

Supporting Information for

The diverse structures of Cd(II) coordination polymers with 1,3,5-benzenetricarboxate tuned by organic bases

Hua Xiang, Wen-Yang Gao, Di-Chang Zhong, Long Jiang,* and Tong-Bu Lu*

Table S1 Selected bond lengths (Å) and angles (°) for **1-4^a**.

1					
Cd(1)-O(1)	2.233(6)	Cd(1)-O(3)#2	2.444(6)	Cd(1)-O(4)#2	2.372(5)
Cd(1)-O(5)#1	2.437(14)	Cd(1)-O(6)#1	2.304(15)	Cd(1)-O(7)	2.565(7)
Cd(2)-O(2)	2.185(5)	Cd(2)-O(4)#2	2.269(6)	Cd(2)-O(7)	2.347(6)
O(1)-Cd(1)-O(8)	87.7(7)	O(1)-Cd(1)-O(6)#1	136.5(3)	O(1)-Cd(1)-O(4)#2	95.0(2)
O(1)-Cd(1)-O(5)#1	82.5(3)	O(1)-Cd(1)-O(3)#2	148.2(2)	O(1)-Cd(1)-O(7)	79.8(2)
O(2)-Cd(2)-O(4)#4	94.8(2)	O(2)-Cd(2)-O(4)#2	85.2(2)	O(2)-Cd(2)-O(7)#3	86.4(2)
O(2)-Cd(2)-O(7)	93.6(2)	O(3)#2-Cd(1)-O(7)	97.1(2)	O(4)#2-Cd(1)-O(7)	74.9(2)
O(4)#2-Cd(2)-O(7)	98.8(2)	O(4)#2-Cd(2)-O(7)	81.2(2)	O(4)#2-Cd(1)-O(5)#1	162.1(4)
O(4)#2-Cd(1)-O(3)#2	54.2(2)	O(5)#1-Cd(1)-O(3)#2	129.2(3)	O(5)#1-Cd(1)-O(7)	87.3(4)
O(6)#1-Cd(1)-O(3)#2	75.0(3)	O(6)#1-Cd(1)-O(5) #1	54.3(4)	O(6)#1-Cd(1)-O(7)	92.2(4)
O(6)#1-Cd(1)-O(4)#2	124.3(4)	O(8)-Cd(1)-O(6)#1	97.3(8)	O(8)-Cd(1)-O(4)#2	105.8(7)
O(8)-Cd(1)-O(5)#1	91.8(8)	O(8)-Cd(1)-O(3)#2	93.1(7)	O(8)-Cd(1)-O(7)	167.5(7)
2					
Cd(1)-O(1)	2.392(3)	Cd(1)-O(2)	2.359(3)	Cd(1)-O(3)#4	2.350(4)
Cd(1)-O(4)#4	2.455(4)	Cd(1)-O(5)#3	2.483(4)	Cd(1)-O(6)#3	2.307(3)
Cd(1)-N(1)	2.294(3)				
O(2)-Cd(1)-O(1)	54.84(11)	O(3)#4-Cd(1)-O(4)#4	54.07(12)	O(6)#3-Cd(1)-O(5)#3	54.65(13)
N(1)-Cd(1)-O(1)	85.70(12)	N(1)-Cd(1)-O(4)#4	92.79(16)	N(1)-Cd(1)-O(5)#3	86.53(13)

