

Electronic Supplementary Information (ESI) for:

Two d¹⁰ luminescent metal organic frameworks as dual functional luminescent sensors for (Fe³⁺, Cu²⁺) and 2,4,6-trinitrophenol(TNP) with high selectivity and sensitivity

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Table S1. Selected bond distances (Å) and angles (°) for **1**

Cd1-O1	2.187(4)	Cd2-O5 ⁱⁱⁱ	2.228(3)
Cd1-O5 ⁱ	2.284(3)	Cd2-O5	2.228(3)
Cd1-N2	2.314(4)	Cd2-O2 ^{iv}	2.261(4)
Cd1-N3	2.321(4)	Cd2-O2 ^v	2.261(4)
Cd1-O4 ⁱⁱ	2.437(4)	Cd2-O4 ^{vi}	2.288(4)
Cd1-O3 ⁱⁱ	2.443(4)	Cd2-O4 ^{vii}	2.288(4)
O1-Cd1-O5 ⁱ	104.49(15)	O5 ⁱⁱⁱ -Cd2-O5	180.0
O1-Cd1-N2	165.48(15)	O5 ⁱⁱⁱ -Cd2-O2 ^{iv}	86.50(14)
O5 ⁱ -Cd1-N2	82.81(15)	O5-Cd2-O2 ^{iv}	93.50(14)
O1-Cd1-N3	95.32(16)	O5 ⁱⁱⁱ -Cd2-O2 ^v	93.50(14)
O5 ⁱ -Cd1-N3	124.17(14)	O5-Cd2-O2 ^v	86.50(14)
N2-Cd1-N3	70.33(16)	O2 ^{iv} -Cd2-O2 ^v	180.0
O1-Cd1-O4 ⁱⁱ	102.48(14)	O5 ⁱⁱⁱ -Cd2-O4 ^{vi}	103.78(13)
O5 ⁱ -Cd1-O4 ⁱⁱ	72.30(13)	O5-Cd2-O4 ^{vi}	76.21(13)
N2-Cd1-O4 ⁱⁱ	91.65(15)	O2 ^{iv} -Cd2-O4 ^{vi}	87.44(16)
N3-Cd1-O4 ⁱⁱ	151.79(14)	O2 ^v -Cd2-O4 ^{vi}	92.56(16)
O1-Cd1-O3 ⁱⁱ	93.29(16)	O5 ⁱⁱⁱ -Cd2-O4 ^{vii}	76.22(13)
O5 ⁱ -Cd1-O3 ⁱⁱ	125.45(13)	O5-Cd2-O4 ^{vii}	103.79(13)
N2-Cd1-O3 ⁱⁱ	92.47(16)	O2 ^{iv} -Cd2-O4 ^{vii}	92.56(16)
N3-Cd1-O3 ⁱⁱ	104.30(15)	O2 ^v -Cd2-O4 ^{vii}	87.44(16)
O4 ⁱⁱ -Cd1-O3 ⁱⁱ	53.46(13)	O4 ^{vi} -Cd2-O4 ^{vii}	180.0

Symmetry transformations used to generate equivalent atoms: (i) $x+1, y, z$; (ii) $x+1/2, -y+3/2, z+1/2$; (iii) $-x-1/2, -y+3/2, -z+1$; (iv) $-x+1/2, -y+3/2, -z+1$; (v) $x-1, y, z$; (vi) $x-1/2, -y+3/2, z+1/2$; (vii) $-x, y, -z+1/2$; (viii) $x-1/2, -y+3/2, z-1/2$;

