

SUPPORTING INFORMATION

Triazine functionalized nanoporous metal-organic framework for selective adsorption and chromatographic separation of transition metal ions and cationic dyes and white-light emission by Ln³⁺ ions encapsulation.

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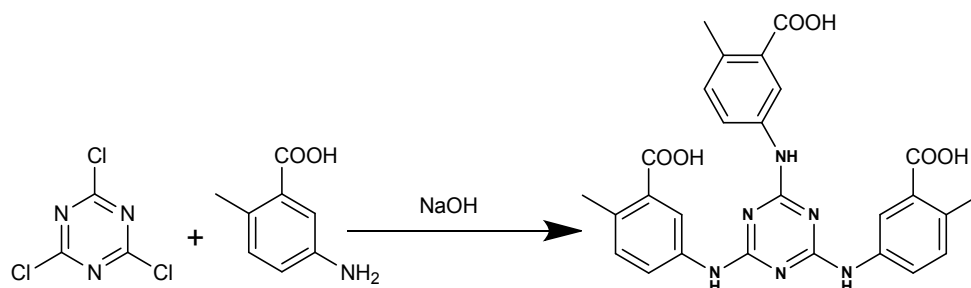
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Synthesis of Ligand 5,5',5''-((1,3,5-triazine-2,4,6-triyl)tris(azanediyl))tris(3-methylbenzoic acid)



Ligand 5,5',5''-((1,3,5-triazine-2,4,6-triyl)tris(azanediyl))tris(2-methylbenzoic acid) was synthesized by a procedure similar to the previously reported one for the synthesis of H₆TATPT.[1] Cyanuric chloride (1.84 g, 0.01 mol) was added to H₂O (30 ml) and then was stirred at 0 °C for 30 min. After that a mixture of 5-amino-2-methylbenzoic acid (1.51 g, 0.01 mol) and NaOH (0.5 g, 0.0125 mol) was added dropwise into the aqueous solution and stirred at 0 °C for 1.5 h. Then a solution of 5-amino-2-methylbenzoic acid (3.02 g, 0.02 mol) and sodium hydroxide (1g) in H₂O (25 ml) was added and the reaction mixture was stirred at room temperature. After stirring at room temperature for 2 h, the mixture was heated slowly to boiling and refluxed for 3 h. During this period, the pH of the mixture was maintained between 10 and 11 by the addition of sodium hydroxide solution. After cooling, the volume was increased to approximately 500 ml by adding water (300 ml). The solution was acidified with concentrated hydrochloric acid where upon a crystalline solid precipitated out. The mixture was allowed to cool to room temperature and filtered.

After washing thoroughly with cold water, the product was dried at 65°C in a vacuum oven. Yield: 80%. ¹H-NMR (500 MHz, DMSO-d₆) δ = 2.48(s, 9H), 7.38 (s, 3H), 7.56 (s, 3H), 8.16 (s, 3H), 8.2 (s, 3H), 9.36 (s, 3H), 12.73 (s, 3H); ¹³C NMR (150 MHz, DMSO-d₆): δ = 169.3, 165.7, 142.2, 139.1, 130.93, 126.04, 120.4, 111.6, 21.3

[1] C. Y. Sun, X. L. Wang, C. Chao, J. L. Jin, Z. M. Su, P. Huang and K. Z. Shao, Solvatochromic Behavior of Chiral Mesoporous MetalOrganic Frameworks and Their Applications for Sensing Small Molecules and Separating Cationic Dyes, Chem. Eur. J. 19 (2013) 3639.

Table S1. Crystal data and structure refinement for MOF1

	C_{38}
Empirical formula	$Cd_2N_{12}O_8H_{28}$
Formula weight	977.30
Crystal system	Monoclinic
Space group	$C12/m1$
a (Å)	38.99 (2)
b (Å)	21.8182(14)
c (Å)	21.818
α (°)	90.00
β (°)	124.03
γ (°)	90
V (Å ³)	15382.4(13)
Z	8
ρ_{calc} (mg cm ⁻³)	0.844
F(000)	3776
Reflections collected	40201
Crystal size	0.24 x 0.22 x 0.2 mm
R1	0.2445
wR2	0.4935

$$R_1 = \frac{\sum |F_0| - |F_c|}{\sum |F_0|}, \text{bw}R_2 = \left[\frac{\sum w (F_0^2 - F_c^2)}{\sum w (F_0^2)} \right]^{1/2}$$

