Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

A robust porous pillar-chained Cd-framework with selective sorption for CO_2 and guest-driven tunable luminescence

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Content

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

	1	**1a**	**1b**
Chemical formula	$C_{18}H_{16}Cd_2N_6O_7$	$C_9H_7CdN_3O_3$	$C_9H_7CdIN_3O_3$
M	653.17	317.58	444.48
Crystal system	Tetragonal	Triclinic	Triclinic
Space group	*P*4(2)/*n*	*P*4(2)/*n*	*P*4(2)/*n*
a /Å	20.872(8)	20.8164(13)	21.23(6)
b /Å	20.872(8)	20.8164(13)	21.23(6)
c /Å	5.882(2)	5.8701(4)	6.029(17)
V/Å^3	2562.4(16)	2543.6(3)	2717(13)
Z	4	8	8
T /*K*	298(2)	298(2)	298(2)
F(000)	1272	1232	1656
D_{calcd} / gcm^{-3}	1.693	1.659	2.173
μ /mm^{-1}	1.705	1.712	3.879
λ /Å	0.71073	0.71073	0.71073
R_{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
R_1 [$I = 2\sigma(I)$][a]	0.0429	0.0313	0.0611
wR_2 [$I = 2\sigma(I)$][b]	0.1184	0.0865	0.1790
R_1 [all data][a]	0.0657	0.0390	0.0830
wR_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] $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

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)

[a]Symmetry 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.

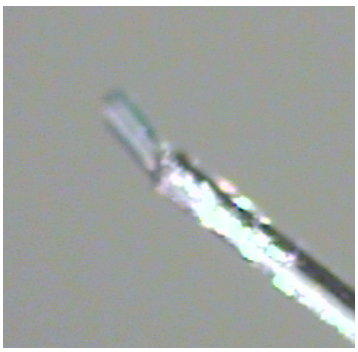
Table S**3** Distances (Å) and angles (°) of hydrogen bonds for compounds **1, 1a** and **1b**.

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; [a]Distances between the protons and centroids of benzene rings in ligand Hcpt.

Figure S1

(a)



(b)