Table S2. Selected bond distances (Å) and angles (°) for **2**

Zn1-O2 ⁱ	2.018(2)	Zn2-O4 ⁱⁱⁱ	1.983(3)
Zn1-O2	2.018(2)	Zn2-O1	2.010(2)
Zn1-O3 ⁱⁱ	2.103(2)	Zn2-O5 ^v	2.107(2)
Zn1-O3 ⁱⁱⁱ	2.103(2)	Zn2-N1	2.115(3)
Zn1-O5 ^{iv}	2.160(2)	Zn2-N2	2.189(3)
Zn1-O5 ^v	2.160(2)	Zn2-O6 ^v	2.381(3)
O2 ⁱ -Zn1-O2	179.999(1)	O4 ⁱⁱⁱ -Zn2-O1	97.55(11)
O2 ⁱ -Zn1-O3 ⁱⁱ	92.83(10)	O4 ⁱⁱⁱ -Zn2-O3 ⁱⁱ	98.32(10)
O2-Zn1-O3 ⁱⁱⁱ	87.17(10)	O1-Zn2-O5 ^v	103.51(9)
O2 ⁱ -Zn1-O3 ⁱⁱⁱ	87.17(10)	O4 ⁱⁱⁱ -Zn2-N1	110.29(12)
O2-Zn1-O3 ⁱⁱⁱ	92.83(10)	O1-Zn2-N1	92.47(11)
O3 ⁱⁱ -Zn1-O3 ⁱⁱⁱ	180.0	O5 ^v -Zn2-N1	145.06(11)
O2 ⁱ -Zn1-O5 ^{iv}	91.93(9)	O4 ⁱⁱⁱ -Zn2-N2	86.21(12)
O2-Zn1-O5 ^{iv}	88.07(9)	O1-Zn2-N2	168.04(11)
O3 ⁱⁱ -Zn1-O5 ^{iv}	92.29(9)	O5 ⁱ -Zn2-N2	87.08(10)
O3 ⁱⁱⁱ -Zn1-O5 ^{iv}	87.71(9)	N1-Zn2-N2	75.59(12)
O2 ⁱ -Zn1-O5 ^v	88.07(9)	O4 ⁱⁱⁱ -Zn2-O6 ^v	156.16(10)
O2-Zn1-O5 ^v	91.93(9)	O1-Zn2-O6 ^v	93.76(10)
O3 ⁱⁱ -Zn1-O5 ^v	87.71(9)	O5 ^v -Zn2-O6 ^v	58.50(9)
O3 ⁱⁱⁱ -Zn1-O5 ^v	92.29(9)	N1-Zn2-O6 ^v	90.03(11)
O5 ^{iv} -Zn1-O5 ^v	180.00(14)	N2-Zn2-O6 ^v	87.01(10)

Symmetry transformations used to generate equivalent atoms: (i) $-x+1, -y+1, -z+1$; (ii) $-x+2, -y+1, -z+1$; (iii) $x-1, y, z$; (iv) $-x+1, -y, -z+1$; (v) $x, y+1, z$; (vi) $x, y-1, z+1/2$; (vii) $x+1, y, z$.

