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### Supporting Information for CrystEngComm 2021

### Two Cd(II)-based metal-organic frameworks for the highly effective

detection of Fe<sup>3+</sup> ions and levofloxacin in aqueous media

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## Section 1. Experimental Section

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#### 1. Materials and methods

All chemical reagents were obtained directly from commercial sources and used directly without purification. L ligand was purchased from Jinan Henghua Sci. & Tec. Co. Ltd. (Jinan, China). Elemental analysis (C, H, and N) was recorded with a Perkin-Elmer 240C analyzer. FTIR spectra were measured on a Bruker VERTEX 80V FTIR spectrophotometer (4000–400 cm<sup>-1</sup>). Thermogravimetric analyses (TGA) were performed on a Netzsch STA449 F1 thermal analyzer and heated from room temperature to 800 °C at a rate of 10 °C/min. The solid-state UV-Vis diffuse-reflectance spectra were measured using a UV-Vis Puxi T9 ultraviolet-visible spectrophotometer. Powder X-Ray diffraction (PXRD) patterns were measured using a Rigaku D/Max-2500 diffractometer equipped with a copper target tube operated at 40 kV and 40 mA ( $\lambda$  = 1.5418 Å). The luminescence spectra were recorded on Edinburgh instruments FS5 spectrophotometer.

#### 2. X-ray crystallography

Crystallographic data for **1** and **2** were collected at 293 K on a Rigaku XtaLabMini diffractometer using graphite-monochromated Mo-K $\alpha$  radiation ( $\lambda = 0.71073$  Å) by a  $\omega$ -scan technique.<sup>1</sup> The reflection data were obtained using the CrysAlisPro program (version 1.171.38.43). The crystal structure was solved with the Olex2.solve and further refined by full-matrix least square method on  $F^2$  by using SHELXL (v. 2018/3).<sup>2</sup> All non-hydrogen atoms were refined by anisotropic thermal parameters. The H atoms of water molecules were located from difference Fourier maps. The other hydrogen atoms were generated geometrically and refined isotropically using the riding model.<sup>3</sup> The main crystallographic data are summarized in Table S1. Selected bond distances and angles are supplied in Table S2.

#### 3. Stability experiments

Add 4 mg of evenly ground powder 1 and 2 to 4 mL of different pH solutions (pH = 3-12), and let stand at room temperature for 30 min to fully penetrate. Then, the fluorescence intensity experiments of 1 and 2 were carried out. Finally, the sample was washed and dried for PXRD measurements to evaluate the stability of 1 and 2 toward different pH solutions.

#### 4. Sensing experiments

Anti-interference tests were carried out in the presence of various other metal ions and Fe<sup>3+</sup> ions with an equal concentration of  $5 \times 10^{-4}$  mol·L<sup>-1</sup>. Competition tests were carried out in the presence of various other antibiotics and LVX with an equal concentration of  $1 \times 10^{-4}$  mol·L<sup>-1</sup>. The recoverability of **1** and **2** for sensing analytes was also discussed. The samples after the first sensing experiment was collected by centrifuged, washed and dried and then use it for the cyclic quenching experiment. The time-dynamic fluorescence response spectra for **1** and **2** were also further measured. After adding LVX with a concentration of 2.0 µmol·L<sup>-1</sup> to **1** and **2**, the fluorescence intensity was measured every 5 s, and record the time required to reach a stable value.

#### 5. Electrochemical measurement

The photoelectrochemical properties were studied on an electrochemical station (CHI660E, Chenhua, Shanghai, China) linked with computer. The Ag/AgCl electrode, platinum foil, and  $Na_2SO_4$  (0.2 mol·L<sup>-1</sup>) were employed as reference electrode, counter electrode, and electrolyte solution, respectively. The frequency was 1500, 2000, and 2500 Hz.

### References

- [1] Agilent, CrysAlis PRO, Agilent Technologies Ltd, Yarnton, Oxfordshire, England, 2014.
- [2] G. M. Sheldrick, Acta Crystallogr., Sect. C: Struct. Chem., 2015, 71, 3-8.
- [3] A. L. Spek, Acta Crystallogr., Sect. D: Biol. Crystallogr., 2009, 65, 148–155.