Table S2. Selected Bonds Lengths (Å) and Angles (°) for **MOF1**

The bond lengths of compound 1			
Cd(1)-N(2)	2.820(9)	Cd(2)-N(1)	2.813(2)
Cd(1)-N(4)	2.141(11)	Cd(2)-N(2)	2.804(9)
Cd(1)-N(6)	2.215(6)	Cd(2)-N(3)	2.210(13)
Cd(1)-N(9)	2.812(2)	Cd(2)-N(5)	2.201(7)
Cd(1)-O(1)#1	2.304(13)	Cd(2)-O(3)#3	2.341(12)
Cd(1)-O(2)#2	2.318(12)	Cd(2)-O(4)#1	2.341(14)
Cd(1)-O(5)#1	2.564(11)	Cd(2)-O(7)#3	2.536(12)
Cd(1)-O(6)#2	2.563(11)	Cd(2)-O(8)#1	2.512(13)

The bond angles of compound 1			
N(4)-Cd(1)-N(2)	88.8(4)	N(2)-Cd(2)-N(1)	88.9(3)
N(4)-Cd(1)-N(6)	127.4(4)	N(3)-Cd(2)-N(1)	52.0(4)
N(4)-Cd(1)-O(1)#1	139.4(4)	N(3)-Cd(2)-N(2)	88.4(4)
N(4)-Cd(1)-O(2)#2	84.0(4)	N(3)-Cd(2)-O(3)#3	84.6(5)
N(4)-Cd(1)-N(9)	51.9(4)	N(3)-Cd(2)-O(4)#1	139.7(5)
N(4)-Cd(1)-O(5)#1	90.0(4)	N(3)-Cd(2)-O(7)#3	113.2(4)
N(4)-Cd(1)-O(6)#2	110.7(4)	N(3)-Cd(2)-O(8)#1	89.7(5)
N(6)-Cd(1)-N(2)	51.4(3)	N(3)-Cd(2)-C(7)#3	102.1(5)
N(6)-Cd(1)-O(1)#1	84.2(4)	N(5)-Cd(2)-N(1)	86.4(4)
N(6)-Cd(1)-O(2)#2	140.6(4)	N(5)-Cd(2)-N(2)	52.5(3)
N(6)-Cd(1)-N(9)	89.2(4)	N(5)-Cd(2)-N(3)	125.1(4)
N(6)-Cd(1)-O(5)#1	110.3(3)	N(5)-Cd(2)-O(3)#3	139.8(4)
N(6)-Cd(1)-O(6)#2	90.0(3)	N(5)-Cd(2)-O(4)#1	87.0(4)
N(9)-Cd(1)-N(2)	87.9(3)	N(5)-Cd(2)-O(7)#3	89.0(4)

#1 -x+1/2,-y+3/2,-z+1 #2 -x+1,y,-z+2 #3 -x+1,y,-z+1.

Table S3. ICP results of MOF1 for single metal ion adsorption in DMF solvent containing different metal ions (0.01M) after 12 h immersing

Metal ions (M)	M/Cd Concentration ratio (µg/ml)	M/Cd Mol ratio (calculation)
Cu ²⁺	0.4586/0.5925	0.77
Co ²⁺	0.0328/0.7125	0.074
Ni ²⁺	0.0182/0.7241	0.05
Mn ²⁺	0.0011/0.7452	0.0014
Zn ²⁺	0.0013/0.7369	0.0017

Table S4. ICP results for selective metal ion adsorption in mixed metal ions system in MOF1

Metal ions (M)	M/Cd Concentration ratio (µg/ml)	M/Cd Mol ratio (calculation)
Cu ²⁺	0.5402/0.71	0.78
Co ²⁺	0.0373/0.71	0.094
Ni ²⁺	0.0189/0.71	0.054

