

Supplementary Information

3,8-connected Cd(II)-based metal-organic framework as an apt luminescent sensor for antibiotic sulfasalazine

Table of Contents

Table S1. Crystal data and structure refinement parameters of 1	2
Table S2. Partial bond lengths (Å) and bond angles (°) of 1	3
Figure S1. Coordination mode of L ⁴ ligand.....	3
Figure S2. PXRD simulation pattern of 1 , PXRD pattern of 1 after sensing SLA and PXRD pattern of 1 after four sensing cycles.....	4
Figure S3. TGA analysis of 1	4
Figure S4. N ₂ adsorption and desorption isotherms at 77 K.....	5
Figure S5. view of the PL intensity of sample 1	5
Figure S6. The SEM pattern of morphology of 1 before and after the fluorescent probe test.....	6
Figure S7. UV-spectra of antibiotic SLA and 1	6
Figure S8. FT-IR of ligand H ₄ L, and 1	7

Table S1. Crystal data and structure refinement parameters of **1**

Compound	1
Formula	C ₄₄ H ₂₆ Cd ₄ O ₁₉
Formula weight	1308.5
Temperature (K)	293(2)
Crystal system	Monoclinic
Space group	<i>C2/c</i>
<i>a</i> (Å), <i>b</i> (Å), <i>c</i> (Å)	25.4577(11), 11.0140(7), 14.1461(12)
α (°), β (°), γ (°)	90, 92.376(5), 90
<i>V</i> (Å ³)	3963.0(5)
<i>Z</i>	4
<i>D</i> _{calc} (Mg m ⁻³)	2.193
μ (mm ⁻¹)	17.739
<i>F</i> (000)	2536.0
Crystal size (mm)	0.05× 0.02× 0.02
θ range (°)	3.475 to 67.06
Index ranges	-30 ≤ <i>h</i> ≤ 23 -11 ≤ <i>K</i> ≤ 13 -16 ≤ <i>L</i> ≤ 16
Reflections collected	12248
Independent reflection	3507 [<i>R</i> _{int} = 0.2003]
Data/restraints/parameters	3507/229/342
Final <i>R</i> ₁ , <i>wR</i> ₂ indices [<i>I</i> > 2σ (<i>I</i>)]	0.1633, 0.3734
<i>R</i> ₁ , <i>wR</i> ₂ indices (all data)	0.1784, 0.3825
<i>GOF</i>	1.073
$\Delta\rho_{\text{max,min}}$ (e Å ⁻³)	1.60/-2.1

Table S2. Bond length (Å) and bond angle (°) of **1**

1					
Cd1-O(10)	2.342(17)	Cd1#2-O(2)	2.36(2)	Cd1#4-O(1)	2.08(2)
Cd2-O(8)#1	2.360(17)	Cd2-O(3)#2	2.145(19)	Cd1#5-O11	2.425(17)
Cd2#6-O(3)	2.145(19)	Cd3-O(6)#1	2.333(18)	Cd3-O(5)	1.70(5)
O(10)-Cd(1)-O(4)#9	88.0(6)	O(10)-Cd(1)-O(11)#9			54.6(6)
O(10)-Cd(1)-O(2)#7	100.4(7)	O(2)#7Cd(1)-O(2)			78.2(6)
O(8)-Cd(2)-O(8)#1	76.5(8)	O(10)-Cd(2)-O(8)#1			76.5(6)
O(3)#2Cd(2)-O(8)	164.6(7)	O(3)#3-Cd(2)-O(8)			88.1(7)
O(3)#3-Cd(2)-O(10)	100.1(7)	O(3)#2-Cd(2)-O(10)#1			95.9(7)
O(6)#1-Cd(3)-O(8)#1	52.3(6)	O(6)#1-Cd(3)-O(5)#1			93.1(10)
O(7)-Cd(3)-O(6)	113.4(12)	O(7)-Cd(3)-O(8)			92.0(12)
O(9)-Cd(3)-O(6)	102.0(18)				
Symmetry codes for #1 1-x,+y,-1/2-z; #2 1/2+x,1/2+y,+z; #3 1/2-x,1/2+y,-1/2-z; #4 -1/2+x,1/2-y,-1/2+z; #5 -1/2+x,1/2+y,+z; #6-1/2+x,-1/2+y,+z; #7 1-x,1-y,-z;					

