Electronic supplementary information (ESI)

Synthesis, characterization and selective hysteretic sorption property of metal-organic frameworks with 3,5-di(pyridine-4-yl)benzoate

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Table S1. Selected bond lengths (Å) and angles ( ) for 1 - 3.

Compound **1**			
Zn1-N2	2.083(2)	Zn1-N1^{i}	2.087(2)
Zn1-O4	2.098(2)	Zn1-O1^{ii}	2.1688(18)
Zn1-O1W	2.176(2)	Zn1-O2^{ii}	2.230(2)
N2-Zn1-N1^{i}	109.12(8)	N2-Zn1-O4	94.16(9)
N1^{i}-Zn1-O4	86.31(9)	N2-Zn1-O1^{ii}	154.21(7)
N1-Zn1-O1^{ii}	96.12(8)	O4-Zn1-O1^{ii}	92.64(8)
N2-Zn1-O1W	86.86(9)	N1^{i}-Zn1-O1W	92.43(9)
O4-Zn1-O1W	178.59(8)	O1^{ii}-Zn1-O1W	86.85(8)
N2-Zn1-O2^{ii}	95.10(7)	N1^{i}-Zn1-O2^{ii}	155.77(8)

O4-Zn1-O2^{ii}	92.77(9)	O1^{ii}-Zn1-O2^{ii}	59.70(6)
O1W-Zn1-O2 ^{ii}	88.11(8)		
Symmetry codes: (i) x-1/2, −y+3/2, z-1/2; (ii) x-1/2, −y+5/2, z-1/2; (iii) x+1/2, -y+5/2, z+1/2; (iv) x+1/2,-y+3/2,z+1/2.			
Compound **2**			
Cd1-N2^{i}	2.317(3)	Cd1-O3^{ii}	2.327(2)
Cd1-O2 ^{iii}	2.365(3)	Cd1-N3	2.375(3)
Cd1-N1	2.396(3)	Cd1-O1^{iii}	2.459(3)
Cd1-O4^{ii}	2.542(3)		
N2^{i}-Cd1-O2^{iii}	136.73(9)	N2^{i}-Cd1-O2^{iii}	137.40(9)
O3^{ii}-Cd1-O2^{iii}	85.80(9)	N2^{i} -Cd1-N3	90.84(11)
O3^{ii}-Cd1-N3	86.57(10)	O2^{iii}-Cd1-N3	94.95(10)
N2^{i}-Cd1-N1	95.81(10)	O3^{ii}-Cd1-N1	84.78(9)
O2 ^{iii} -Cd1-N1	83.91(9)	N3-Cd1-N1	171.34(10)
N2^{i}-Cd1-O1 ^{iii}	82.89(9)	O3^{ii}-Cd1-O1^{iii}	140.02(9)
O2^{iii} -Cd1-O1^{iii}	54.54(8)	N3-Cd1-O1^{iii}	100.40(11)
N1-Cd1-O1 ^{iii}	85.97(10)	N2^{i} -Cd1-O4^{ii}	82.68(9)
O3^{ii} -Cd1-O4^{ii}	54.05(8)	O2^{iii} -Cd1-O4^{ii}	139.79(8)
N3-Cd1-O4 ^{ii}	85.58(11)	N1-Cd1-O4^{ii}	89.75(10)
O1^{iii}-Cd1-O4^{ii}	164.45(9)		
Symmetry codes: (i) -x+3/2, y-1/2, z; (ii) x, -y+1, z+1/2; (iii) -x+5/2, -y+1/2, z-1/2; (iv) x,-y+1,z-1/2; (v) -x+5/2,-y+1/2,z+1/2; (vi) -x+3/2,y+1/2,z.			
Compound **3**			
Co1-O3	2.009(3)	Co1-N1^{i}	2.116(3)