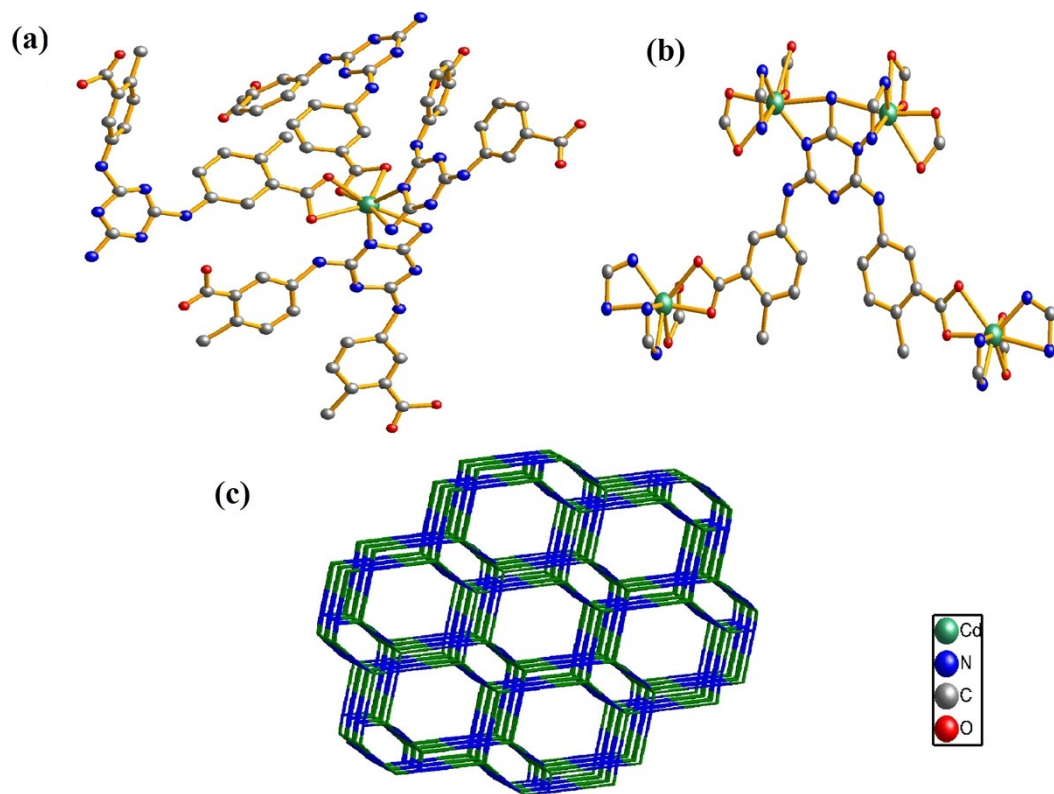


Fig. S1. (a) Coordination environment of Cd²⁺ ions; (b) connectivity of ligand (C grey, O red, N blue, Cd green); (c) Topology of MOF1.

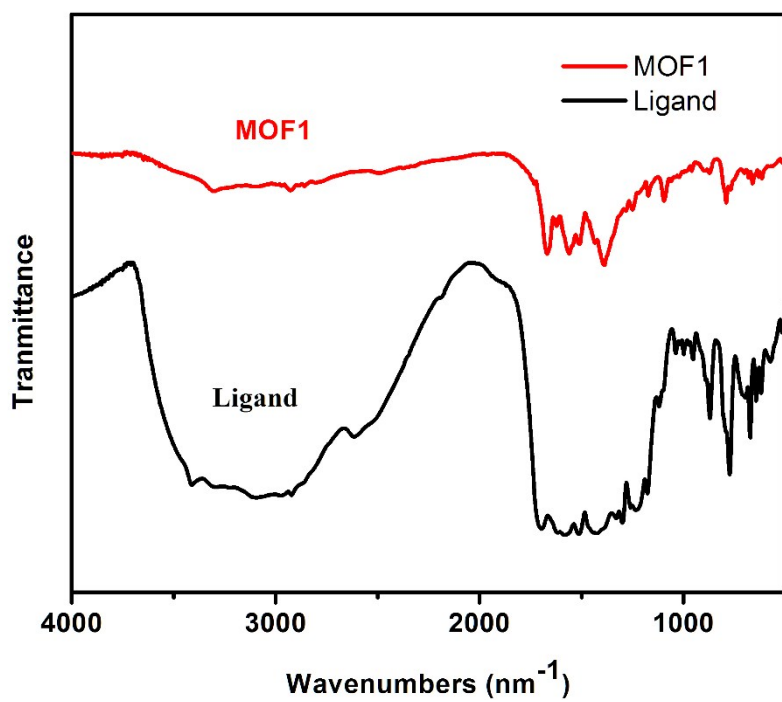


Fig. S2. IR spectrum of Ligand and MOF1.

