

Supporting Information

A robust porous pillar-chained Cd-framework with selective sorption for CO₂ and guest-driven tunable luminescence

Teng Li,^{a,b} Jian Yang,^a Xu-Jia Hong,^a Yan-Jun Ou,^a
Zhi-Gang Gu^{*c} and Yue-Peng Cai^{*a,b}

^aSchool of Chemistry and Environment, South China Normal University; Key Laboratory of the Energy Conversion and Energy Storage Materials, Guangzhou 510006, P.R. China.

^bKey Laboratory of Theoretical Chemistry of Environment, Ministry of Education, Guangzhou 510006, P.R. China

^cInstitute of Functional Interface (IFG), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

Content

Table S1 Crystal data and structure refinement of three compounds **1**, **1a** and **1b**.

Table S2 Selected bond lengths and angles for three compounds **1**, **1a** and **1b**.

Table S3 Distances (Å) and angles (°) of hydrogen bonds for three compounds **1**, **1a** and **1b**.

Figure S1 (a) Photo picture of the colorless and transparent single crystals of compound **1**.

(b) Coordination environment of Cd^{II} ion and coordination mode **I** of ligand cpt ion in **1**.

Figure S2 The TGA curves of compounds **1**, **1a** and **1b**.

Figure S3 PXRD patterns of as-prepared and dehydrated samples of **1** and **1a** in comparison with the simulations from the single-crystal data.

Figure S4 VT-PXRD patterns of as-prepared samples and the simulations from the single-crystal data of **1**.

Figure S5 The TGA and DSC curves of compound **1**.

Figure S6 Solvent-free 3-D pillar-chained MOF with 1-D channels after dehydration of complex **1**.

Figure S7 Photographs showing the color change of compound **1** before and after I₂ adsorption in vapor state, (a) for a single-crystal sample; (b) for bulk samples.

Figure S8 3-D pillar-chained MOF-**1b** with 1-D channels captured molecular iodine.

Figure S9 The molecular I₂ encapsulated in 1-D channels in MOF-**1b** is stabilized in the channels through I···N and I···I interactions.

Figure S10 (a) The I₂ dissociation process when crystals of **1** were immersed in H₂O. (b) PXRD patterns of **1**, its I₂-loaded samples at 0, 1, 6, 24, 48h (namely, regenerated MOF-**1**).

Table S1 Crystal data and structure refinement of three compounds **1**, **1a** and **1b**.

	1	1a	1b
Chemical formula	C ₁₈ H ₁₆ Cd ₂ N ₆ O ₇	C ₉ H ₇ CdN ₃ O ₃	C ₉ H ₇ CdIN ₃ O ₃
<i>M</i>	653.17	317.58	444.48
Crystal system	Tetragonal	Triclinic	Triclinic
Space group	<i>P4(2)/n</i>	<i>P4(2)/n</i>	<i>P4(2)/n</i>
<i>a</i> / Å	20.872(8)	20.8164(13)	21.23(6)
<i>b</i> / Å	20.872(8)	20.8164(13)	21.23(6)
<i>c</i> / Å	5.882(2)	5.8701(4)	6.029(17)
<i>V</i> / Å ³	2562.4(16)	2543.6(3)	2717(13)
<i>Z</i>	4	8	8
<i>T</i> / K	298(2)	298(2)	298(2)
<i>F</i> (000)	1272	1232	1656
<i>D</i> _{calcd} / gcm ⁻³	1.693	1.659	2.173
<i>μ</i> / mm ⁻¹	1.705	1.712	3.879
<i>λ</i> / Å	0.71073	0.71073	0.71073
<i>R</i> _{int}	0.0683	0.0000	0.0603
data/restraint/parm	2173 / 4 / 167	2288 / 48 / 136	2284 / 0 / 167
GOF	1.089	1.081	1.086
<i>R</i> ₁ [<i>I</i> = 2σ(<i>I</i>)] ^a	0.0429	0.0313	0.0611
<i>wR</i> ₂ [<i>I</i> = 2σ(<i>I</i>)] ^b	0.1184	0.0865	0.1790
<i>R</i> ₁ [all data] ^a	0.0657	0.0390	0.0830
<i>wR</i> ₂ [all data] ^b	0.1351	0.0904	0.2029
Largest diff. peak and hole (e·Å ⁻³)	0.847 and -0.663	0.759 and -0.758	1.098 and -0.992

