Electronic Supplementary Information

From two-dimensional networks to three-dimensional metal-organic frameworks mediated by solvent ratio: Luminescence and gas adsorption properties

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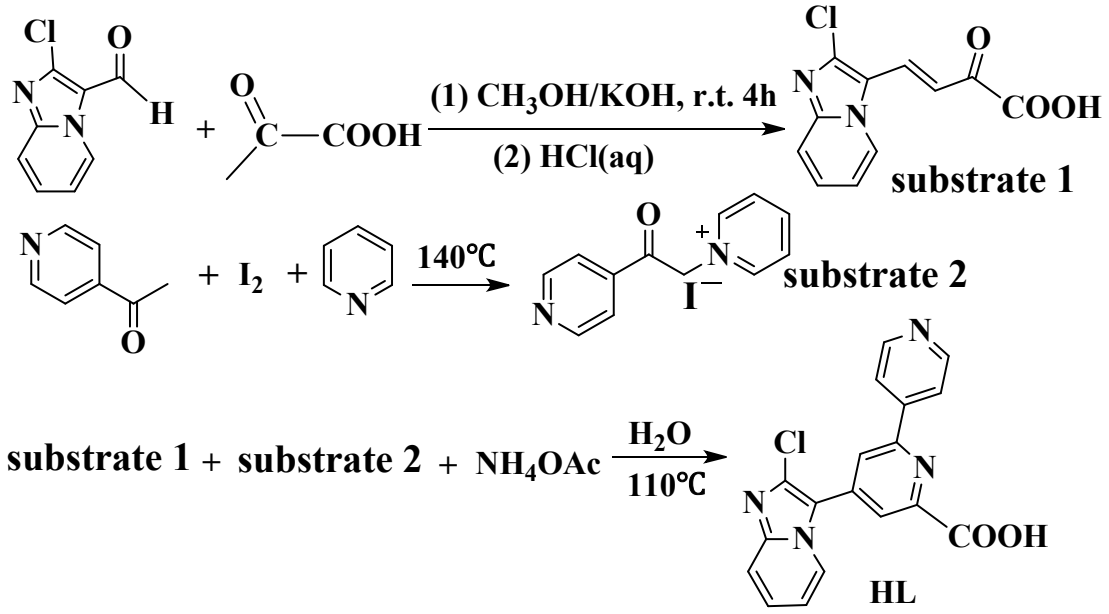
Table S1 Selected bond distances (Å) and angles (º) for **1**−**3**.[a]

1		**2**		**3**	
Co(1)-O(1)	2.004(7)	Co(1)-O(1)	2.049(3)	Co(1)-O(1)	2.0458(18)
Co(1)-O(1)#2	2.004(7)	Co(1)-O(3)	2.050(3)	Co(1)-O(2)#15	2.1240(18)
Co(1)-N(3)	2.229(8)	Co(1)-O(6)	2.071(3)	Co(1)-O(3)	2.170(2)
Co(1)-N(3)#2	2.229(8)	Co(1)-N(3)	2.213(3)	Co(1)-O(6)	2.1072(19)
Co(1)-N(8)	2.218(7)	Co(1)-N(4)#2	2.154(3)	Co(1)-N(3)	2.192(2)
Co(1)-N(8)#2	2.218(7)	Co(1)-N(7)	2.223(3)	Co(1)-N(4)#10	2.121(2)
Co(2)-O(3)	1.998(7)	Co(2)-O(2)	2.139(2)	O(1)-Co(1)-O(2)#15	91.97(7)
Co(2)-O(3)#2	1.998(7)	Co(2)-O(2)#2	2.139(2)	O(1)-Co(1)-O(3)	93.48(9)
Co(2)-N(4)	2.234(8)	Co(2)-O(5)	2.056(3)	O(1)-Co(1)-O(6)	86.51(8)
Co(2)-N(4)#2	2.234(8)	Co(2)-O(5)#2	2.056(3)	O(1)-Co(1)-N(3)	77.92(7)
Co(2)-N(7)	2.258(8)	Co(2)-N(8)	2.193(3)	O(1)-Co(1)-N(4)#10	173.39(8)
Co(2)-N(7)#2	2.258(8)	Co(2)-N(8)#2	2.193(3)	O(2)#15-Co(1)-O(3)	173.30(9)
O(1)-Co(1)-O(1)#2	180.0	O(1)-Co(1)-O(3)	87.34(13)	O(2)#15-Co(1)-O(6)	94.17(8)
O(1)-Co(1)-N(3)	79.8(3)	O(1)-Co(1)-O(6)	97.36(13)	O(2)#15-Co(1)-N(3)	91.17(7)
O(1)-Co(1)-N(3)#2	100.2(3)	O(1)-Co(1)-N(3)	76.92(11)	O(2)#15-Co(1)-N(4)#10	88.21(8)
O(1)-Co(1)-N(8)	90.5(3)	O(1)-Co(1)-N(4)#2	171.15(12)	O(3)-Co(1)-O(6)	90.06(9)
O(1)-Co(1)-N(8)#2	89.5(3)	O(1)-Co(1)-N(7)	84.21(11)	O(3)-Co(1)-N(3)	86.16(8)
O(1)#2-Co(1)-N(3)	100.2(3)	O(3)-Co(1)-O(6)	175.24(12)	O(3)-Co(1)-N(4)#10	86.84(9)
O(1)#2-Co(1)-N(3)#2	79.8(3)	O(3)-Co(1)-N(3)	90.13(11)	O(6)-Co(1)-N(3)	163.70(8)
O(1)#2-Co(1)-N(8)	89.5(3)	O(3)-Co(1)-N(4)#2	88.87(12)	O(6)-Co(1)-N(4)#10	86.89(8)