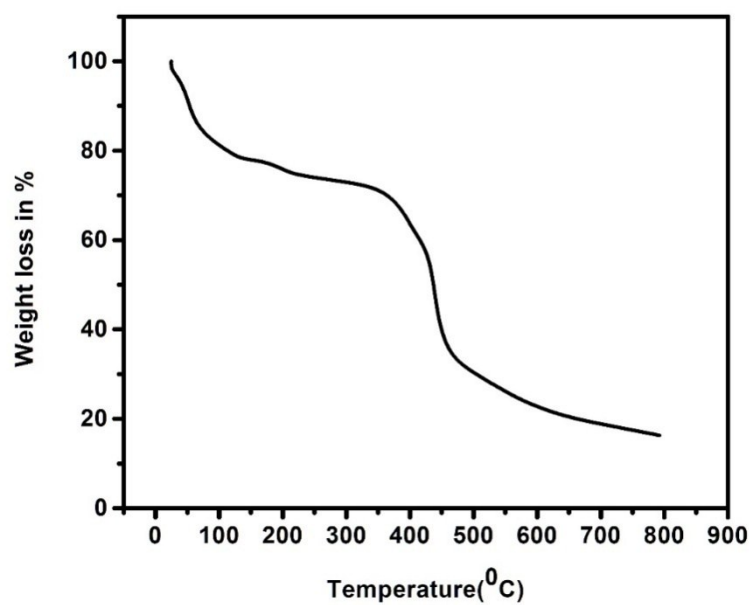


Fig. S3. TG curve of MOF1.

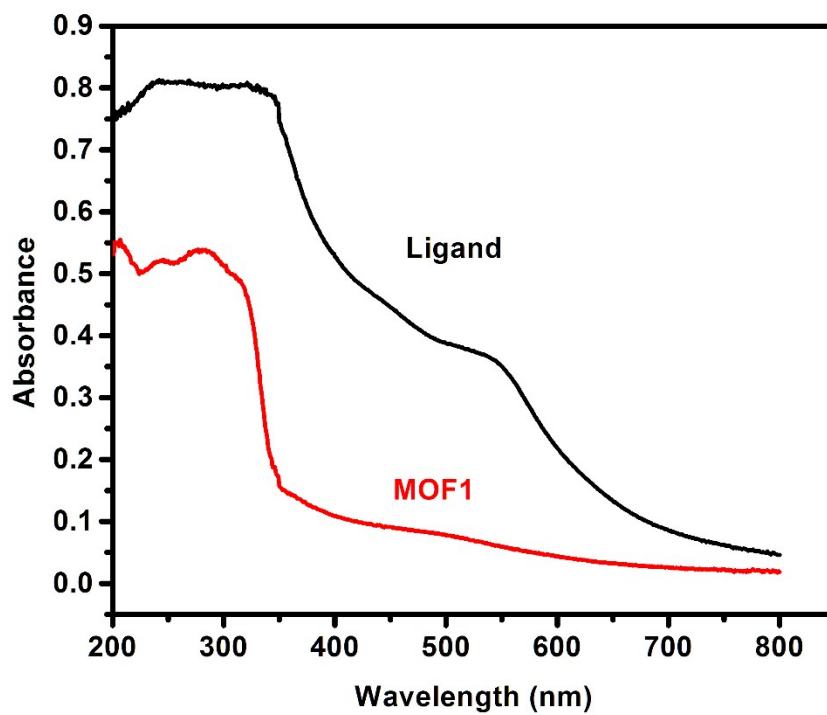


Fig. S4. UV spectrum of Ligand and MOF1.

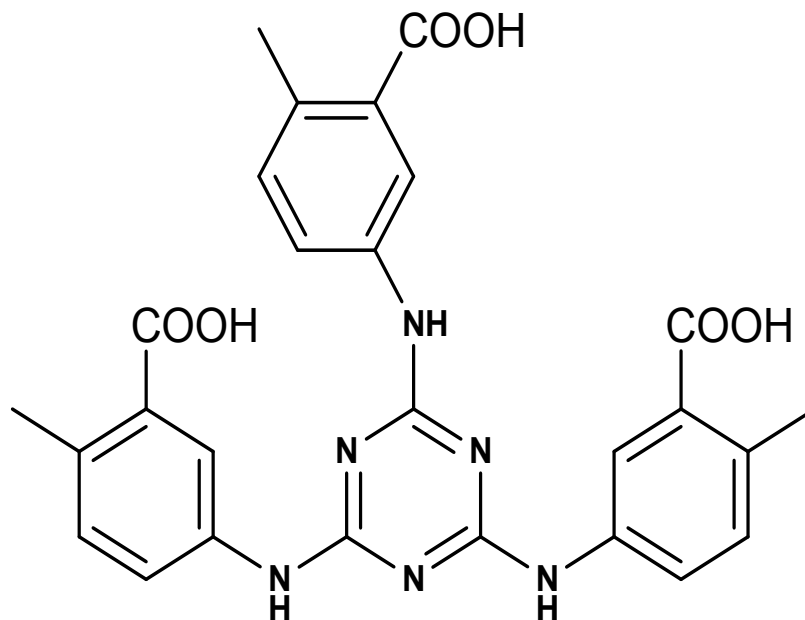


Fig. S5. The structure of Ligand.