3

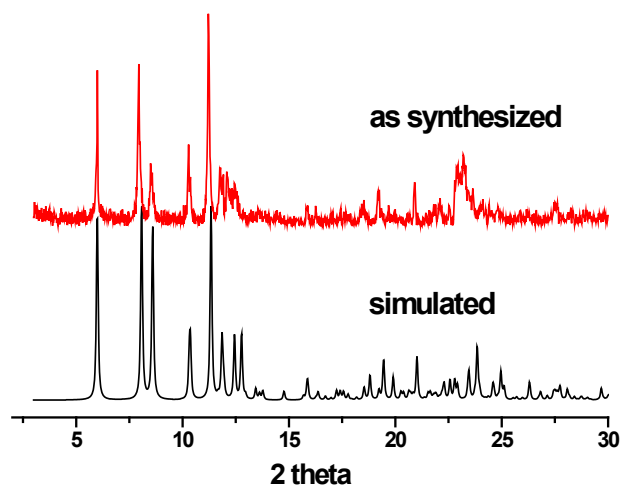
Cd(1)-O(1)	2.335(3)	Cd(1)-O(2)	2.337(2)	Cd(1)-O(7)	2.518(3)
Cd(1)-O(8)	2.319(3)	Cd(2)-O(3)	2.285(3)	Cd(2)-O(4)	2.519(3)
Cd(1)-N(1)	2.337(3)	Cd(1)-O(11)#2	2.492(3)	Cd(1)-O(12)#2	2.317(3)
Cd(2)-O(5)#4	2.406(3)	Cd(2)-O(6)#4	2.336(3)	Cd(2)-O(9)#1	2.378(3)
Cd(2)-O(10)#1	2.479(3)	Cd(2)-N(2)#3	2.324(3)		
O(2)-Cd(1)-O(1)	55.81(10)	O(8)-Cd(1)-O(7)	53.68(10)	O(4)-Cd(2)-O(3)	53.94(10)
N(1)-Cd(1)-O(1)	89.11(11)	N(1)-Cd(1)-O(7)	86.06(11)	N(1)-Cd(1)-O(8)	99.23(13)
O(11)#2-Cd(1)-O(12)#2	54.54(10)	O(6)#4-Cd(2)-O(5)#4	55.10(10)	O(9)#1-Cd(2)-O(10)#1	53.77(11)
N(2)#3-Cd(2)-O(4)	84.72(11)	N(2)#3-Cd(2)-O(5)#4	85.17(11)	N(2)#3-Cd(2)-O(10)#1	85.77(12)

4

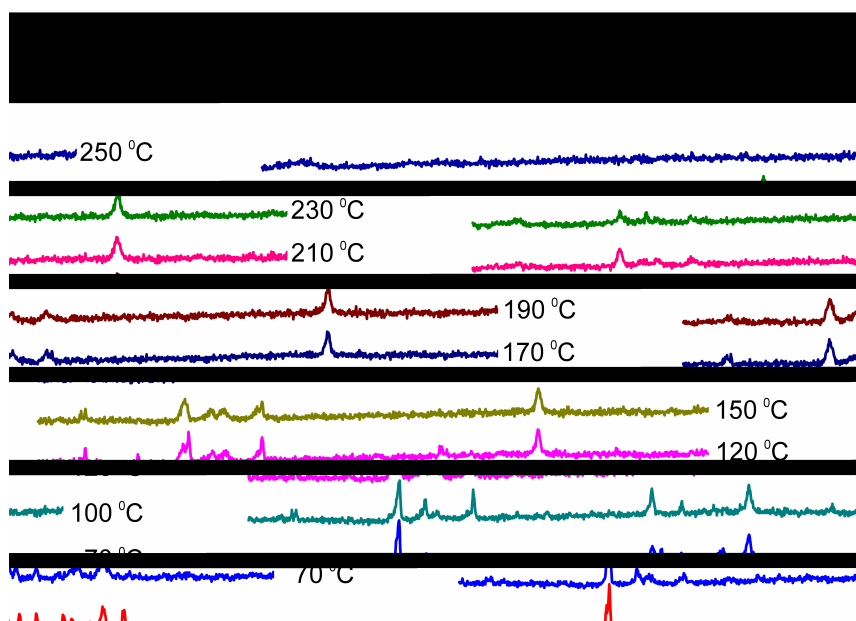
Cd(1)-O(1)	2.458(7)	Cd(1)-O(2)	2.374(7)	Cd(1)-O(3)#2	2.403(7)
Cd(1)-O(4)#2	2.305(7)	Cd(1)-O(6)#1	2.250(6)	Cd(1)-N(1)	2.220(9)
Cd(2)-N(3)	2.338(9)	Cd(2)-N(5)	2.321(9)	Cd(2)-O(1W)	2.354(7)
O(2)-Cd(1)-O(1)	54.5(2)	O(4)#2-Cd(1)-O(3)#2	55.7(2)	O(6)#1-Cd(1)-O(1)	86.2(2)
O(6)#1-Cd(1)-O(3)#2	89.6(2)	N(1)-Cd(1)-O(2)	95.3(3)	N(1)-Cd(1)-O(4)#2	90.8(3)
N(1)-Cd(1)-O(6)#1	107.7(3)	O(1W)-Cd(2)-O(1W)#3	177.6(3)	N(3)-Cd(2)-O(1W)	86.3(3)
N(3)-Cd(2)-N(3)#3	85.3(4)	N(5)-Cd(2)-O(1W)	88.7(3)	N(5)-Cd(2)-N(3)	92.0(3)