^a *R*₁ = Σ||*F*_o| - |*F*_c||/Σ|*F*_o|, ^b *wR*₂ = [Σ*w*(*F*_o² - *F*_c²)²/Σ*w*(*F*_o²)²]^{1/2}, where *w* = 1/[σ²(*F*_o²) + (*aP*)₂ + *bP*]. *P* = (*F*_o² + 2*F*_c²)/3.

Table S2. Selected atomic distances (Å) and bond angles (°) for compounds **1**, **1a** and **1b**^a.

1			
Cd(1)-O(3)	2.234(5)	O(3)-Cd(1)-O(3)#1	102.53(16)
Cd(1)-O(3)#1	2.259(4)	O(3)-Cd(1)-O(3)#2	100.12(15)
Cd(1)-O(3)#2	2.337(4)	O(3)#1-Cd(1)-O(3)#2	71.83(17)
Cd(1)-O(2)#3	2.338(5)	O(3)-Cd(1)-O(2)#3	94.99(17)
Cd(1)-N(1)	2.398(6)	O(3)#1-Cd(1)-O(2)#3	162.42(17)
Cd(1)-O(1)#3	2.463(5)	O(3)#2-Cd(1)-O(2)#3	103.91(17)
O(3)#2-Cd(1)-N(1)	165.90(18)	O(3)-Cd(1)-N(1)	86.36(18)
O(2)#3-Cd(1)-N(1)	87.83(18)	O(3)#1-Cd(1)-N(1)	94.63(18)
O(3)-Cd(1)-O(1)#3	145.74(15)	O(2)#3-Cd(1)-O(1)#3	54.50(17)
O(3)#1-Cd(1)-O(1)#3	108.96(16)	N(1)-Cd(1)-O(1)#3	78.13(18)
O(3)#2-Cd(1)-O(1)#3	102.16(15)		
1a			
Cd(1)-O(3)#4	2.230(3)	O(3)#5-Cd(1)-O(2)#6	104.13(12)
Cd(1)-O(3)	2.251(3)	O(3)#4-Cd(1)-N(3)	86.39(12)
Cd(1)-O(3)#5	2.323(3)	O(3)-Cd(1)-N(3)	94.65(12)
Cd(1)-O(2)#6	2.342(3)	O(3)#5-Cd(1)-N(3)	165.77(12)
Cd(1)-N(3)	2.386(4)	O(2)#6-Cd(1)-N(3)	87.70(12)
Cd(1)-O(1)#6	2.451(3)	O(3)#4-Cd(1)-O(1)#6	145.74(10)
O(3)#4-Cd(1)-O(3)	102.45(11)	O(3)-Cd(1)-O(1)#6	108.91(11)
O(3)#4-Cd(1)-O(3)#5	100.18(10)	O(3)#5-Cd(1)-O(1)#6	102.43(10)
O(3)-Cd(1)-O(3)#5	71.69(12)	O(2)#6-Cd(1)-O(1)#6	54.61(11)
O(3)#4-Cd(1)-O(2)#6	95.02(11)	N(3)-Cd(1)-O(1)#6	77.79(12)
O(3)-Cd(1)-O(2)#6	162.48(11)		
1b			
Cd(1)-O(3)#7	2.302(8)	O(3)#7-Cd(1)-O(3)#4	72.3(2)
Cd(1)-O(3)	2.313(9)	O(3)-Cd(1)-O(3)#4	99.9(2)
Cd(1)-O(3)#4	2.377(8)	O(3)#7-Cd(1)-O(1)	163.1(2)
Cd(1)-O(1)	2.385(10)	O(3)-Cd(1)-O(1)	94.8(2)
Cd(1)-N(3)#8	2.428(10)	O(3)#4-Cd(1)-O(1)	104.7(2)
Cd(1)-O(2)	2.509(8)	O(3)#7-Cd(1)-N(3)#8	94.0(2)
I(1)-I(2)	2.74(3)	O(3)-Cd(1)-N(3)#8	85.9(2)
O(3)#7-Cd(1)-O(3)	102.2(2)	O(3)#4-Cd(1)-N(3)#8	165.9(2)
O(3)#7-Cd(1)-O(2)	109.0(3)	O(1)-Cd(1)-N(3)#8	87.6(2)
O(3)#4-Cd(1)-O(2)	102.6(2)	O(3)-Cd(1)-O(2)	145.8(2)
N(3)#8-Cd(1)-O(2)	78.4(2)	O(1)-Cd(1)-O(2)	54.8(2)

