Electronic supplementary information

New metal-organic frameworks with 2,6-di(1H-imidazol-1-yl)naphthalene and dicarboxylate ligands: Synthesis, crystal structure and photoluminescence sensing property

LIU Zhi-Qiang[1,2] CAO Shi-Hu[1] ZHANG Zhe[1] WU Jun-Feng[1] ZHAO Yue[2] SUN Wei-Yin*[,2]

([1]*School of Chemistry and Chemical Engineering, AnHui Province Key Laboratory of Functional Optical, Electrical and Magnetic Materials, Key Laboratory of Functional Coordination Compounds and Nano Materials of Anhui Higher Education Institutes, Anqing Normal University, Anqing 246011, China*)

([2] *State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, China*)

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

Compound **1**			
Co(1)-O(1)	0.19837(15)	Co(1)-N(1)	0.20329(19)
O(1)-Co(1)-O(1)^{i}	96.41(9)	O(1)^{i}-Co(1)-N(1)	107.06(7)
O(1)-Co(1)-N(1)	118.25(7)	N(1)-Co(1)-N(1)^{i}	109.77(11)
Symmetry transformations used to generate equivalent atoms:			
^{i} -x,y,-z+1/2.			
Compound **2**			
Co(1)-O(2)	0.20244(13)	Co(1)-N(4)^{ii}	0.21388(16)
Co(1)-O(1)^{i}	0.20467(13)	Co(1)-O(3)^{iii}	0.21548(13)
Co(1)-N(1)	0.21258(16)	Co(1)-O(4)^{iii}	0.22451(14)
O(2)-Co(1)-O(1)^{i}	111.15(5)	N(1)-Co(1)-O(3)^{iii}	93.34(6)
O(2)-Co(1)-N(1)	86.75(6)	N(4)#2-Co(1)-O(3)^{iii}	88.69(6)
O(1)^{ii}-Co(1)-N(1)	86.71(6)	O(2)-Co(1)-O(4)^{iii}	155.52(6)
O(2)-Co(1)-N(4)^{ii}	91.52(6)	O(1)^{i}-Co(1)-O(4)^{iii}	93.18(5)

$O(1)^{i}$-Co(1)-$N(4)^{ii}$	92.18(6)	N(1)-Co(1)-$O(4)^{iii}$	92.21(6)
N(1)-Co(1)-$N(4)^{ii}$	177.45(6)	$N(4)^{ii}$-Co(1)-$O(4)^{iii}$	90.14(6)
O(2)-Co(1)-$O(3)^{iii}$	95.99(5)	$O(3)^{iii}$-Co(1)-$O(4)^{iii}$	59.63(5)
$O(1)^{i}$-Co(1)-$O(3)^{iii}$	152.81(5)		

Symmetry transformations used to generate equivalent atoms:

^{i} -x+1,-y+1,-z+2 ^{ii} x-1,y-1,z+1 ^{iii} -x,-y+1,-z+2.

Compound **3**

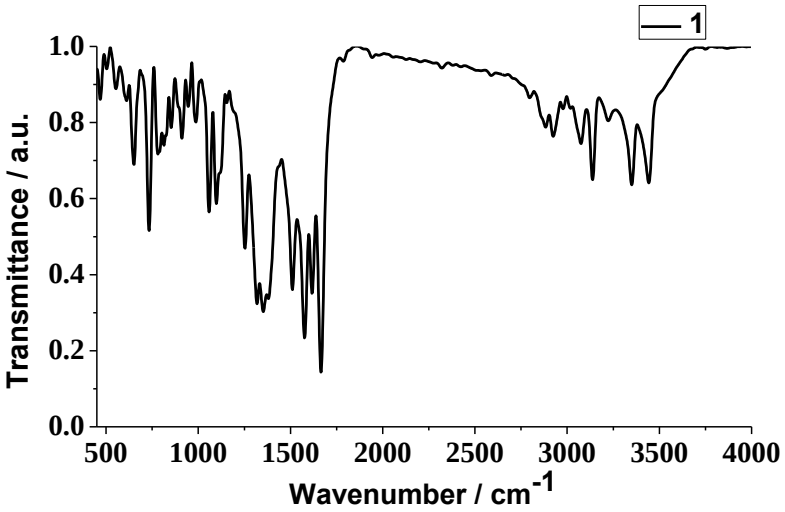
Co(1)-O(6)	0.20335(17)	Co(1)-N(1)	0.21477(19)
Co(1)-O(1)	0.21022(15)	Co(1)-$N(4)^{i}$	0.21556(18)
Co(1)-O(5)	0.21051(16)	Co(1)-$O(5)^{ii}$	0.22437(16)
O(6)-Co(1)-O(1)	91.58(7)	O(5)-Co(1)-$N(4)^{i}$	94.17(7)
O(6)-Co(1)-O(5)	168.30(7)	N(1)-Co(1)-$N(4)^{i}$	99.73(8)
O(1)-Co(1)-O(5)	87.49(6)	O(6)-Co(1)-$O(5)^{ii}$	89.04(7)
O(6)-Co(1)-N(1)	96.99(8)	O(1)-Co(1)-$O(5)^{ii}$	82.33(6)
O(1)-Co(1)-N(1)	82.85(7)	O(5)-Co(1)-$O(5)^{ii}$	79.27(6)
O(5)-Co(1)-N(1)	94.47(7)	N(1)-Co(1)-$O(5)^{ii}$	164.14(7)
O(6)-Co(1)-$N(4)^{i}$	86.24(7)	N(4)#1-Co(1)-$O(5)^{ii}$	95.29(7)
O(1)-Co(1)-$N(4)^{i}$	176.80(7)		

