

Selective detection of trinitrophenol by a Cd(II)-based coordination compound

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Supporting Information

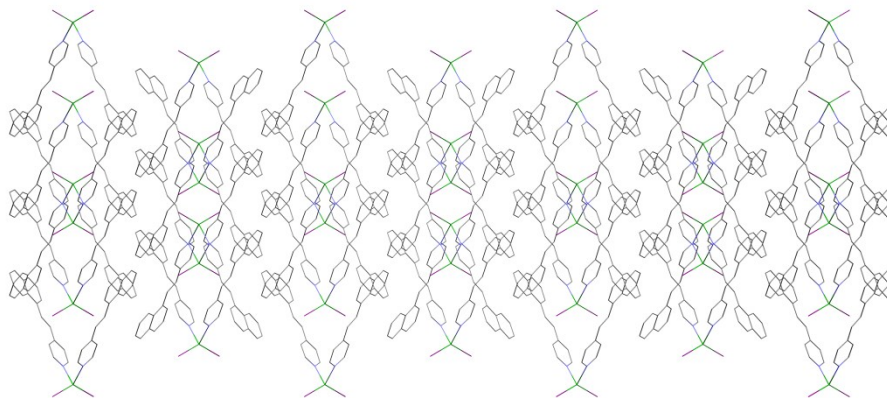


Fig. S1 3D supramolecular assembly of compound **1** viewed along *c*-axis.

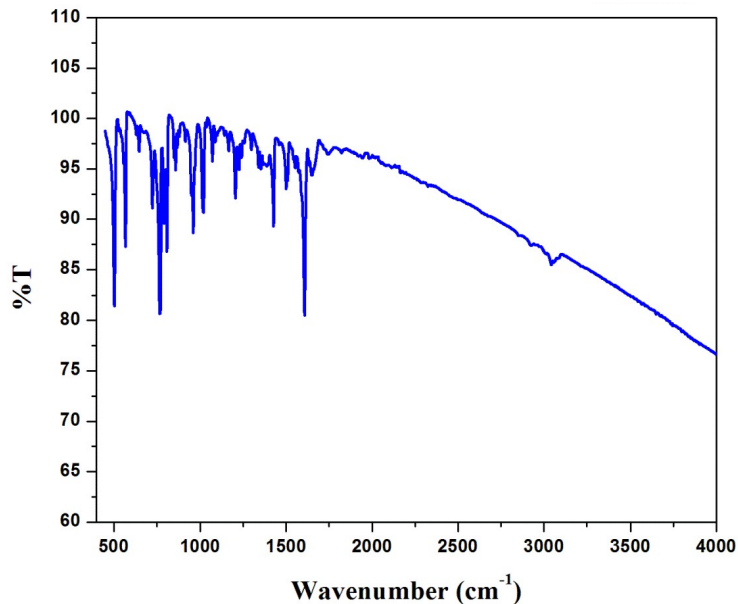


Fig. S2 FT-IR spectrum of compound **1**.

Table S1. Crystal data and refinement parameters for compound **1**

Formula	$C_{34}H_{26}CdI_2N_2$ (1)
fw	828.78
crystalsyst	monoclinic
space group	$C2/c$
a (Å)	28.4498(19)
b (Å)	7.4390(5)
c (Å)	17.7851(12)
α (deg)	90
β (deg)	125.191(2)
γ (deg)	90
V (Å ³)	3076.1(4)
Z	4
D_{calcd} (g/cm ³)	1.790
μ (mm ⁻¹)	2.742
λ (Å)	0.71073
data[$I > 2\sigma(I)$]/params	2703/177
GOF on F^2	1.088
final R indices[$I > 2\sigma(I)$] ^{a,b}	$R1 = 0.0329$ $wR2 = 0.0887$