^aSymmetry transformations used to generate equivalent atoms: #1 $y-1/2, -x+1, z+1/2$; #2 $-y+1, x+1/2, z+1/2$; #3 $y, -x+3/2, -z+1/2$; #4 $-y+1, x+1/2, z-1/2$; #5 $-x+1/2, -y+3/2, z$; #6 $y, -x+1/2, -z+1/2$; #7 $y-1/2, -x+1, z-1/2$; #8 $-y+3/2, x, -z+3/2$.

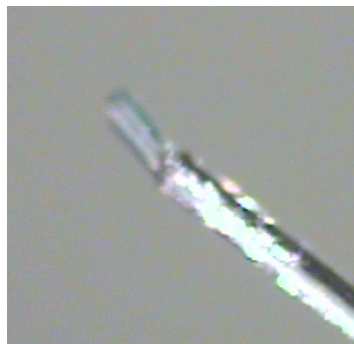
Table S3 Distances (Å) and angles (°) of hydrogen bonds for compounds **1**, **1a** and **1b**.

D-H...A	Distance (D-H)	Distance (H...A)	Distance(D...A)	Angle (D-H...A)
1				
O(3)-H3...O1#1	0.84(6)	1.95(3)	2.770(6)	165(9)
O4-H4B... π^a	0.85(6)	3.70(5)	4.052(7)	118(8)
O4-H4A... π^a	0.84(7)	3.72(6)	4.052(7)	111(9)
1a				
O(3)-H(3A)...O(1)#2	0.84(5)	1.97(6)	2.771(4)	161(5)
1b				
O(3)-H(3A)...O(2)#3	0.85(10)	2.00(11)	2.806(10)	162(8)
I1...I2#4		3.01(3)		
I1...N2		3.68(6)		
N2...I2#5		3.85(6)		
I1...I2		3.43(6)		

*Symmetry transformation used to generate equivalent atoms: #1 $y, -x+3/2, -z-1/2$; #2 $-x, -y+1, -z$; #3 $x, y, z+1$; #4 $y, 1.5-x, 1.5-z$; #5 $x, y, -1+z$; ^aDistances between the protons and centroids of benzene rings in ligand Hcpt.

Figure S1

(a)



(b)