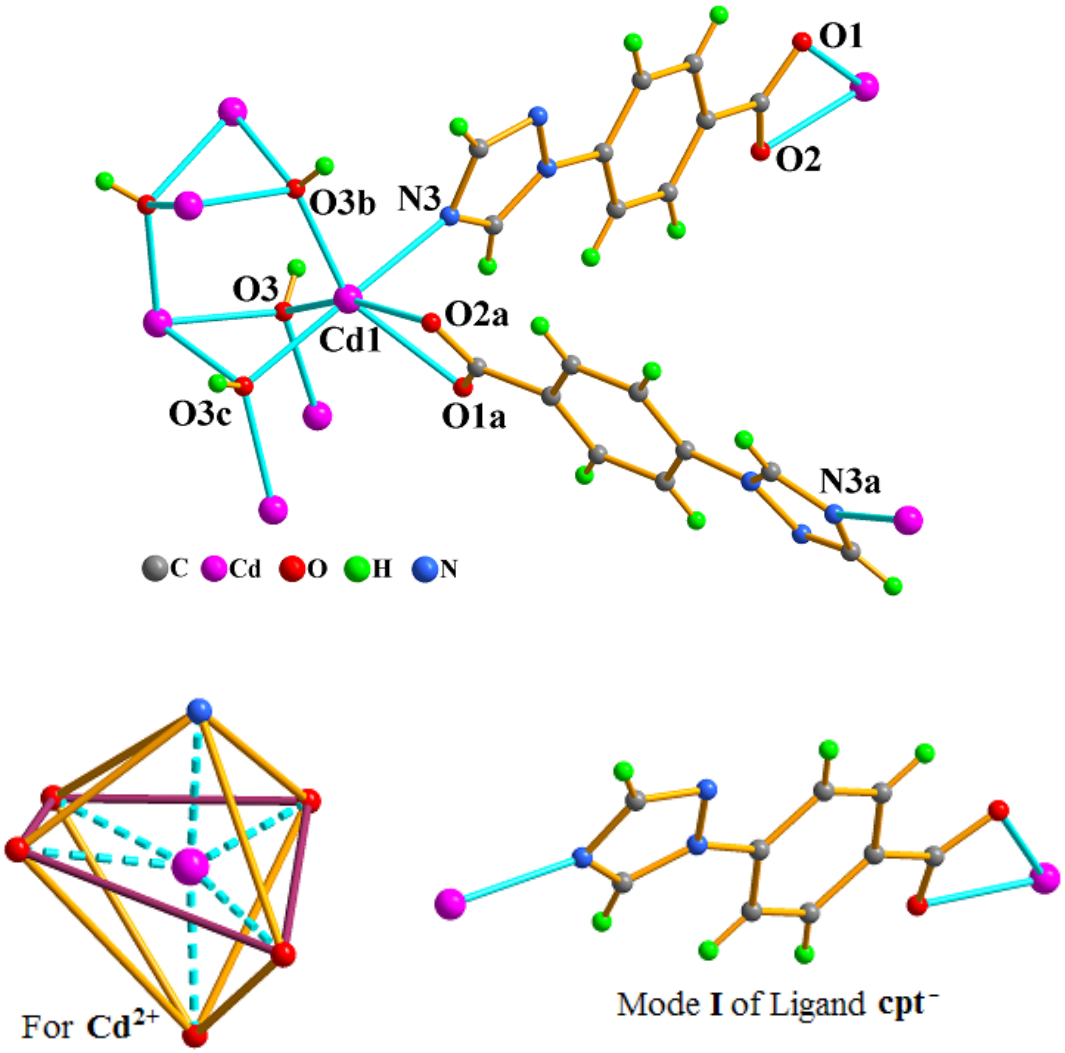

O1
O2
O3b
N3
O3
Cd1
O2a
O3c
O1a
N3a
C Cd O H N
For Cd2+
Mode I of Ligand cpt-

Figure S2

