Electronic supplementary information (ESI)

Metal-organic frameworks with 1,4-di(1H-imidazol-4-yl)benzene and varied carboxylate ligands for selectively sensing Fe(III) Ion and ketone molecules

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Table S1. Selected bond lengths (Å) and angles (°) for **1** - **4**.

Compound **1**			
Zn(1)-N(1)	2.006(3)	Zn(1)-O(2)	2.444(3)
Zn(1)-O(1)	2.048(3)		
N(1)-Zn(1)-N(1)#1	109.7(2)	N(1)#1-Zn(1)-O(2)	90.79(13)
N(1)-Zn(1)-O(1)#1	104.30(13)	O(1)#1-Zn(1)-O(2)	89.40(11)
N(1)#1-Zn(1)-O(1)#1	98.66(12)	O(1)-Zn(1)-O(2)	57.91(10)
O(1)#1-Zn(1)-O(1)	139.62(16)	O(2)-Zn(1)-O(2)#1	76.61(15)
N(1)-Zn(1)-O(2)	152.86(12)		

Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,-z+1/2.

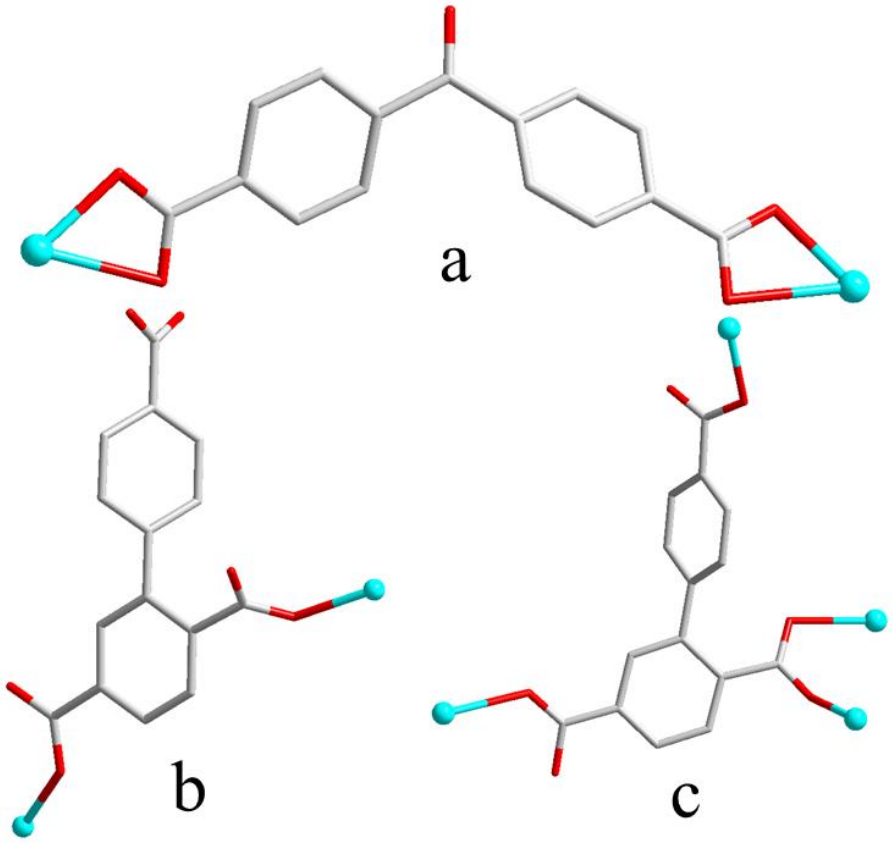
Compound **2**			
Co(1)-N(3)	2.0389(15)	Co(1)-O(3)#1	2.0812(13)
Co(1)-N(1)	2.0633(15)	Co(1)-O(2)	2.3351(14)
Co(1)-O(1)	2.0784(14)	Co(1)-O(4)#1	2.3513(16)
N(3)-Co(1)-N(1)	102.84(7)	O(1)-Co(1)-O(2)	58.60(5)
N(3)-Co(1)-O(1)	138.17(6)	O(3)#1-Co(1)-O(2)	169.10(5)
N(1)-Co(1)-O(1)	99.78(6)	N(3)-Co(1)-O(4)#1	92.55(6)
N(3)-Co(1)-O(3)#1	102.37(6)	N(1)-Co(1)-O(4)#1	151.23(6)