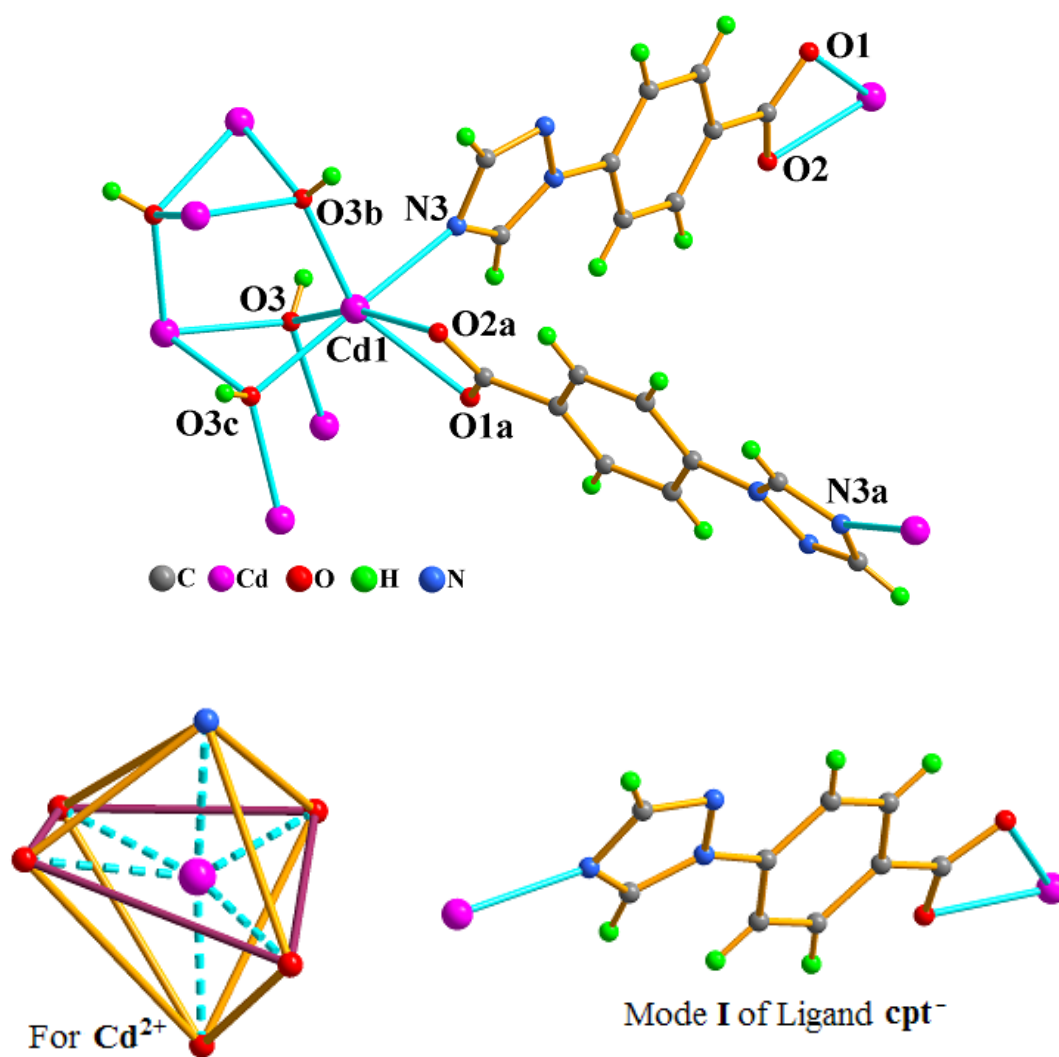


Figure S2

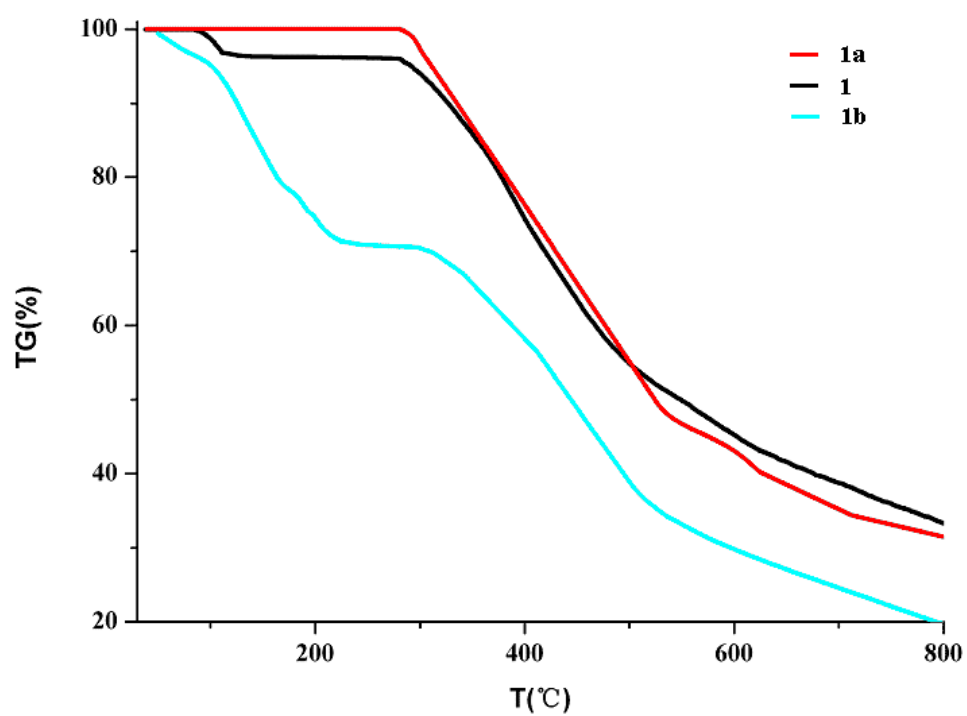