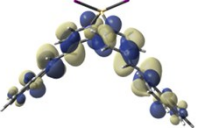
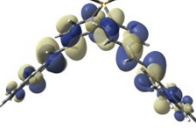
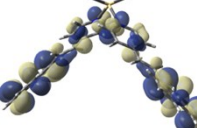
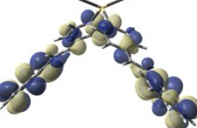
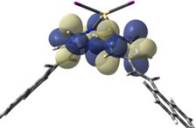
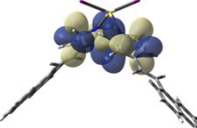
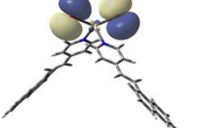
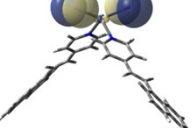
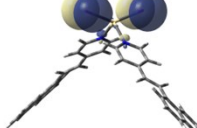
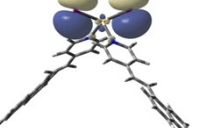
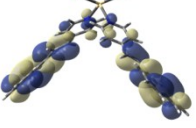
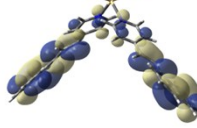
$$^a R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, \quad ^b wR2 = \left[\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2} \right]^{1/2}$$

Table S2. Selected bond lengths and bond angles in **1**

I(1) - Cd(1)	2.6915(4)	Cd(1)-N(1)-C(5)-C(4)	166.6(5)
Cd(1) - N(1)	2.306(4)	C(3)-C(4)-C(5)-N(1)	1.0(10)
Cd(1) - N(1)a	2.306(4)	Cd(1)-N(1)-C(1)-H(1)	12
I(1) - Cd(1) - N(1)	105.24(11)	C(1)-N(1)-C(5)-H(5)	179
N(1) - Cd(1) - I(1)a	110.10(11)	N(1)a-Cd(1)-N(1)-C(1)	63.7(4)
Cd(1) - N(1) - C(1)	118.4(3)	I(1)-Cd(1)-N(1)-C(5)	5.5(5)
I(1) - Cd(1) - I(1)a	131.34(2)	I(1)a-Cd(1)-N(1)-C(5)	151.4(4)
N(1)- Cd(1) - N(1)a	85.22(16)	I(1)-Cd(1)-N(1)-C(1)	173.3(4)
Cd(1) - N(1) - C(5)	123.3(4)	I(1)a - Cd(1) - N(1)a	105.24(11)
I(1) - Cd(1) - N(1)a	110.10(11)	C(15)-C(16)-C(17)-H(17)	178