N(1)-Co(1)-O(3)#1	94.13(6)	O(1)-Co(1)-O(4)#1	83.73(6)
O(1)-Co(1)-O(3)#1	110.61(5)	O(3)#1-Co(1)-O(4)#1	58.51(5)
N(3)-Co(1)-O(2)	86.75(6)	O(2)-Co(1)-O(4)#1	115.77(5)
N(1)-Co(1)-O(2)	89.56(6)		
Symmetry transformations used to generate equivalent atoms:			
#1 x+1, y, z+1.			
Compound **3**			
Ni(1)-N(3)	2.044(2)	Ni(2)-O(9)	2.059(2)
Ni(1)-O(3)	2.0644(17)	Ni(2)-O(1)	2.0643(19)
Ni(1)-O(10)	2.122(2)	Ni(2)-O(12)	2.100(2)
Ni(2)-O(8)	2.032(2)	Ni(2)-O(7)	2.114(2)
Ni(2)-N(1)	2.045(2)		
O(12)-Ni(2)-O(7)	87.46(9)	O(8)-Ni(2)-O(1)	89.03(8)
N(3)-Ni(1)-O(3)	90.25(7)	N(1)-Ni(2)-O(1)	176.79(8)
N(3)#1-Ni(1)-O(3)	89.75(7)	O(9)-Ni(2)-O(1)	92.33(8)
N(1)-Ni(2)-O(9)	87.66(8)	O(8)-Ni(2)-O(12)	171.36(8)
N(3)-Ni(1)-O(10)	87.97(8)	N(1)-Ni(2)-O(12)	90.63(8)
N(3)#1-Ni(1)-O(10)	92.03(8)	O(9)-Ni(2)-O(12)	94.38(9)
O(3)-Ni(1)-O(10)	90.66(8)	O(1)-Ni(2)-O(12)	86.17(8)
O(3)#1-Ni(1)-O(10)	89.34(8)	O(8)-Ni(2)-O(7)	85.24(9)
O(1)-Ni(2)-O(7)	88.44(8)	N(1)-Ni(2)-O(7)	91.67(9)
O(8)-Ni(2)-N(1)	94.18(8)	O(9)-Ni(2)-O(7)	178.05(8)
O(8)-Ni(2)-O(9)	92.98(8)		
Symmetry transformations used to generate equivalent atoms:			
#1 -x+2, -y, -z+1.			