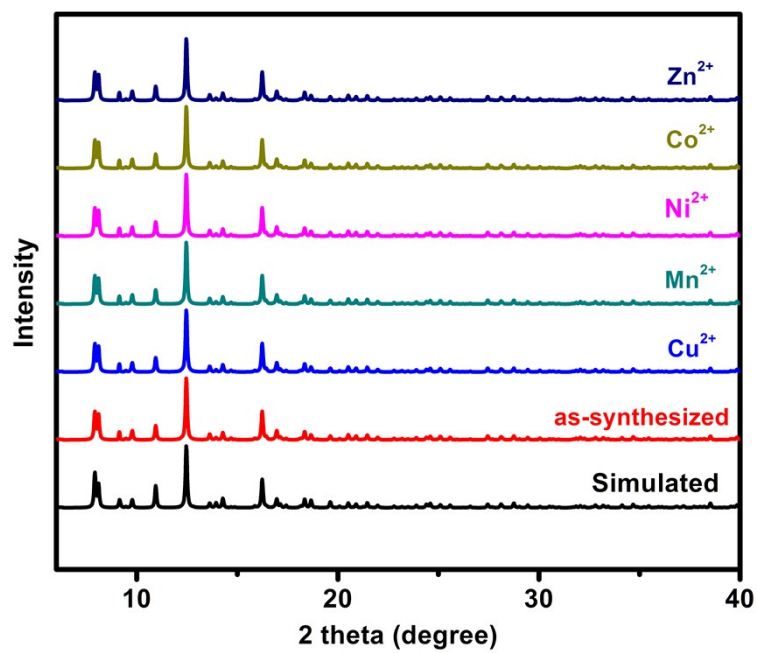


Fig. S6. PXRD patterns of simulated MOF1 and immersed in different metal ions DMF solution.

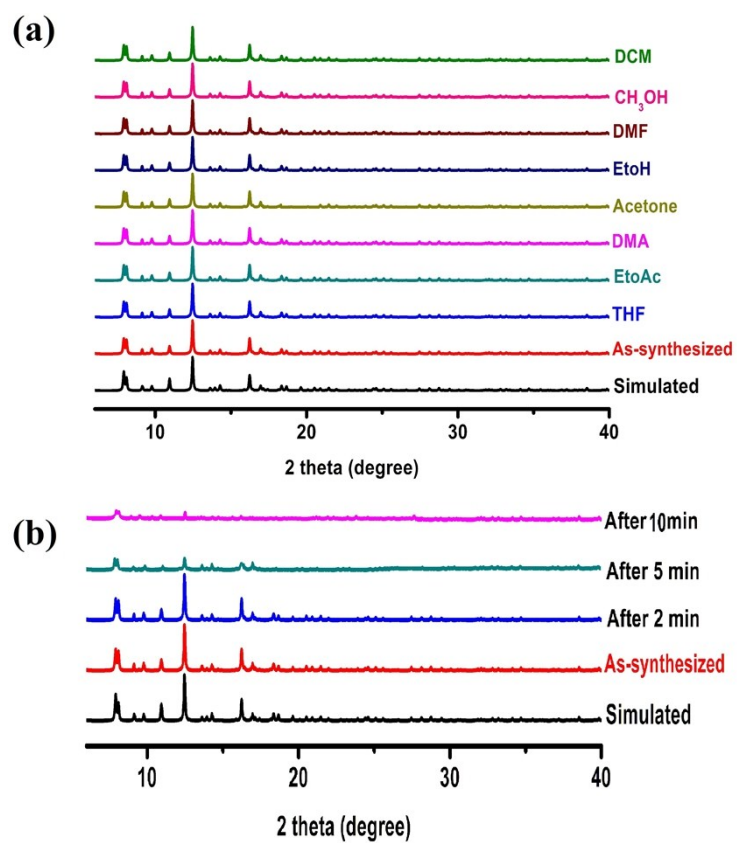


Fig. S7. PXRD patterns of simulated MOF1 immersed in different solvents (a) and in water (b) .

