Electronic Supplementary Information *for*

Guest-induced single-crystal-to-single-crystal transformations of a new 4-connected 3D cadmium(II) metal–organic framework

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Table S1. Selected bond distances /Å and bond angles /° for **1** and **1a**.

1			
Cd(1)-O(2)	1.95(3)	Cd(1)-O(4)	2.322(12)
Cd(1)-O(3)#1	2.489(15)	Cd(1)-O(6)#2	2.492(13)
Cd(1)-O(5)#2	2.500(12)	Cd(1)-N(1)#3	2.508(13)
O(2)-Cd(1)-O(4)	105.9(10)	O(2)-Cd(1)-O(3)#1	93.0(10)
O(4)-Cd(1)-O(3)#1	158.0(4)	O(2)-Cd(1)-O(6)#2	170.7(10)
O(4)-Cd(1)-O(6)#2	83.3(4)	O(3)#1-Cd(1)-O(6)#2	77.7(4)
O(2)-Cd(1)-O(5)#2	126.7(14)	O(4)-Cd(1)-O(5)#2	81.3(4)
O(3)#1-Cd(1)-O(5)#2	78.3(4)	O(6)#2-Cd(1)-O(5)#2	52.5(4)
O(2)-Cd(1)-N(1)#3	98.2(14)	O(4)-Cd(1)-N(1)#3	83.2(5)
O(3)#1-Cd(1)-N(1)#3	105.6(5)	O(6)#2-Cd(1)-N(1)#3	83.9(4)
O(5)#2-Cd(1)-N(1)#3	135.0(4)		
1a			
Cd(1)-O(1)#1	2.298(18)	Cd(1)-O(4)	2.435(18)
Cd(1)-O(3)	2.431(15)	Cd(1)-N(1)#2	2.547(17)

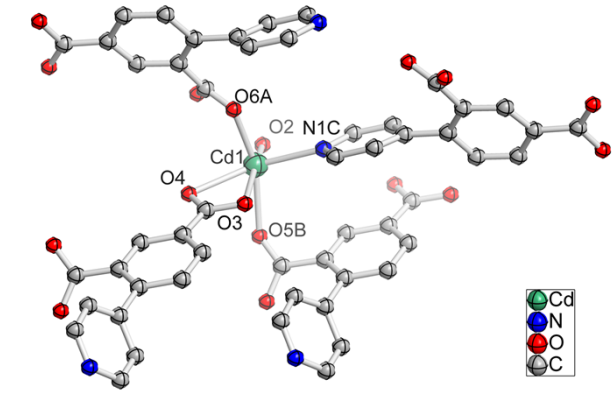
Cd(1)-O(2)#3	2.597(13)		
O(1)#1-Cd(1)-O(4)	80.4(5)	O(1)#1-Cd(1)-O(3)	81.4(5)
O(4)-Cd(1)-O(3)	53.1(5)	O(1)#1-Cd(1)-N(1)#2	81.3(6)
O(4)-Cd(1)-N(1)#2	81.7(6)	O(3)-Cd(1)-N(1)#2	133.6(6)
O(1)#1-Cd(1)-O(2)#3	155.7(6)	O(4)-Cd(1)-O(2)#3	76.8(6)
O(3)-Cd(1)-O(2)#3	78.3(5)	N(1)#2-Cd(1)-O(2)#3	103.2(5)

Symmetry operations: Complex **1**: #1: $y + 1, -x + y + 1, -z + 2$; #2: $y + 1, -x + y + 1, -z + 1$; #3: $-x + 5/3, -y + 1/3, -z + 7/3$; Complex **1a**: #1: $y - 1/3, -x + y + 1/3, -z + 4/3$; #2: $-y + 4/3, x - y + 5/3, z - 4/3$; #3: $x, y, z - 1$.