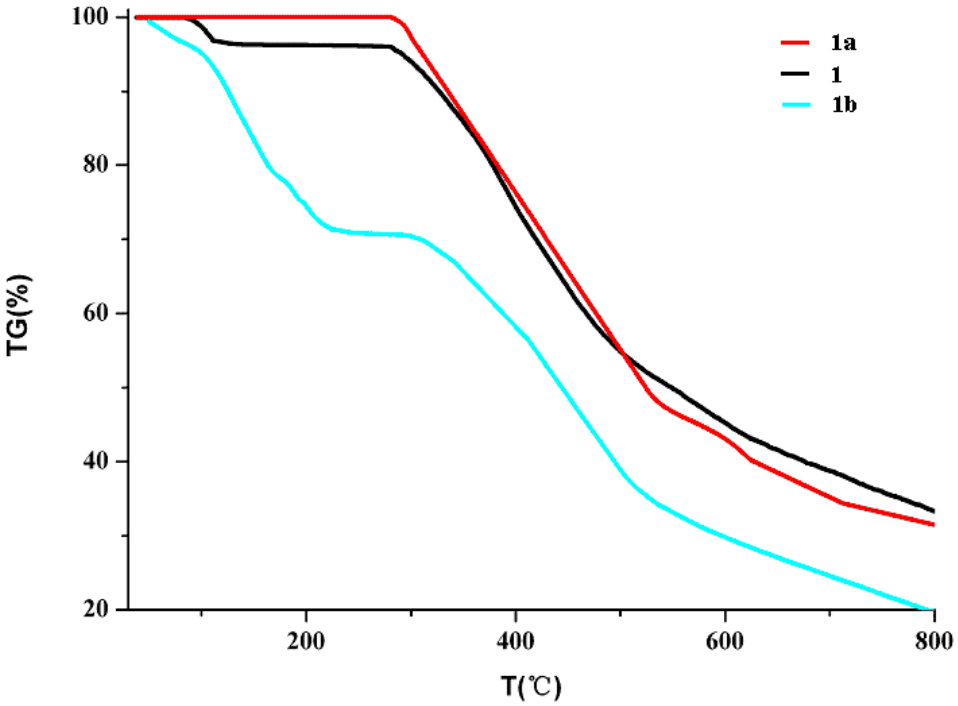


Figure S3

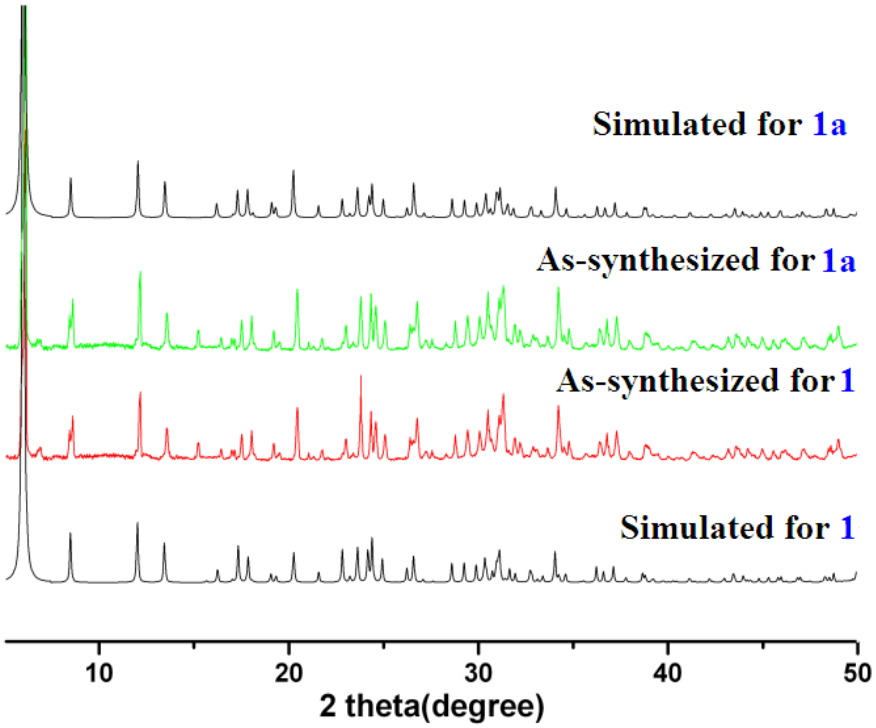


Figure S4

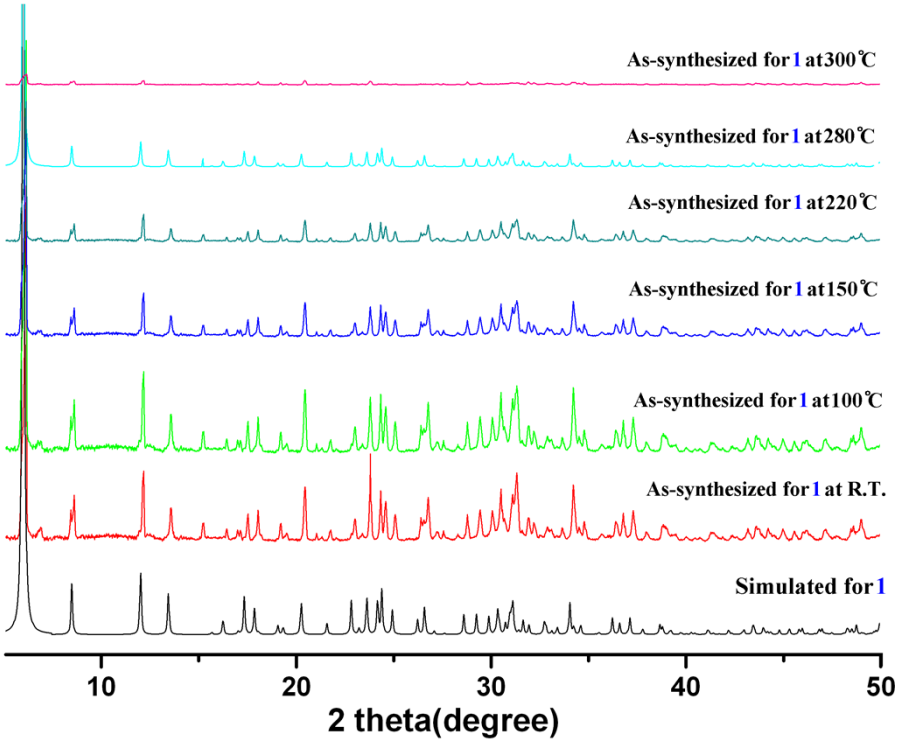