Symmetry transformations used to generate equivalent atoms:

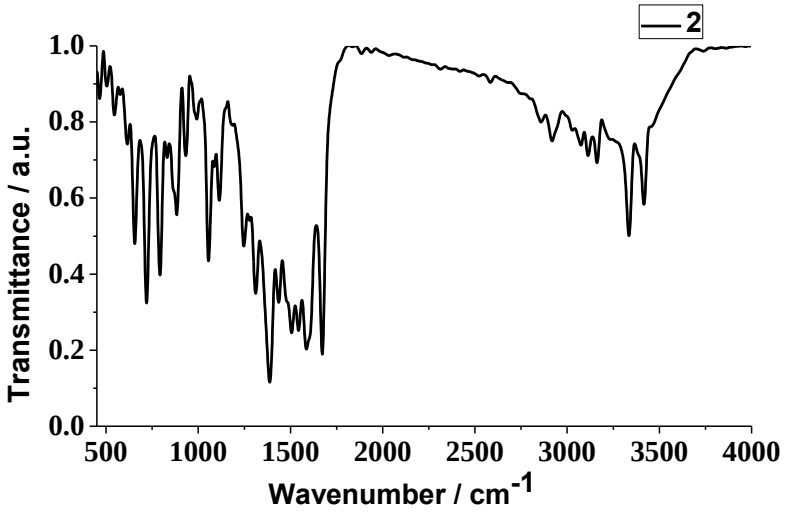
^{i} x,y+1,z-1 ^{ii} -x,-y+2,-z.

Table S2. Parameters of hydrogen bonds for 1 - 3.

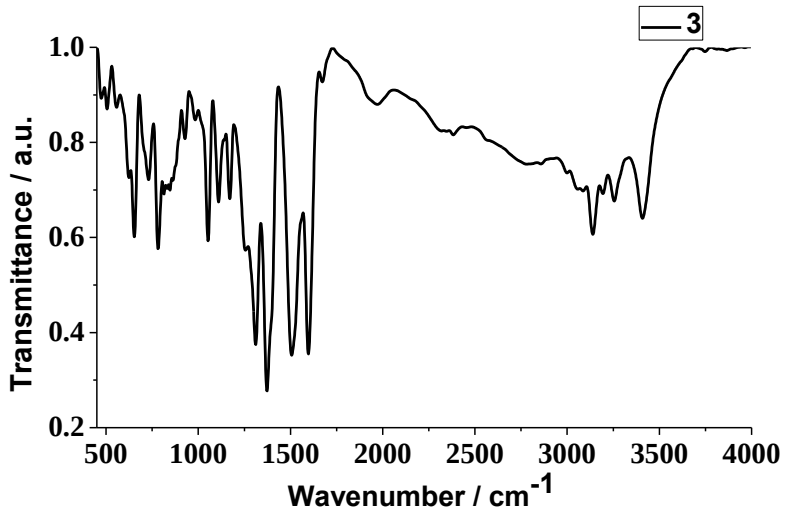
Complex **1**				
D-H---*A*	*D*-H (nm)	H---*A* (nm)	*D*---*A* (nm)	*D*-H---*A* (°)
C(16)-H(16)...O(1)^{iv}	0.093	0.237	0.3289(3)	168
C(13)-H(13)...O(5)^{v}	0.093	0.232	0.3239(3)	169
C(9)-H(9)...O(2)^{i}	0.093	0.242	0.3001(3)	121
N(5)-H(5A)...O(5)^{vi}	0.084	0.231	0.3072(3)	151
Complex **2**				
D-H---*A*	*D*-H (nm)	H---*A* (nm)	*D*---*A* (nm)	*D*-H---*A* (°)
C(4)-H(4)...O(5)^{v}	0.093	0.244	0.3228(4)	143
N(5)-H(5B)...O(4)^{vi}	0.089	0.215	0.3008(2)	163
N(5)-H(5A)...O(1)^{vii}	0.089	0.251	0.3071(2)	122
Complex **3**				
D-H---*A*	*D*-H (nm)	H---*A* (nm)	*D*---*A* (nm)	*D*-H---*A* (°)
C(27)-H(27)...O(4)	0.093	0.226	0.3119(3)	154
C(15)-H(15)...O(4)^{v}	0.093	0.228	0.3094(3)	146
O(6)-H(6B)...O(3)^{i}	0.096	0.184	0.2776(3)	165
O(6)-H(6A)...N(6)	0.096	0.175	0.2664(3)	159
N(7)-H(7A)...O(1W)	0.086	0.205	0.2843(3)	153
C(21)-H(21)...O(4)	0.093	0.261	0.3524(3)	169



(a)



(b)



(c)

Fig. S1 IR spectra of **1** - **3**.