O(1)#2-Co(1)-N(8)#2	90.5(3)	O(3)-Co(1)-N(7)	78.75(11)	N(3)-Co(1)-N(4)#10	108.68(8)
N(3)-Co(1)-N(3)#2	180.0	O(6)-Co(1)-N(3)	91.68(12)		
N(3)-Co(1)-N(8)	98.5(3)	O(6)-Co(1)-N(4)#2	86.37(12)		
N(3)-Co(1)-N(8)#2	81.5(3)	O(6)-Co(1)-N(7)	100.88(11)		
N(3)#2-Co(1)-N(8)	81.5(3)	N(3)-Co(1)-N(4)#2	111.10(11)		
N(3)#2-Co(1)-N(8)#2	98.5(3)	N(3)-Co(1)-N(7)	158.54(11)		
N(8)-Co(1)-N(8)#2	180.0	N(4)#2-Co(1)-N(7)	87.21(11)		
O(3)-Co(2)-O(3)#2	180.0(4)	O(2)-Co(2)-O(2)#2	180.0		
O(3)-Co(2)-N(4)	92.0(3)	O(2)-Co(2)-O(5)	86.65(11)		
O(3)-Co(2)-N(4)#2	88.0(3)	O(2)-Co(2)-O(5)#2	93.35(11)		
O(3)-Co(2)-N(7)	78.2(3)	O(2)-Co(2)-N(8)	92.08(11)		
O(3)-Co(2)-N(7)#2	101.9(3)	O(2)-Co(2)-N(8)#2	87.92(11)		
O(3)#2-Co(2)-N(4)	88.0(3)	O(2)#2-Co(2)-O(5)	93.35(11)		
O(3)#2-Co(2)-N(4)#2	92.0(3)	O(2)#2-Co(2)-O(5)#2	86.65(11)		
O(3)#2-Co(2)-N(7)	101.8(3)	O(2)#2-Co(2)-N(8)	87.92(11)		
O(3)#2-Co(2)-N(7)#2	78.1(3)	O(2)#2-Co(2)-N(8)#2	92.08(11)		
N(4)-Co(2)-N(4)#2	180.0	O(5)-Co(2)-O(5)#2	180.0		
N(4)-Co(2)-N(7)	85.3(3)	O(5)-Co(2)-N(8)	93.19(12)		
N(4)-Co(2)-N(7)#2	94.8(3)	O(5)-Co(2)-N(8)#2	86.81(12)		
N(4)#2-Co(2)-N(7)	94.8(3)	O(5)#2-Co(2)-N(8)	86.81(12)		
N(4)#2-Co(2)-N(7)#2	85.2(3)	O(5)#2-Co(2)-N(8)#2	93.19(12)		
N(7)-Co(2)-N(7)#2	180.0	N(8)-Co(2)-N(8)#2	180.0		

[a] Symmetry code for **1** and **2**: #2= -x, -y, -z; symmetry code for **3**: #10= -x, -y, -z, #15= x-y+2/3, x+1/3, -z+1/3.