Symmetry codes: #1 $x, y+1, z$, #2 $x-1/2, y+1/2, z$, #3 $-x+3/2, -y+3/2, -z+1$, #4 $-x+2, -y+1, -z+1$, for **1**; #1 $-x+3/2, y-1/2, -z+3/2$, #2 $-x+1/2, y-1/2, -z+1/2$, #3 $-x+1/2, y+1/2, -z+1/2$, #4 $-x+3/2, y+1/2, -z+3/2$, for **2**; #1 $-x+1, y+1/2, -z+1/2$, #2 $-x+1, y-1/2, -z+1/2$, #3 $-x, -y+1, -z$, #4 $-x, y+1/2, -z-3/2$, for **3**; #1 $-x, y-1/2, -z-3/2$, #2 $-x+1, y+1/2, -z+1/2$, #3 $-x+1, y-1/2, -z+1/2$, #4 $-x, -y+1, -z$, #5 $-x, y+1/2, -z-3/2$, for **4**.

(a)



(b)



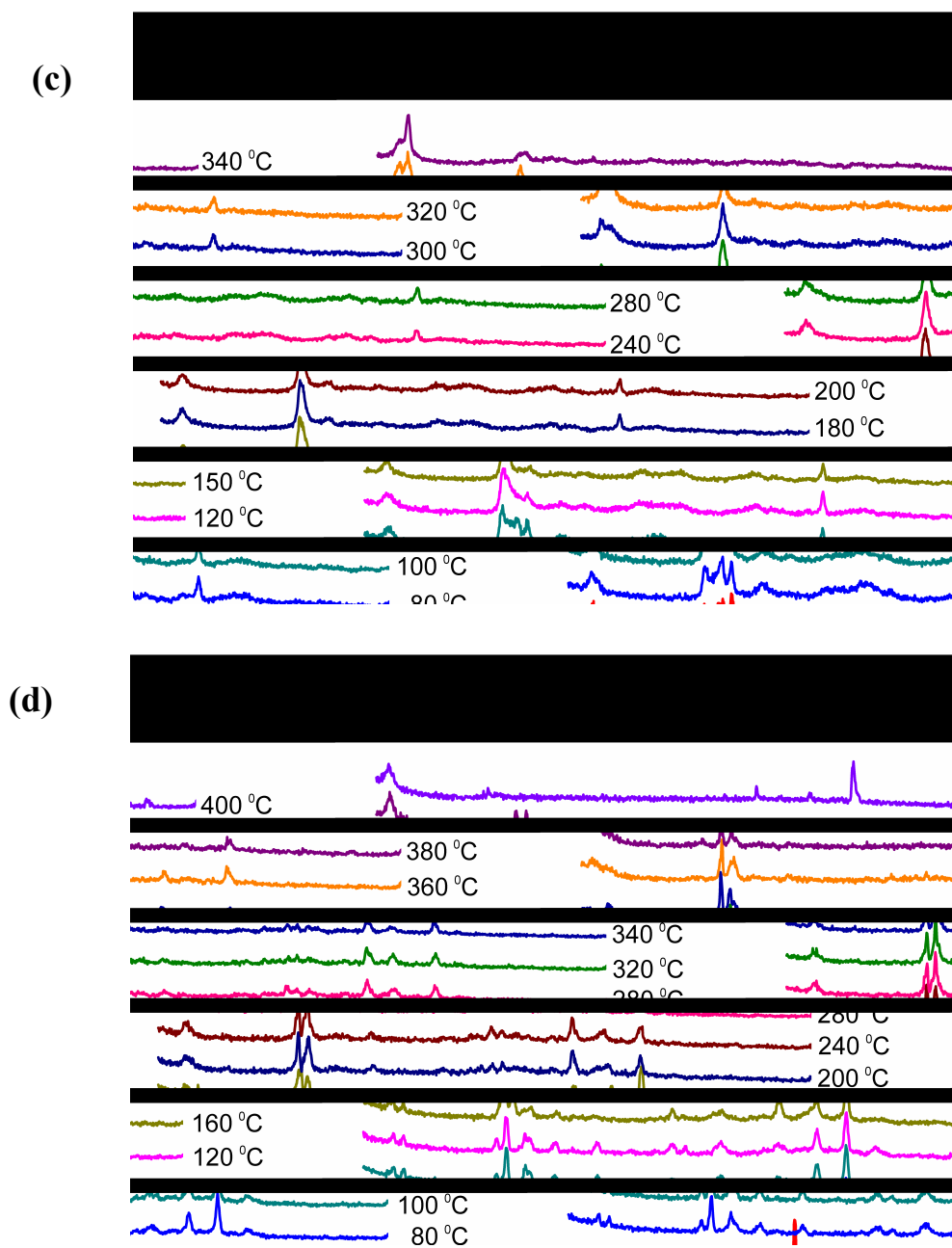


Fig. S1 The XPRD pattern for **1** (a), and the variable temperature PXRD patterns for **2** (b), **3** (c), and **4** (d), respectively.

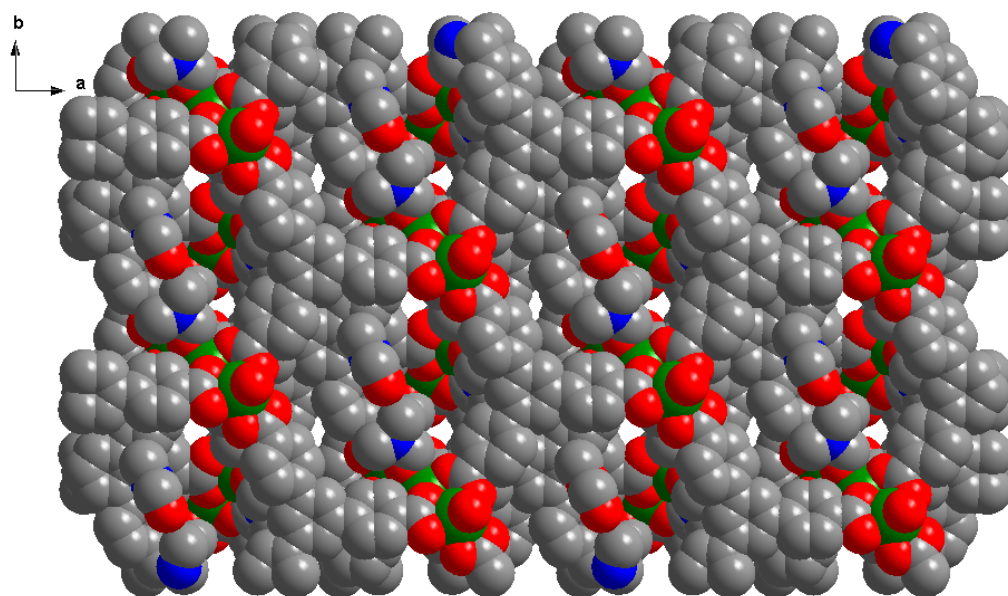


Fig. S2 The 3D structure of **1**, showing there is almost no pores.