Figure S3

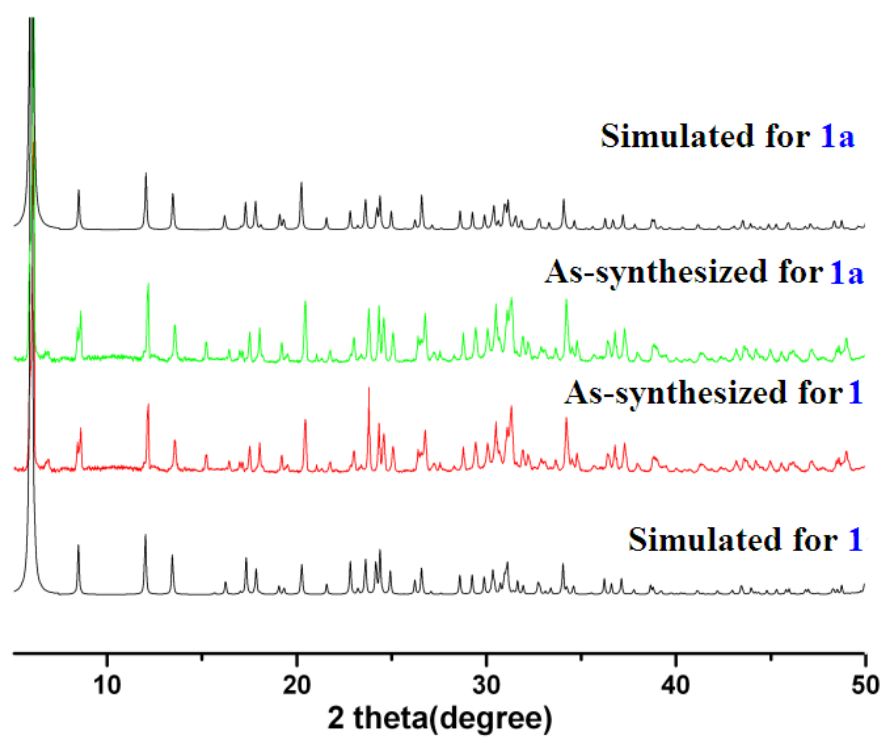


Figure S4

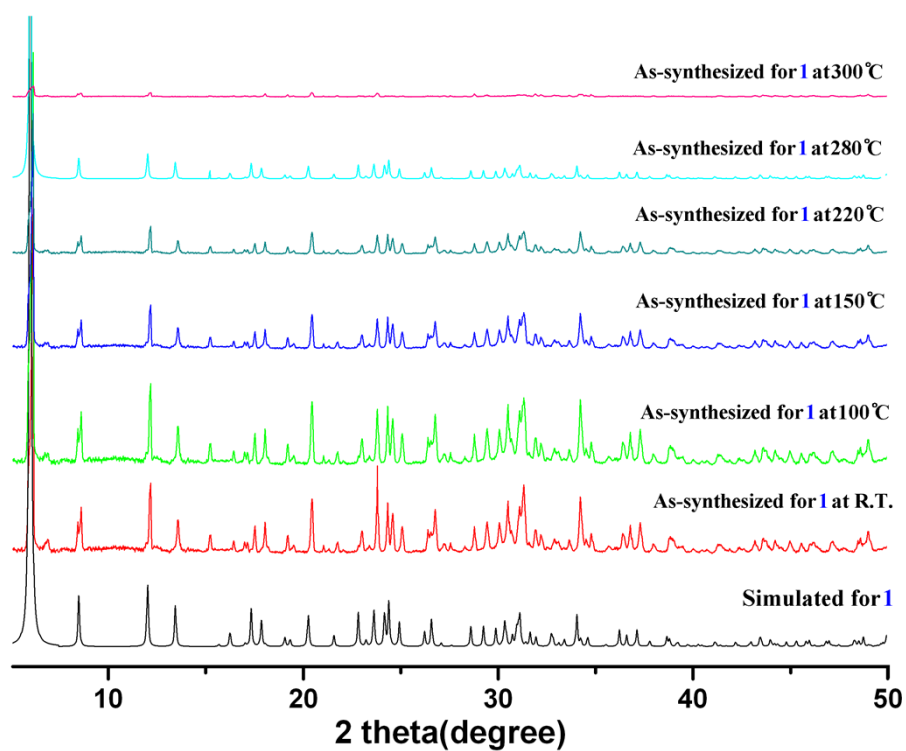