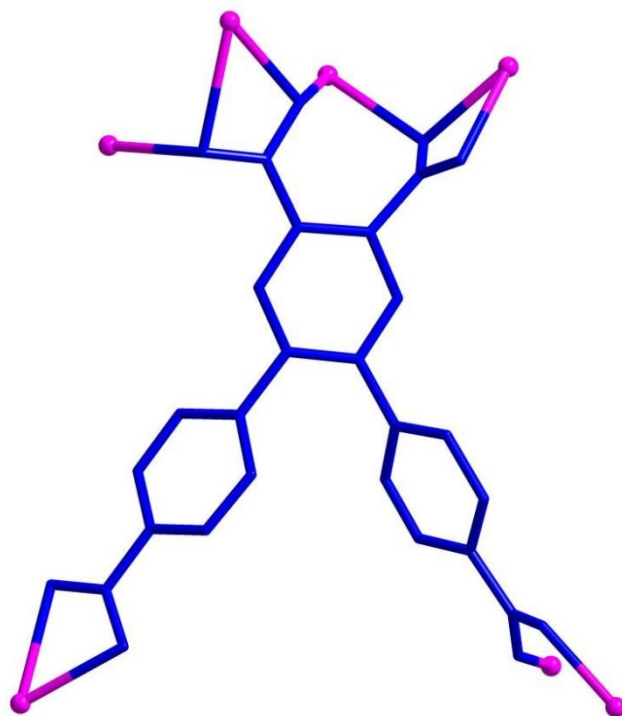


Figure S1. Coordination mode of L^4 ligand

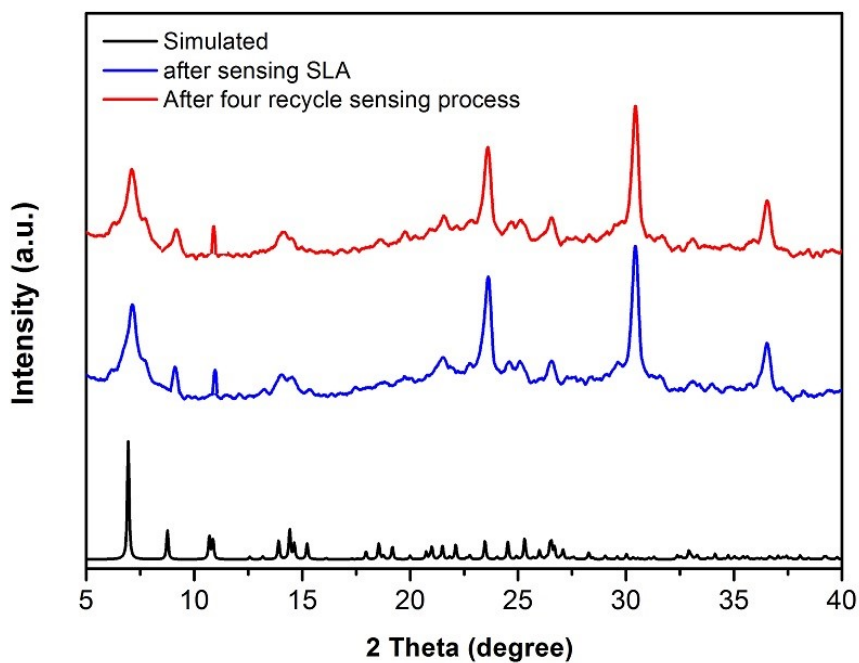


Figure S2. PXRD simulation pattern of **1**, PXRD pattern of **1** after sensing SLA and PXRD pattern of **1** after four sensing cycles.