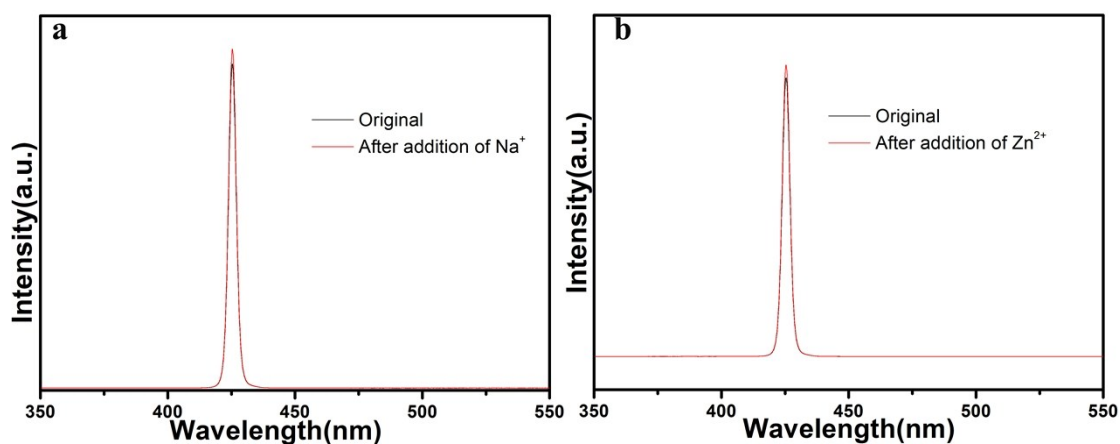


Fig.S1 a) The emission of the original compound **1** emulsion and after the addition of 1000 μL Na^+ (0.01 M) solution; **b)** The emission of the original compound **1** emulsion and after the addition of 1000 μL Zn^{2+} (0.01 M) solution

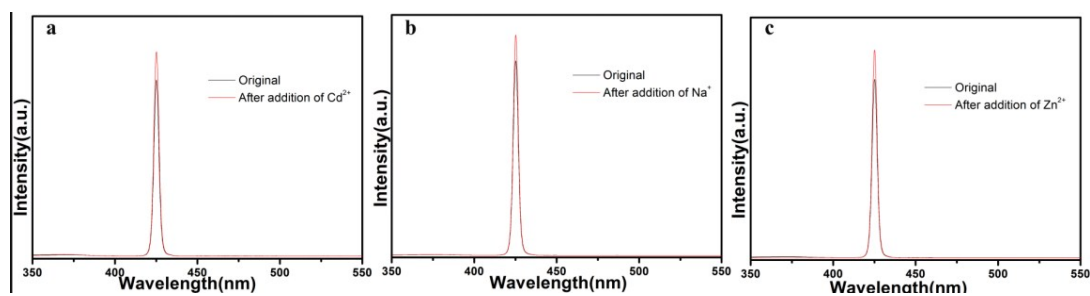


Fig.S2 a) The emission of the original compound 2 emulsion and after the addition of 1000 μL Cd^{2+} (0.01 M) solution; b) The emission of the original compound 2 emulsion and after the addition of 1000 μL Na^+ (0.01 M) solution; c) The emission of the original compound 2 emulsion and after the addition of 1000 μL Zn^{2+} (0.01 M) solution

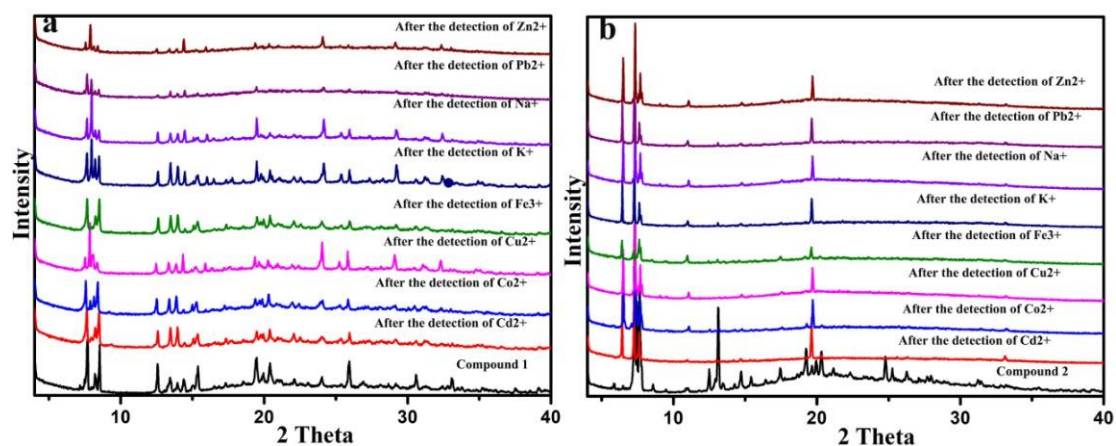


Fig.S3 a) The PXRD of compound 1 and after the detection of the metal ions; b) The PXRD of compound 2 and after the detection of the metal ions