Figure S5

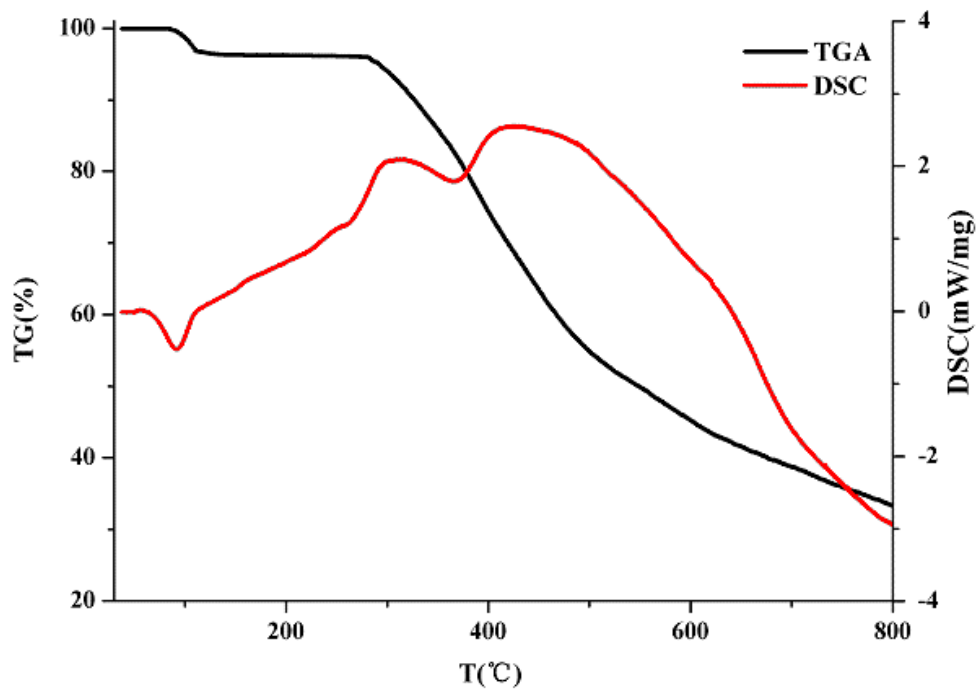


Figure S6