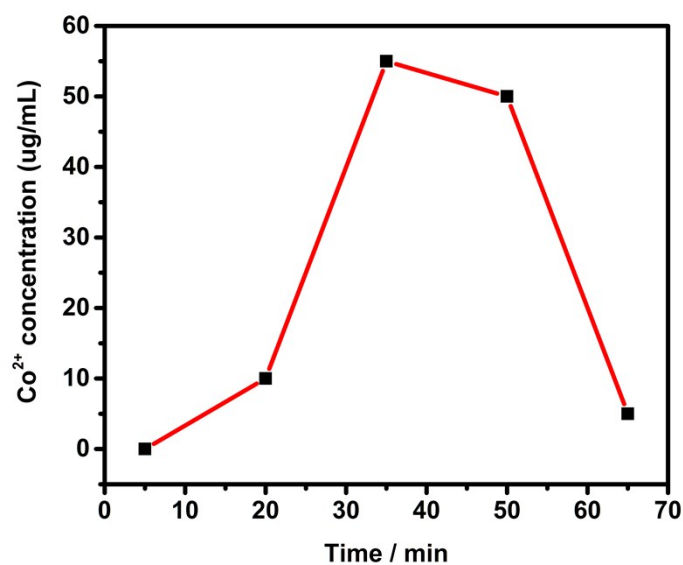


Fig. S8. The Co^{2+} concentration of eluting agent (DMF) at given time.

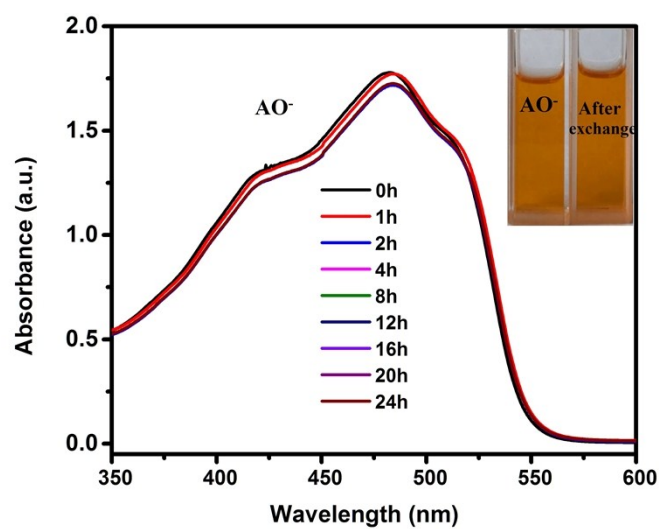


Fig. S9. UV-vis spectra of DMF solution of AO^- dye with **MOF1**.

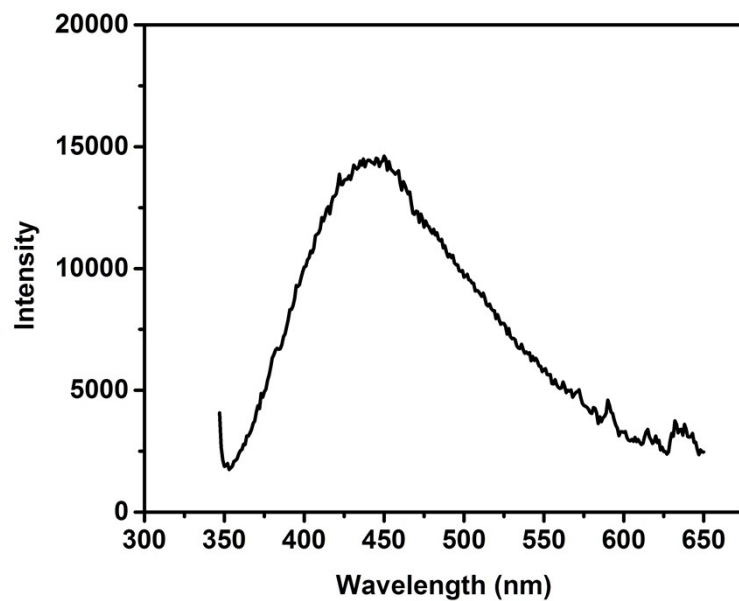


Fig. S10. Emission spectra of free ligand ($\lambda_{\text{ex}} = 289$ nm) in the solid state at room temperature.