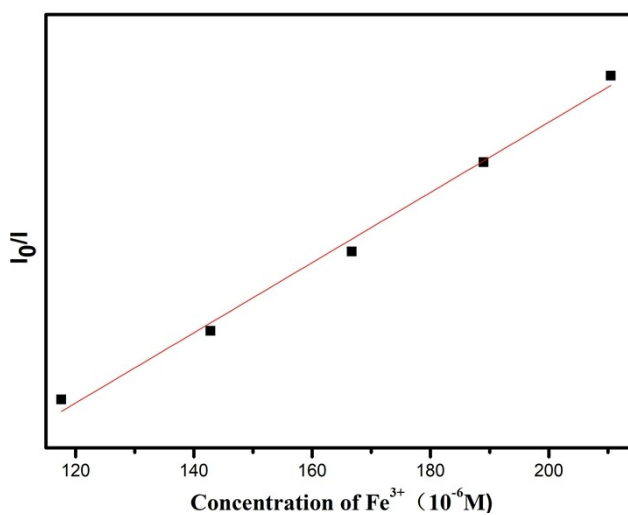


Fig. S4 Stern-Volmer plots of I_0/I vs. the concentration of Fe^{3+} ion of compound 1

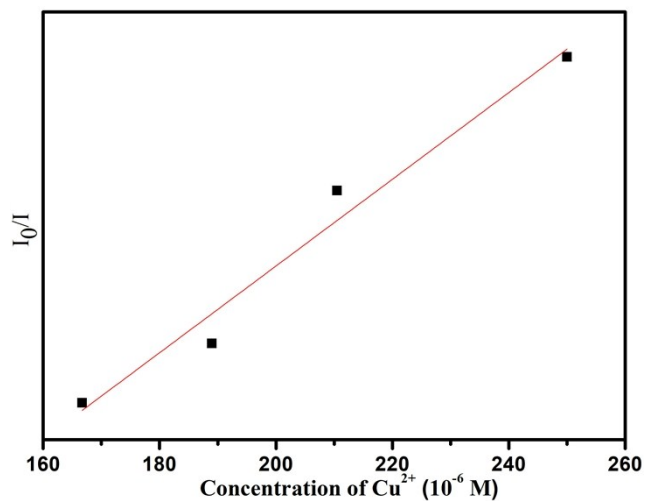


Fig. S5 Stern-Volmer plots of I_0/I vs. the concentration of Cu^{2+} ion of compound 1

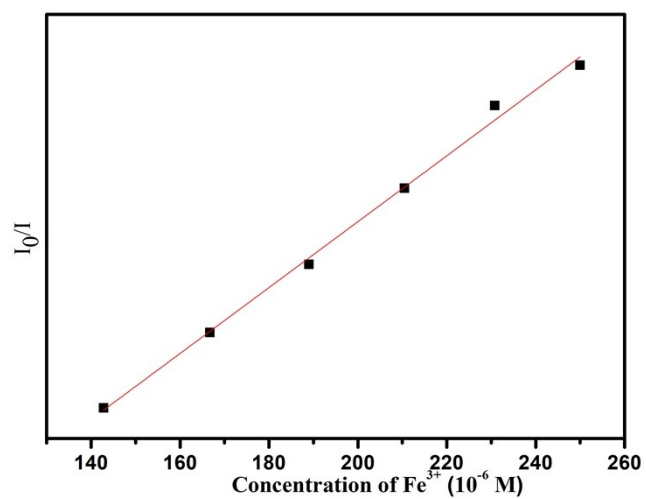


Fig. S6 Stern-Volmer plots of I_0/I vs. the concentration of Fe^{3+} ion of compound 2