Figure S5

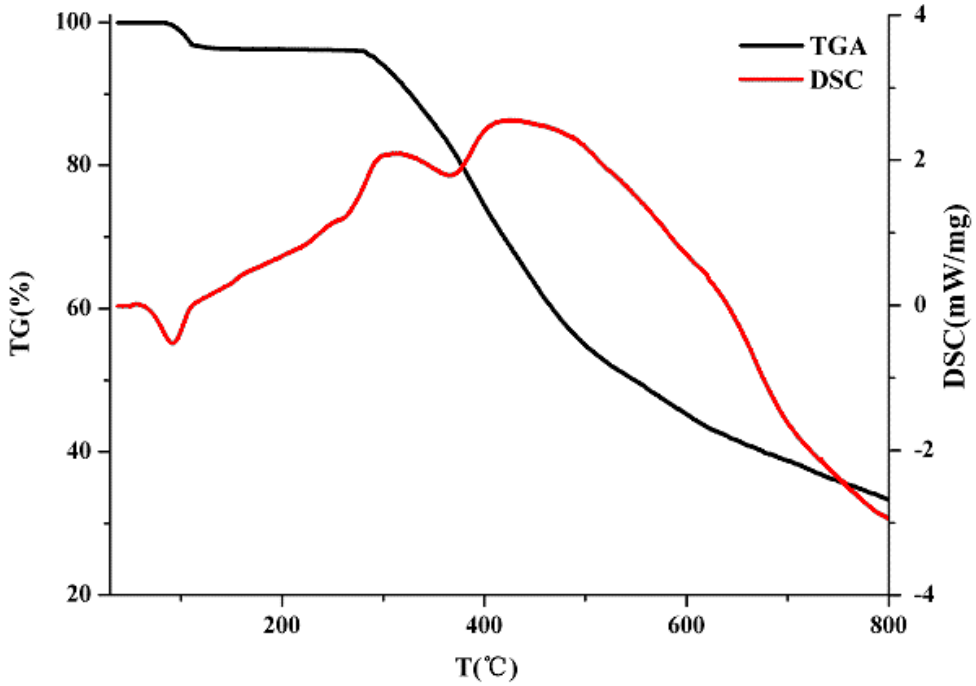


Figure S6

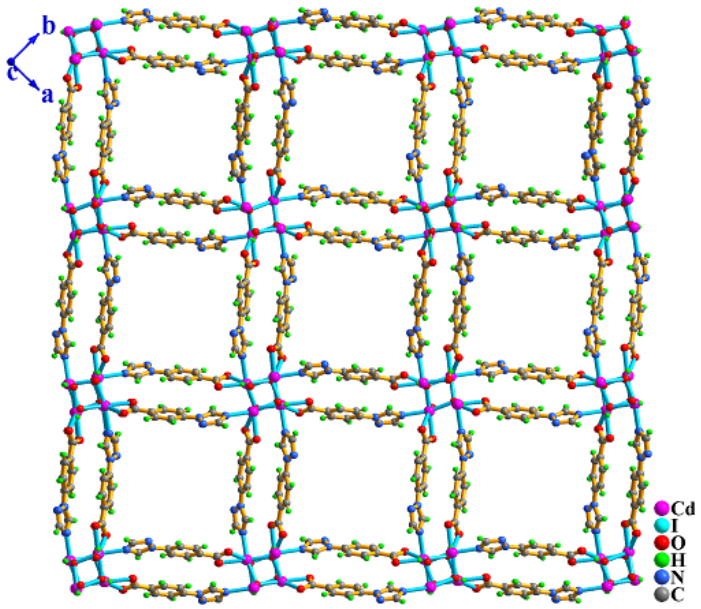
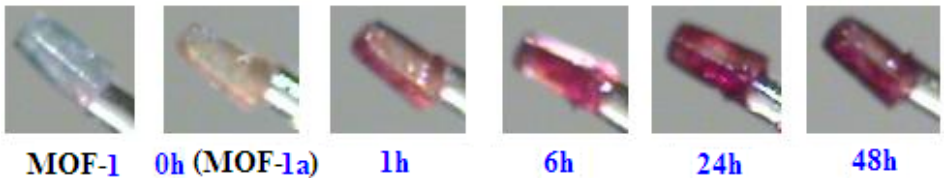