## Section 2. Supplementary Tables and Figures

Table Titles:

 Table S1. Crystallographic data and refinement parameter for 1 and 2.

Table S2. Selected bond lengths (Å) and angles (°) for 1 and 2.

CPs	1	2	
Chemical formula	C <sub>15</sub> H <sub>13</sub> CdN <sub>2</sub> O <sub>5</sub> S	C <sub>15</sub> H <sub>10</sub> CdNO <sub>4</sub>	
Formula weight	445.73	380.64	
Crystal system	Triclinic	Triclinic	
Space group	Pī	Pī	
<i>a</i> (Å)	6.26(3)	7.52(6)	
<i>b</i> (Å)	10.77(4)	9.85(8)	
<i>c</i> (Å)	12.39(4)	10.31(9)	
α (°)	111.32(3)	62.37(8)	
β (°)	96.57(3)	76.21(7)	
γ (°)	105.52(4)	67.71(7)	
$V(Å^3)$	729.15(5)	624.13(10)	
Ζ	2	2	
$D_{\text{calcd}}$ (g/cm <sup>3</sup> )	2.030	2.025	
Absorption coefficient, mm <sup>-1</sup>	1.672	1.765	
<i>F</i> (000)	442	374	
Crystal size, mm	0.22×0.20×0.18	0.22×0.20×0.18	
$\theta$ range, deg	4.342-52.044	4.472-60.888	
Index range <i>h</i> , <i>k</i> , <i>l</i>	-7/7, -13/13, -15/15	-10/10, -14/13, -14/14	
Reflections collected	16486	17532	
Independent reflections $(R_{int})$	2856(0.0357)	3598(0.0618)	
Data/restraint/parameters	2856 / 0 / 222	3598 / 0 / 190	
Goodness-of-fit on $F^2$	1.128	1.074	
Final R <sub>1</sub> , $w$ R <sub>2</sub> ( $I > 2\sigma(I)$ )	0.0208, 0.0545	0.0326, 0.0776	
Largest diff. peak and hole	0.34, -0.75	0.87, -1.22	

Table S1 Crystallographic data and refinement parameter for 1 and 2  $\,$ 

Parameter	Value	Parameter	Value
1			
Cd(1)-O(4)A	2.355(2)	Cd(1)–O(2)	2.342(2)
Cd(1)–O(2)B	2.436(2)	Cd(1)–O(1)W	2.233(2)
Cd(1)–N(1)	2.245(2)	O(2)Cd(1)O(4)A	108.49(6)
O(4)A-Cd(1)-O(2)B	81.22(6)	O(2)Cd(1)O(2)B	74.19(6)
O(1)W-Cd(1)-O(4)A	120.97(7)	O(1)W-Cd(1)-O(2)B	77.94(7)
O(1)W-Cd(1)-O(2)	117.45(7)	O(1)W-Cd(1)-N(1)	120.14(7)
N(1)Cd(1)O(4)A	91.89(6)	N(1)-Cd(1)-O(2)B	161.32(7)
N(1)Cd(1)O(2)	91.83(7)		
2			
Cd(1)–O(2)A	2.550(2)	Cd(1)–O(2)B	2.426(2)
Cd(1)–O(3)B	2.263(2)	Cd(1)–O(1)A	2.385(2)
Cd(1)–O(4)	2.258(2)	Cd(1)–N(1)	2.255(3)
O(2)ACd(1)O(2)B	71.39(8)	O(3)A-Cd(1)-O(2)A	77.14(7)
O(3)ACd(1)O(2)B	96.96(7)	O(3)A-Cd(1)-O(1)B	150.10(8)
O(1)B-Cd(1)-O(2)A	93.94(7)	O(1)B-Cd(1)-O(2)B	53.34(7)
O(4)Cd(1)O(2)B	83.04(8)	O(4)Cd(1)O(2)A	151.80(8)
O(4)Cd(1)O(3)A	94.84(8)	O(4)Cd(1)O(1)B	79.55(8)
N(1)-Cd(1)-O(2)B	141.77(9)	N(1)-Cd(1)-O(2)A	101.51(8)
N(1)-Cd(1)-O(3)A	118.55(9)	N(1)Cd(1)O(1)B	91.08(8)
N(1)-Cd(1)-O(4)	105.98(9)		

Table S2 Selected bond lengths (Å) and angles (°) for 1 and 2

symmetry code for 1: A = x, 1+y, +z, B = 1-x, 2-y, 2-z, C = 2-x, 2-y, 1-z.

symmetry code for **2**: A = 1+x, +y, +z, B = 1-x, 1-y, 2-z, C = 1-x, -y, 2-z, D = 1-x, 1-y, 1-z.

