

Supporting Information for

Photoelectric properties and potential nitro derivatives sensing by a highly luminescent of Zn (II) and Cd (II) metal-organic frameworks assembled by the flexible hexapodal ligand,1,3,5-triazine-2,4,6-triamine hexaacetic acid

Shuang Li,^a Jian Song,^a Jue Chen Ni,^a Zhi Nan Wang,^a Xue Gao,^a Zhan Shi,^b Feng Ying Bai,^a Yong Heng Xing^{*a}

^a College of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian City, 116029, China. E-mail: xingyongheng2000@163.com

^b State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun 130012, P.R. China

Supplementary Index

1. Infrared Spectra	pS2
2. TG analyses	pS2
3. PXRD	pS3
4. UV-vis Spectra	pS3
5. Band gap	pS4
6. Fluorescence Spectroscopy	pS5
7. Table for bond angles	pS8

1. Infrared spectra

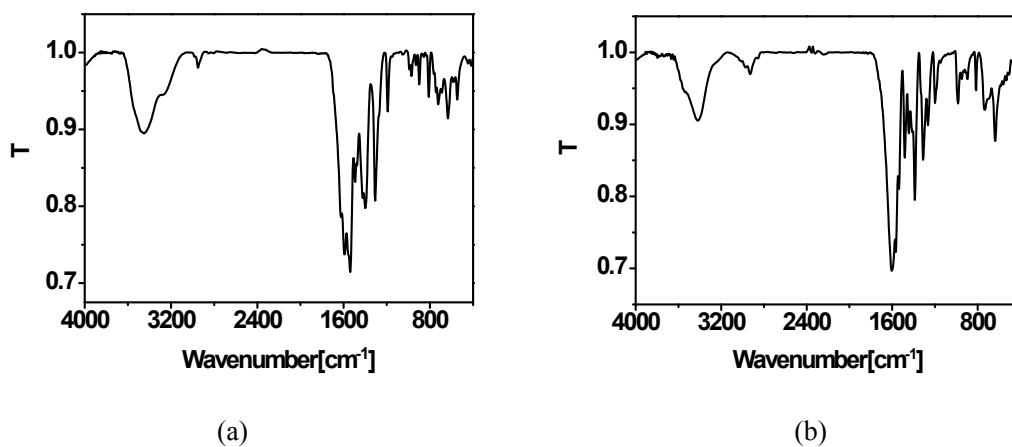


Figure S1. IR spectra of coordination polymers: (a) for 1, (b) for 2

2. TG analyses

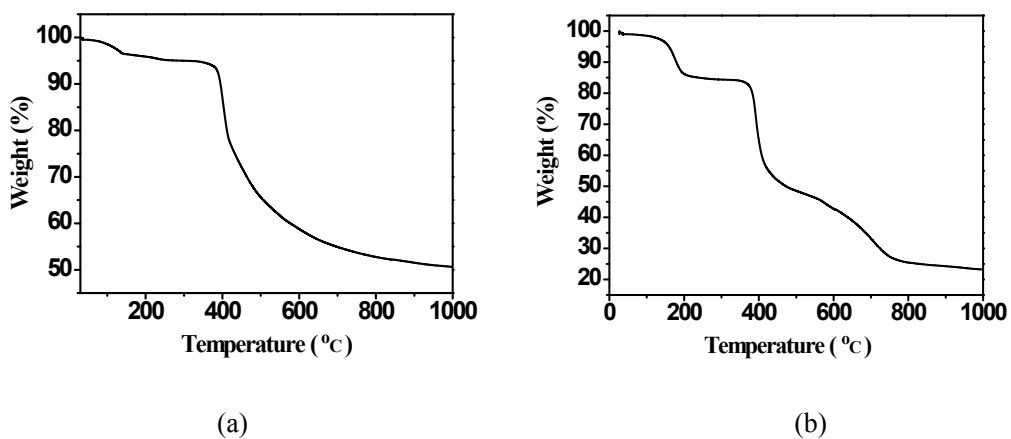


Figure S2. TG curves of coordination polymers: (a) for 1, (b) for 2

3. PXRD

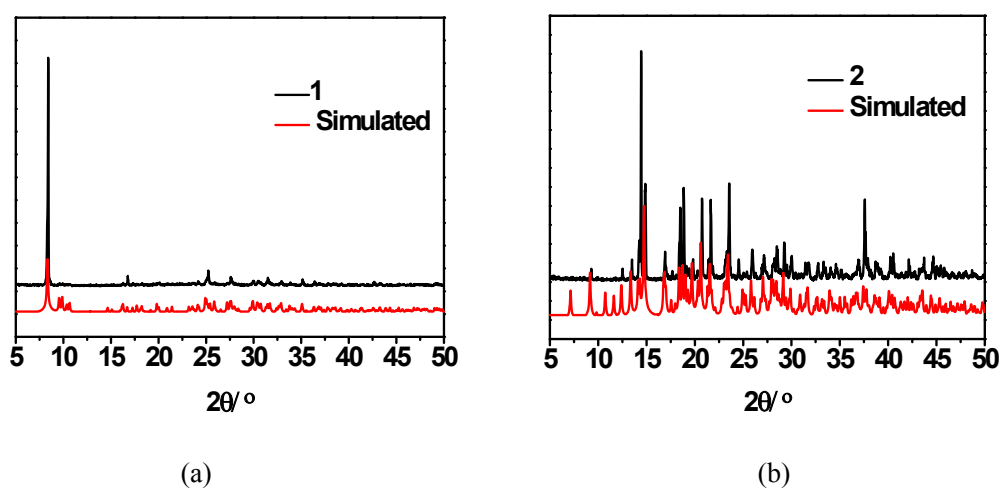


Figure S3. Powder X-ray diffraction patterns for coordination polymers: (a) for 1, (b) for 2.

4. UV-vis Spectroscopy

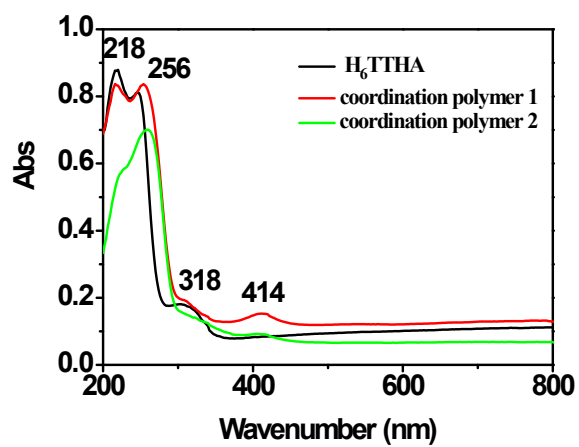
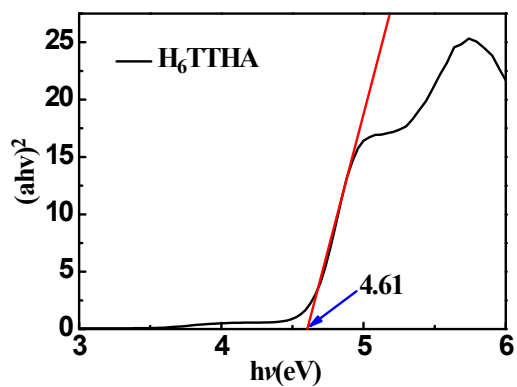
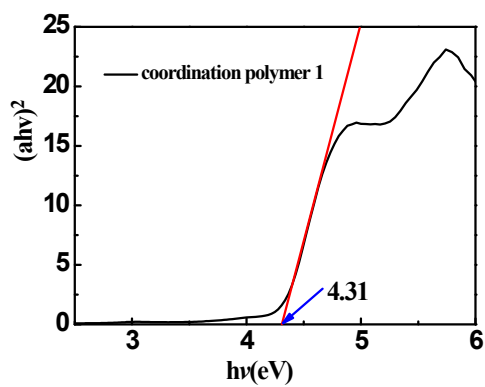


Figure S4. Solid-state UV-vis absorption spectra of the ligand H_6TTHA and coordination polymers 1 and 2.