Symmetry Code: a = 1-x, y, 1/2-z

Table 3. Energy of different MOs from DFT calculation

		
LUMO -2.72eV	LUMO+1 -2.7eV	LUMO+2 -1.7eV
		
LUMO+3 -1.66eV	LUMO+4 -1.6eV	LUMO+5 -1.52eV
		
HOMO -4.93eV	HOMO-1 -5.23eV	HOMO-2 -5.44eV
		
HOMO-3 -5.51eV	HOMO-4 -5.86eV	HOMO-5 -6.17eV

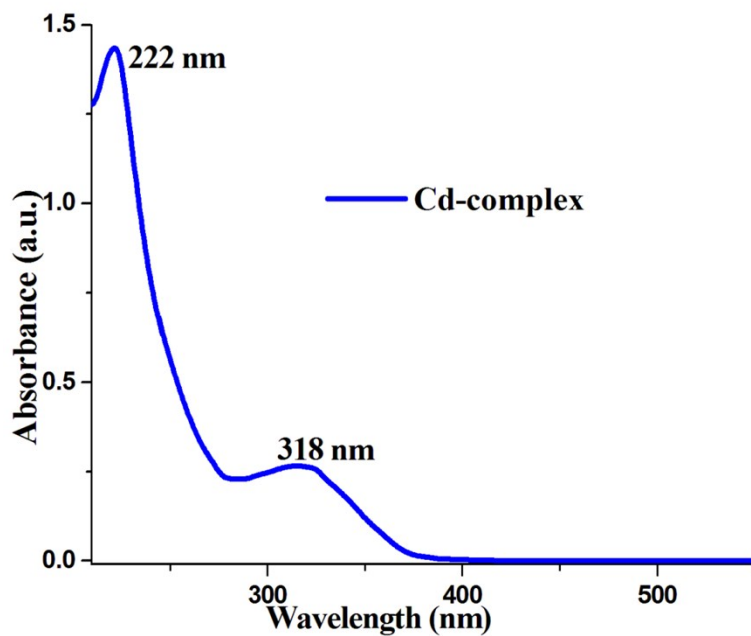


Fig. S3 UV-vis spectrum of **1** in acetonitrile.

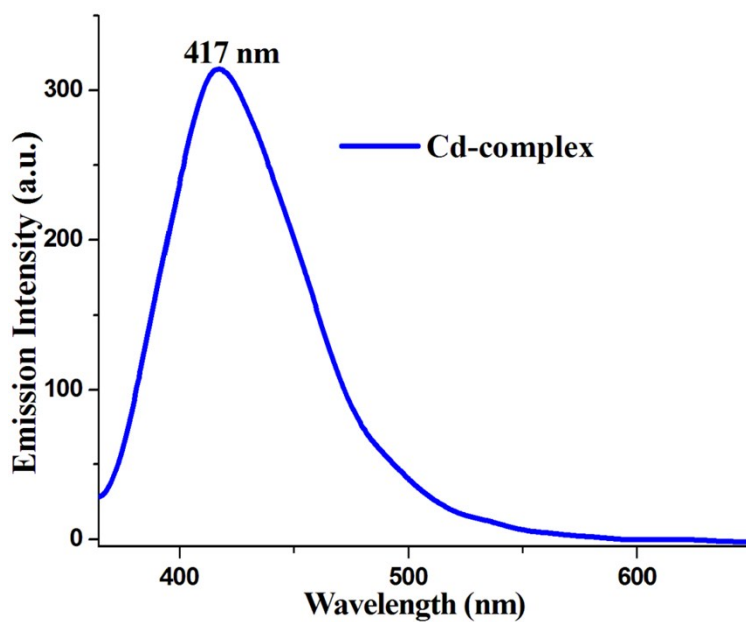


Fig. S4 Fluorescence spectrum of **1** in acetonitrile (λ_{ex} 320).

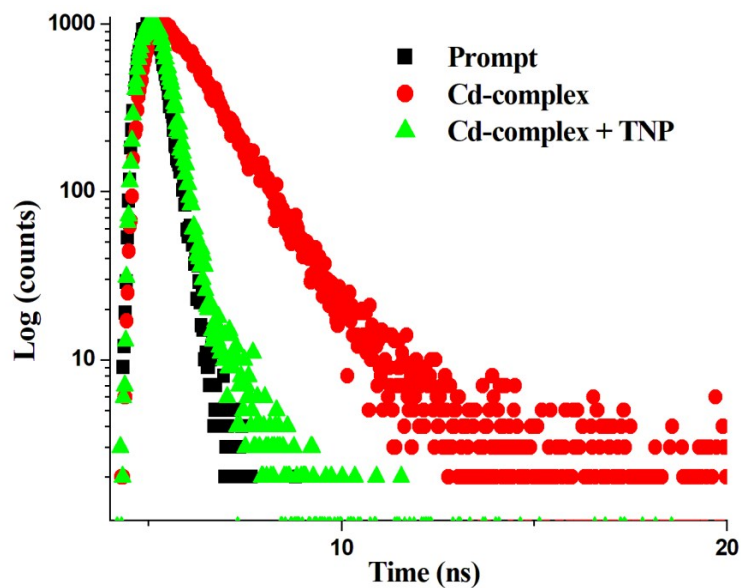


Fig. S5 Fluorescence decay profile of compound **1** and compound **1** with TNP.