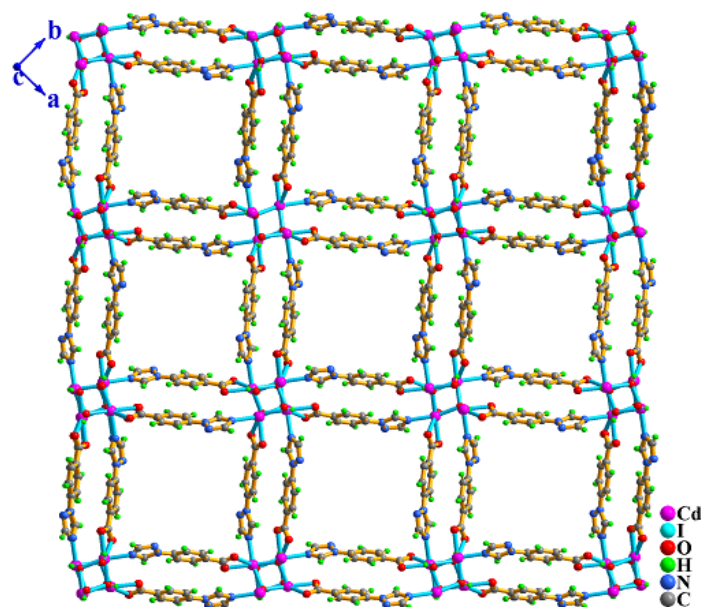
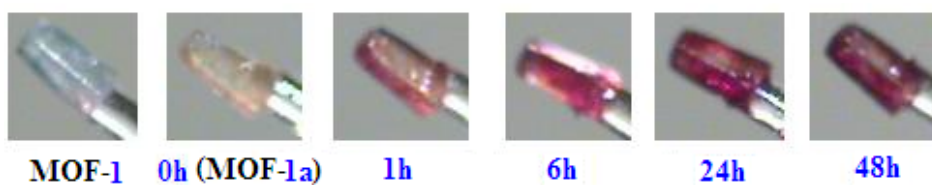


Figure S7

(a)



(b)

