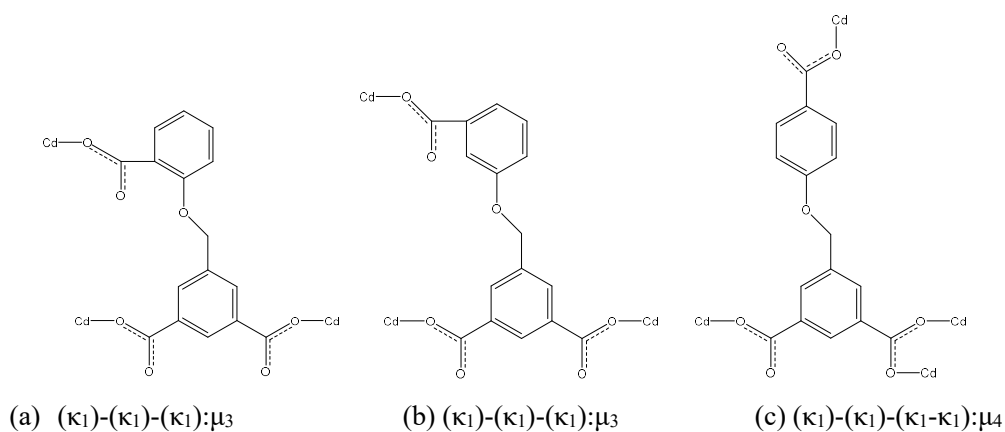


# Highly sensitive fluorescent sensing for nitrobenzene of Cd<sup>II</sup> complexes based on three isomers and a bis-imidazole ligand

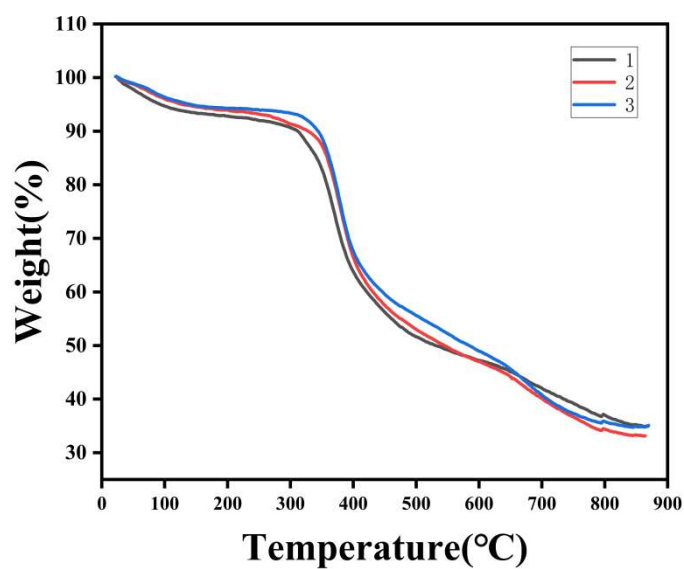
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Materials, Shaanxi Key Laboratory of Chemical Reaction Engineering, Yan'an University,  
Yan'an 716000, P. R. China