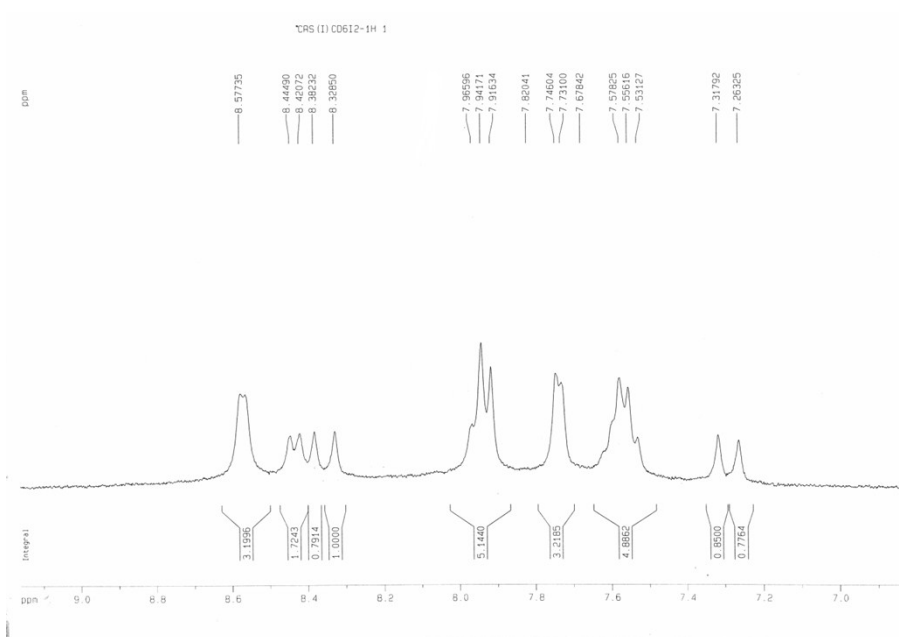


Fig. S6 ¹H NMR spectrum of **1** in DMSO-d₆ solvent.

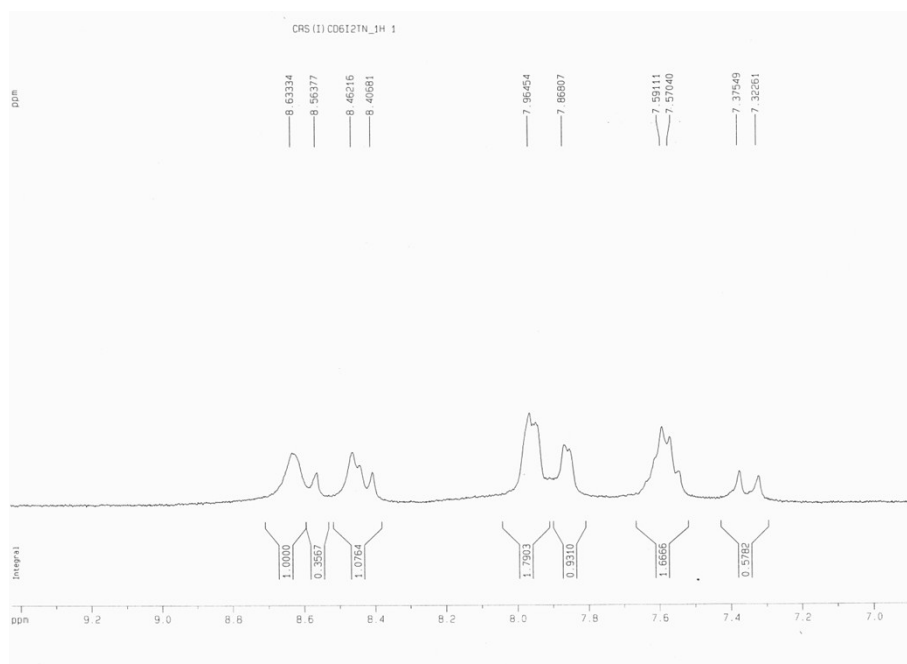


Fig. S7 ^1H NMR spectrum of **1** with trinitrophenol (TNP) in DMSO-d_6 .