Compound **4**			
Cd(1)-N(1)	2.208(5)	Cd(1)-O(4)#2	2.266(4)
Cd(1)-O(1)	2.207(4)	Cd(1)-O(6)#3	2.507(4)
Cd(1)-O(3)#1	2.219(4)		
N(1)-Cd(1)-O(1)	145.95(16)	O(3)#1-Cd(1)-O(4)#2	110.48(15)
N(1)-Cd(1)-O(3)#1	111.55(17)	N(1)-Cd(1)-O(6)#3	81.27(15)
O(1)-Cd(1)-O(3)#1	95.32(15)	O(1)-Cd(1)-O(6)#3	79.65(13)
N(1)-Cd(1)-O(4)#2	84.78(16)	O(3)#1-Cd(1)-O(6)#3	86.95(14)
O(1)-Cd(1)-O(4)#2	105.62(15)	O(4)#2-Cd(1)-O(6)#3	160.85(16)
Symmetry transformations used to generate equivalent atoms:			
#1 -x, -y+2, -z+1; #2 x+1, y, z; #3 x+1, y, z-1.			

Table S2. The parameters of hydrogen bonds for **2** and **3**.

Complex **2**				
D-H---*A*	*D*-H	H---*A*	*D*---*A*	*D*-H---*A*
O(1W)-H(1WB)...O(1)	0.85	2.57	3.094(3)	121
O(1W)-H(1WA)...O(4)#1	0.85	2.23	3.018(3)	154
N(4)-H(4)...O(2)#5	0.86	1.93	2.775(2)	167
N(2)-H(2A)...O(3)#6	0.86	1.98	2.785(2)	155
Symmetry codes: #1 -x, -y-1, -z+2; #5 x+1, y+1, z; #6 -x+1, -y+1, -z+1.				
Complex **3**				
D-H---*A*	*D*-H	H---*A*	*D*---*A*	*D*-H---*A*
O(12)-H(12B)...O(11)#6	0.88	1.88	2.744(4)	169
O(11)-H(11C)...O(2)#7	0.85	1.91	2.735(4)	163
O(10)-H(10A)...O(4)#8	0.86	2.18	2.908(3)	143
O(10)-H(10B)...O(4)#1	0.82	2.00	2.733(3)	149
O(9)-H(9B)...O(5)#9	0.89	1.94	2.830(3)	175
O(9)-H(9A)...O(2)	0.82	1.84	2.582(3)	150
O(8)-H(8B)...O(6)#8	0.74	2.13	2.807(3)	153
O(8)-H(8A)...O(6)#9	0.82	1.85	2.608(3)	153
O(7)-H(7A)...O(5)#10	0.84	2.04	2.874(3)	173
N(4)-H(4)...O(5)#11	0.86	2.18	3.014(3)	162
N(2)-H(2)...O(4)#6	0.86	2.08	2.872(3)	152

Symmetry codes: #1 -x+2, -y, -z+1; #4 -x+1, -y, -z+2; #5 -x+2, -y, -z+2; #6 x, y, z+1; #7 x+1, y, z-1; #8 x+1, y, z; #9 -x, -y+1, -z+2; #10 -x+1, -y+1, -z+2; #11 x+1, y-1, z.



Scheme S1. Coordination modes of carboxylate ligands appeared in **1** - **4**.

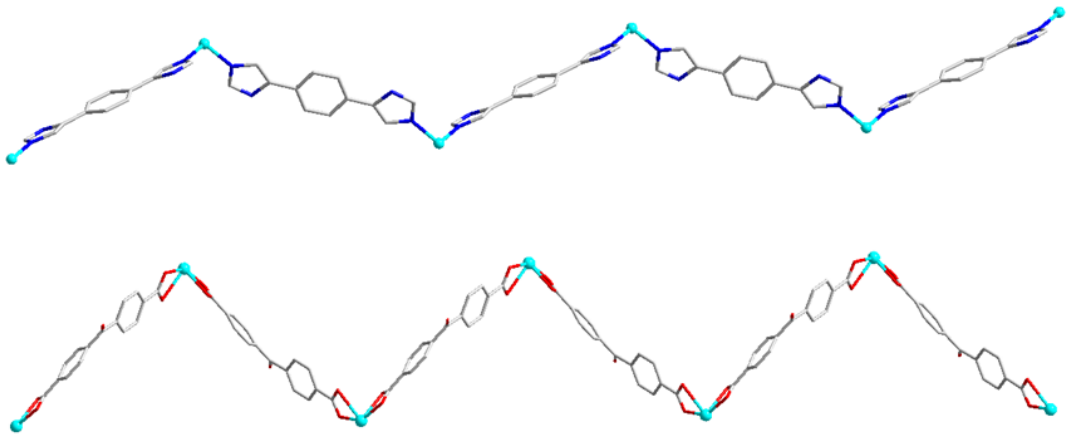


Fig. S1. The 1D zigzag chains of Zn(II)-L and Zn(II)-bpdc^{2-} in **1**.