Scheme S1 The synthesis procedure for HL ligand.

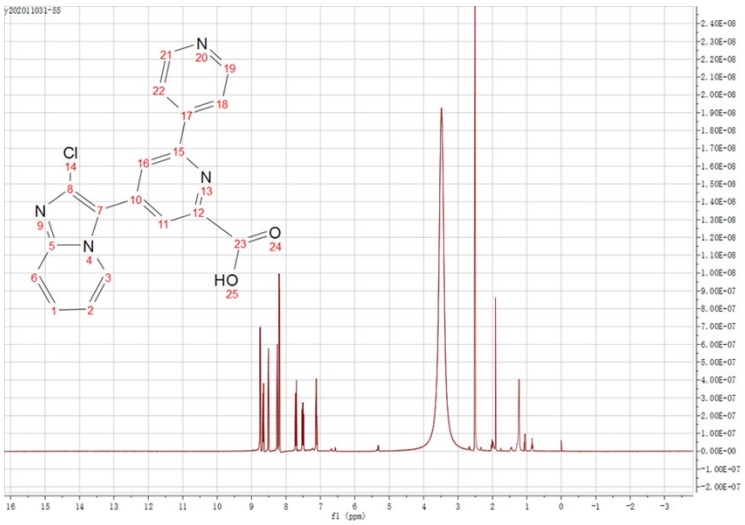


Fig. S1 ^{1}H NMR (400 MHz, dmso-d_6) of HL ligand.

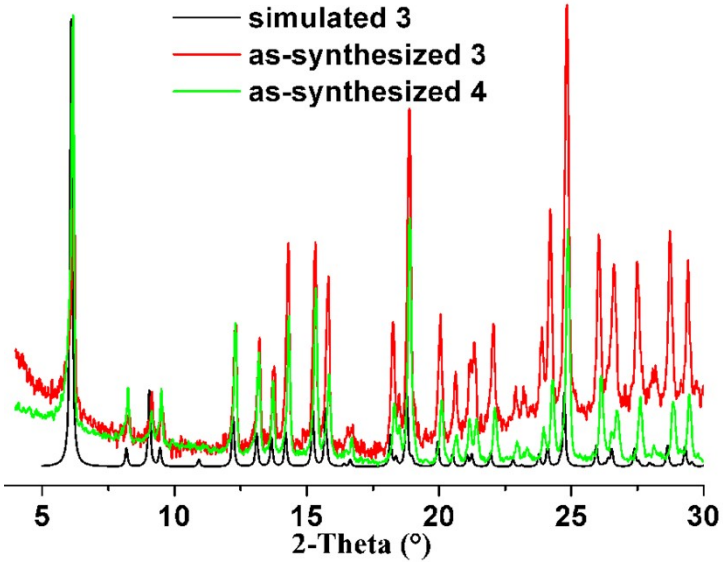


Fig. S2 Powder XRD profiles of **3** and **4**.

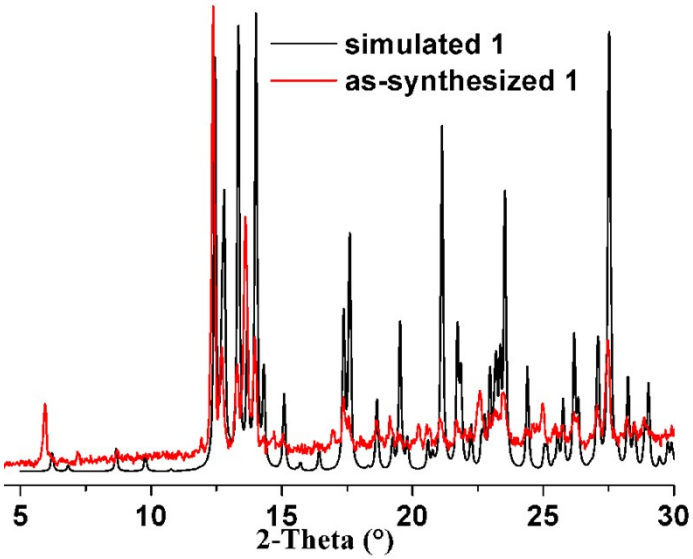


Fig. S3 Powder XRD profiles of **1**.