Figure S7

(a)



(b)

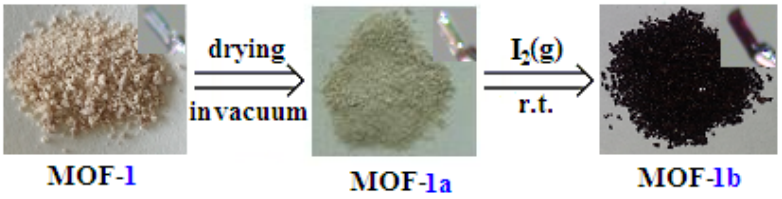


Figure S8

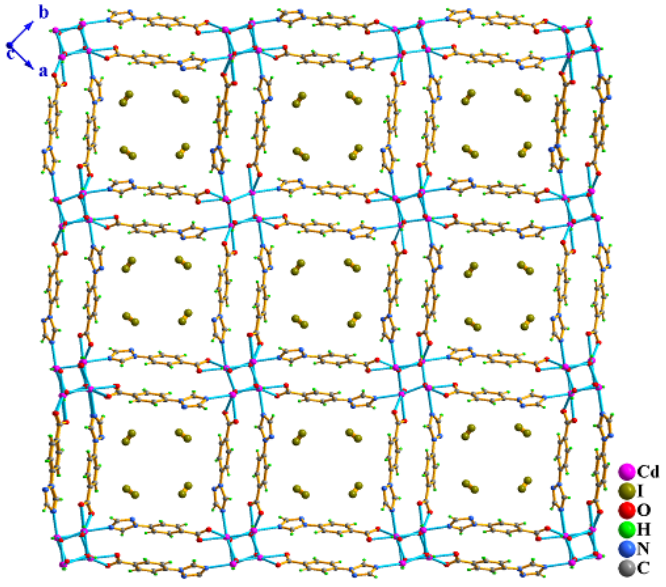
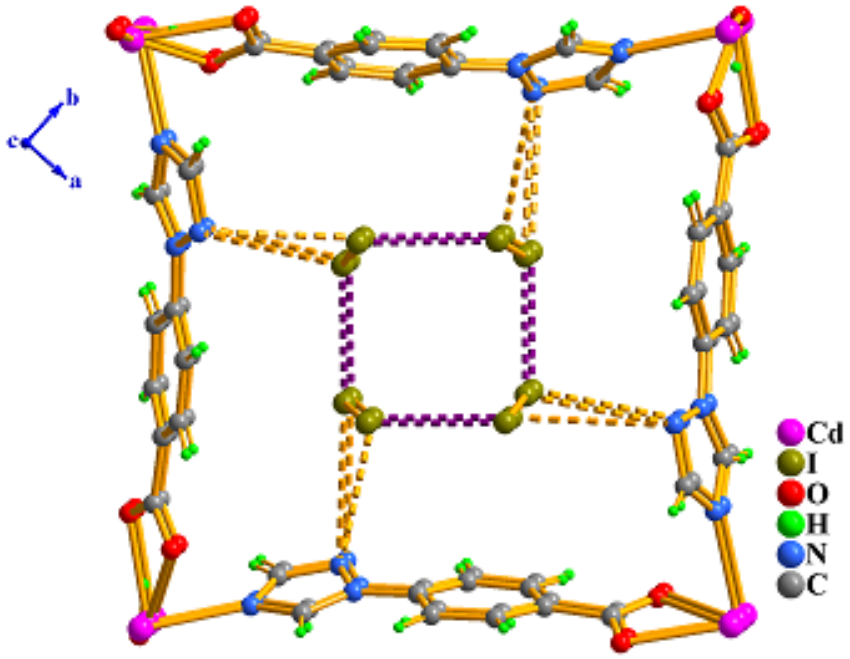
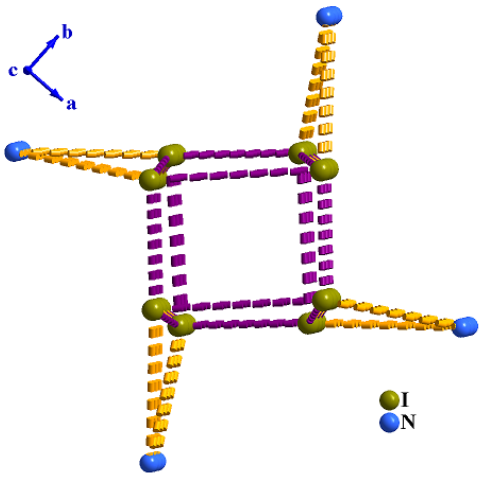