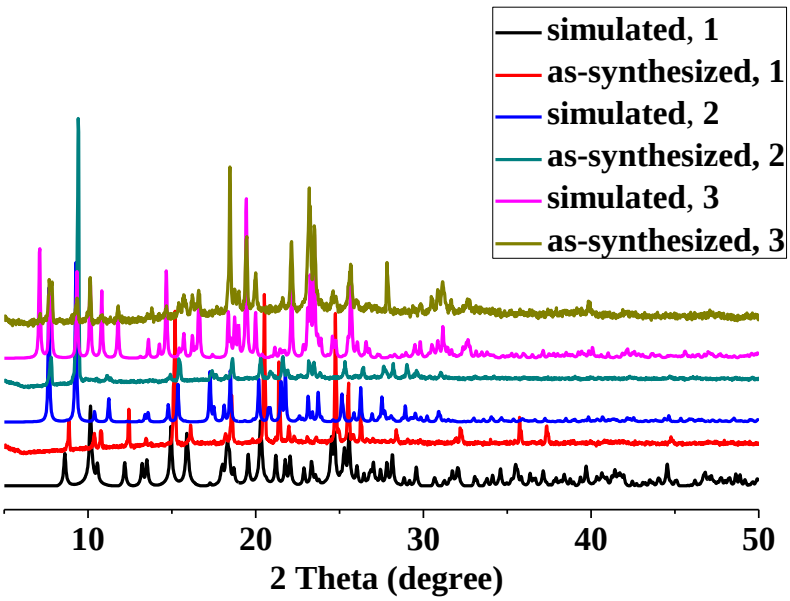


Fig. S2 PXRD patterns of **1** - **3**.

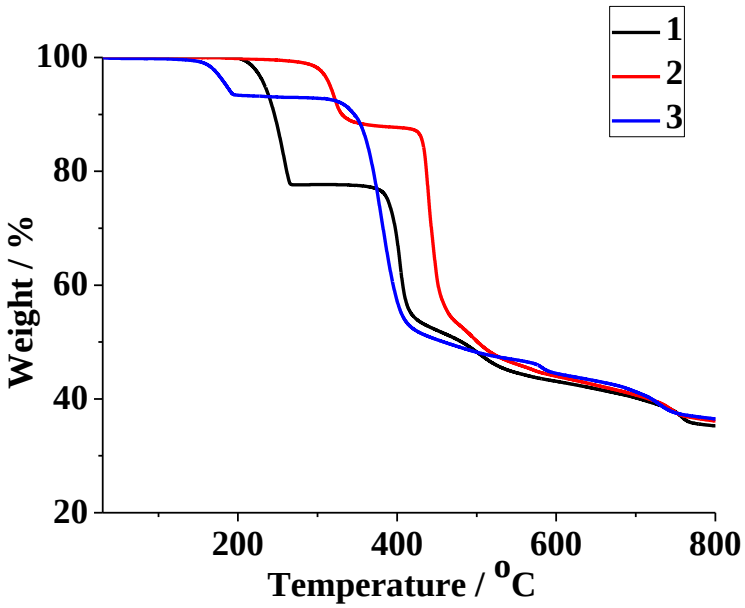


Fig. S3 The TGA curves of **1** - **3**.

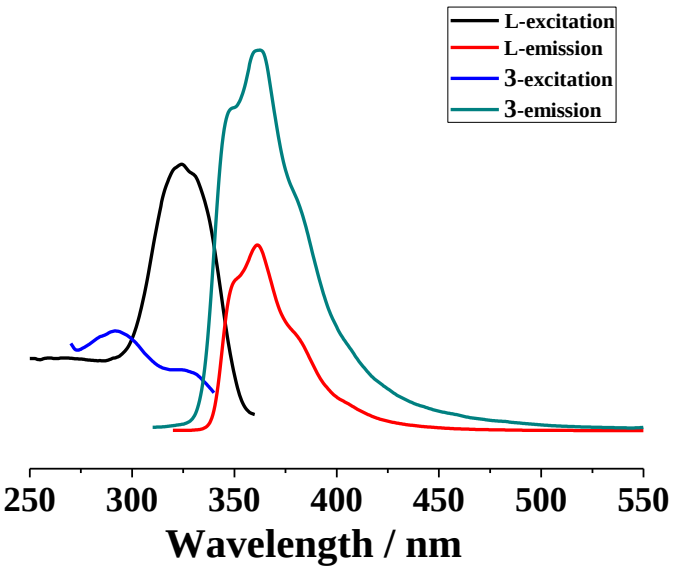


Fig. S4 Emission and excitation spectra of L and **3** in the solid state at room temperature.