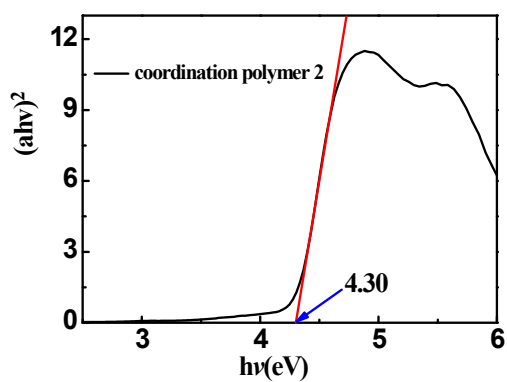
5. Band gap



(a)



(b)



(c)

Figure S5. The band gap of the H₆TTHA ligand and the two coordination polymers:(a) for the H₆TTHA ligand, (b) for 1, (c) for 2.

6. Fluorescence Spectroscopy

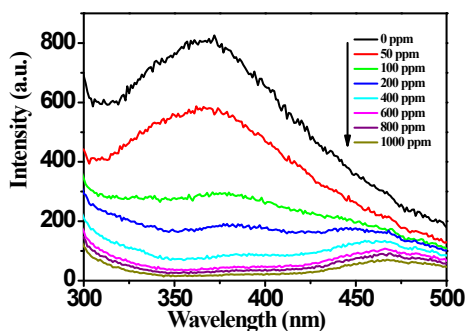
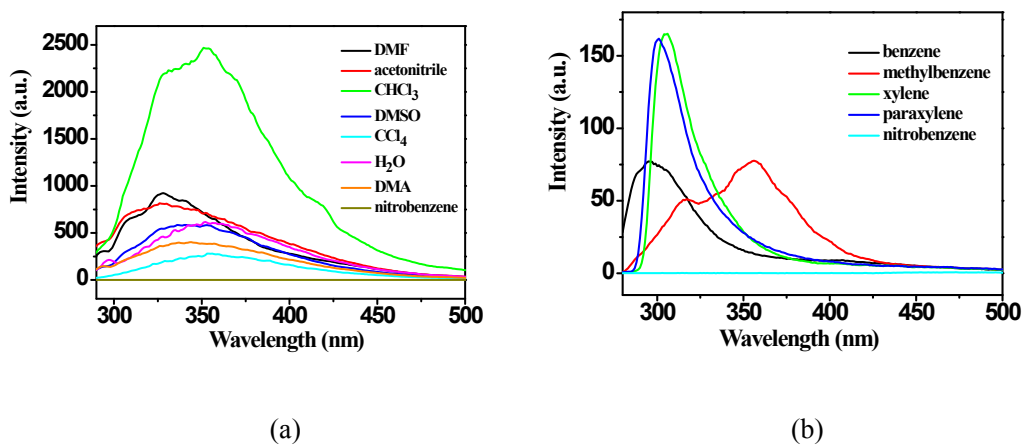
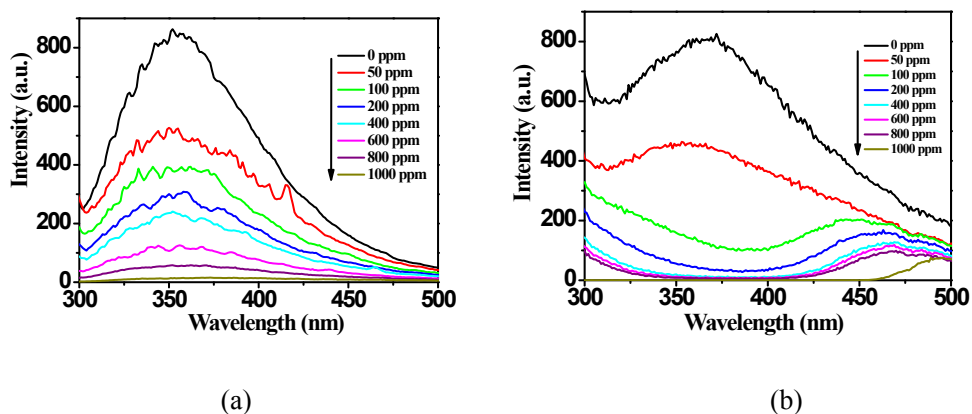
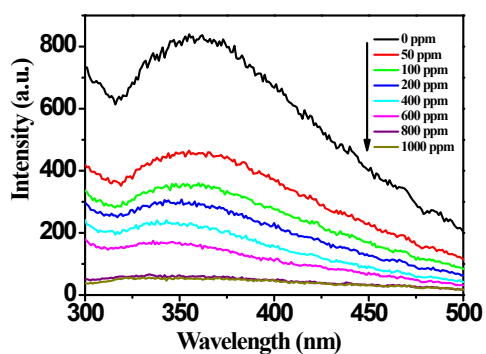
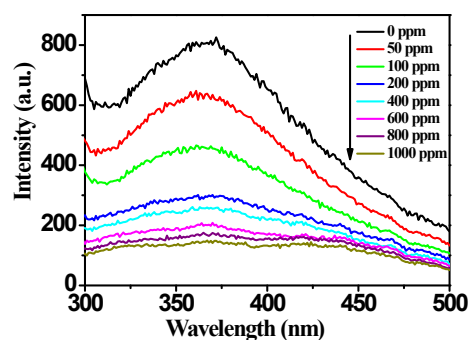