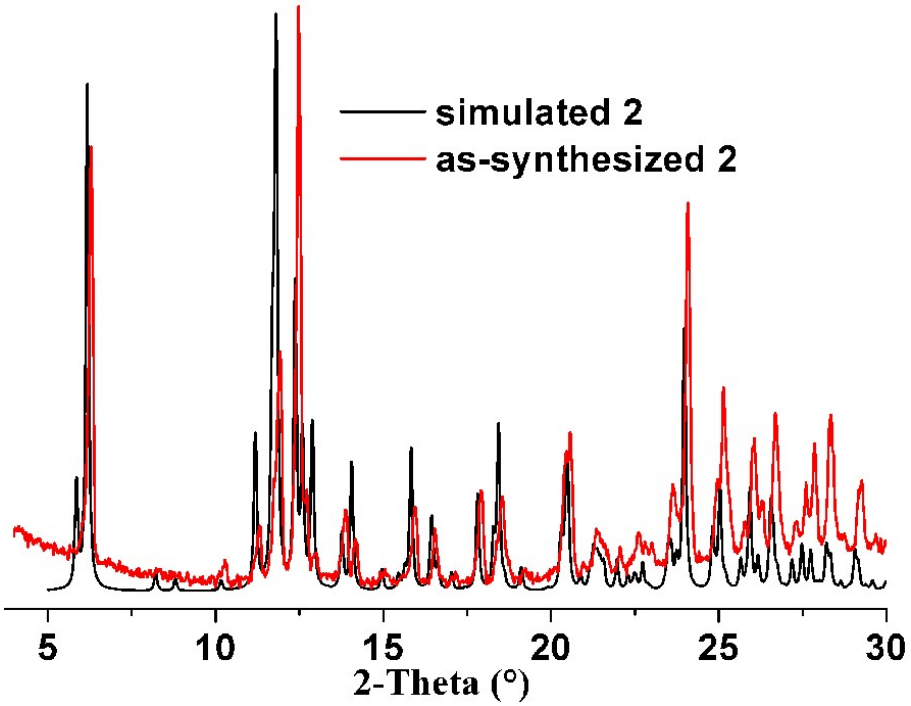


Fig. S4 Powder XRD profiles of **2**.