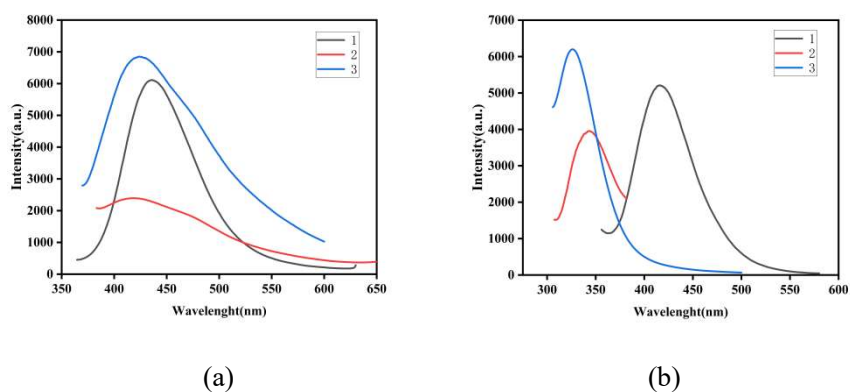
For  
Molecules



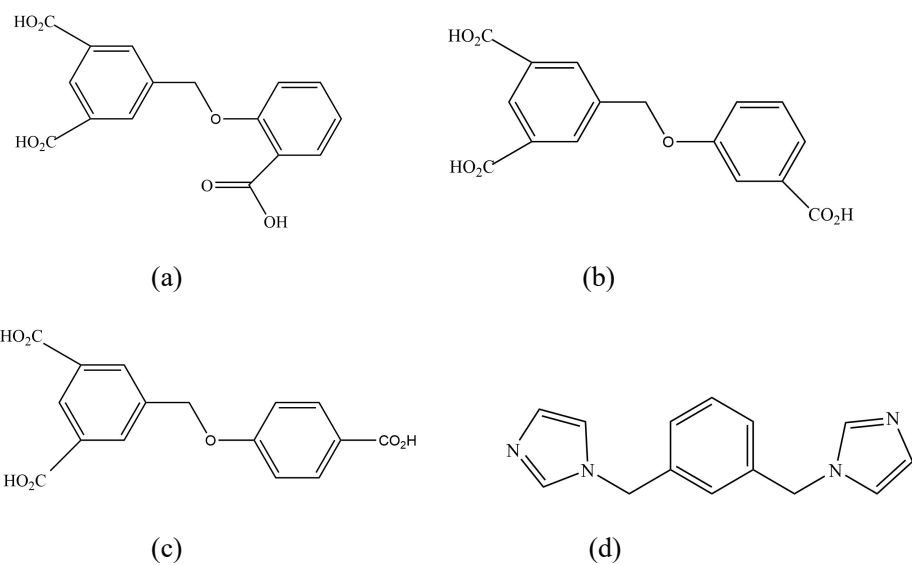
**Chart S1** The coordination modes of *n*-(3,5-dicarboxylato benzyloxy) benzoic acids  
(*n* = 2, 3 or 4-H<sub>3</sub>DBB)



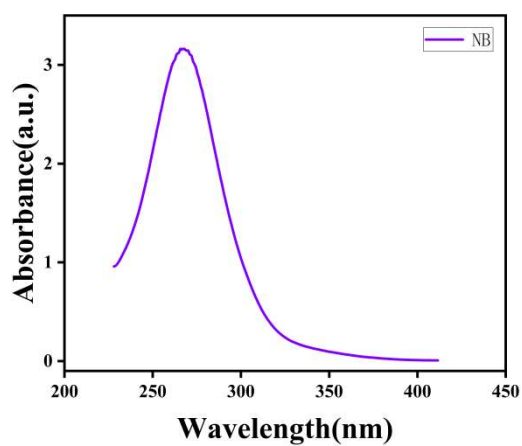
**Figure S1** TG curves for complexes 1-3.



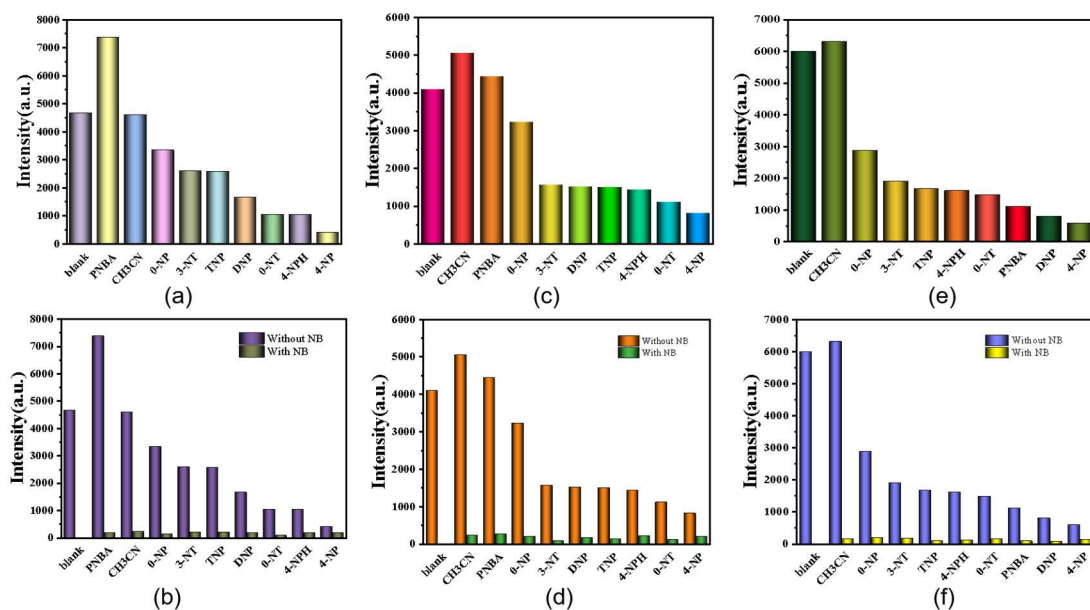
**Figure S2** The emission spectra of the coordination polymers **1-3** in solid state(a) and solution (b).



