

Supplementary Materials for the Manuscript:
**Study on Fluorescence Recognition of Fe³⁺, Cr₂O₇²⁻ and
p-Nitrophenol by a Cadmium Complex and
Related Mechanism**

Lu Liu ¹, Jian-Min Li ², Hui-Jie Wang ¹, Meng-Di Zhang ¹, Yu Xi ¹, Jie Xu ¹, Yuan-Yuan Huang ¹, Bo Zhang ¹, Ying Li ¹, Zhen-Bei Zhang ¹, Zi-Fang Zhao ¹ and Cheng-Xing Cui ^{1,*}

¹ School of Chemistry and Chemical Engineering, Henan Institute of Science and Technology, Xinxiang, 453003, China

² School of Resources and Environment, Henan Institute of Science and Technology, Xinxiang 453003, China

* Correspondence: chengxingcui@hist.edu.cn

Table S1 Crystal Data and Structure Refinement Details for 1.

Complex	1
formula	C ₈₂ H ₆₆ Cd ₂ N ₁₂ O ₁₃ S ₄
fw	1780.50
T/K	293(2)
λ (Cu K α), Å	1.54184
Cryst syst	triclinic
Space group	<i>P</i> -1
a (Å)	12.8204(5)
b (Å)	12.9684(5)
c (Å)	13.2324(5)
α (°)	107.995(3)
β (°)	95.395(3)
γ (°)	110.667(4)
V (Å ³)	1906.10(14)
Z	1
<i>D</i> _{calcd.} (g·cm ⁻³)	1.551
abs coeff/mm ⁻¹	6.103
<i>F</i> (000)	906.0
2 θ (°)	7.214–141.906
GOF	1.048
<i>R</i> ₁ (<i>I</i> > 2sigma(<i>I</i>)) ^a	0.0497
<i>wR</i> ₂ (<i>I</i> > 2sigma(<i>I</i>)) ^b	0.0584

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

Table S2. Selected Bond Lengths (Å) and Bond Angles (deg) for 1^a.

Complex 1					
Cd(1)-N(1)	2.349(3)	Cd(1)-N(2)	2.378(3)	Cd(1)-N(5)¹	2.419(3)
Cd(1)-N(6) ¹	2.391(4)	Cd(1)-O(1)	2.325(3)	Cd(1)-O(6) ¹	2.240(3)
Cd(1) ¹ -N(5)	2.419(3)	Cd(1) ¹ -N(6)	2.391(4)	Cd(1) ² -O(6)	2.240(3)
N(1)-Cd(1)-N(2)	69.96(12)	N(1)-Cd(1)-N(5) ¹	98.73(12)	N(1)-Cd(1)-N(6) ¹	161.48(12)
N(2)-Cd(1)-N(5) ¹	81.43(12)	N(2)-Cd(1)-N(6) ¹	95.13(12)	N(6) ¹ -Cd(1)-N(5) ¹	67.32(12)
O(1)-Cd(1)-N(1)	90.52(14)	O(1)-Cd(1)-N(2)	150.63(14)	O(1)-Cd(1)-N(5) ¹	80.12(12)
O(1)-Cd(1)-N(6) ¹	98.56(14)	O(6) ² -Cd(1)-N(5) ¹	142.44(13)	O(6) ² -Cd(1)-N(6) ¹	81.37(13)
O(6) ² -Cd(1)-O(1)	84.79(15)				

^a Symmetry transformations used to generate equivalent atoms in complex (1): ¹ 2-x,3-y,2-z; ² 1-x,1-y,1-z.