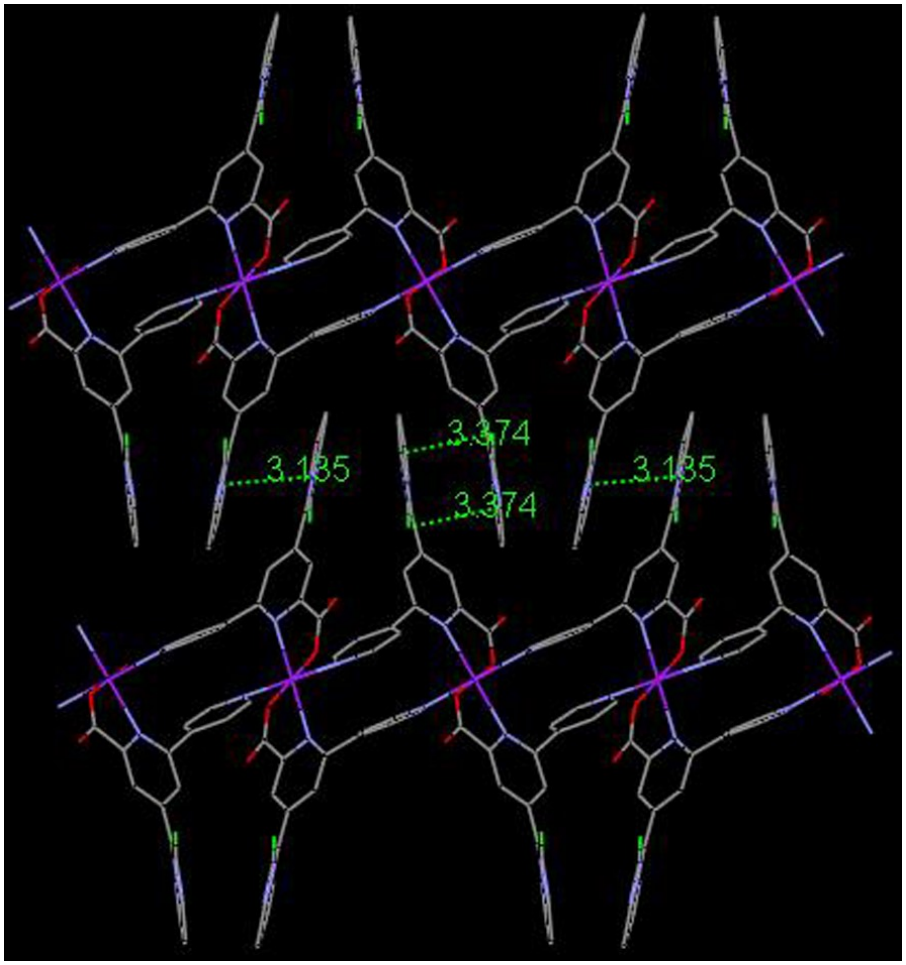


Fig. S5 The 3D supramolecular structure of **1**.