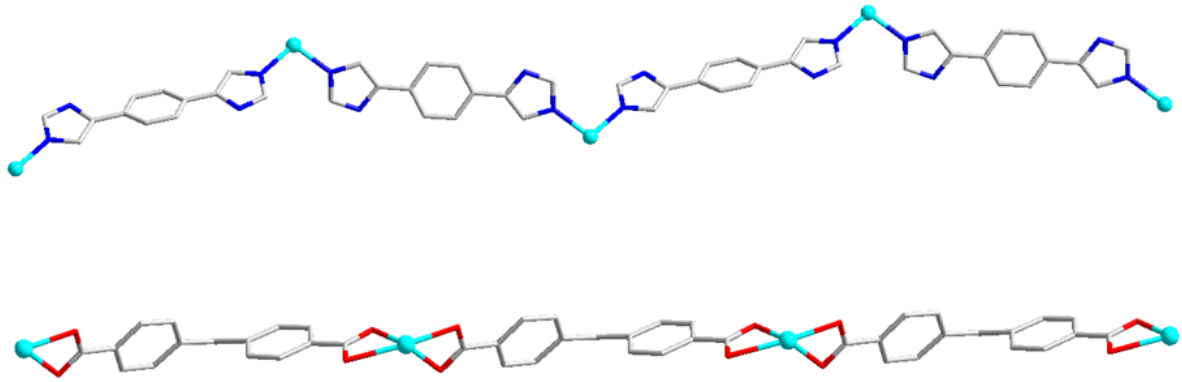


Fig. S2. 1D zigzag chains of Co(II)-L and Co(II)-bpdc^{2-} in **2**.

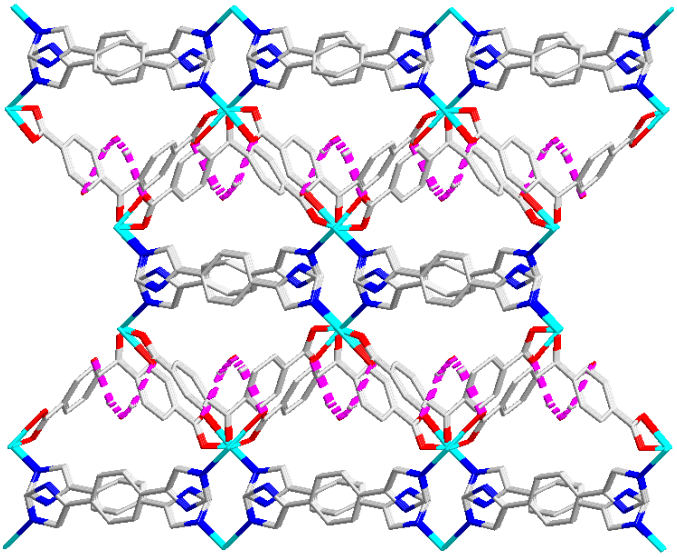


Fig. S3. 3D structure of **2** with hydrogen bonds indicated by dashed lines.

Fig. S4. 1D zigzag chain of Ni(II)-L in **3**.

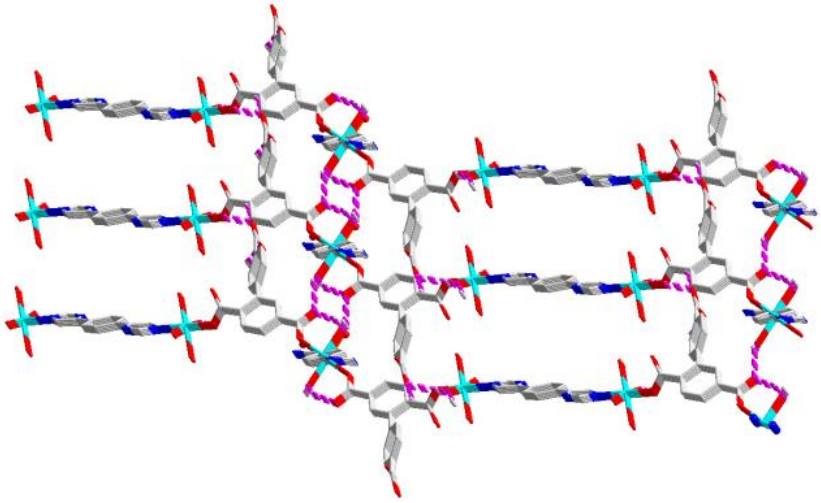


Fig. S5. 3D structure of **3** with hydrogen bonds indicated by dashed lines.