Figure S6. (a) Emission spectra of coordination polymer **1** in different solvents. (b) Emission spectra of **1** in benzene, methylbenzene, xylene, and paraxylene. (c) Luminescence quenching of **1** dispersed in H₂O by gradually increasing TNP concentration.



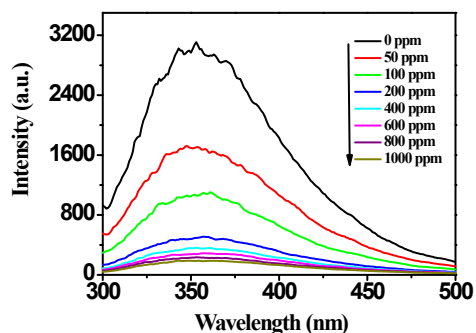


(c)

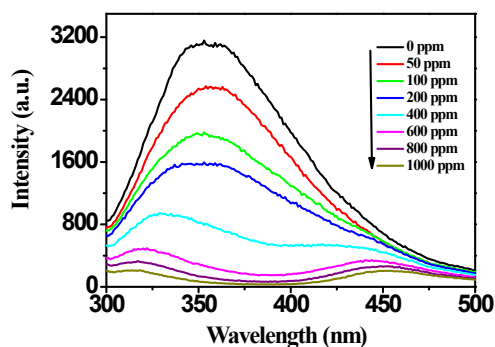


(d)

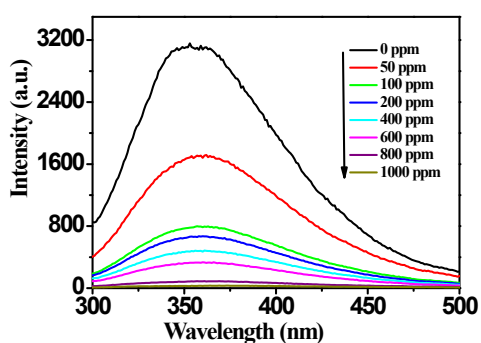
Figure S7. Luminescence quenching of coordination polymer **1** dispersed in H₂O by gradually increasing different quenchers' concentration: (a) NB, (b) p-Nitroaniline, (c) m-Dinitrobenzene, (d) sodium nitrobenzene sulfonate.



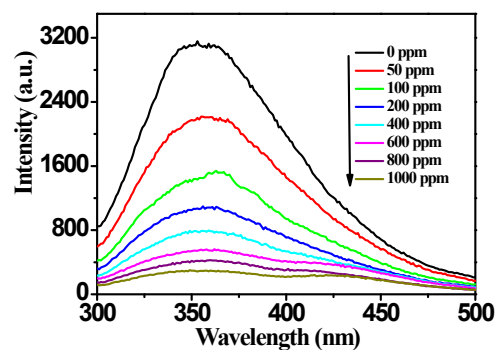
(a)



(b)



(c)



(d)

Figure S8. Luminescence quenching of coordination polymer **2** dispersed in H₂O by gradually increasing different quenchers' concentration: (a) NB, (b) p-Nitroaniline, (c) m-Dinitrobenzene, (d) sodium nitrobenzene sulfonate.