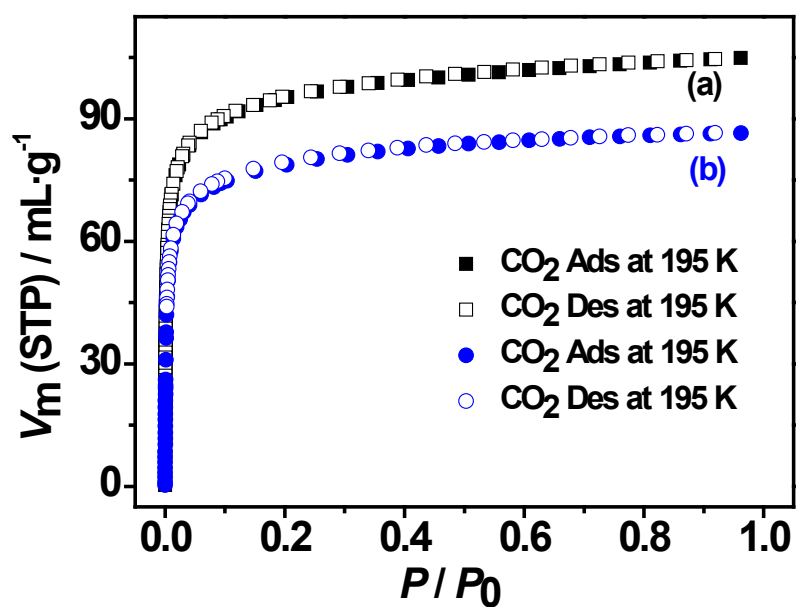


Fig. S3 The gas sorption isotherms of CO₂ for desolvated **3** degassed at 513 K (a) and 383 K (b), respectively.

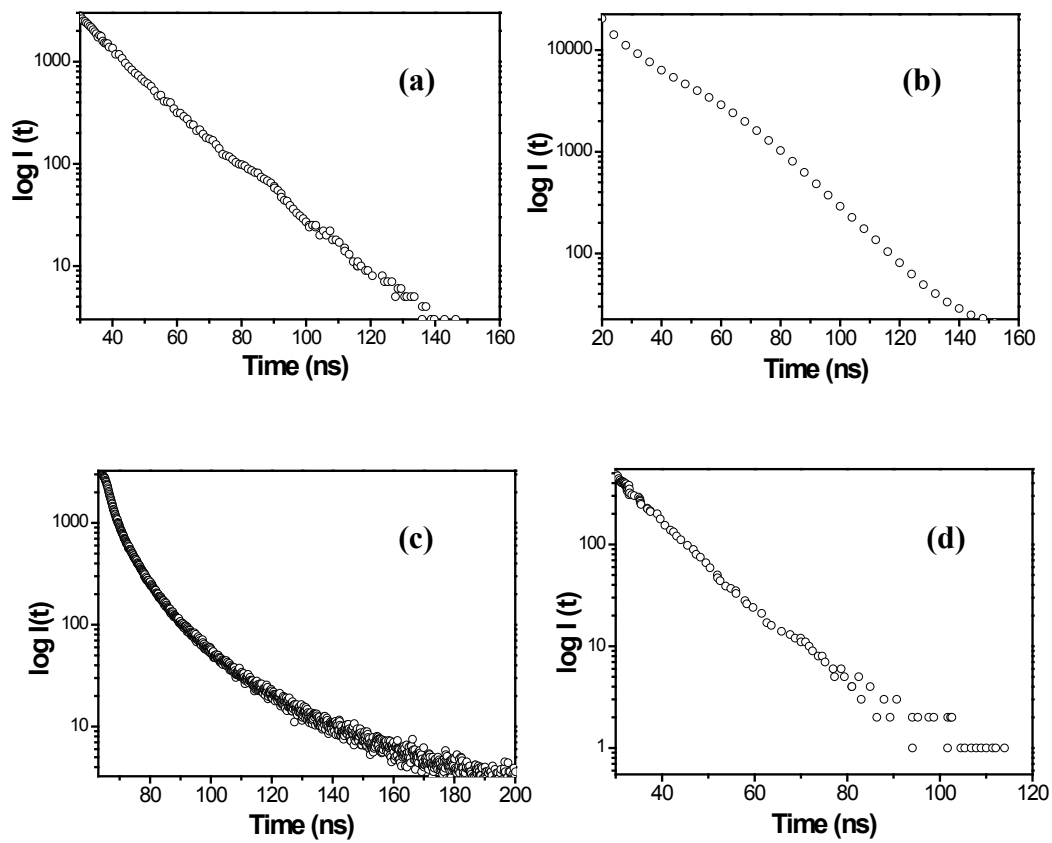


Fig. S4 The Emission decay patterns for **1** (a), **2** (b), **3** (c) and **4** (d).