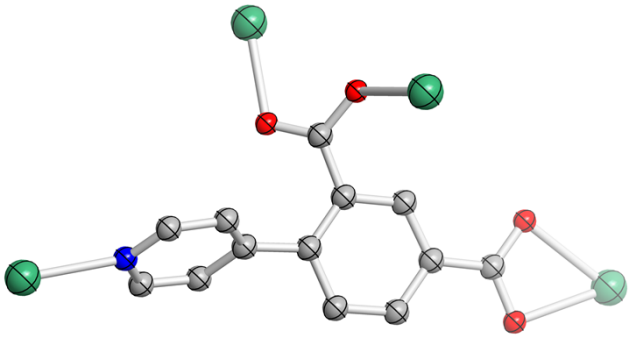
Table S2. Distance (Å) and angles (°) of hydrogen bonding for **1**[a].

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
O(2)-H(4W)···O(5)#6	1.35	2.04	2.91(3)	116.9
O(2)-H(3W)···O(3)#1	1.21	2.58	3.24(4)	112.5
O(2)-H(3W)···O(1)#6	1.21	1.90	2.61(5)	111.7
O(1)-H(2W)···O(5)#2	0.85	1.97	2.82(3)	178.3
O(1)-H(1W)···O(1)#5	0.85	1.96	2.81(3)	176.4

[a] Symmetry codes: #1, $y + 1, -x + y + 1, -z + 2$; #2, $y + 1, -x + y + 1, -z + 1$; #5, $x - y, x - 1, -z + 1$; #6, $x, y, z + 1$.



(a)



(b)

Fig. S1. View of the local coordination geometry of Cd(II) atom (a) and pic ligand (b) in **1**. Hydrogen atoms are omitted for clarity. Symmetry codes, A = y, $-x + y$, $-z + 2$; B = x, y, $z + 1$; C = $-y + 2/3$, $x - y + 1/3$, $z + 4/3$.

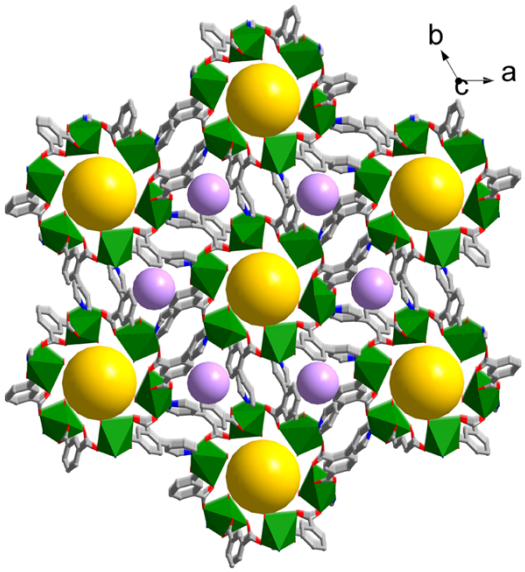
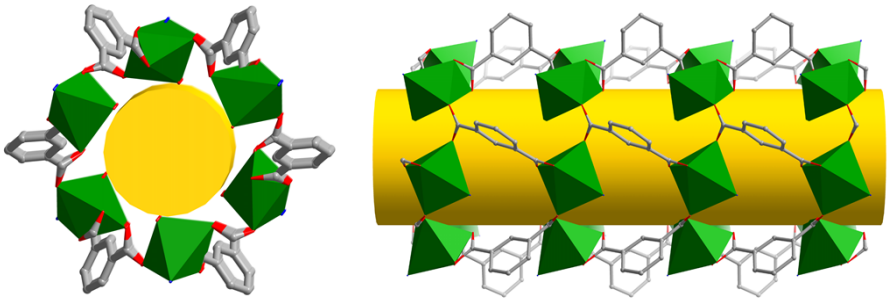
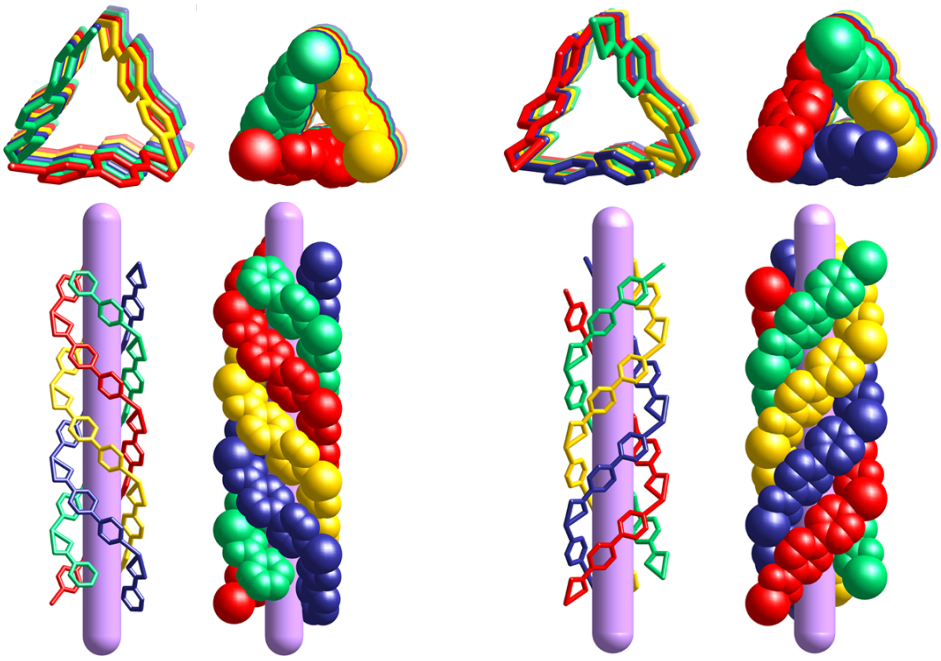