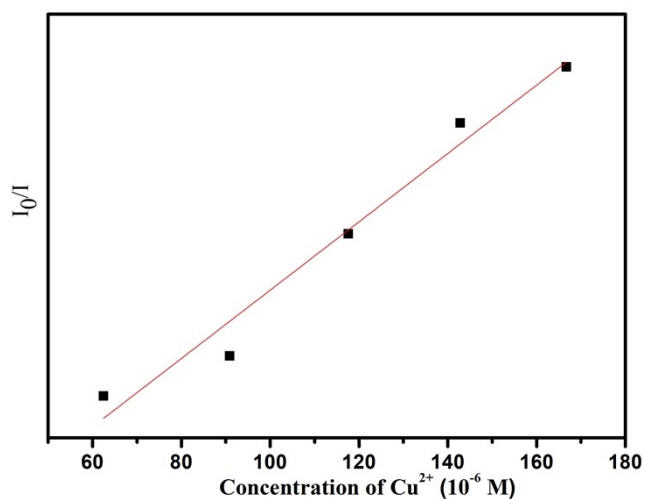


Fig. S7 Stern-Volmer plots of I_0/I vs. the concentration of Cu^{2+} ion of compound 2

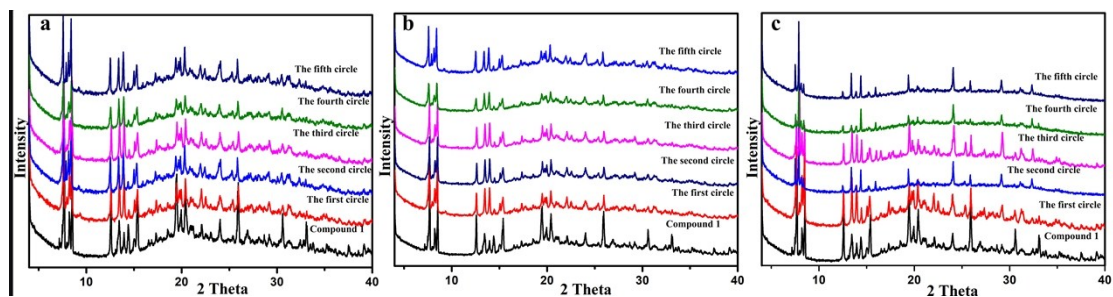


Fig. S8 a) Five circle PXRD experiments of compound 1 after sensing Fe^{3+} ; b) Five circle PXRD experiments of compound 1 after sensing Cu^{2+} ; c) Five circle PXRD experiments of compound 1 after sensing TNP

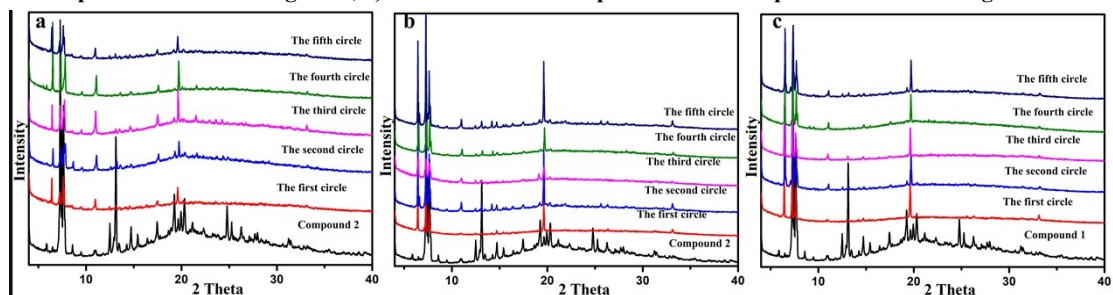


Fig. S9 a) Five circle PXRD experiments of compound 2 after sensing Fe^{3+} ; b) Five circle PXRD experiments of compound 2 after sensing Cu^{2+} ; c) Five circle PXRD experiments of compound 2 after sensing TNP

