Supporting Information

Three-dimensional Cd(II) metal–organic framework: a bifunctional luminescence sensor for benzaldehyde and Fe^{2+} ion

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1. Crystallographic Data

X-Ray crystallography. Crystallographic data were collected at 293 K (for **1**) on an Agilent SuperNova (Dual, Cu at zero, AtlasS2, CCD) diffractometer equipped with graphite-monochromated Mo-Kα radiation (λ = 1.54184 Å), using the φ–ω scan technique. Semiempirical multiscan absorption corrections were applied by SCALE3 ABSPACK, and the programs CrysAlisPro were used for integration of the diffraction profiles. The structures were solved by direct methods with the ShelXT-2015 structure solution program and refined using least squares minimization by with the ShelXL-2015 refinement package. Some restraints are employed, such as ISOR (anisotropic parameter), DFIX (restricting the distance between two atoms) to solve the disorder of the O atoms. All non-hydrogen atoms were refined anisotropically, and hydrogen atoms were located geometrically and refined isotropically. Crystallographic data are listed in Table S1.

Table S1. Crystallographic Data and Structure Refinement Details for **1**

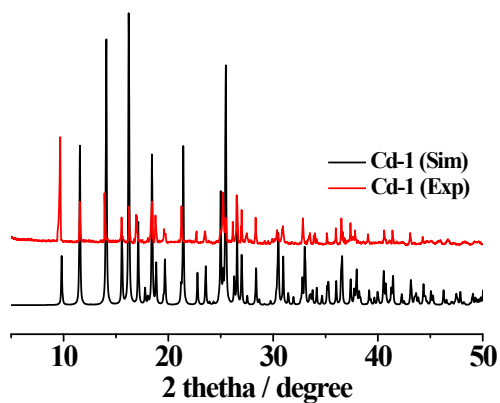|	**1**
formula	$C_{22}H_{14}CdN_{12}O_4$
Mr	622.85
crystal system	monoclinic
space group	$P2_1/c$
a (Å)	9.1685(7)
b (Å)	11.3729(12)
c (Å)	10.5397(7)
α(°)	90
β(°)	101.086(7)
γ(°)	90
V (Å³)	1078.50(15)
Z	2
ρcalc (Mg/m³)	1.918
μ (mm⁻¹)	1.077
F(000)	620.0
θ range(°)	2.264~25.01
limiting indices	$-8 \leq h \leq 10$, $-13 \leq k \leq 10$, $-12 \leq l \leq 12$
Reflns collected	4567
GOF on F^2	1.038
R_1/wR_2 [$I > 2\sigma(I)$]	$R_1 = 0.0405$, $wR_2 = 0.0763$
R_1/wR_2 (all data)	$R_1 = 0.0613$, $wR_2 = 0.0862$

2 Powder X-ray Diffraction
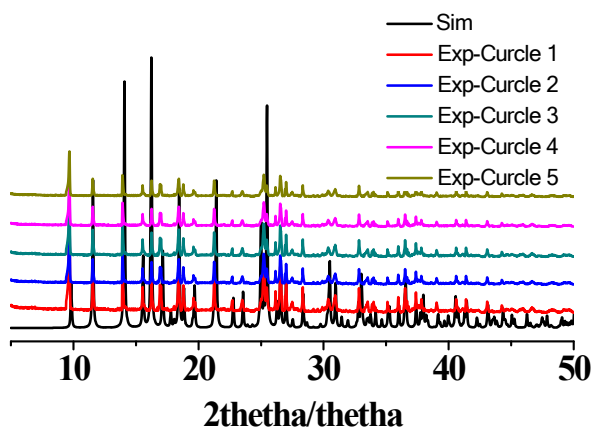

Figure S1. XRD patterns of complex **1**.

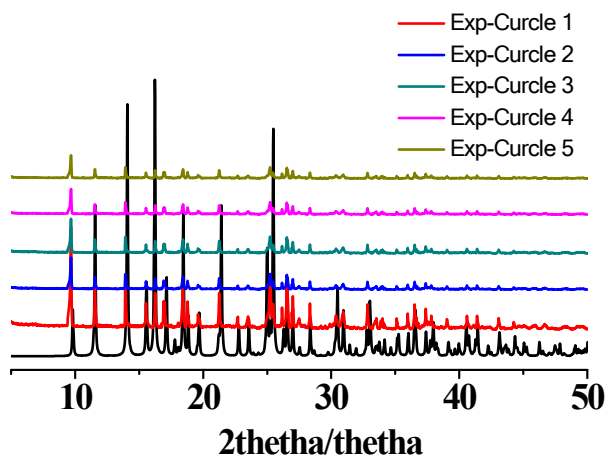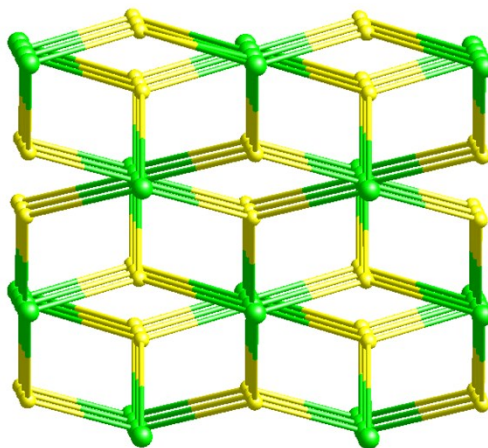**Figure S2.** XRD patterns of **1** toward PhCHO after cyclic experiments