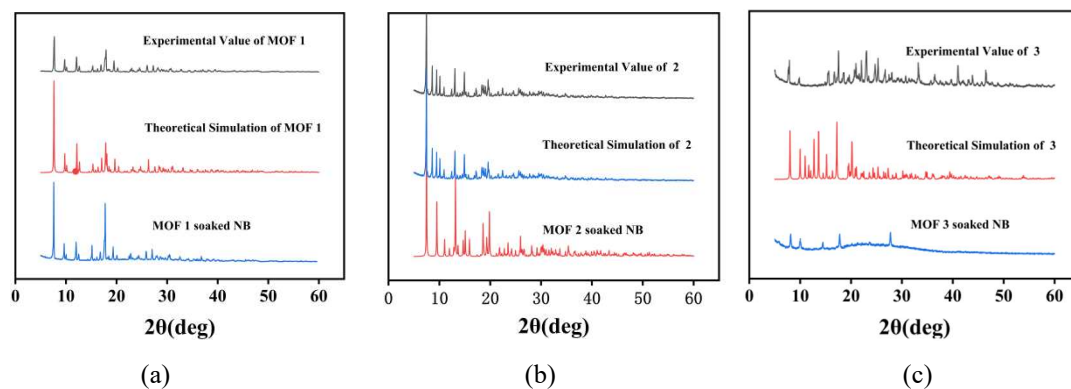
**Figure S3** The structures of ligands [n-(3,5-dicarboxylato benzyloxy) benzoic acid (n = 2, 3 or 4-H3DBB) (a-c) and a linear N-donor ligand: 3-bis(imidazole-1-ylmethyl) benzene (3-bibz)] (d)



**Figure S4** The UV-vis absorption spectrum of nitrobenzene



**Figure S5** Fluorescence sensing characterization of complexes 1-3 for nitro explosives (a-c);  
Anti-jamming experiment of p-nitrobenzene (b-f).



**Figure S6** Theoretical and experimental values of complexes 1-3 (a-c) and PXRD patterns of soaked NB

**Table S1** Crystal data and structure refinement details for **1-3**

complexes 1-3	1	2	3
Formula	$C_{30}H_{23}Cd_{1.50}N_4O_7$	$C_{46}H_{27}Cd_3N_4O_{14}$	$C_{30}H_{24}Cd_2N_4O_8$
Formula weight	720.12	1196.91	793.35
Crystal system	Monoclinic	Triclinic	Orthorhombic
Space group	$C2/c$	$P-1$	$Pna2_1$
$a$ (Å)	31.351(18)	9.3533(16)	14.836(6)
$b$ (Å)	9.891(6)	9.7956(18)	9.759(4)

<i>c</i> (Å)	23.440(14)	12.0920(18)	22.293(9)
$\alpha$ (°)	90	99.495(4)	90
$\beta$ (°)	131.531(7)	92.055(6)	90
$\gamma$ (°)	90	103.023(6)	90
<i>V</i> (cm <sup>3</sup> )	5441(6)	1061.5(3)	3228(2)
$\rho$ (g cm <sup>-3</sup> )	1.758	1.872	1.633
<i>Z</i>	8	1	4
F(000)	2872	587	1568.0
Goof			
<i>R</i> <sub>1</sub> , w <i>R</i> <sub>2</sub> (I>2σ(I))	<i>R</i> <sub>1</sub> = 0.0500, w <i>R</i> <sub>2</sub> = 0.1367	<i>R</i> <sub>1</sub> = 0.0515, w <i>R</i> <sub>2</sub> = 0.1039	<i>R</i> <sub>1</sub> = 0.0645, w <i>R</i> <sub>2</sub> = 0.1837
<i>R</i> <sub>1</sub> , w <i>R</i> <sub>2</sub> (all data)	<i>R</i> <sub>1</sub> = 0.1561, w <i>R</i> <sub>2</sub> = 0.2098	<i>R</i> <sub>1</sub> = 0.1041, w <i>R</i> <sub>2</sub> = 0.1198	<i>R</i> <sub>1</sub> = 0.4968, w <i>R</i> <sub>2</sub> = 0.5858