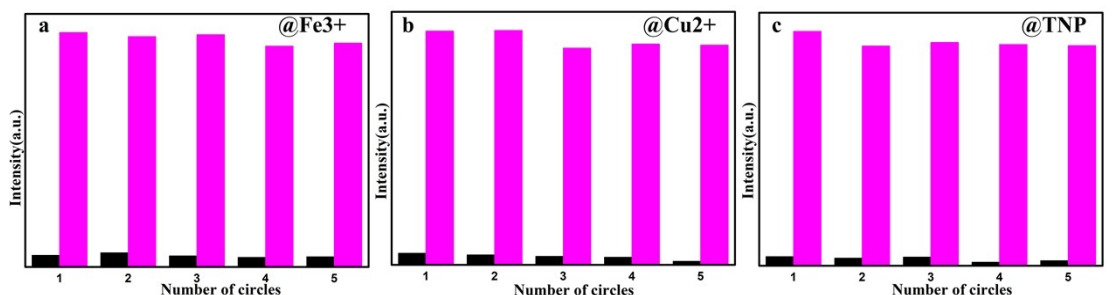


Fig. S10 a) Five circle test of compound 1a towards sensing Fe^{3+} in DMF; b) Five circle test of compound 1a towards sensing Cu^{2+} in DMF; c) Five circle test of compound 1a towards sensing TNP in DMF

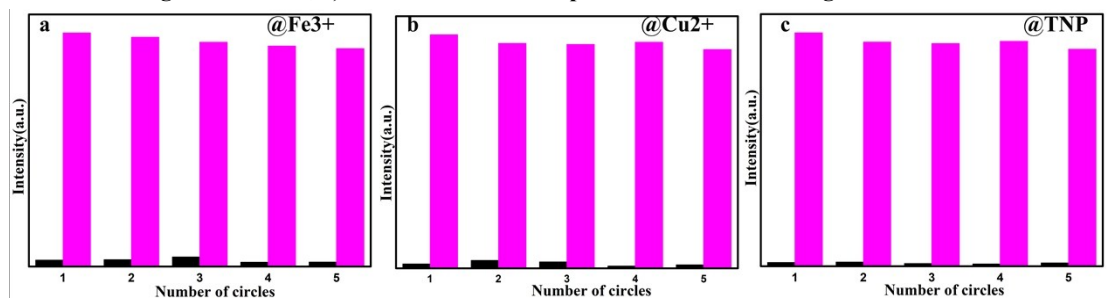


Fig. S11 a) Five circle test of compound 1b towards sensing Fe^{3+} in DMF; b) Five circle test of compound 1b towards sensing Cu^{2+} in DMF; c) Five circle test of compound 1b towards sensing TNP in DMF