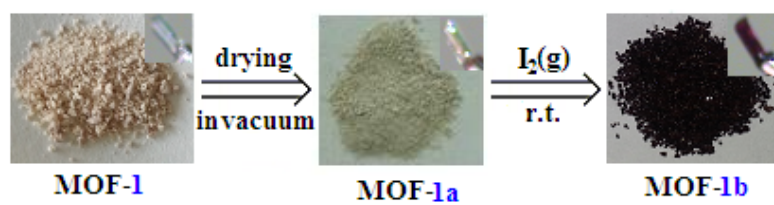


Figure S8

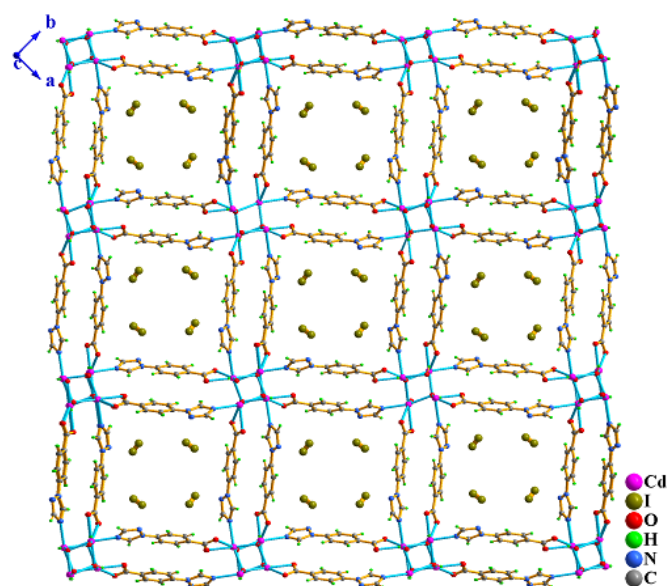
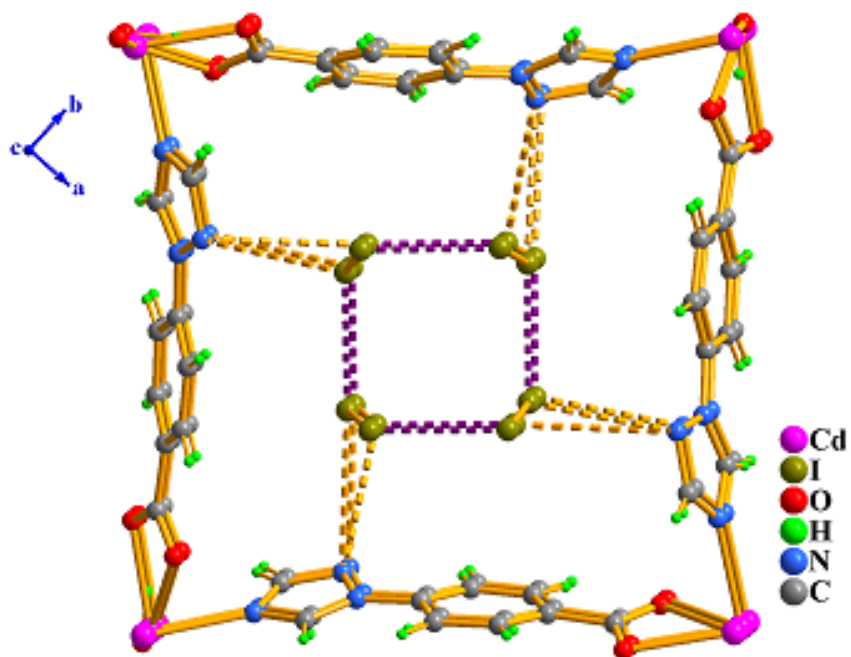
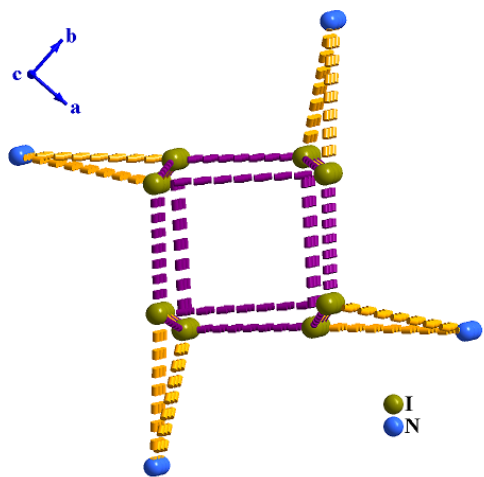


Figure S9

(a)



(b)



(c)

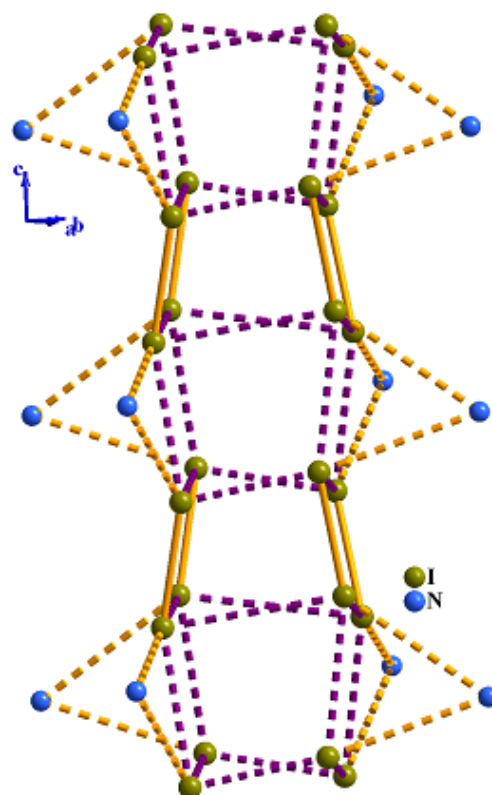


Figure S10

