Electronic Supplementary Information (ESI) for

Two Cdmium(II) Coordination Polymers as Luminescent Sensors for the Detection of Nitrofuran/Nitroimidazole Antibiotics

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Comment S1: Materials and characterization for CPs 1 and 2.

Chemical reagents were purchased commercially and were used as received without further purification. FT-IR spectra of the compounds were recorded in the range of 400–4000 cm⁻¹ on a 750FT-IR spectrometer with KBr pellets. Elemental (C, H, N) analyses were carried out with a Perkin Elmer 240C elemental analyzer. Powder X-ray diffraction (XRD) data were collected using Cu-K α radiation (1.5418 Å) on a Bruker-AXS D8 Advance X-ray diffractometer in the angular range $2\theta = 5$ – 50° at room temperature, in which the X-ray tube was operated at 40 kV and 40 mA. Thermogravimetric analysis (TGA) data were recorded with a PerkinElmer STA6000 thermal analyzer from 25 °C to 1000 °C with a heating rate of 10 °C min⁻¹ in an N₂ atmosphere (a flow rate of 20 mL min⁻¹). Fluorescent spectra were recorded on a Hitachi F-4600 fluorescence spectrophotometer. UV-vis spectra were obtained at room temperature using a Shimadzu UV-3600 double monochromator spectrophotometer.

Comment S2: Syntheses of CPs 1 and 2.

For CP 1: A mixture of H₄tptc (1.6 mg, 0.004 mmol), *o*-bimb (1.9 mg, 0.008 mmol), CdCl₂·2.5H2O (1.8 mg, 0.008 mmol) in DMF/H₂O (1.0 mL, v/v, 1/1) was sealed in a hard glass tube and then was added into one drop of NaOH (0.2 M), then the mixed solution was sealed in a vacuum environment and heated to 130 °C for 3000 minutues, and then cooled to room temperature at a rate of 10 °C per hour. The colourless blocky crystals that formed was collected by filtration, washed with mother liquor and pure water for three times, and then dried at room temperature to give CP 1 with a yield of 47% (based on H₄tptc). Anal. (%) calcd. for C₂₅H₁₉CdN₄O₄: C, 54.41; H, 3.47; N, 10.15. Found: C, 54.36; H, 3.87; 10.13. IR (KBr pellet, cm⁻¹): 3451 (m), 1566 (vs), 1521 (m), 1425 (vs), 1390 (s), 1348 (s), 1241 (s), 1109 (s), 1087 (s), 1022 (w), 897 (w), 859 (s), 778 (s), 727 (s), 618 (m), and 589 (w).

For CP **2**: CP **2** was assembled under a similar condition of CP **1**, except without the addition of NaOH, and the *m*-bimb replaced *o*-bimb ligand. After heated and cooled, the colourless blocky crystals of CP **2** were obtained and collected by filtration, washed with mother liquor and ethanol for three times, and then dried at room temperature to give 1 with a yield of 51% (based on H₄tptc). Anal. (%) calcd. for $C_{25}H_{20}CdClN_4O_4$: C, 51.04; H, 3.43; N, 9.52. Found: C, 50.97; H, 3.47; N, 9.57. IR (KBr pellet, cm⁻¹): 3437 (m), 1691 (m), 1562 (s), 1520 (m), 1402 (s), 1352 (s), 1293 (s), 1226 (s), 1112 (m), 1083 (s), 982 (m), 929 (m), 838 (s), 755 (s), 725 (m), 686 (w), and 578 (w).

Comment S3: Preparation of samples for luminescence measurements.

Each milled sample of the CPs 1 or 2 (1.0 mg) was immersed in 2.0 mL DMF solution to form uniform suspensions after ultrasonication for 30 min. Then the gradient detections of ABXs were tested by injection 1 mM ABXs into the colorimetric dish to test the fluorescence properties.

Comment S4: X-ray crystallography for CPs 1 and 2.

Structural integrity single crystals of **1** and **2** were carefully selected under an optical microscope and fixed to thin glass fibers. After that, single-crystal X-ray diffraction analyses was performed on a Siemens SMART diffractometer using Mo-K α radiation (λ =0.71073Å) at 293(2) K. The structures of CPs **1** and **2** were solved by direct methods, with the non-hydrogen atoms refined anisotropially by using the SHELXTL package with F^2 values based full-matrix least-squares procedure and Olex 2.0 [1,2]. All the hydrogen atoms except those for water molecules were generated geometrically with fixed isotropic thermal parameters, and included in the structure factor calculations. And the hydrogen atoms attached to oxygen were refined with O–H=0.85Å and U_{iso}(H) =1.2U_{eq}(O). The crystallographic data, the details of the crystal structures, as well as the CCDC number for CPs **1** and **2** are listed in Table S1. Selected bond lengths and angles for CPs **1** and **2** are shown in Table S2.