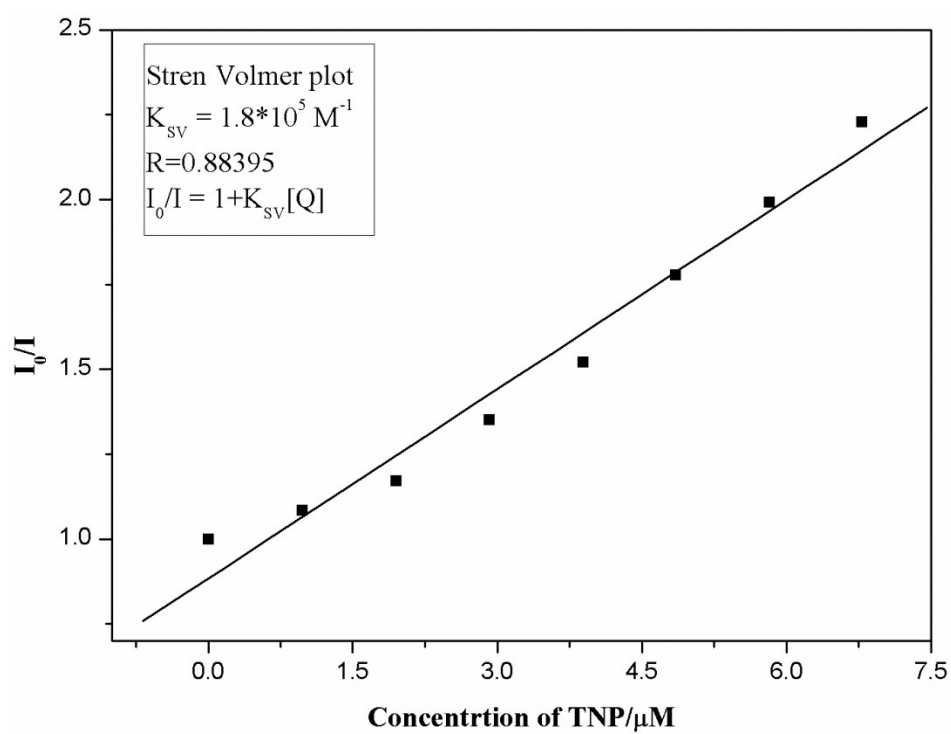


Fig. S8 Plot of I_0/I against the concentration of TNP.

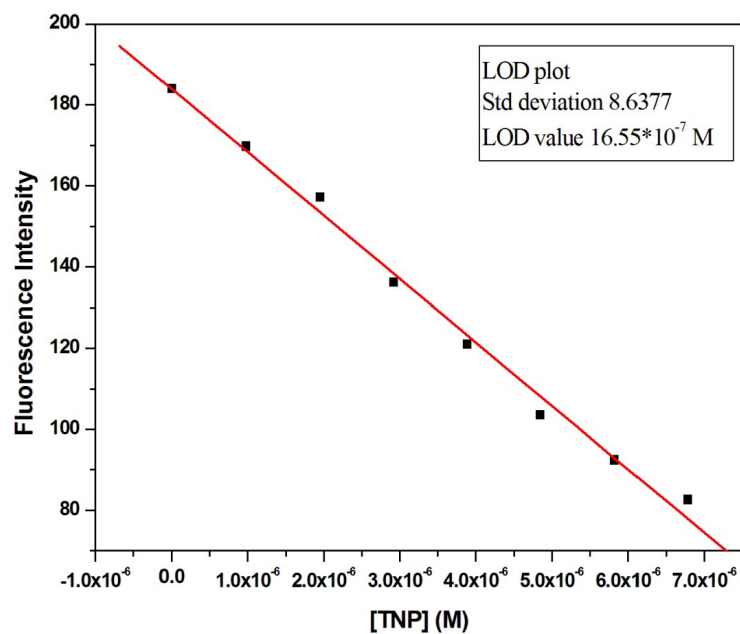


Fig. S9 Limit of detection (LOD) plot for TNP using 3σ method.