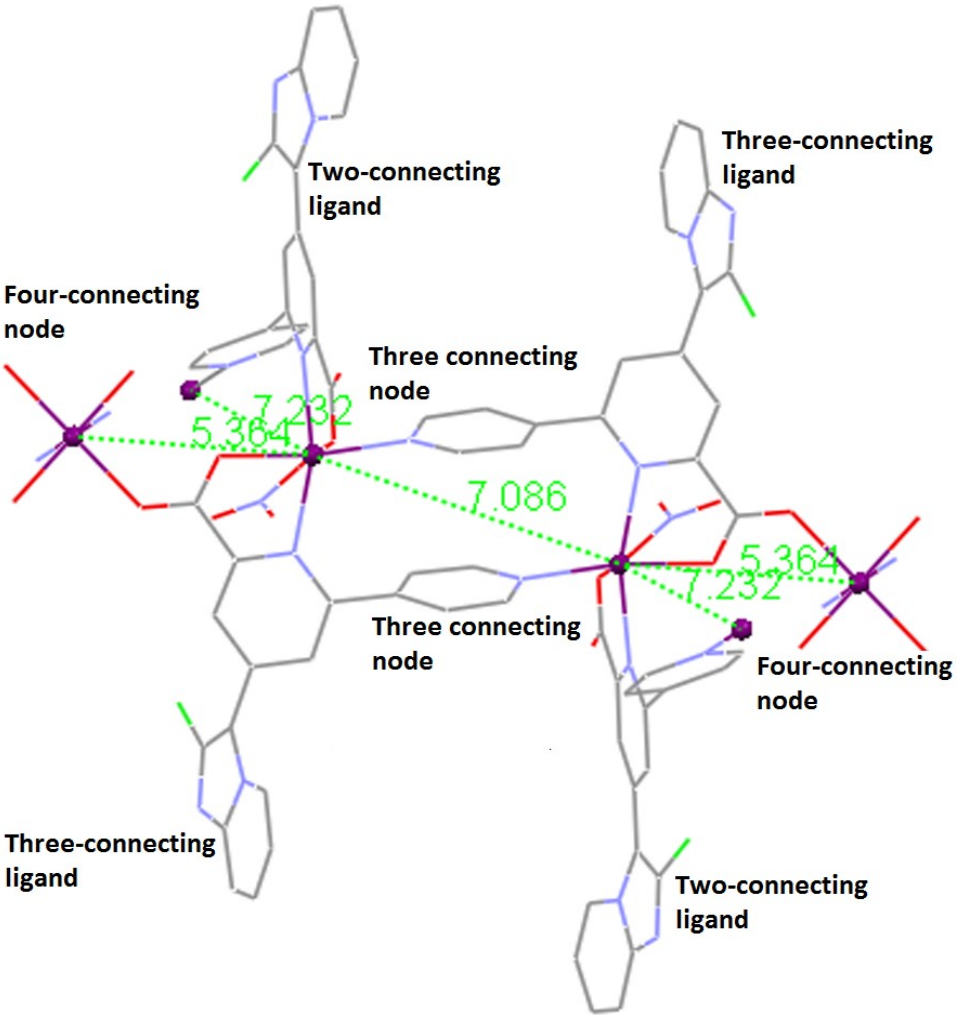


Fig. S6 The two- and three-connecting ligands in **2**.

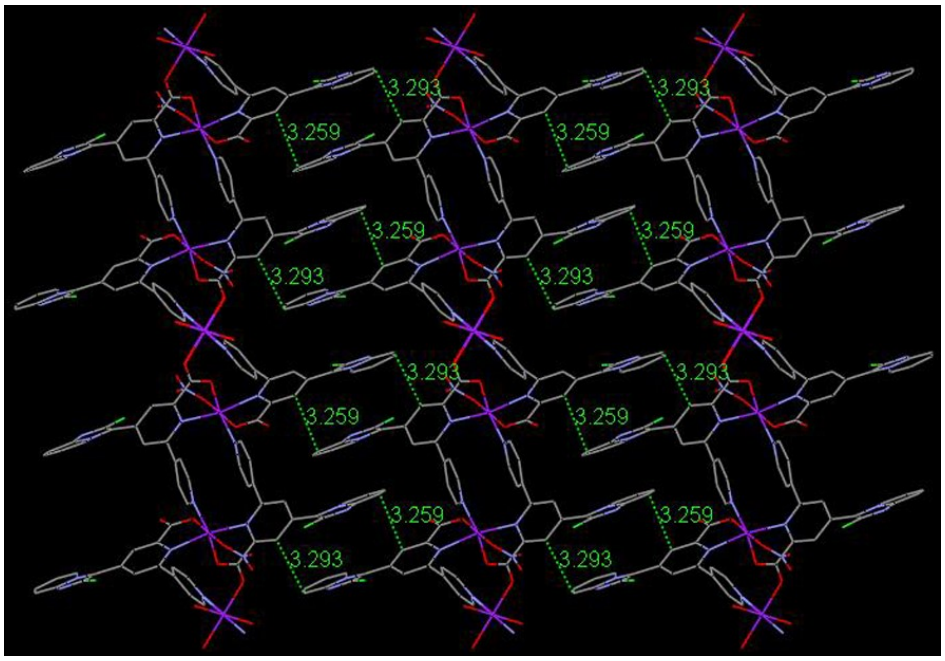


Fig. S7 The 3D supramolecular structure of **2**.