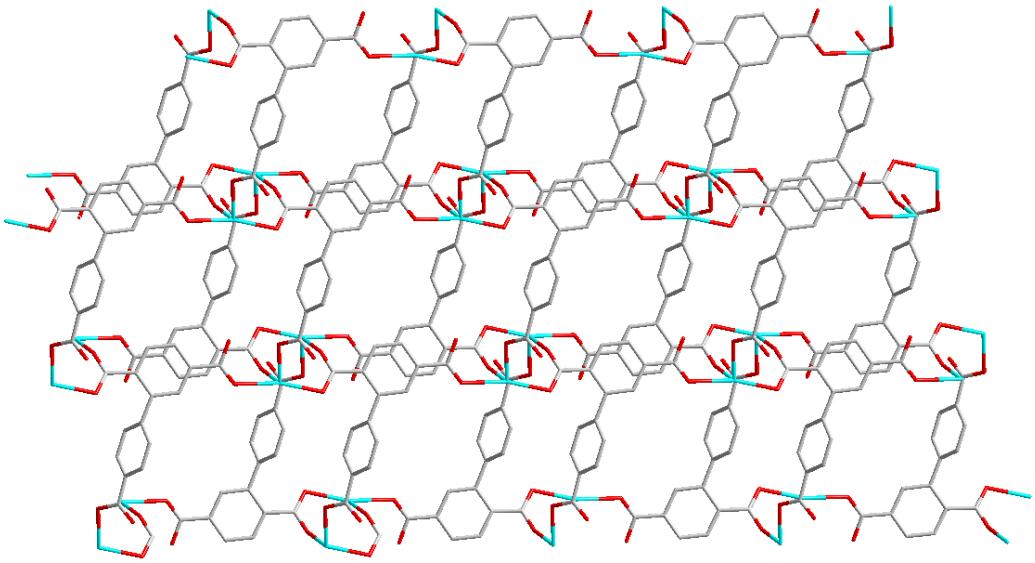


Fig. S6. The 2D network of Cd(II)-$Hbptc^{2-}$ in **4**.