Fig. S2. View of the 3D framework shows two different channels, which are highlighted as semitransparent colored spheres (yellow and pink spheres has a diameter of 7.4 and 4.0 Å, respectively).



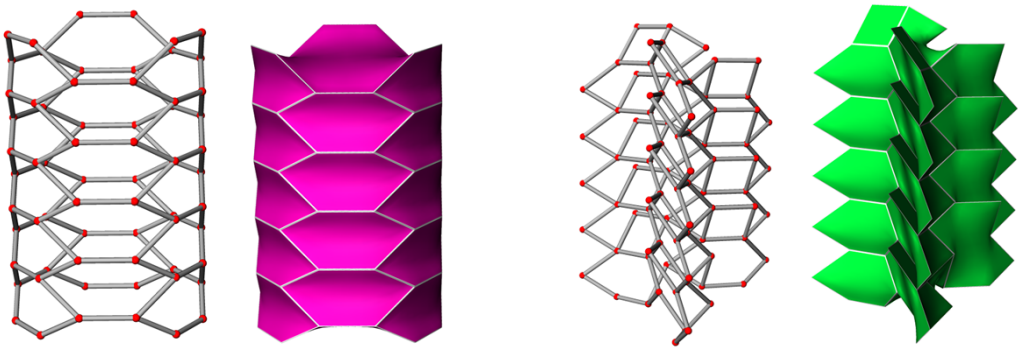
(a) (b)

Fig. S3. Top (a) and side (b) view of the star-like channel.



(a) (b)

Fig. S4. Stick and space-filling view of the four-fold left- (a) and right-handed helical channels (b).



(a) (b)

Fig. S5. Topological and tilling views of (a) ($6^3.12^2$) cage, and (b) ($4.6.8^3$) cage.