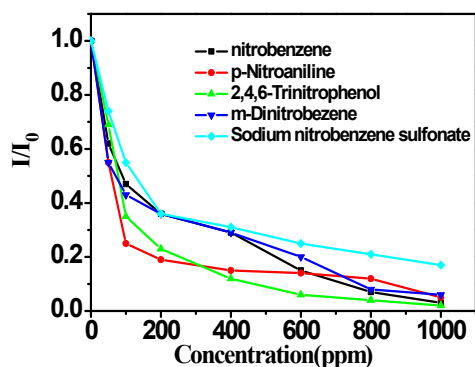
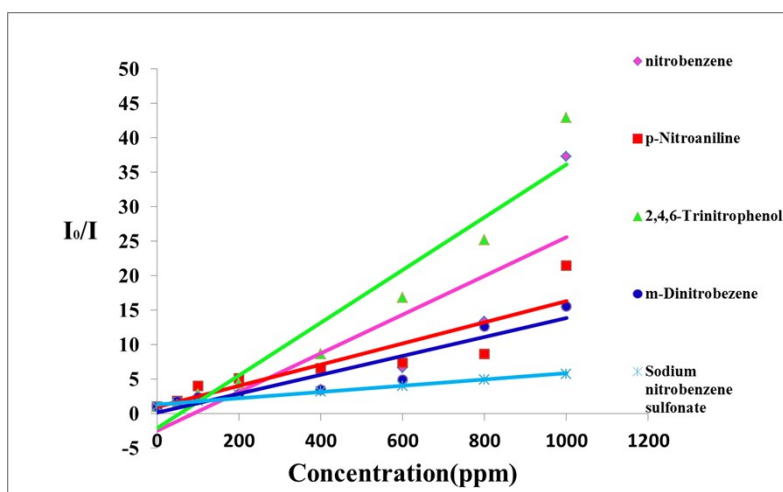
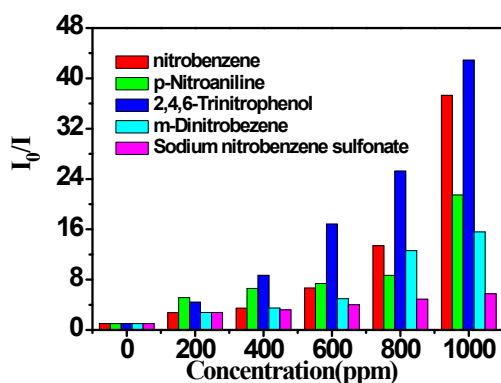


Figure S9. Plot of fraction of luminescence intensity of **1** vs. concentration of analytes. I_0 and I are the luminescence intensities in the absence and presence of analyte, respectively.



(a)



(b)

Figure S10. For **1**, (a) linear relationships of the quenching are fluorescence intensity ratio and quencher concentration; (b) at different concentrations, the value of the fluorescence intensities and the quencher ratios.