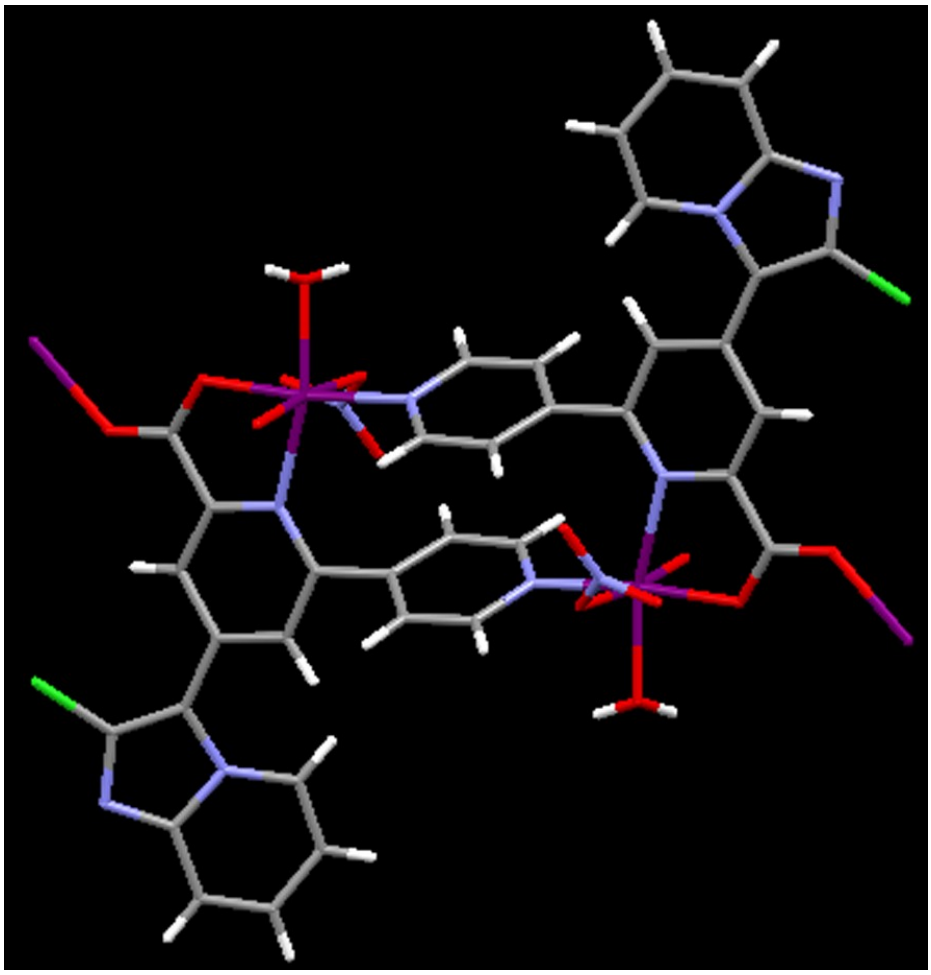


Fig. S8 The quasi-rectangular SBU in **3**.

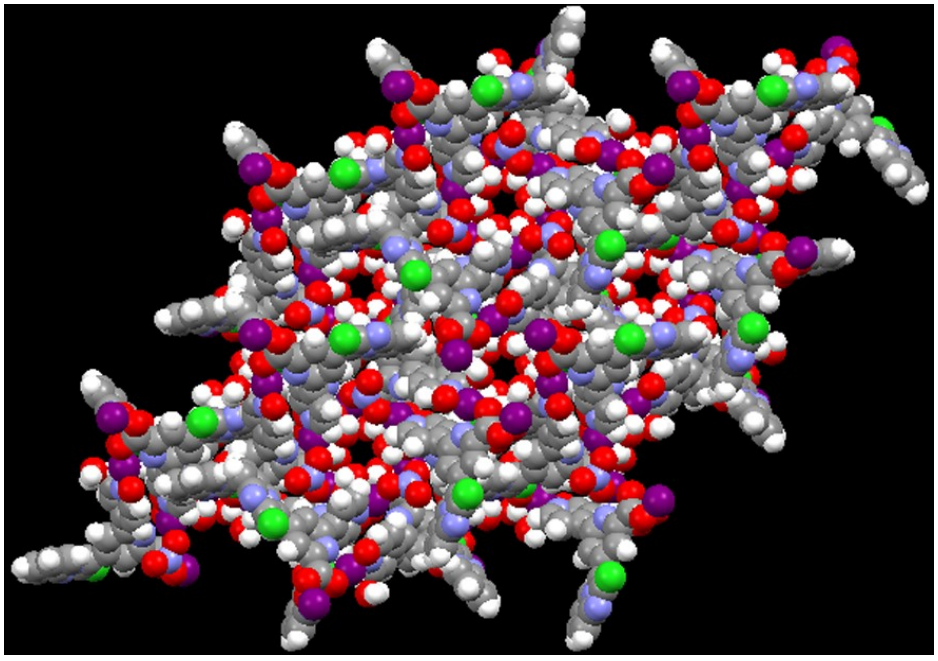


Fig. S9 Space-filling representation of **3**, showing guest-free small hexagonal channels.