 Table S1. Crystal data, experimental conditions, and structure refinement parameters of CPs 1 and 2.

		-			
	CP 1	CP 2			
Empirical formula	$C_{25}H_{19}CdN_4O_4$	$C_{25}H_{20}CdClN_4O_4$			
Formula weight	551.84	588.30			
Crystal system	Monoclinic	Monoclinic			
Space group	$P2_1/n$	$P2_1/c$			
a [Å]	6.972 (3)	9.431(4)			
<i>b</i> [Å]	17.311 (9)	13.316(4)			
c [Å]	17.837 (8)	18.540(7)			
β [°]	93.913 (14)	91.891(13)			
$V[Å^3]$	2147.7 (17)	2326.9(14)			
Ζ	4	4			
$Dc/(g \cdot cm^{-3})$	1.707	1.679			
F(000)	1108	1180			
μ (Mo K α)/mm ⁻¹	1.059	1.094			
θ range (°)	3.07-27.1	3.251-26.022			
R _{int}	0.0451	0.0264			
Refinement method	Full-matrix least-squares on F ²				
Goodness-of-fit on F^2	0.998	1.101			
$R_1, wR_2 [I > 2\sigma(I)]^{a,b}$	0.0425, 0.0859	0.0293, 0.0740			
R_1 , wR_2 (all data) ^{a,b}	0.0522, 0.0852	0.0312, 0.0754			
CCDC number	1943131	1876336			

a) $R_1 = \Sigma ||Fo| - |Fc| / \Sigma ||Fo|$. b) $wR_2 = \{ [\Sigma w (Fo^2 - Fc^2)^2 / \Sigma w (Fo^2)^2] \}^{1/2}$.

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

CP 1								
Cd(1)-O(1)	2.420(3)	Cd(1)-O(2)	2.327(3)	Cd(1)-N(3)	2.237(3)	$Cd(1)-N(4)^{\#1}$	2.275(4)	
Cd(1)-O(3)#2	2.420(4)	Cd(1)-O(4)#2	2.376(4)	O(1)-Cd(1)-O(2)	54.72(10)	O(2)-Cd(1)-O(3)#2	124.39(14)	
O(2)-Cd(1)-O(4) ^{#2}	89.71(14)	O(1)-Cd(1)-N(3)	86.56(12)	O(2)-Cd(1)-N(3)	127.07(12)	N(3)-Cd(1)-N(4)#1	102.86(14)	
N(3)-Cd(1)-O(3)#2	107.99(14)	N(3)-Cd(1)-O(4)#2	119.35(15)	$N(4)-Cd(1)-O(1)^{\#1}$	136.17(12)	N(4)-Cd(1)-O(2)#1	87.81(12)	
N(4)#1-Cd(1)-O(3)#2	87.21(13)	N(4)#1-Cd(1)-O(4)#2	127.84(14)	O(3)#2-Cd(1)-O(1)	130.91(12)	O(4)#2-Cd(1)-O(1)	78.78(12)	
O(4)#2-Cd(1)-O(3)#2	52.93(12)							
Symmetry codes: #1 -	1/2-x, $1/2+y$, $1/2+y$	/2-z; #2 -1/2+x, 3/2-y, -1	$/2+_{Z}$.					
CP 2								
Cd(1)-O(1)	2.3725(18)	Cd(1)-O(2)	2.4045(18)	Cd(1)-N(1)	2.253(2)	$Cd(1)-N(4)^{\#1}$	2.283(2)	
Cd(1)-Cl(1)	2.5596(9)	Cd(1)-Cl(1)#2	2.7181(11)	O(1)-Cd(1)-O(2)	54.55(6)	O(1)-Cd(1)-Cl(1)	162.95(5)	
O(1)-Cd(1)-Cl(1)#2	88.19(5)	O(2)-Cd(1)-Cl(1)#2	83.55(5)	O(2)-Cd(1)-Cl(1)	108.76(5)	O(1)-Cd(1)-N(1)	95.20(7)	
O(2)-Cd(1)-N(1)	148.67(7)	N(1)-Cd(1)-N(4)#1	98.62(8)	N(1)-Cd(1)-Cl(1)	100.66(7)	N(1)-Cd(1)-Cl(1)#2	87.99(6)	
N(4)#1-Cd(1)-O(1)	92.10(8)	$N(4)^{\#1}-Cd(1)-O(2)$	91.19(8)	N(4)#1-Cd(1)-Cl(1)#2	173.33(6)	N(4)#1-Cd(1)-Cl(1)	91.69(6)	
$Cl(1)^{\#1}-Cd(1)-Cl(1)$	86.15(2)							
Symmetry codes: $\#1 - x_1 - 1/2 + y_1 - 1/2 - z_1 + y_2 - 1 - z_1 - y_2 - 1 - z_1 - z_2$								

Table S3 The hydrogen bonding interactions of CP 2.