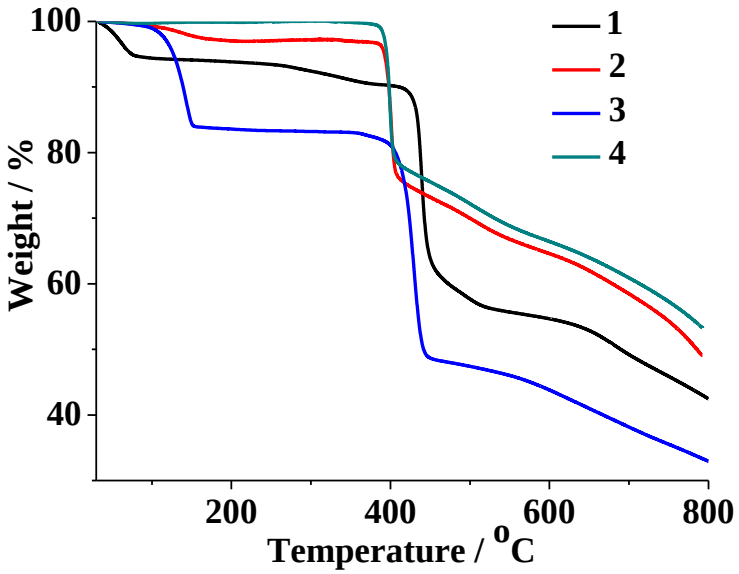
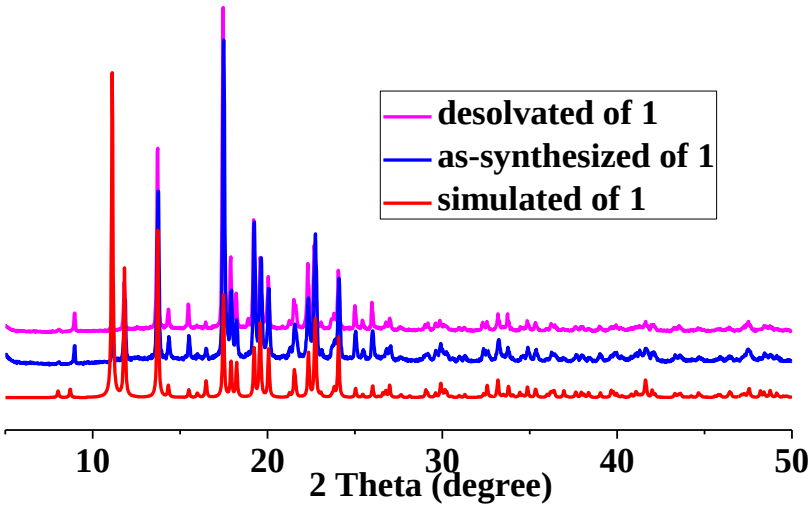
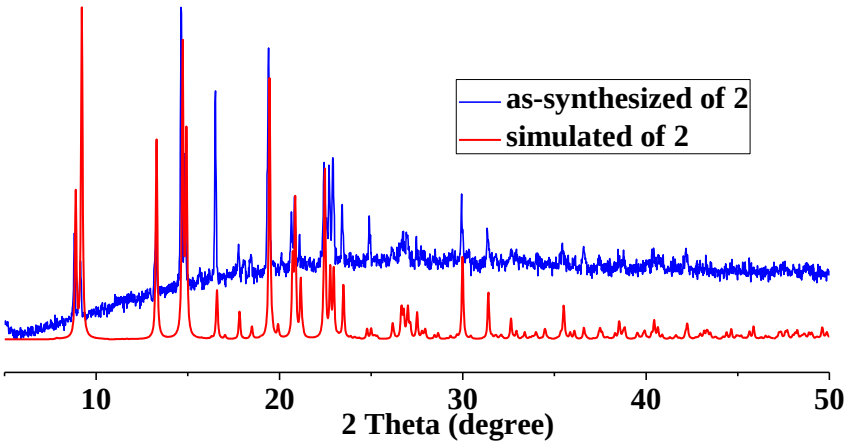


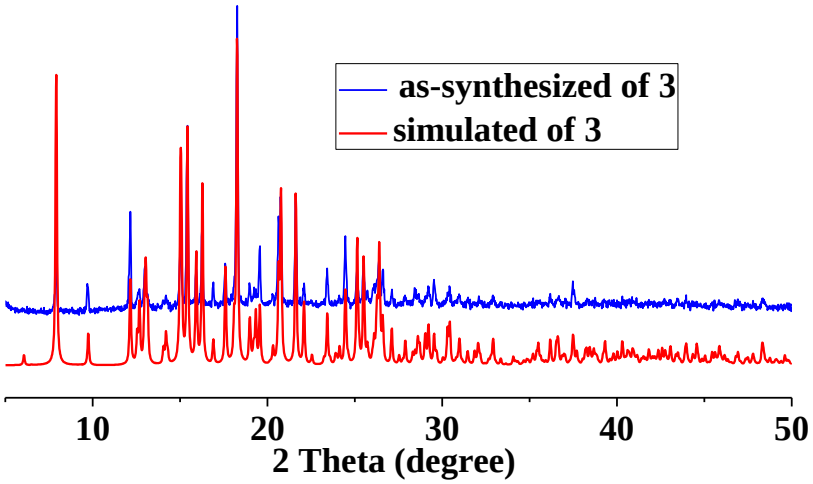
Fig. S7. TG curves of **1** - **4**.


desolvated of 1
as-synthesized of 1
simulated of 1
10
20
30
40
50
2 Theta (degree)

