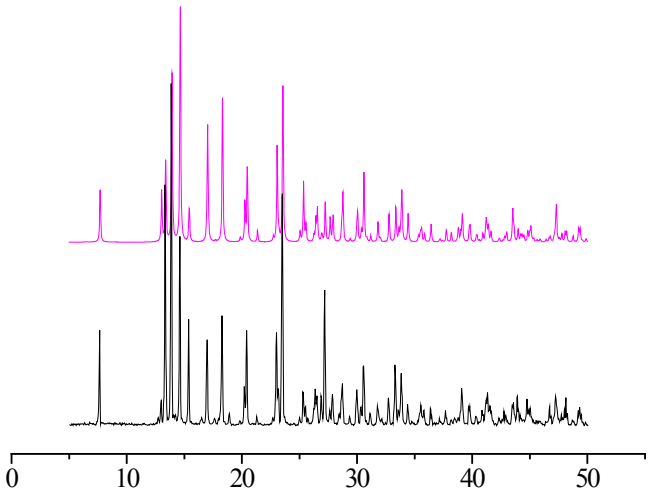

Fig. S2 The simulated X-ray powder diffraction patterns (upper) and the measured one (lower) of compound **1**

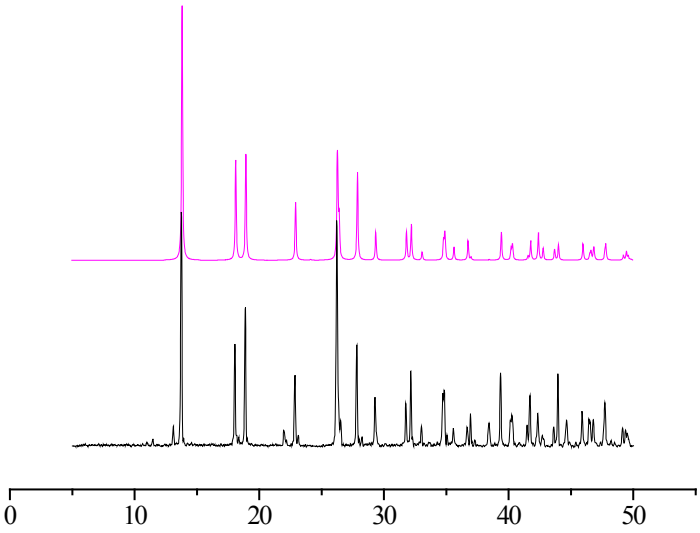

Fig. S3 The simulated X-ray powder diffraction patterns (upper) and the measured one (lower) of compound **2**

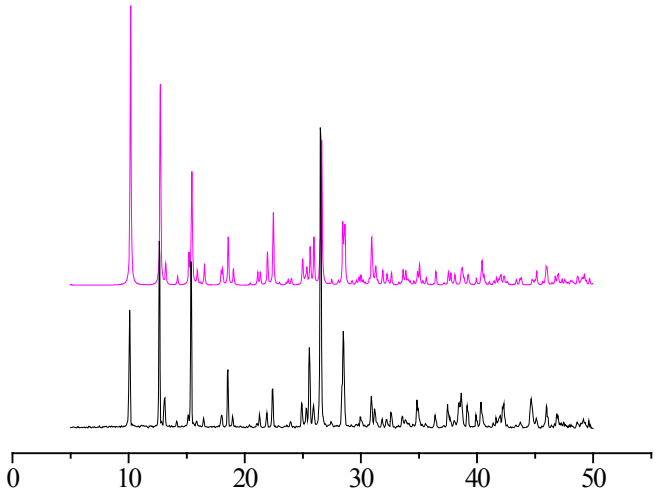

Fig. S4 The simulated X-ray powder diffraction patterns (upper) and the measured one (lower) of compound **3**

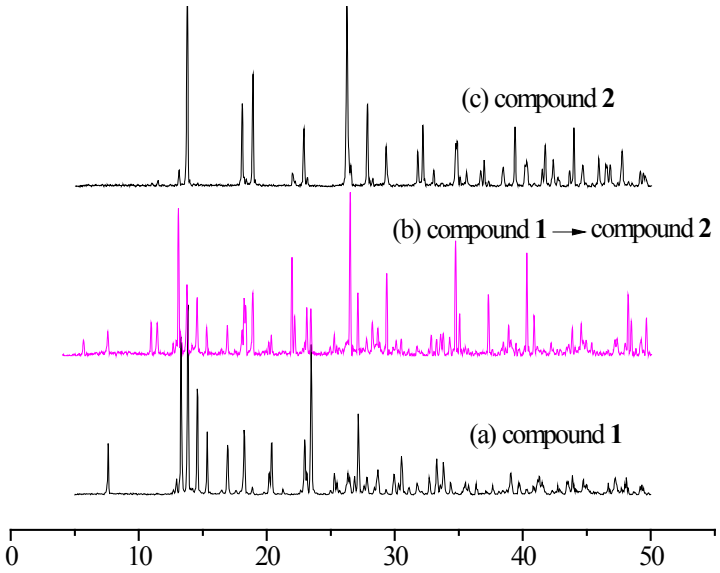

Fig. S5 Powder X-ray diffraction patterns of (a) compound **1**. (b) after the reaction of **1** with $NaClO_4$. (c) compound **2**.