Figure Titles:

- Fig. S1. 1D double chain formed by tdc<sup>2-</sup> ligand and Cd(II) center for 1.
- Fig. S2. Simulated and experimental PXRD patterns for 1 and 2.
- Fig. S3. PXRD patterns for 1 and 2 in different pH aqueous solutions.
- Fig. S4. TGA curves of 1 and 2.
- Fig. S5. Solid-state luminescence spectra of L ligand, 1 and 2.
- Fig. S6. The emission decay lifetimes of 1 and 2 monitored at 335 nm.
- Fig. S7. Anti-interference experiments of 1 and 2 for  $Fe^{3+}$  ions with different metal ions.
- Fig. S8. The luminescence spectra of (a) 1 and (b) 2 suspended in aqueous solutions with different concentrations of  $Fe^{3+}$  ions.
- Fig. S9. Three cycles experiment to detect  $Fe^{3+}$  ions in 1 and 2.
- Fig. S10. Fluorescence bands of (a) 1 and (b) 2 in various antibiotics.
- **Fig. S11.** Fluorescence intensity *versus* time curve of **1** and **2** when added to LVX solution in Cd(II)-MOF suspensions.
- Fig. S12. Three cycles experiment to detect LVX in 1 and 2.
- Fig. S13. Anti-interference experiments of 1 and 2 for LVX with different antibiotics.
- Fig. S14. PXRD patterns of 1 and 2 after sensing analyte.
- Fig. S15. Mott-Schottky plots of the samples at the frequency of 1500, 2000, and 2500 Hz.
- Fig. S16. Energy levels of LUMO and HOMO orbitals for two Cd(II)-MOFs and antibiotics.
- Fig. S17. The molecular orbital diagram of LVX drawn by VMD 1.9.3 program.
- Fig. S18. UV–Vis spectra of  $Fe^{3+}$  ions/ LVX and emission spectra of 1 and 2.

Fig. S1. 1D double chain formed by  $tdc^{2-}$  ligand and Cd(II) center for 1.



Fig. S2. Simulated and experimental PXRD patterns for 1 and 2.



Fig. S3. PXRD patterns for 1 and 2 in different pH aqueous solutions.



Fig. S4. TGA curves of 1 and 2.



Fig. S5. Solid-state luminescence spectra of L ligand, 1 and 2.



Fig. S6. The emission decay lifetimes of 1 and 2 monitored at 335 nm.



Fig. S7. Anti-interference experiments of 1 and 2 for  $Fe^{3+}$  ions with different metal ions.



Fig. S8. The luminescence spectra of (a) 1 and (b) 2 suspended in aqueous solutions with different concentrations of  $Fe^{3+}$  ions.



Fig. S9. Three cycles experiment to detect  $Fe^{3+}$  ions in 1 and 2.



Fig. S10. Fluorescence bands of (a) 1 and (b) 2 in various antibiotics.



Fig. S11. Fluorescence intensity versus time curve of 1 and 2 when added to LVX solution in

Cd(II)-MOF suspensions.



Fig. S12. Three cycles experiment to detect LVX in 1 and 2.



Fig. S13. Anti-interference experiments of 1 and 2 for LVX with different antibiotics.



Fig. S14. PXRD patterns of 1 and 2 after sensing analyte.



Fig. S15. Mott-Schottky plots of the samples at the frequency of 1500, 2000, and 2500 Hz.



Fig. S16. Energy levels of LUMO and HOMO orbitals for two Cd(II)-MOFs and antibiotics.



Fig. S17. The molecular orbital diagram of LVX drawn by VMD 1.9.3 program.



Fig. S18. UV–Vis spectra of  $Fe^{3+}$  ions/ LVX and emission spectra of 1 and 2.