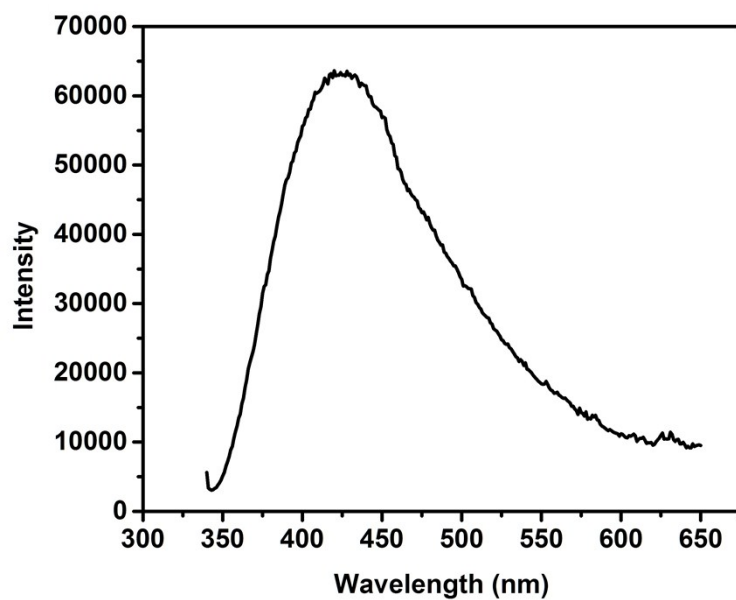


Fig. S11. Emission spectra of **MOF1** ($\lambda_{\text{ex}} = 289$ nm) in the solid state at room temperature.

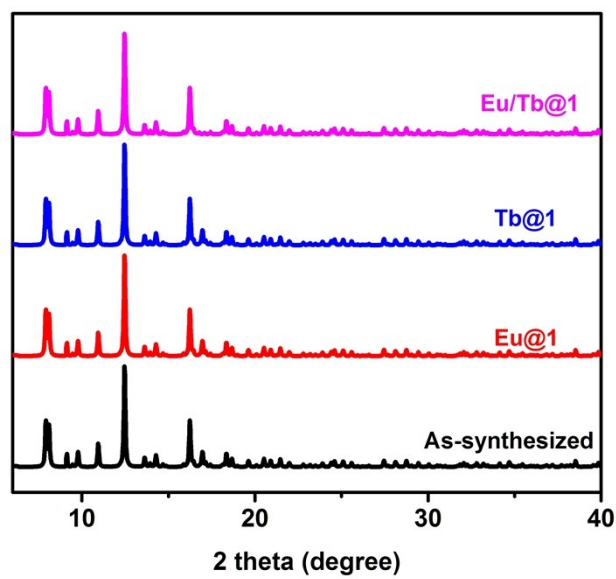


Fig. S12. PXRD patterns of MOF1 before and after lanthanide encapsulation.

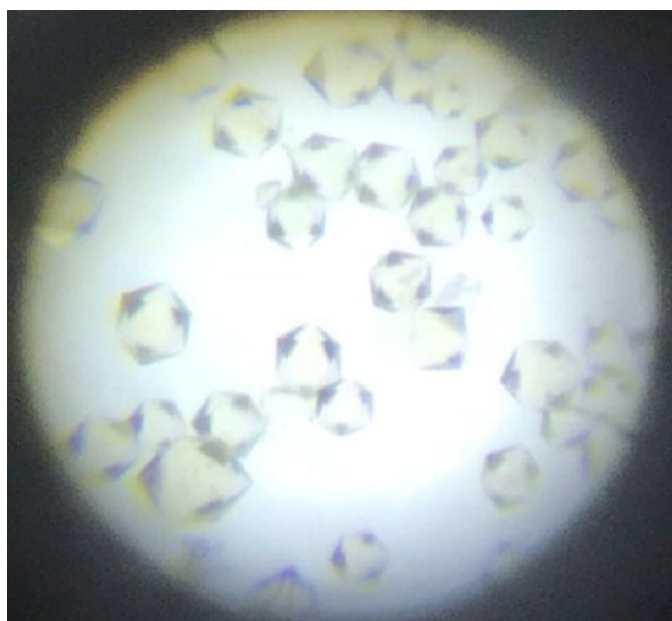
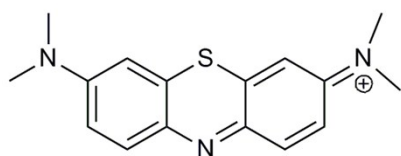
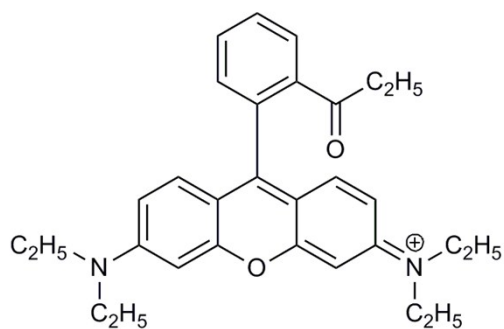


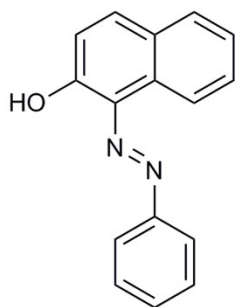
Fig. S13. Photograph of crystals of MOF1.