Co1-N2^{ii}	2.124(3)	Co1-O1W	2.134(3)
Co1-O2	2.169(3)	Co1-O1	2.232(3)
O3-Co1- N1^{i}	99.52(13)	O3-Co1-N2^{ii}	85.55(12)
N1^{i}-Co1-N2^{ii}	112.77(13)	O3-Co1-O1W	171.52(11)
N1^{i}-Co1-O1W	84.85(12)	N2^{ii}-Co1-O1W	86.05(12)
O3-Co1-O2	94.01(12)	N1^{i}-Co1-O2	94.66(12)
N2^{ii} -Co1-O2	152.29(12)	O1W-Co1-O2	92.87(11)
O3-Co1-O1	90.76(13)	N1-Co1-O1	153.30(12)
N2^{ii} -Co1-O1	92.43(12)	O1W-Co1-O1	88.40(11)
O2-Co1-O1	59.86(9)		
Symmetry codes: (i) x+1/2, y-1/2, z; (ii) x+1/2, y+1/2, z; (iii) -x+1/2, -y+1/2, -z+2; (iv) x-1/2,y+1/2,z; (v) x-1/2,y-1/2,z.			

Table S2. The parameters of hydrogen bonds for 1 – 3.

Complex **1**				
D—H ··*A*	*D*—H	H ··*A*	*D* ··*A*	*D*—H ··*A*
O1W—H1WA ··O1	0.85	2.02	2.868 (3)	171
O1W—H1WB ··O5	0.84	1.94	2.755 (4)	165
C1—H1 ··O2W	0.93	2.53	3.231(10)	132
C1—H1 ··O5	0.93	2.54	3.271(4)	135
Symmetry codes: (i) 1/2- x, 5/2-y, 1-z; (ii) x, 2−y, 1/2+z; (iii) 1-x, 1-y, 1-z; (iv) 1/2+x,-1/2+y, 1+z.				
Compound **2**				
D—H ··*A*	*D*—H	H ··*A*	*D* ··*A*	*D*—H ··*A*
C4—H4A ··O2	0.93	2.55	3.484(4)	176
C5—H5A ··O3	0.93	2.32	3.023(4)	133
C13—H13A ··O4	0.93	2.42	3.048(4)	125
C14—H14A ··O2	0.93	2.48	3.389(5)	167
C17—H17A ··O1	0.93	2.43	3.090(4)	128
C18—H18A ··O3	0.93	2.47	3.121(5)	127
Symmetry codes: (i) -1/2+x,1/2+y,3/2-z; (ii) x,1-y,1/2+z; (iii) 3/2-x,3/2-y,1/2+z; (iv) -1/2+x,1/2+y,3/2-z; (v) -1+x,1-y,-1/2+z; (vi) x,1-y,1/2+z.				
Compound **3**				
D—H ··*A*	*D*—H	H ··*A*	*D* ··*A*	*D*—H ··*A*
O1W—H1WA ··O4	0.85	2.12	2.696 (4)	125
O1W—H1WB ··O1	0.85	2.04	2.812(4)	151
C12—H12 ··O2	0.93	2.58	3.133(6)	118

C13—H13 ··O1	0.93	2.47	3.082(6)	124
Symmetry codes: (i) x, -y,-1/2+z; (ii) 1/2-x, 1/2-y, 1-z; (iii) –1/2+x, 1/2+y, z; (iv) -1/2+x,-1/2+y,z.				

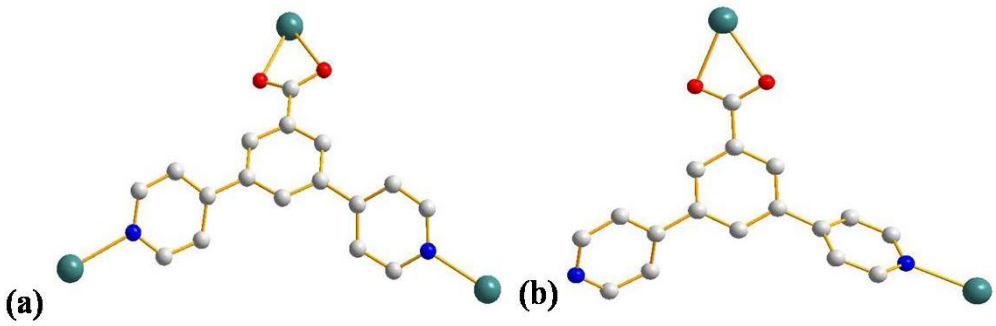


Fig.S1 Coordination modes of L^-: (a) mode I and (b) mode II in complex **2**.