Figure S3. XRD patterns of **1** toward Fe^{2+} ion in DMF solution after cyclic experiments

3 The 3D topological structure of 1

Figure S4. The 3D topological structure of **1** viewed along *a* direction. Color codes: yellow codes, 3-connected TBC$^-$-ligand; green codes, 6-connected Cd^{2+} ions.

4 Thermal Gravimetric Analysis Curves
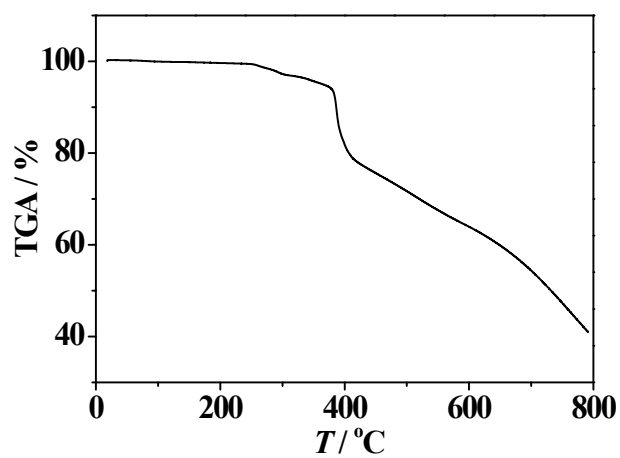
Figure S5. TGA curves of complex **1**.
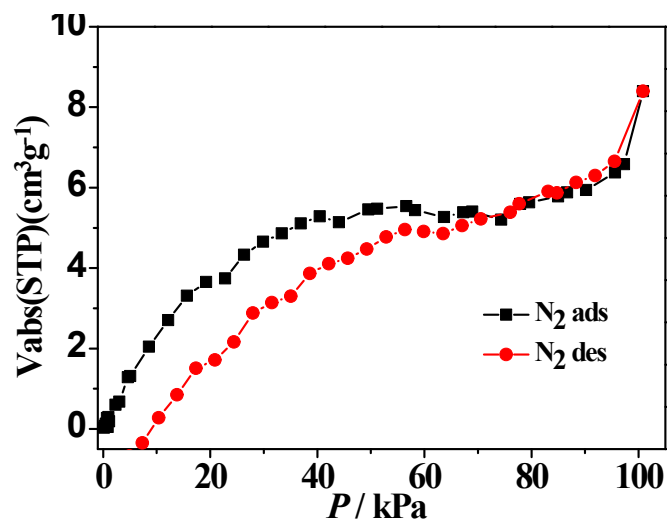
5 Sorption Properties

Figure S6. N2 sorption isotherms of 1 at 295 K.