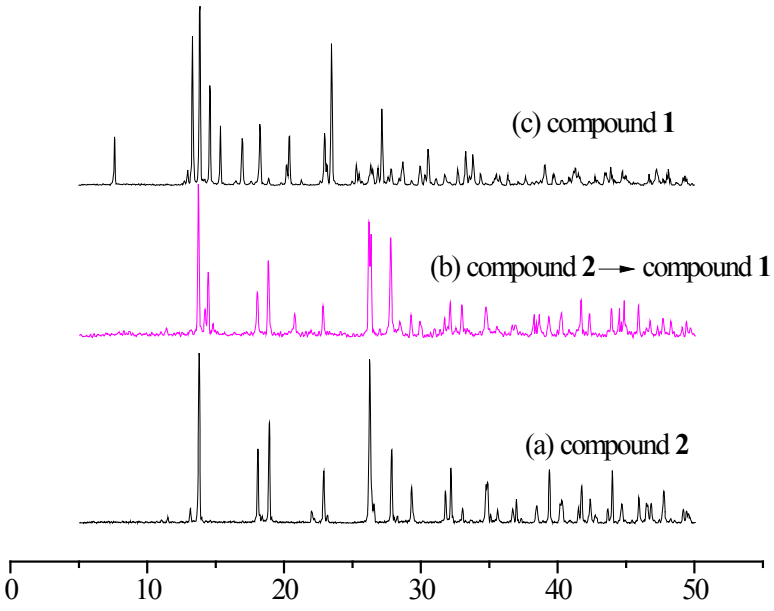

Fig. S6 Powder X-ray diffraction patterns of (a) compond **2**. (b) after the reaction of **2** with $NaNO_3$. (c) compound **1**.

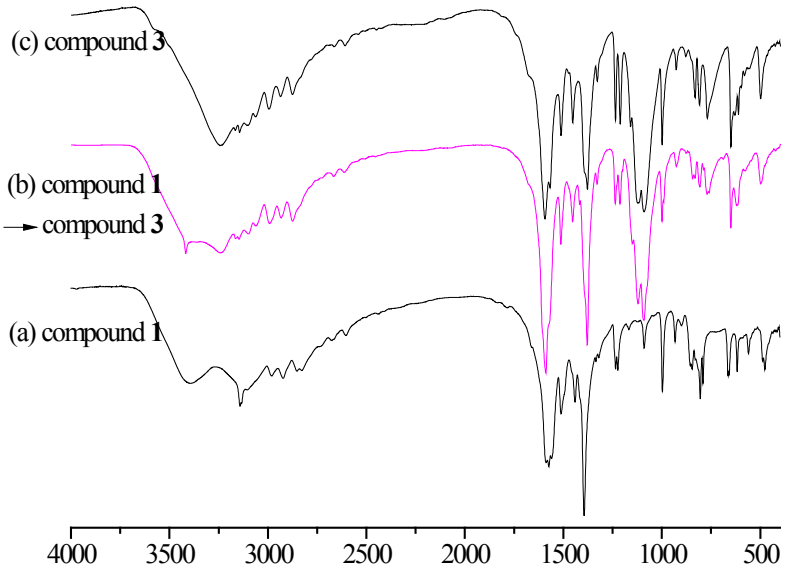

Fig. S7 FT-IR spectrum of (a) compound **1**. (b) after the reaction of **1** with Na_2SO_4. (c) compound **3**.

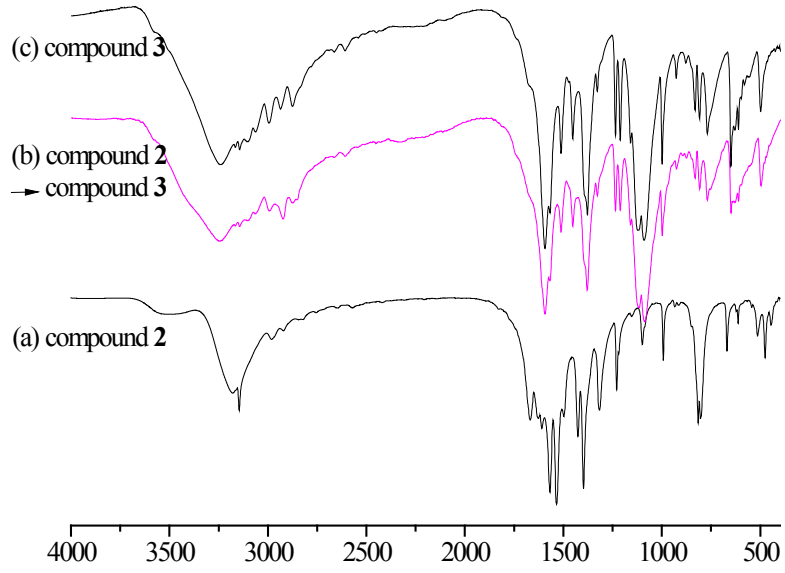

Fig. S8 FT-IR spectrum of (a) compound **2**. (b) after the reaction of **2** with Na_2SO_4. (c) compound **3**.