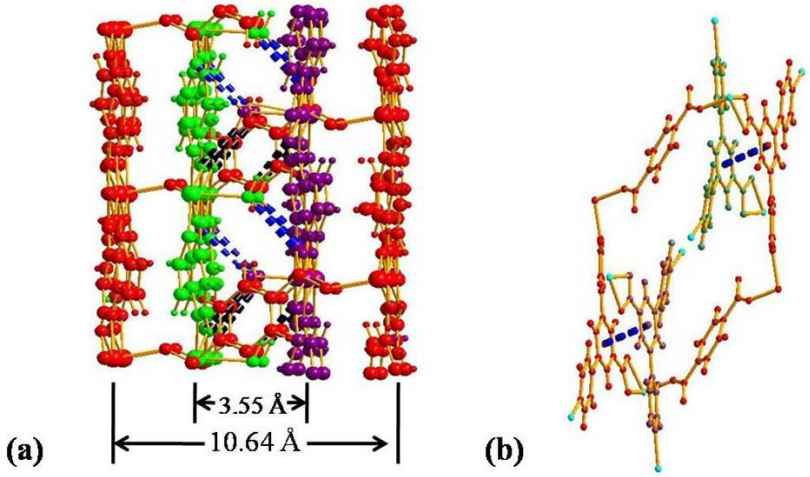


Fig.S2 (a) Hydrogen bonding interactions of complex **3** between different layers (O1W-H1WA ··O4 are shown in blue dash lines, O1W-H1WB ··O1 are shown in black dash lines). (b) The π ··π interactions between the layers in **3** indicated by blue dash lines.

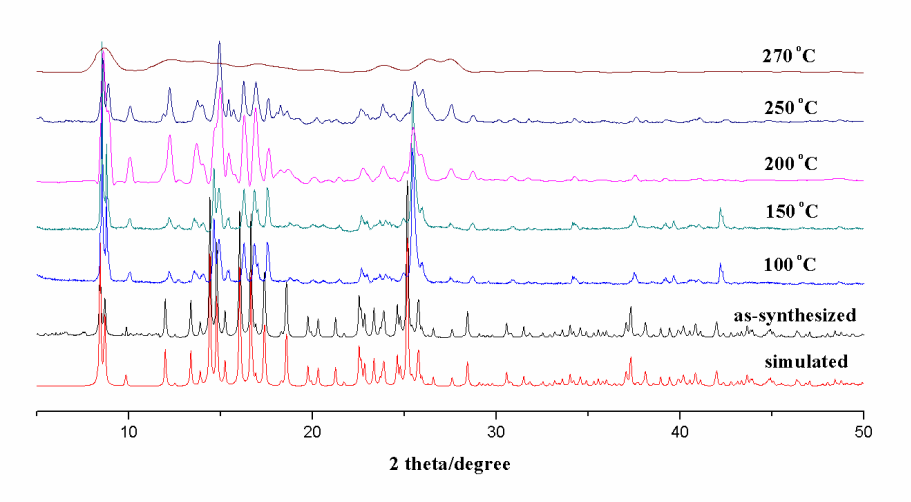


Fig.S3 The PXRD patterns of complex **1** at different temperature.