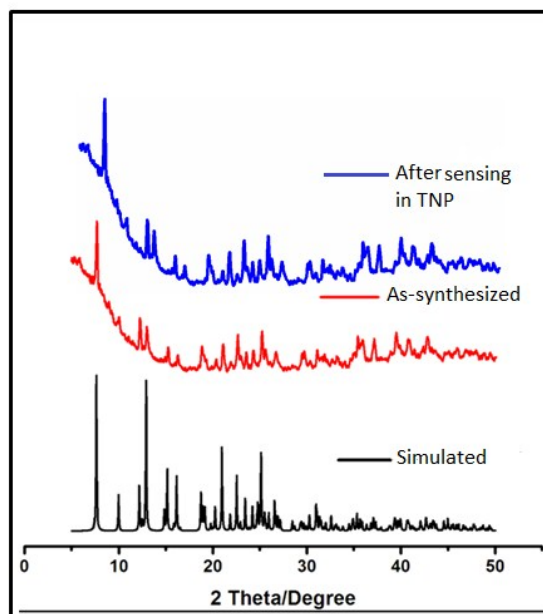


Fig. S10 PXRD patterns of simulated **1** (black), as-synthesized **1** (red) and after sensing of **1** in TNP (blue).

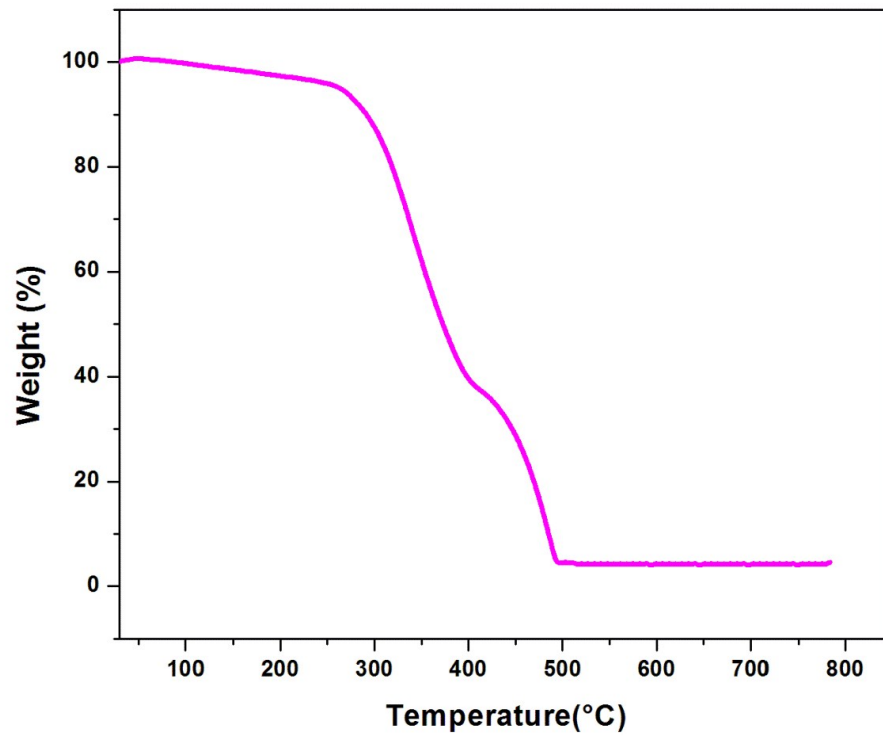


Fig. S11 TGA plot of **1** (pink).