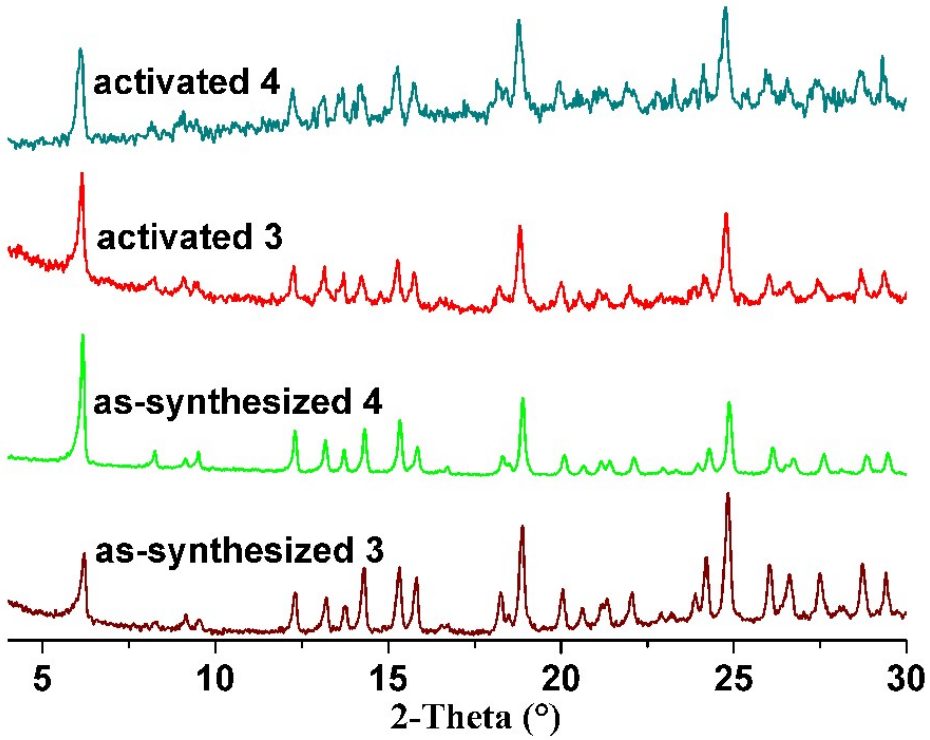


Fig. S10 Powder XRD profiles of as-synthesized and activated **3** and **4**.

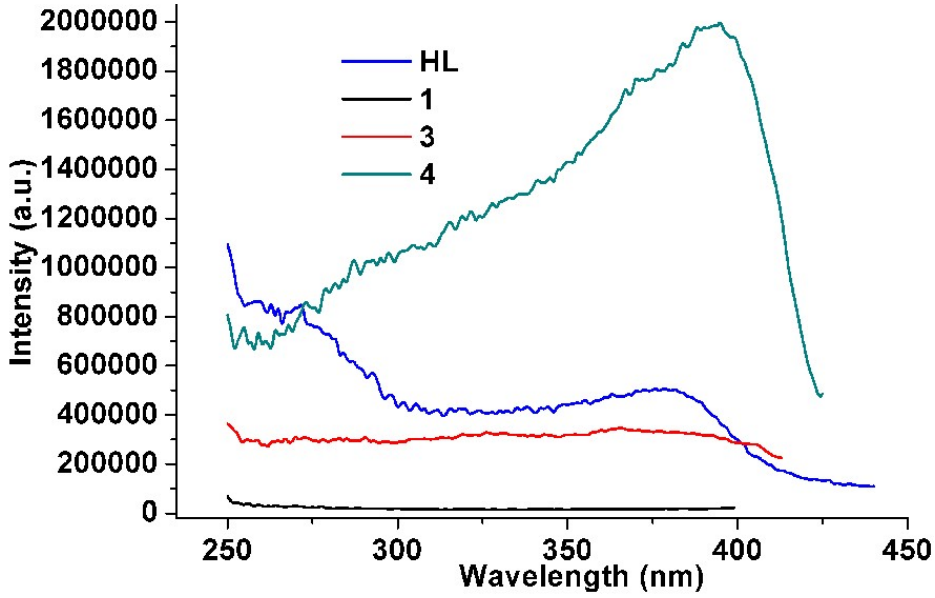


Fig. S11 Solid-state excitation spectra of HL ligand and coordination polymers.