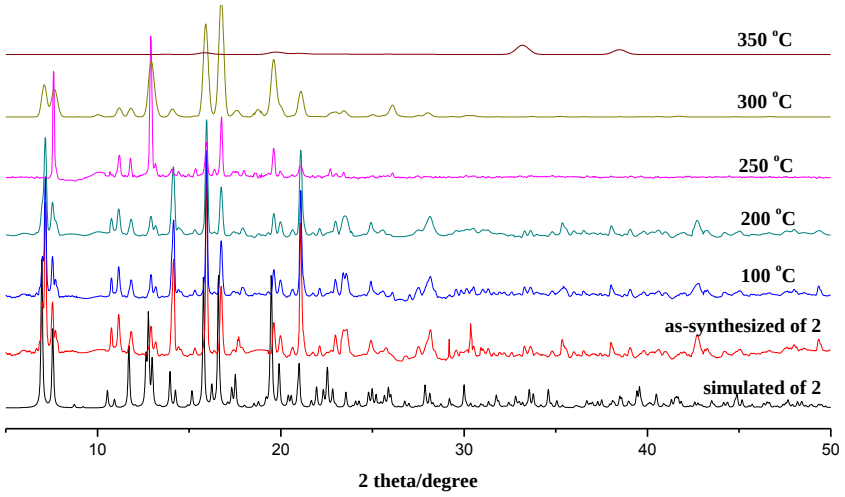


Fig.S4 The PXRD patterns of complex **2** at different temperature.

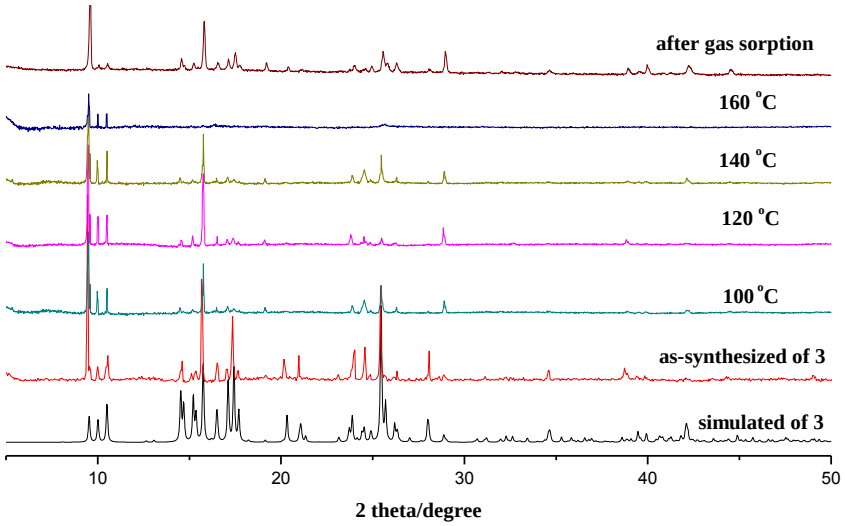


Fig.S5 The PXRD patterns of complex **3** at different temperature and after gas sorption.

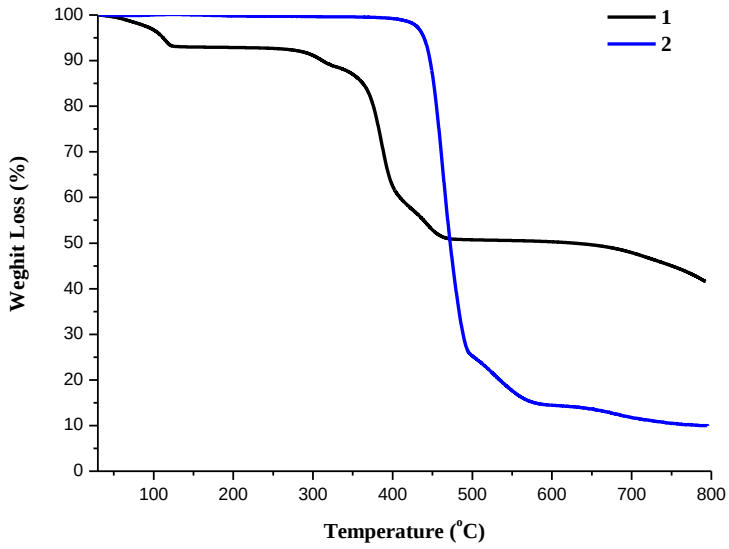


Fig.S6 The TGA curves of complexes **1** and **2**.