Figure S9

(a)



(b)



(c)

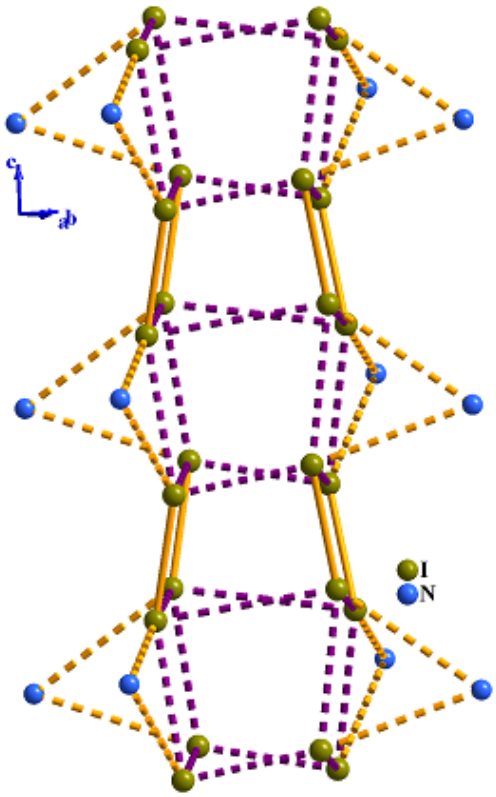
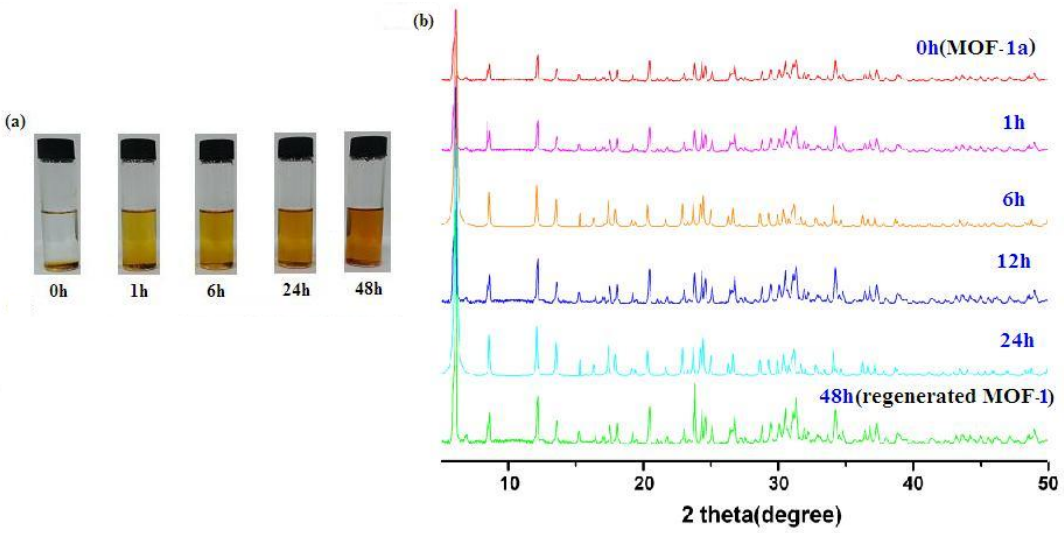


Figure S10


(a)
0h
1h
6h
24h
48h
(b)
0h(MOF-1a)
1h
6h
12h
24h
48h(regenerated MOF-1)
10
20
30
40
50
2 theta(degree)