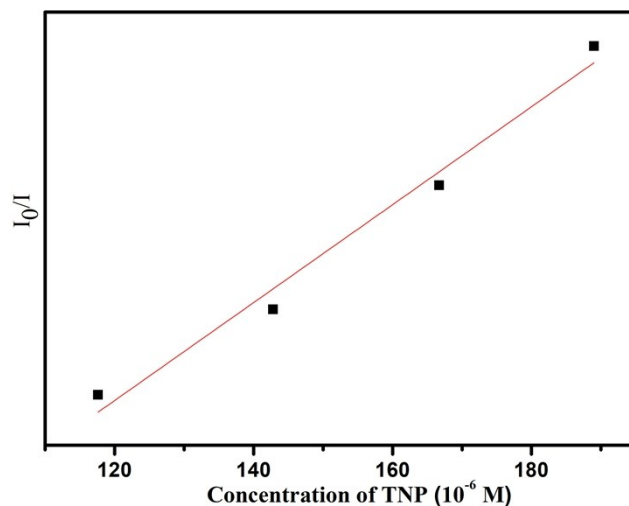


Fig. S12 Stern-Volmer plots of I_0/I vs. the concentration of TNP of compound 1

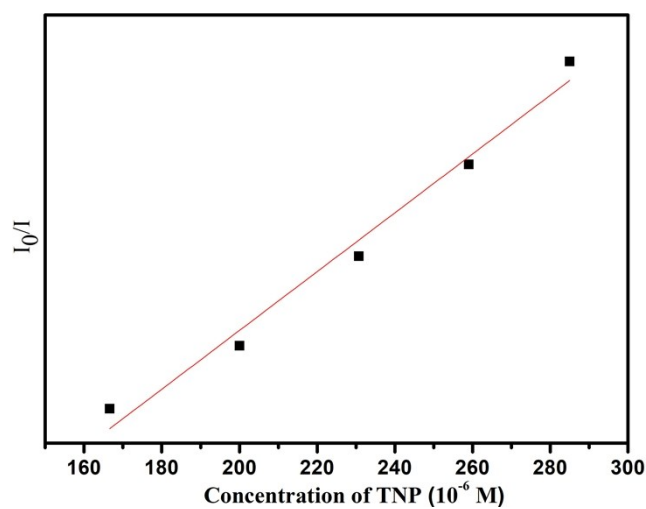


Fig. S13 Stern-Volmer plots of I_0/I vs. the concentration of TNP of compound 2

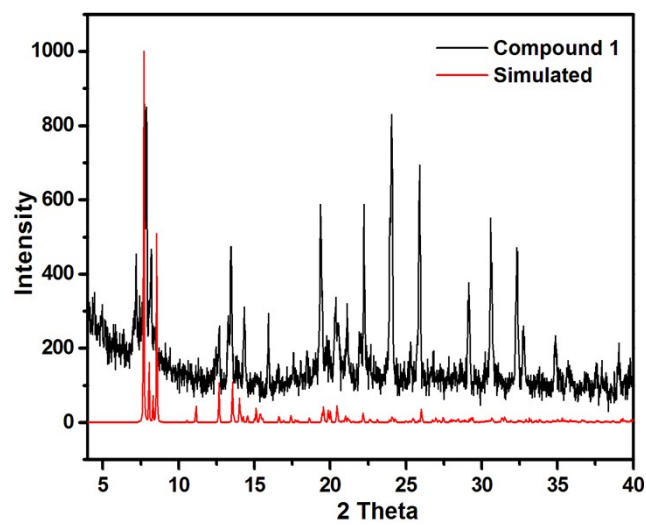


Fig. S14 The PXRD of compound 1

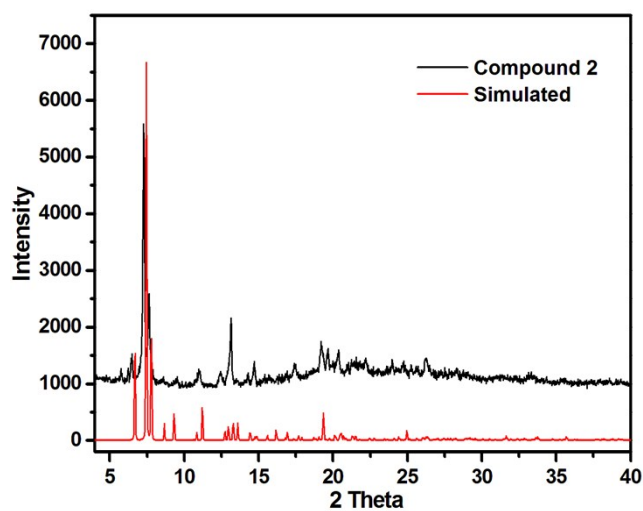


Fig. S15 The PXRD of compound 2

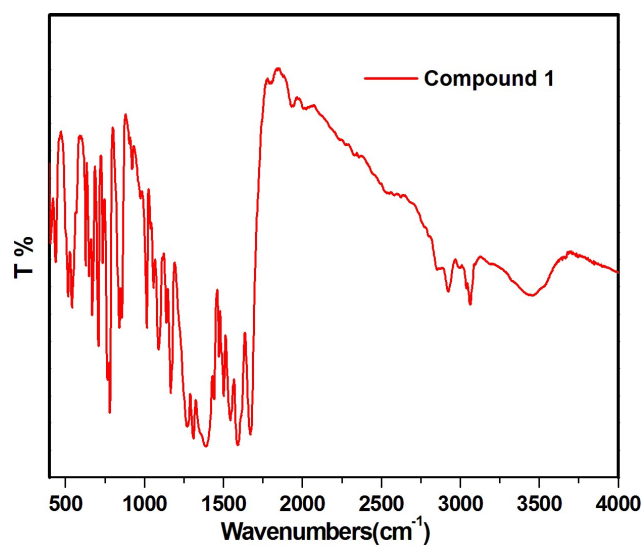


Fig. S16 The IR spectrum of compound 1

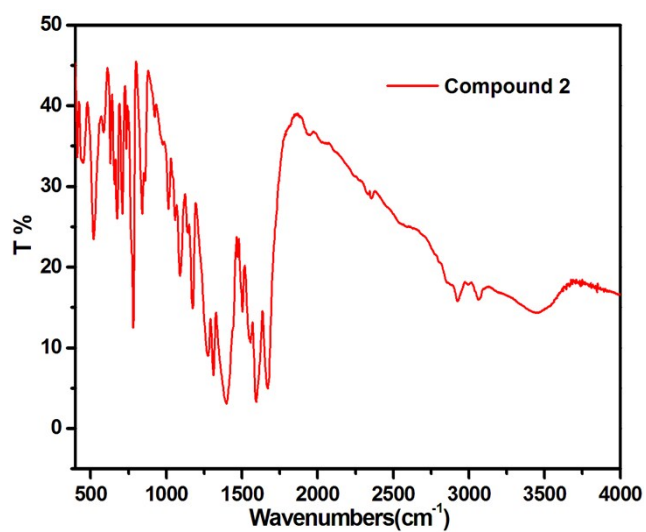


Fig. S17 The IR spectrum of compound 2