7. Table for bond angles

Table S1. Bond angles (deg) for coordination polymers **1** and **2***

Coordination polymer 1					
O12 ^C -Cd1-O1	92.9(2)	O1-Cd1-O1 ^A	84.25(17)	O12 ^C -Cd1-O8	91.4(2)
O1-Cd1-O8	171.6(2)	O1 ^A -Cd1-O8	99.7(2)	O12 ^C -Cd1-O2	83.1(2)
O1-Cd1-O2	84.71(2)	O1 ^A -Cd1-O2	153.16(18)	O8-Cd1-O2	88.6(2)
O12 ^C -Cd1-O13 ^B	154.4(2)	O1-Cd1-O13 ^B	90.42(19)	O1 ^A Cd1-O13 ^B	83.78(18)
O8-Cd1-O13 ^B	82.6(2)	O2-Cd1-O13 ^B	71.91(18)	O5-Cd2-O4	154.82(19)
O5-Cd2-O3	94.2(2)	O4-Cd2-O3	94.5(2)	O5-Cd2-O10 ^D	107.9(2)
O4-Cd2-O10 ^D	96.7(2)	O3-Cd2-O10 ^D	81.1(2)	O5-Cd2-O6 ^D	85.0(2)
O4-Cd2-O6 ^D	106.0(2)	O3-Cd2-O6 ^D	132.29(19)	O10 ^D -Cd2-O6 ^D	54.5(2)
O5-Cd2-O6	89.50(19)	O4-Cd2-O6	74.1(2)	O3-Cd2-O6	158.34(19)
O10 ^D -Cd2-O6	118.0(2)	O6 ^P -Cd2-O6	69.3(2)	O13 ^B -Cd3-O7 ^B	129.2(2)
O7 ^B -Cd3-O5 ^B	117.1(2)	O13 ^B -Cd3-O2	77.6(2)	O7-Cd3-O2	124.71(19)
O5-Cd3-O2 ^B	106.6(2)	O13-Cd3-O7 ^B	152.4(2)	O7-Cd3-O7 ^B	77.1(2)
O5-Cd3-O ^B	79.19(18)	O2 ^B -Cd3-O7 ^B	79.67(19)	O1 ^B -Cd4-O5	107.92(2)
O1 ^B -Cd4-O15 ^B	118.2(2)	O5-Cd4-O15 ^B	91.2(2)	O1 ^B -Cd4-O9 ^D	92.9(2)
O5-Cd4-O9 ^D	158.8(2)	O15 ^B -Cd4-O9 ^D	82.3(2)	O1 ^B -Cd4-O4 ^D	96.74(2)
O5-Cd4-O4 ^D	117.30(19)	O15 ^B -Cd4-O4 ^D	125.8(2)	O9 ^D -Cd4-O4 ^B	54.11(19)
Coordination polymer 2					
O6 ^A -Zn1-O7 ^A	122.64(13)	O6 ^A -Zn1-O1	98.53(13)	O7 ^A -Zn1-O1	121.58(14)
O6 ^A -Zn1-O3 ^B	121.50(12)	O7 ^A -Zn1-O3 ^B	90.17(13)	O1-Zn1-O3 ^B	102.31(12)
O11-Zn2-O9	150.94(12)	O11-Zn2-O15	97.86(12)	O9-Zn2-O15	111.17(13)
O11-Zn2-O4 ^D	88.95(11)	O9-Zn2-O4 ^D	90.70(13)	O15-Zn2-O4 ^D	92.78(13)
O11-Zn2-O16	95.77(12)	O9-Zn2-O16	85.20(12)	O15-Zn2-O16	86.53(13)
O4 ^D -Zn2-O16	175.28(12)	O11-Zn2-N6	75.51(11)	O9-Zn2-N6	75.46(12)
O15-Zn2-N6	173.37(12)	O4 ^D -Zn2-N6	86.99(11)	O16-Zn2-N6	94.24(12)
O13 ^C -Zn3-O13	140.52(12)	O13 ^C -Zn3-O14 ^C	94.84(19)	O13-Zn3-O14 ^C	85.53(18)
O13 ^C -Zn3-O10	96.1(2)	O13-Zn3-O10	123.3(2)	O14 ^C -Zn3-O10	95.17(18)
O13 ^C -Zn3-O14	78.72(16)	O13-Zn3-O14	80.82(15)	O14 ^C -Zn3-O14	148.66(8)
O10-Zn3-O14	115.91(15)	O12-Na1-O8	80.81(12)	O12-Na1-O5 ^E	80.53(12)
O8-Na1-O5 ^E	161.34(14)	O12-Na1-O11 ^F	95.84(12)	O8-Na1-O11 ^F	86.63(11)
O5 ^E -Na1-O11 ^F	95.34(11)	O12-Na1-O16 ^G	165.72(13)	O8-Na1-O16 ^G	109.47(12)
O5 ^E -Na1-O16 ^G	88.90(11)	O11 ^F -Na1-O16 ^G	94.67(11)		

* Symmetry codes: for **1**: A = -x, -y+1, -z; B = -x, -y+1, -z+1; C = x, y, z-1; D = -x+1, -y+1, -z+1; for **2**: A = x+1/2, -y+1/2, -z+1; B = x-1/2, -y+1/2, -z+1; C = -x+2, -y+1, -z-1; D = -x+3/2, y+1/2, z; E = -x+1/2, y+1/2, z; F = x-1/2, y, -z+3/2; G = x-1, y, z.