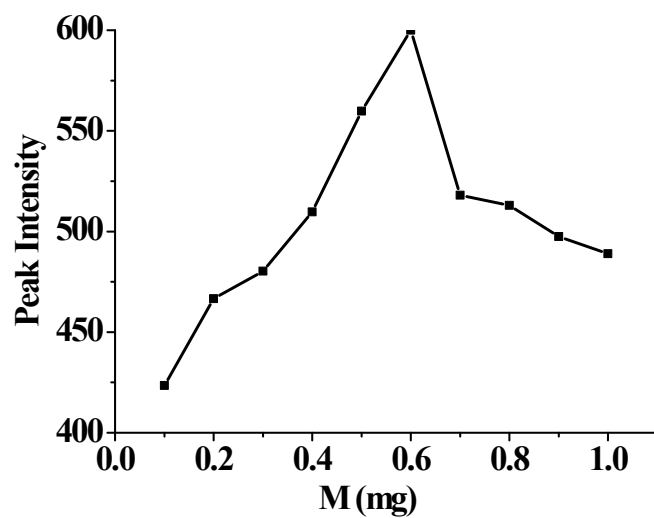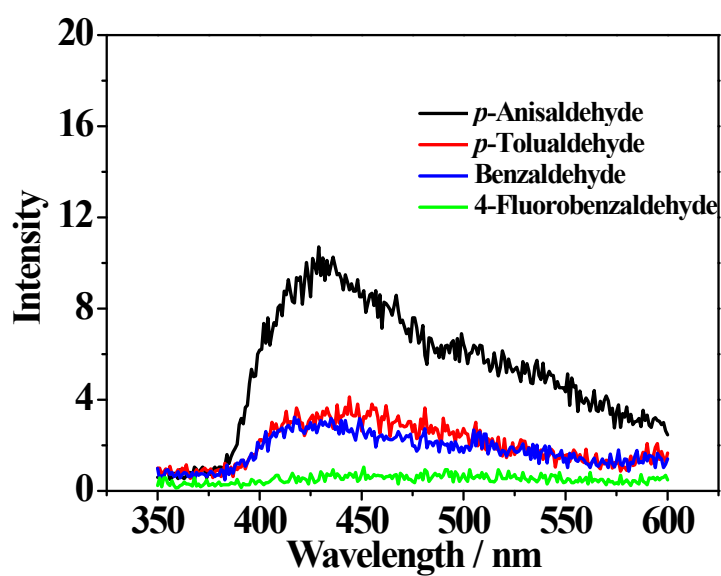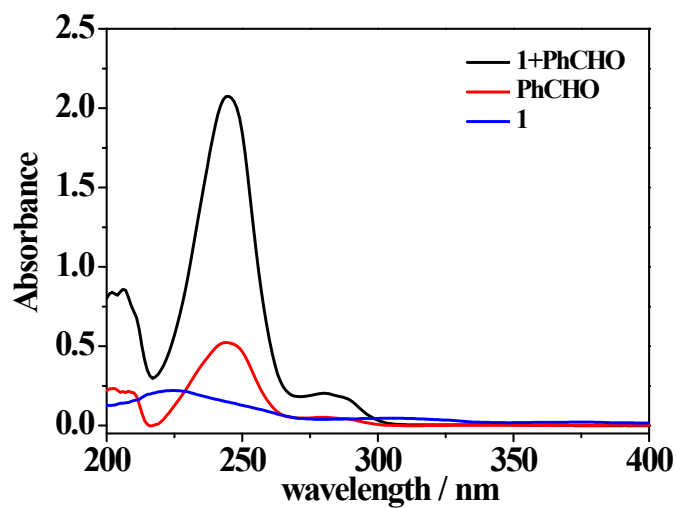# 6 Other Luminescence Properties

Figure S7. The luminescence intensities at 400 nm at different amount of coordination polymer **1** (mg) in 10 ml DMF solution when excited at 335 nm.

Figure S8. The luminescence intensities for coordination polymer **1** in 10 mL DMF solution (0.06 g/L) with different substituted benzaldehydes (100 μL) when excited at 335 nm.

7 UV–vis spectra

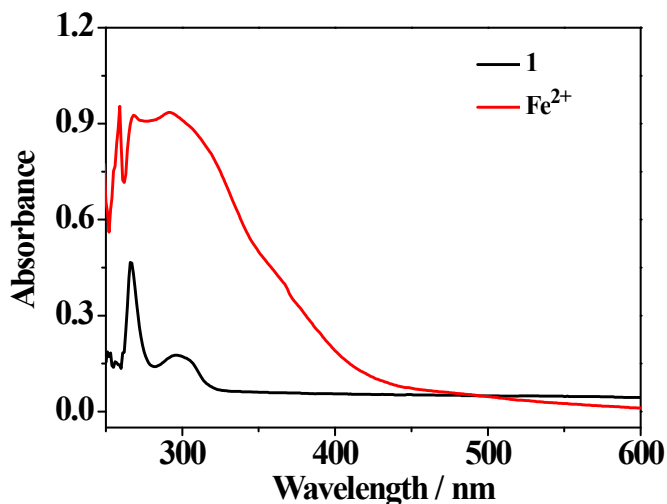**Figure S9.** UV–vis spectra of PhCHO and coordination polymer **1**.

Figure S10. UV–vis spectra of Fe^{2+} and coordination polymer **1**.

8 Tables of Crystal Data

Table S2. Selected bond lengths (Å) and bond angles (°) in complex **1**.

Cd(1)-N(3)#1	2.392(4)	N(3)#2-Cd(1)-N(6)#4	88.60(14)
Cd(1)-N(3)#2	2.392(4)	N(3)#1-Cd(1)-N(6)#4	91.40(14)
Cd(1)-N(6)#3	2.439(4)	N(6)#4-Cd(1)-N(6)#3	180.0
Cd(1)-N(6)#4	2.439(4)	O(1)#5-Cd(1)-N(3)#1	93.47(18)
Cd(1)-O(1)	2.303(7)	O(1)-Cd(1)-N(3)#1	93.47(18)
Cd(1)-O(1)#5	2.303(7)	O(1)-Cd(1)-N(3)#2	86.53(18)
N(3)#1-Cd(1)-N(3)#2	180.00(18)	O(1)#5-Cd(1)-N(3)#2	86.53(18)
N(3)#2-Cd(1)-N(6)#3	91.40(14)	O(1)#5-Cd(1)-N(6)#3	75.79(16)
N(3)#1-Cd(1)-N(6)#3	88.60(14)	O(1)-Cd(1)-N(6)#3	104.21(16)

#1: 1+x, 3/2-y, 1/2+z; #2: 1-x, -1/2+y, 3/2-z; #3: 2-x, 1-y, 1-z; #4: x, y, 1+z; #5: 2-x, 1-y, 2-z.