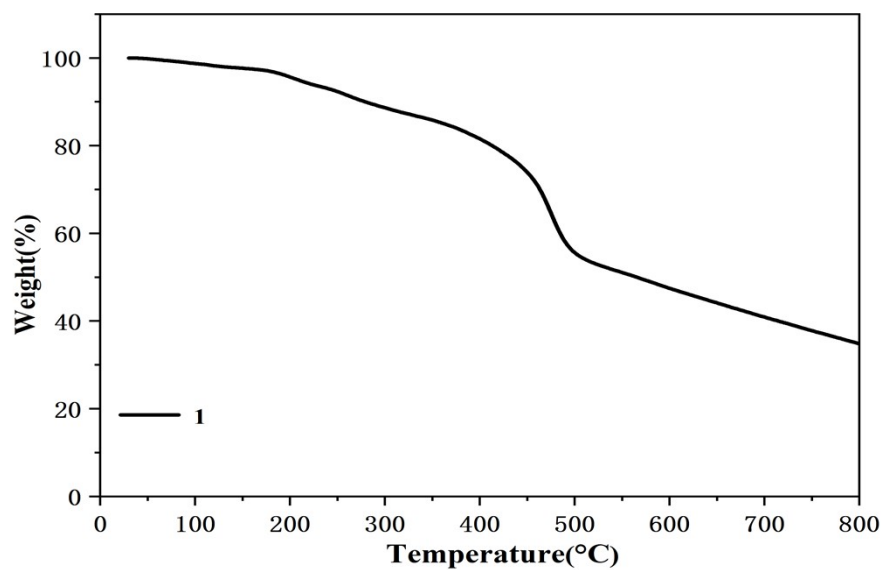


Figure S3. TGA analysis of **1**

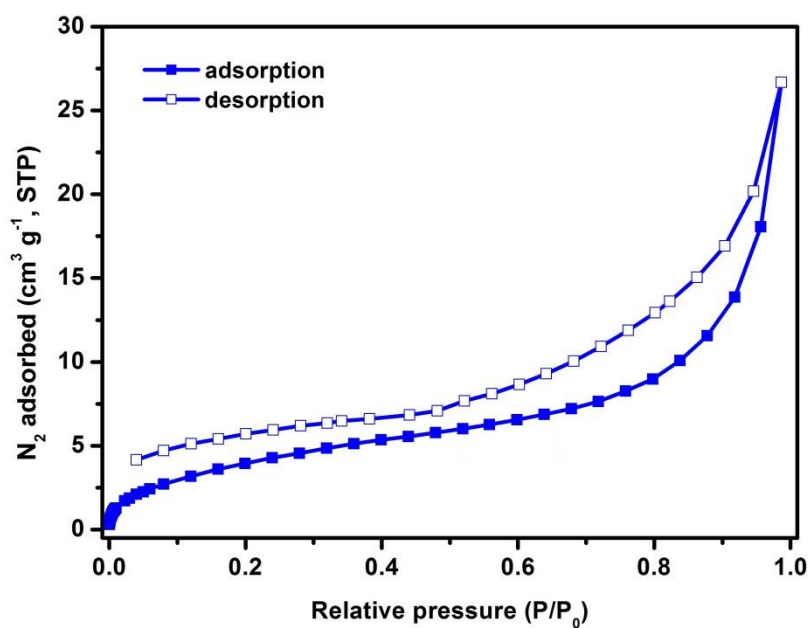


Figure S4. N₂ adsorption and desorption isotherms at 77 K.

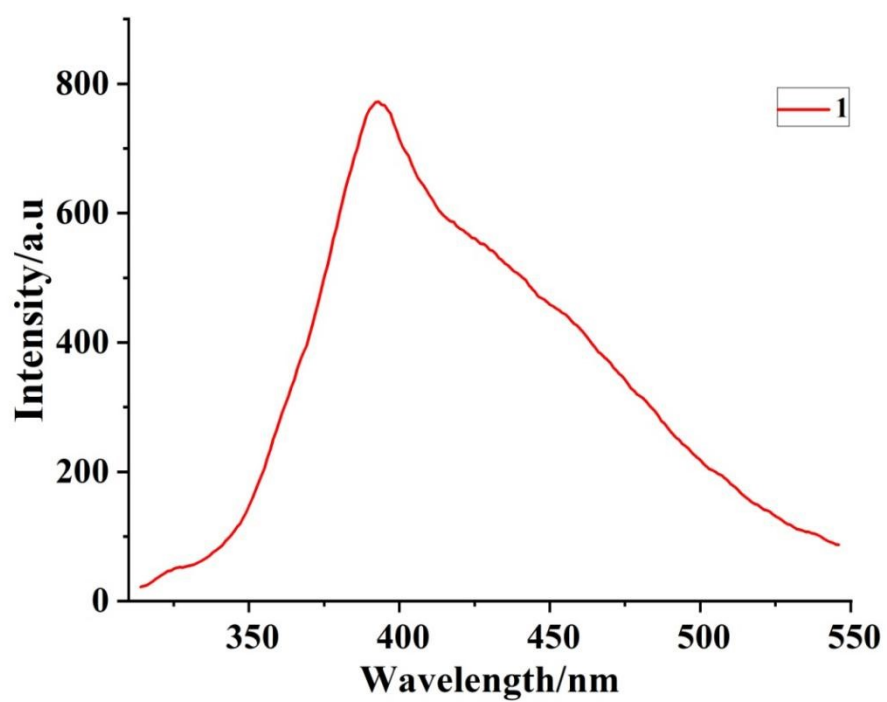


Figure S5. view of the PL intensity of sample **1**.