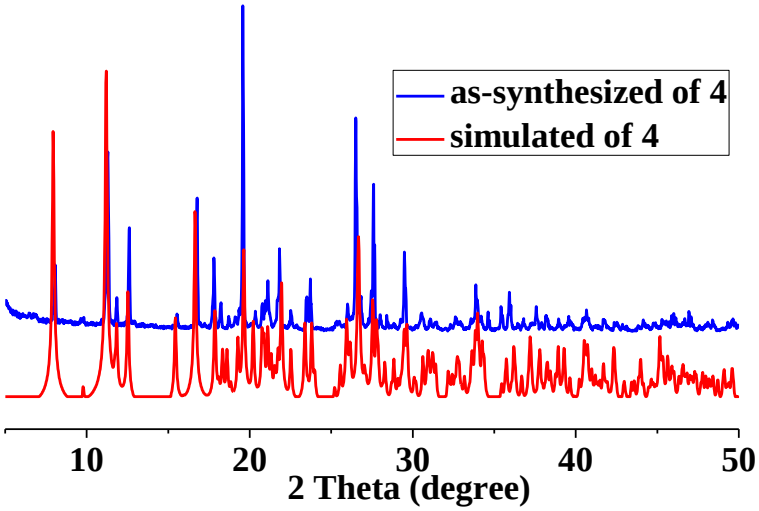
(a)


as-synthesized of 2
simulated of 2
10
20
30
40
50
2 Theta (degree)

(b)



(c)



(d)

Fig. S8. PXRD patterns of **1 - 4**.

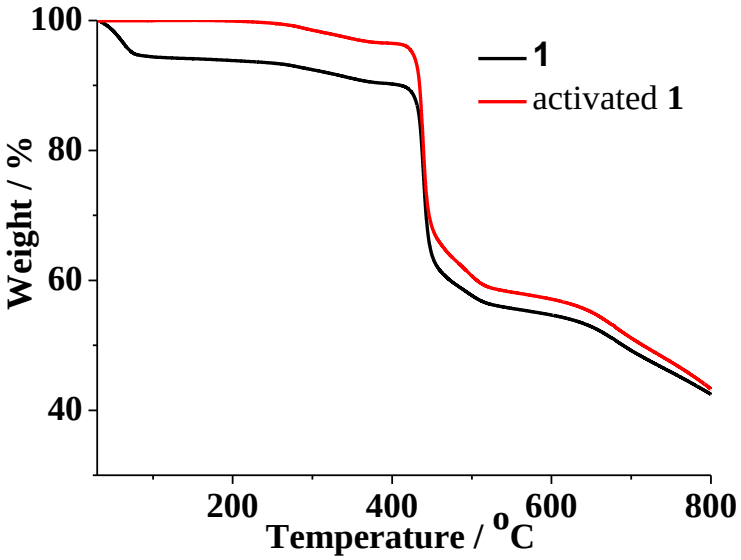


Fig. S9. TG curves of **1**.

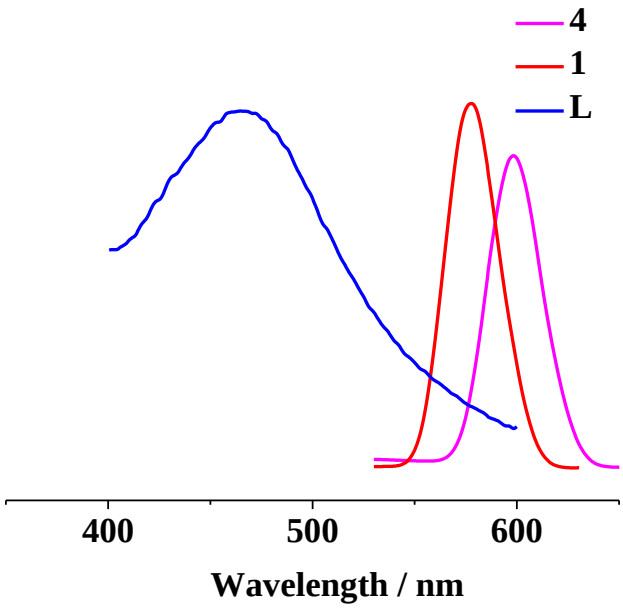


Fig. S10. Emission spectra of **1**, **4** and ligand L in the solid state.