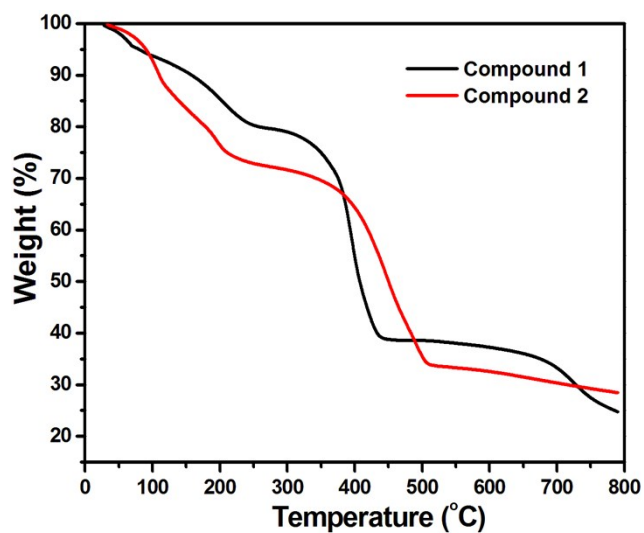


Fig. S18 TGA of compounds 1 and 2

To investigate the thermal stability of compound 1 and 2, thermogravimetric analysis (TGA) was performed under N_2 atmosphere. The results indicate that compound 1 may completely release the guest molecules up to 280 °C. It shows two distinct weight losses of 30-74 °C (5.4 %) and 74-281 °C (13.6 %), attributing to the loss of one water, one CH_3CH_2OH and three DMF molecules, respectively, as to compound 2, it released four DMF, one H_2O , one CH_3CH_2OH molecules at 216 °C (22 %).