$$^a R_1 = \sum(|F_o| - |F_c|) / \sum |F_o|; \quad ^b wR_2 = \{ \sum [w(|F_o|^2 - |F_c|^2)^2] / \sum [w(|F_o|^2)^2] \}^{1/2}.$$

**Table S2** Selected bond lengths (Å) and bond angles (°) of **1**

bond lengths	Å	bond lengths	Å	bond lengths	Å
Cd(1)-O(1)	2.201(5)	Cd(2)-N(1)	2.265(6)	Cd(1)-O(4)	2.335(5)
Cd(1)-O(1)#1	2.201(5)	Cd(2)-O(2)#1	2.279(5)	Cd(2)-O(4)	2.312(5)
Cd(1)-O(7)#2	2.290(6)	Cd(2)-N(4)#4	2.302(6)	Cd(2)-O(5)	2.569(7)
Cd(1)-O(7)#3	2.290(6)	Cd(2)-O(6)#2	2.333(7)	Cd(2)-O(7)#2	2.563(6)
Cd(1)-O(4)#1	2.335(5)				
bond angles	°	bond angles	°	bond angles	°
N(4)#4-Cd(2)-O(6)#2	89.7(2)	O(1)-Cd(1)-O(1)#1	163.6(4)	O(7)#3-Cd(1)-O(4)	167.97(19)
O(4)-Cd(2)-O(6)#2	123.74(19)	O(1)-Cd(1)-O(7)#2	91.4(2)	O(4)#1-Cd(1)-O(4)	114.7(3)
N(1)-Cd(2)-O(7)#2	142.1(2)	O(1)#1-Cd(1)-O(7)#2	99.8(2)	N(1)-Cd(2)-O(2)#1	89.4(2)
O(2)#1-Cd(2)-O(7)#2	99.17(19)	O(1)-Cd(1)-O(7)#3	99.8(2)	N(1)-Cd(2)-N(4)#4	91.5(2)
N(4)#4-Cd(2)-O(7)#2	85.51(19)	O(1)#1-Cd(1)-O(7)#3	91.4(2)	O(2)#1-Cd(2)-N(4)#4	171.1(3)
O(4)-Cd(2)-O(7)#2	71.3(2)	O(7)#2-Cd(1)-O(7)#3	93.8(3)	N(1)-Cd(2)-O(4)	146.4(2)
O(6)#2-Cd(2)-O(7)#2	52.50(19)	O(1)-Cd(1)-O(4)#1	84.1(2)	O(2)#1-Cd(2)-O(4)	85.46(19)
N(1)-Cd(2)-O(5)	93.5(2)	O(1)#1-Cd(1)-O(4)#1	87.1(2)	N(4)#4-Cd(2)-O(4)	88.90(19)
O(2)#1-Cd(2)-O(5)	84.4(2)	O(7)#2-Cd(1)-O(4)#1	167.97(19)	N(1)-Cd(2)-O(6)#2	89.8(2)
N(4)#4-Cd(2)-O(5)	86.7(2)	O(7)#3-Cd(1)-O(4)#1	76.1(2)	O(2)#1-Cd(2)-O(6)#2	99.1(2)
O(4)-Cd(2)-O(5)	52.98(17)	O(1)-Cd(1)-O(4)	87.1(2)	O(7)#2-Cd(2)-O(5)	123.84(18)
O(6)#2-Cd(2)-O(5)	175.16(16)	O(1)#1-Cd(1)-O(4)	84.1(2)	O(7)#2-Cd(1)-O(4)	76.1(2)