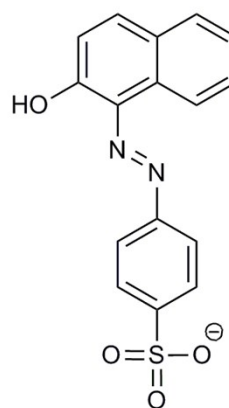
Methylene Blue (MLB⁺)



Butyl rhodamine B (BRB⁺)



Sudan I (SD⁰)



Acidic orange (AO⁻)

Fig. S14. Chemical structures of Dyes used in the manuscript.

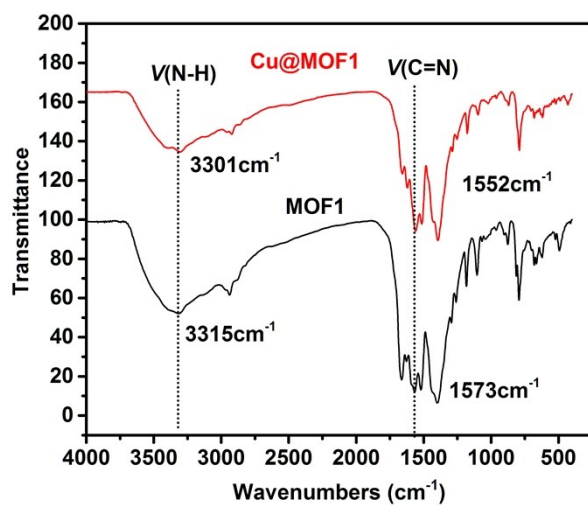


Fig. S15. FT-IR spectra of MOF1 before and after metal loading.

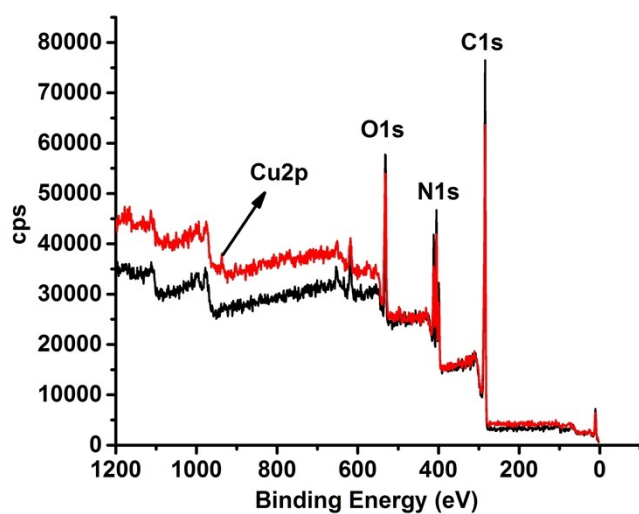


Fig. S16. XPS spectra of MOF1 before (black) and after metal loading (red).

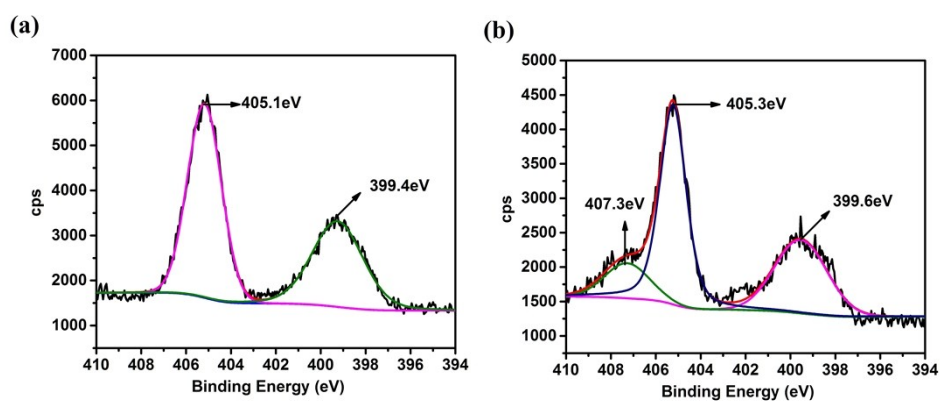


Fig. S17. The N1s XPS spectra of the original MOF1 (a) and Cu-incorporated MOF1(b).