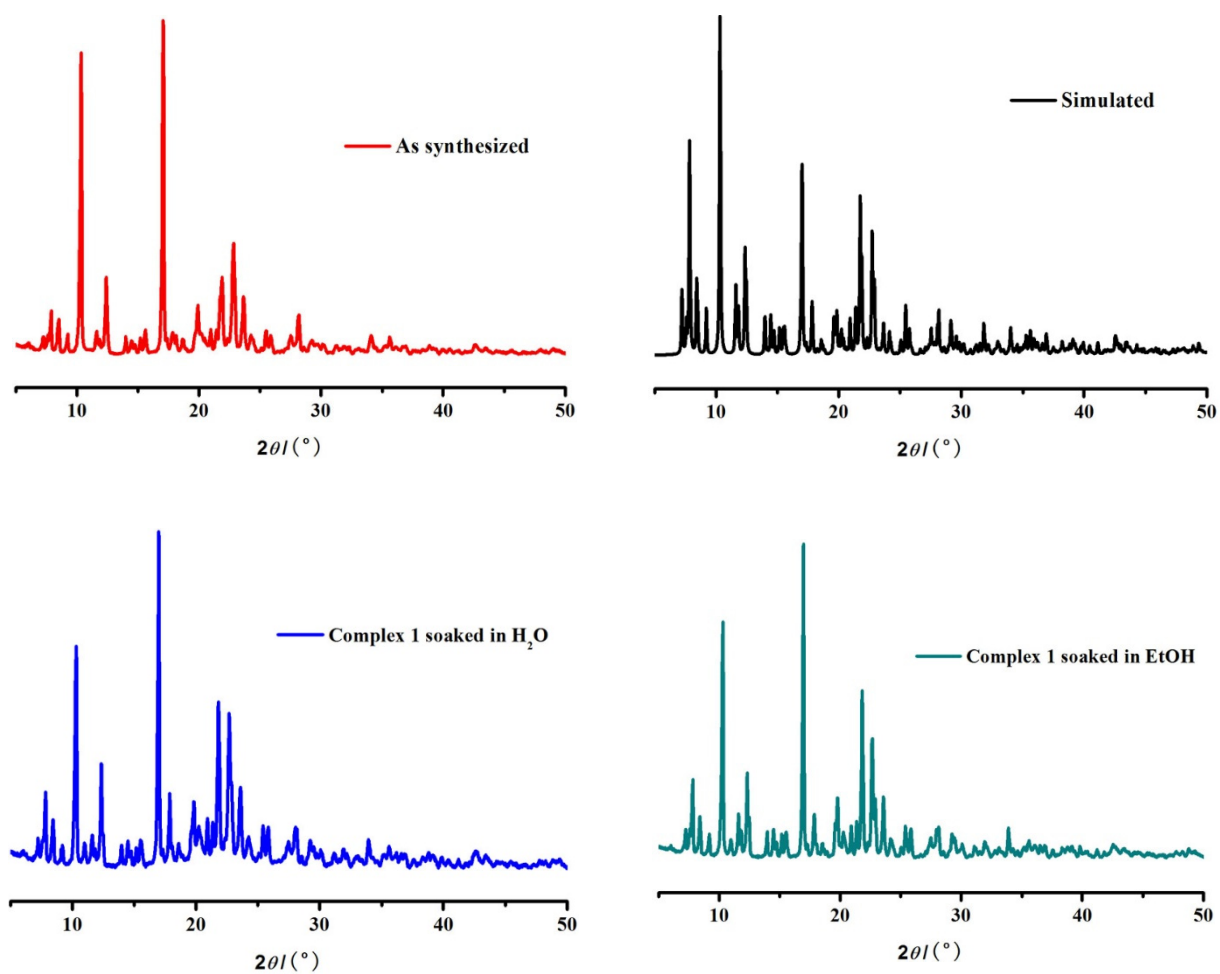


Figure S1. Experimental (red), simulated (black), soaked in H₂O (blue) and soaked in EtOH (cyan) PXRD patterns of complex 1.

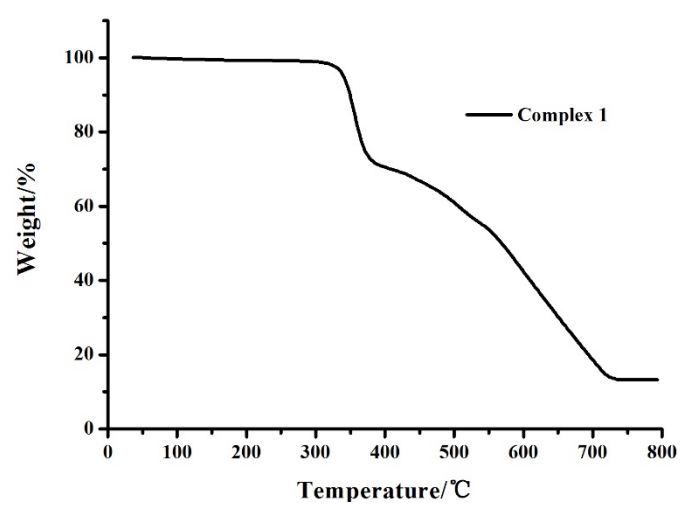
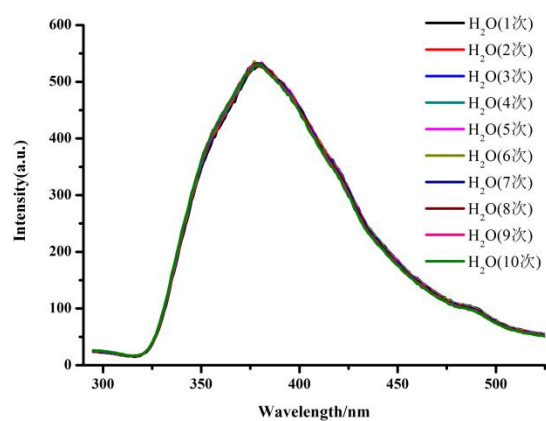
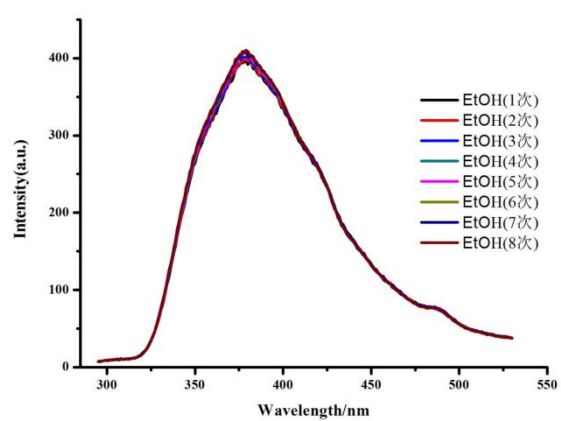