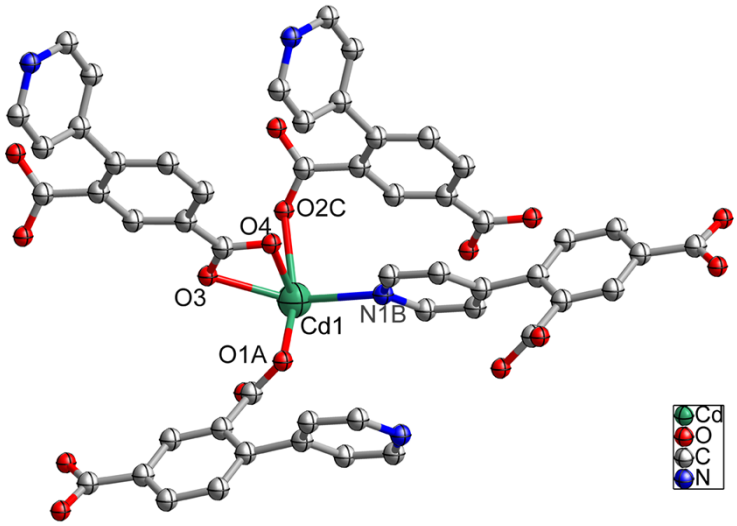
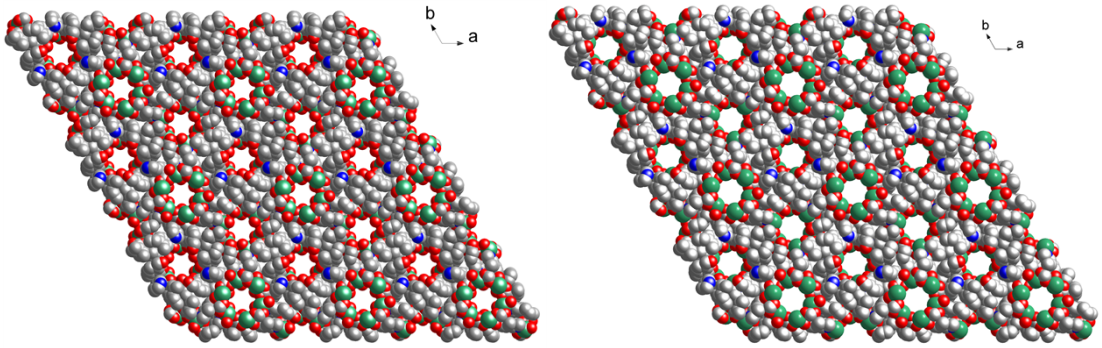


Fig. S6. View of the local coordination geometry of Cd(II) atom in **1a**. Hydrogen atoms are omitted for clarity. Symmetry codes, A = *y* – 1/3, –*x* + *y* + 1/3, –*z* + 4/3; b = –*y* + 4/3, *x* –*y* + 5/3, *z* – 4/3; C = #3 *x*, *y*, *z* – 1.



(a) (b)

Fig. S7. Space-filling view of the 3D porous structures of **1** (a) and **1a** (b).

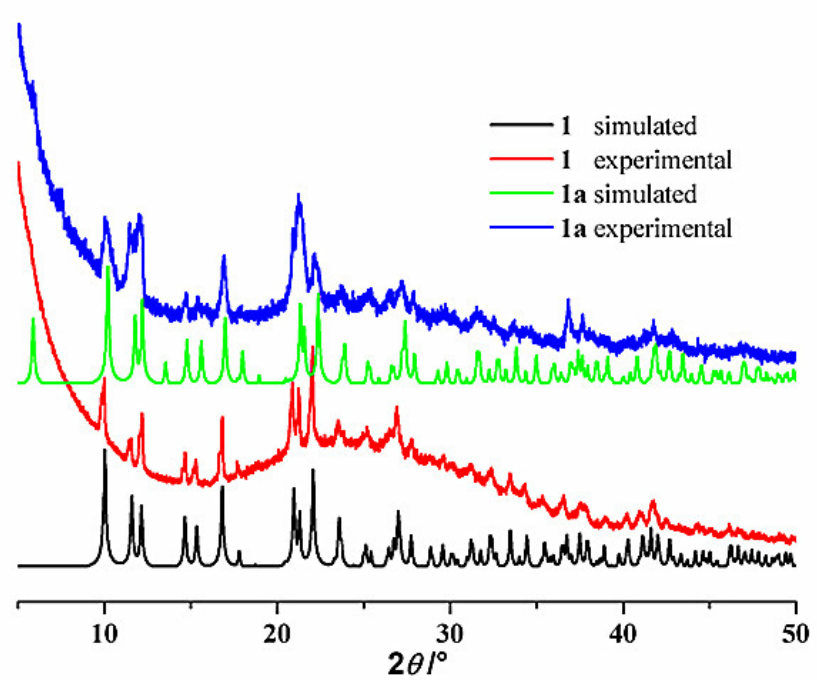


Fig. S8. XRPD patterns of 1 and 1a.