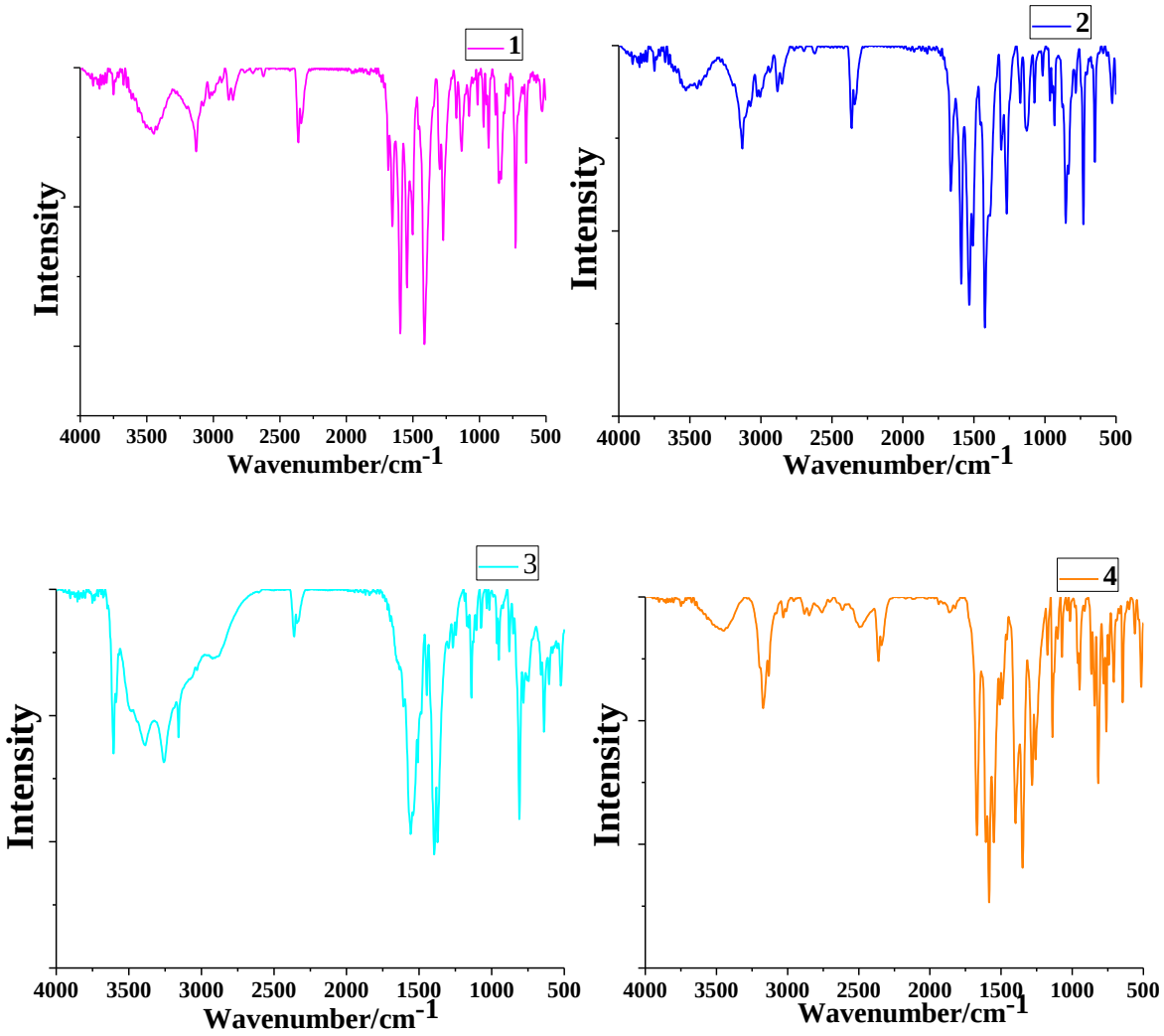


Fig. S11. IR spectra of **1 - 4**.