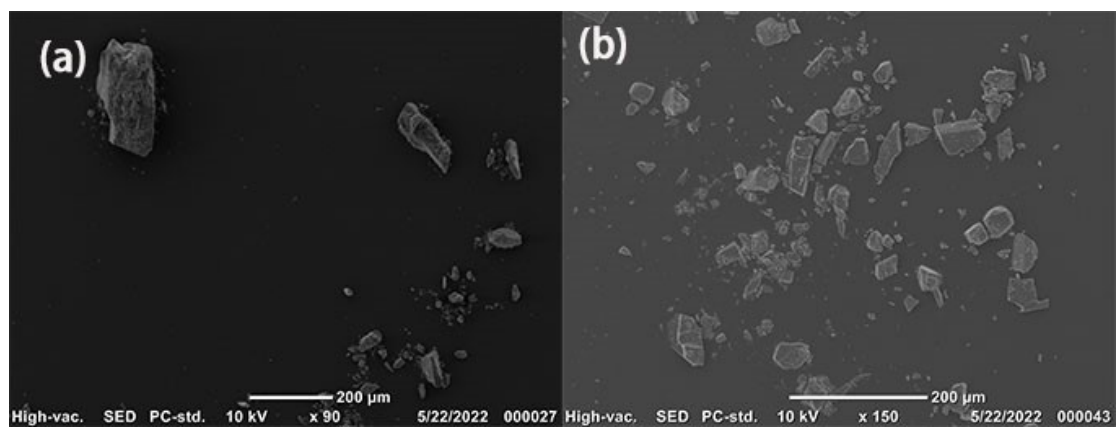


Figure S6. (a) The SEM pattern of morphology of **1** before the fluorescent probe test, (b) The SEM pattern of morphology of **1** after the fluorescent probe test.

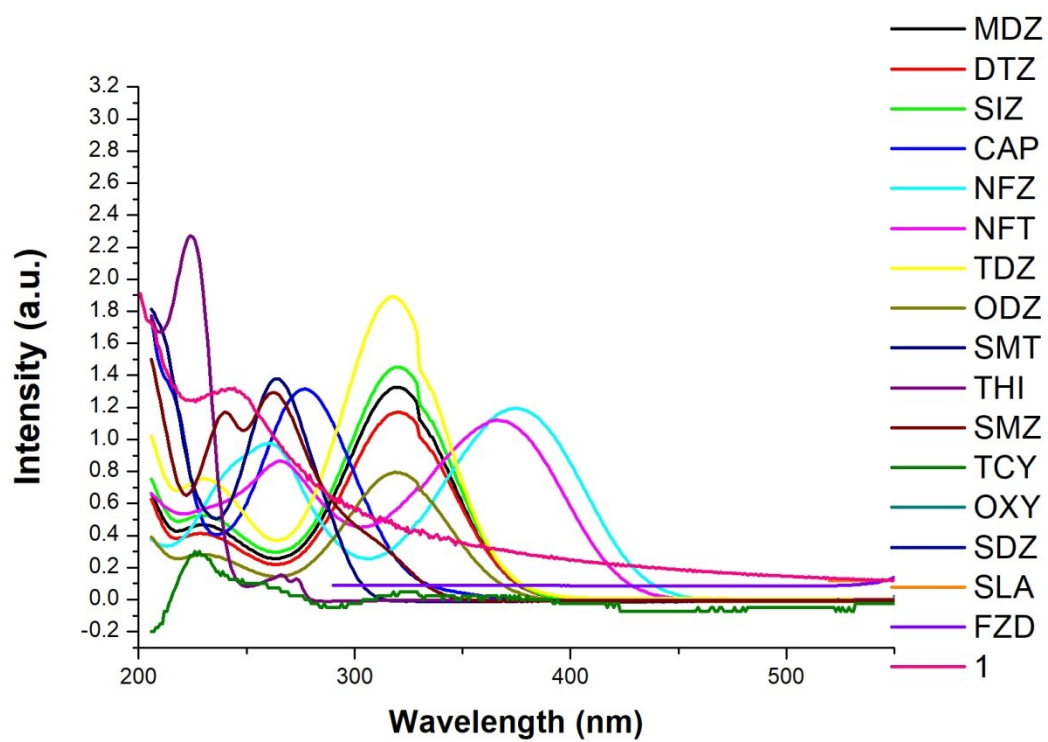


Figure S7. UV-spectra of antibiotics and **1**.

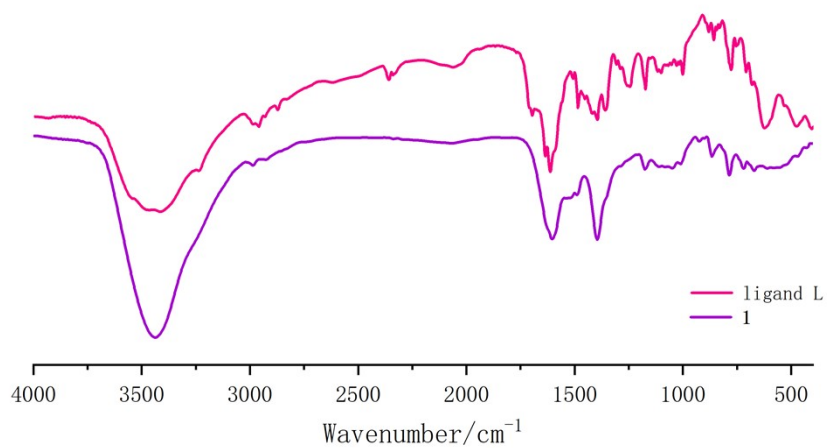


Figure S8. FT-IR of ligand L, and **1**.