	0 0				
D-H···A	D-H (Å)	H…A (Å)	D…A (Å)	∠D-H…A (°)	
O3-H3…O1 ^{#1}	0.84	1.74	2.579(3)	178	
O22-H16…O4 ^{#2}	0.97	2.57	3.501(4)	160	
O24-H19…O4#3	0.93	2.39	3.304(4)	167	
O25-H20··Cl1#4	0.93	2.80	3.415(3)	124	
Symmetry codes: $\#1 - x^+$	1, -v, -z+1; #2 - x+1, -v+1,	-z+1; #3 x-1, $-v+1/2$, z-1/2; #4 -	x, y+1/2, -z+1/2.		



Scheme S1. The selected organic ligands in assembly of CPs 1 and 2.



Scheme S2. The coordination modes of H_4 tptc ligand in assembly of CPs 1 and 2.







Fig. S1 The asymmetric unit of CP **1** with the thermal ellipsoids at 30% probability level (Symmetry codes: i -1/2-x, 1/2+y, 1/2-z; ii - 1/2+x, 3/2-y, -1/2+z; iii 2-x, 1-y, 1-z.).



Fig. S2 The 2D $[Cd_2(tptc)]_n$ sheet in CP 1.



Fig. S3 The right- and left- handed $[Cd(o-bimb)]_n$ helix chains in CP 1.



Fig. S4 The 3D interpenetrating nets of CP 1.



Fig. S5 The asymmetric unit of CP **2** with the thermal ellipsoids at 30% probability level (Symmetry codes: i -*x*, -1/2+*y*, 1/2-*z*; ii -*x*, 1-*y*, 1-*z*; iii -*x*, -*y*, 1-*z*.).



Fig. S6 The binuclear $\{Cd_2Cl_2\}$ SBU in CP 2.



Fig. S7 The 1D $\{Cd_2(H_2tptc)(Cl)_2\}_n$ chain in CP 2.



Fig. S8 The 2D $\{Cd_2(m\text{-bimb})(Cl)_2\}_n$ sheet in CP 2.



Fig. S9 The 3D supermolecular structure of CP 2.



Fig. S10 The TG curves for CPs 1 and 2.



Fig. S11 The fluorescence spectra of free H₄tptc, and CPs 1 and 2 in the solid state at room temperature.



Fig. S12 The luminescence spectra of CP 1 which were dispersed in different solvents.



Fig. S13 The luminescence spectra of CP 2 which were dispersed in different solvents.



Fig. S14 The fluorescence intensities of those emulsions of CP 1 in DMF decreased in different degrees with the concentration of NFZ (a), NFT (b), DND (c), MND (d), RND (e), and OND (f) increases from 0 to 25 μ M.



Fig. S15 The fluorescence intensities of those emulsions of CP 2 in DMF decreased in different degrees with the concentration of NFZ (a), NFT (b), DND (c), MND (d), RND (e), and OND (f) increases from 0 to 25 μ M.



Fig. S16 The Stern-Volumer plots of I_0/I versus the concentration of NFZ (a), NFT (b), DND (c), MND (d), RND (e), and OND (f) for CP 1.



Fig. S17 The Stern-Volumer plots of I_0/I versus the concentration of NFZ (a), NFT (b), DND (c), MND (d), RND (e), and OND (f) for CP 2.





Fig. S19 The quenching rates of CP 2 with the incremental addition of different ABXs.



Fig. S20 The repeatability of CP 1 in detecting NFZ (a), NFT (b), DND (c), MND (d), RND (e), and OND (f).



Fig. S21 The repeatability of CP 2 in detecting NFZ (a), NFT (b), DND (c), MND (d), RND (e), and OND (f).



Fig. S22 The PXRD patterns of CP 1 after three cycles tests of ABXs.



Fig. S23 The PXRD patterns of CP 2 after three cycles tests of ABXs.



Fig. S24 The UV-Vis absorbance spectra of ABXs and CPs 1 and 2 in DMF solution.



Fig. S25 Lifetime decay profile of two CPs before (a for 1, c for 2) and after (b for 1, d for 2) exposure to DND.

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