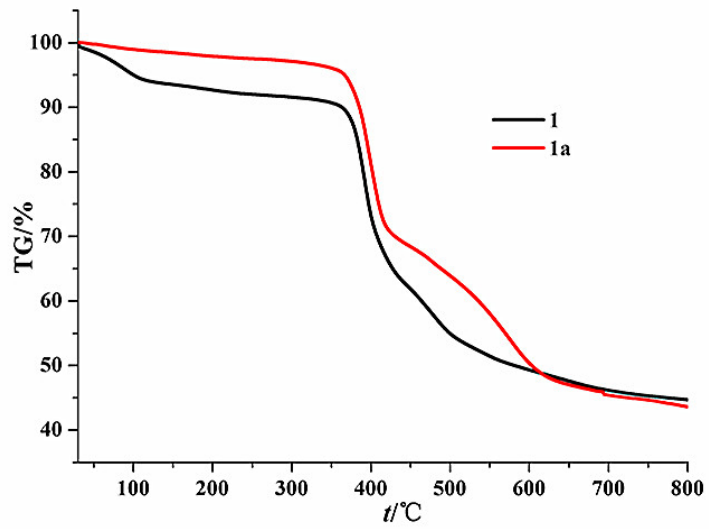


Fig. S9. TGA curve of complexes **1** and **1a**.