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

**Table S3** Selected bond lengths (Å) and bond angles (°) of **2**

bond lengths	Å	bond lengths	Å	bond lengths	Å
Cd(1)-O(1)#1	2.407(4)	Cd(1)-O(4)#3	2.179(4)	Cd(2)-O(1)	2.235(4)
Cd(1)-O(1)	2.407(4)	Cd(1)-O(5)#4	2.251(4)	Cd(2)-O(2)#6	2.463(5)

Cd(1)-O(4)#2	2.179(4)	Cd(2)-O(5)#5	2.416(4)	Cd(2)-O(3)#3	2.596(4)
bond angles	°	bond angles	°	bond angles	°
O(1)-Cd(2)-O(3)#3	107.07(15)	Cd(2)-Cd(1)-Cd(2)#1	180.0	O(4)#2-Cd(1)-O(1)#1	84.66(15)
O(6)#5-Cd(2)-Cd(1)	77.54(11)	O(1)-Cd(1)-Cd(2)#1	139.80(9)	O(4)#2-Cd(1)-O(4)#3	180.0(3)
O(6)#5-Cd(2)-O(5)#5	50.80(14)	O(1)#1-Cd(1)-Cd(2)#1	40.20(9)	O(4)#3-Cd(1)-O(5)#4	90.06(15)
O(2)#6-Cd(2)-Cd(1)	128.18(9)	O(1)#1-Cd(1)-Cd(2)	139.80(9)	O(4)#3-Cd(1)-O(5)#5	89.94(15)
O(2)#6-Cd(2)-O(6)#5	136.48(15)	O(1)-Cd(1)-Cd(2)	40.20(9)	O(4)#2-Cd(1)-O(5)#4	89.94(15)
O(2)#6-Cd(2)-O(5)#5	168.75(13)	O(1)#1-Cd(1)-O(1)	180.0	O(4)#2-Cd(1)-O(5)#5	90.06(15)
O(5)#5-Cd(2)-Cd(1)	40.80(9)	O(4)#2-Cd(1)-Cd(2)#1	66.43(12)	O(5)#4-Cd(1)-Cd(2)	131.11(11)
O(4)#3-Cd(1)-Cd(2)	66.43(12)	O(4)#2-Cd(1)-Cd(2)	113.57(12)	O(4)#3-Cd(1)-O(1)	84.66(15)
O(4)#3-Cd(1)-Cd(2)#1	113.57(12)	O(4)#3-Cd(1)-O(1)#1	95.34(15)	O(4)#2-Cd(1)-O(1)	95.34(15)

Symmetry codes:#1 -x+1,-y+1,-z; #2 -x+1,-y,-z; #3 x,y+1,z; #4 -x+1,-y+1,-z+1; #5 x,y,z-1; #6 -x+2,-y+1,-z

**Table S4** Selected bond lengths (Å) and bond angles (°) of **3**

bond lengths	Å	bond lengths	Å	bond lengths	Å
Cd1-O8	1.971(7)	Cd1-N1	2.015(9)	Cd2-O8#1	1.932(7)
Cd1-O1	1.977(5)	Cd2-O6#2	2.049(8)	Cd2-O3	2.041(6)
Cd1-O4#1	1.999(5)	Cd2-O7#2	2.19(5)	Cd2-N4	2.038(6)
bond angles	°	bond angles	°	bond angles	°
O8-Cd2-O7#2	96.7(6)	O8-Cd1-O1	106.2(3)	O8-Cd2-O3	105.7(3)
O3-Cd2-O7#2	75.0(5)	O8-Cd1-O4#1	106.4(3)	O8-Cd2-N4	112.1(3)
N4-Cd2-O7#2	150.8(6)	O1-Cd1-O4#1	121.3(2)	O3-Cd2-N4	100.4(3)
O6-Cd2-O7#2	57.0(5)	O8-Cd1-N1	118.2(3)	O8-Cd2-O6	115.2(3)
O4#1-Cd1-N1	100.7(3)	N4-Cd2-O6	104.0(3)	O3-Cd2-O6	118.4(4)
O1-Cd1-N1	104.8(3)				

Symmetry codes:#1 x, y+1, z; #2 -x+1, -y, z+1/2.