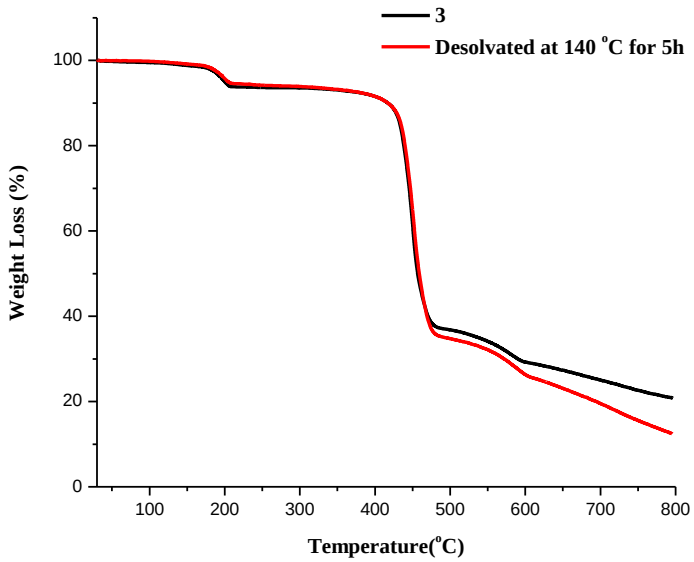
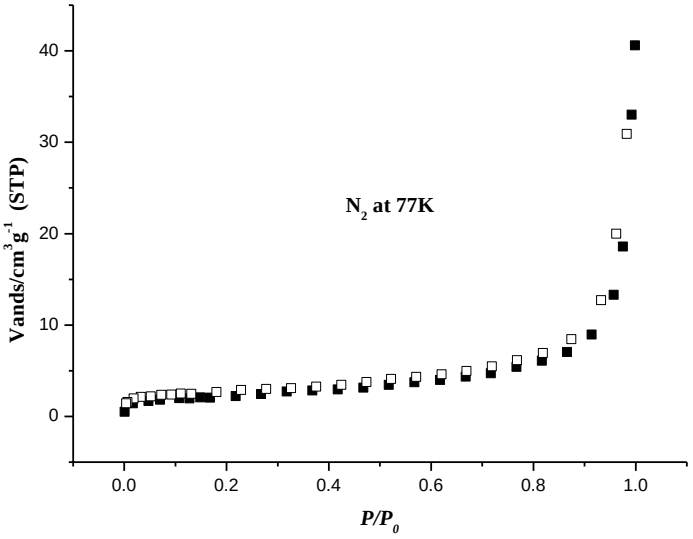
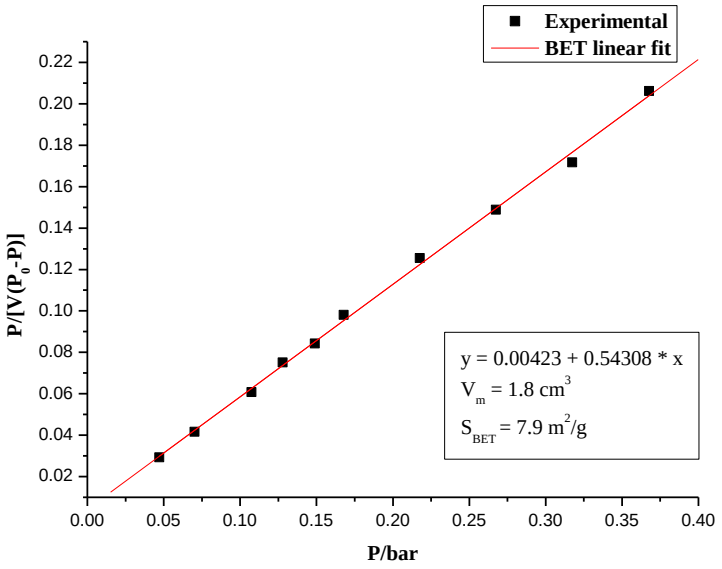


Fig.S7 The TGA curves of complex **3**.



(a)



(b)

Fig.S8 (a) N_2 sorption isotherm at 77 K for **3** (filled shape, adsorption; open shape, desorption). (b) The BET plot calculated from N_2 isotherm at 77K of **3**.