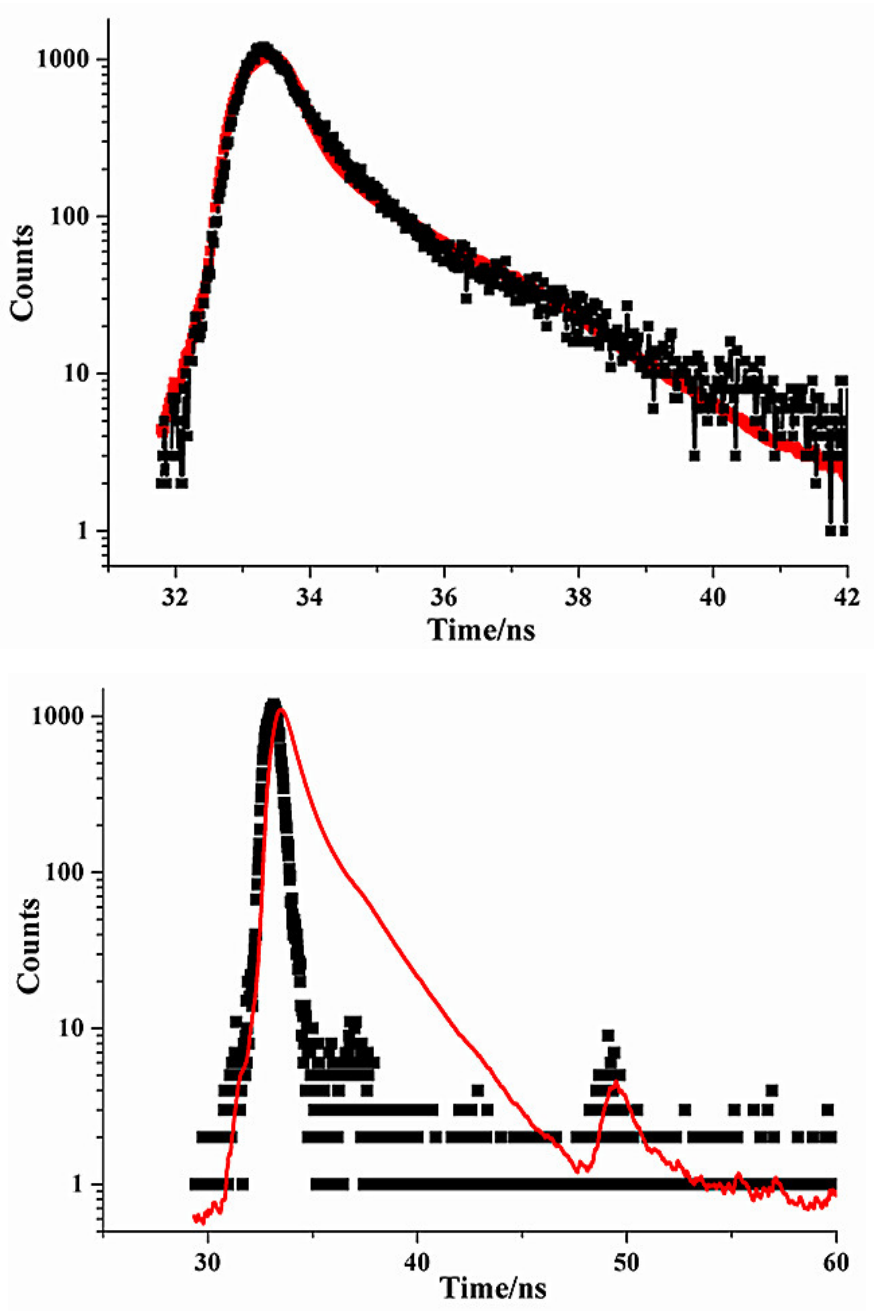


Fig. S10. Fluorescence dacay curves for pristine **1** at 298 K (top) and 77 K (bottom).

Table S2. Photoluminescent lifetime data for **1** at room temperature.

Temp./K	Lifetime (ns)	
	τ_1	τ_2
298	0.1166 (62.49%)	1.604 (37.51%)
77	0.5235 (54.40%)	2.219 (45.602%)

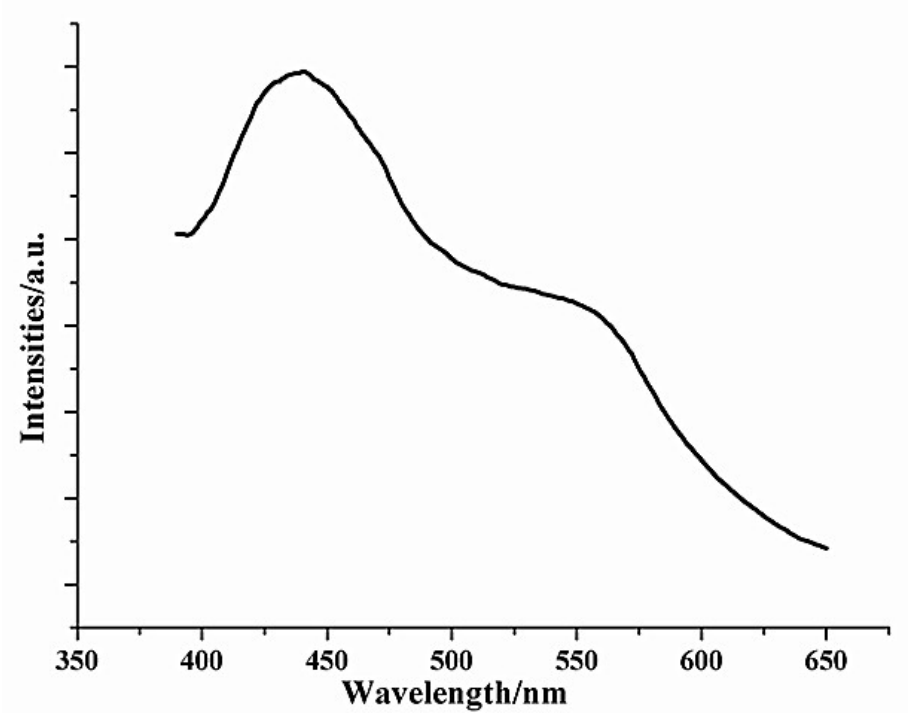


Fig. S11. Emission spectrum for solid **1a** at 298 K (λ_{ex} = 370 nm).