Figure S2. Thermogravimetric curve of complex 1.



(a)



(b)

Figure S3. Fluorescence spectra tested 10 times in water (a) and tested 8 times in EtOH (b) of complex 1.

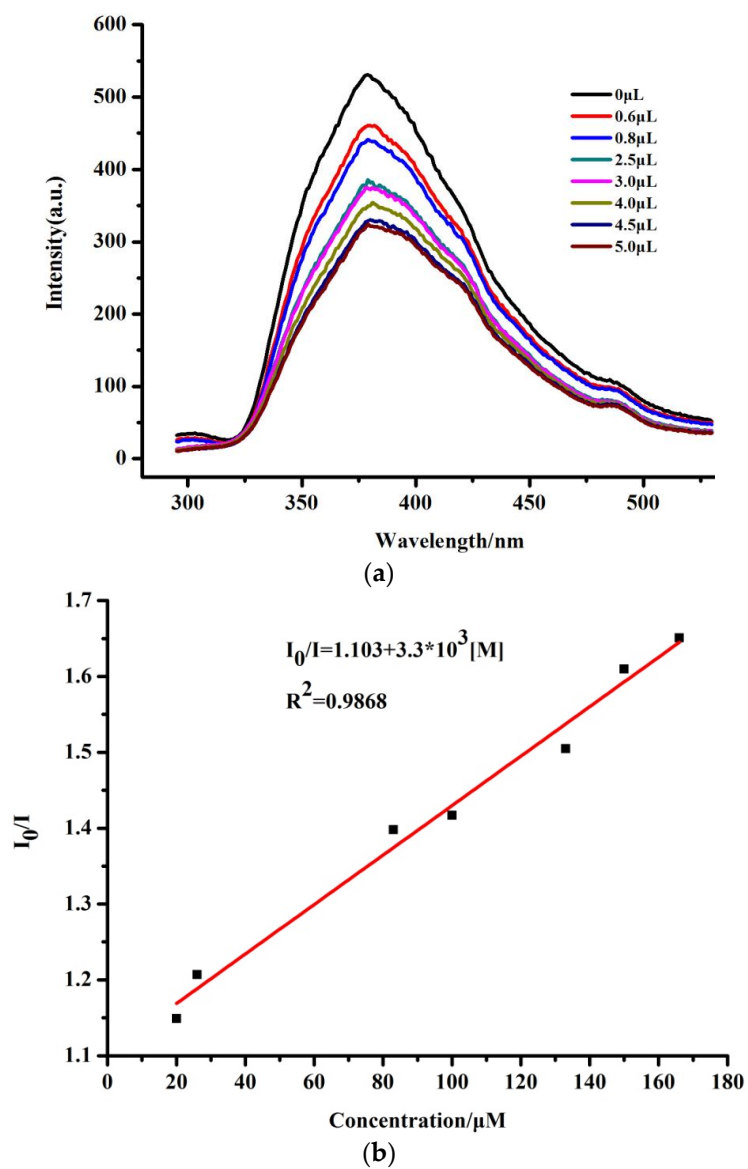


Figure S4. (a) Fluorescence spectra of complex **1** dispersed in aqueous suspension upon incremental addition of Fe^{3+} ions. (b) The linear correlation for the plot of I_0/I vs concentration of Fe^{3+} .

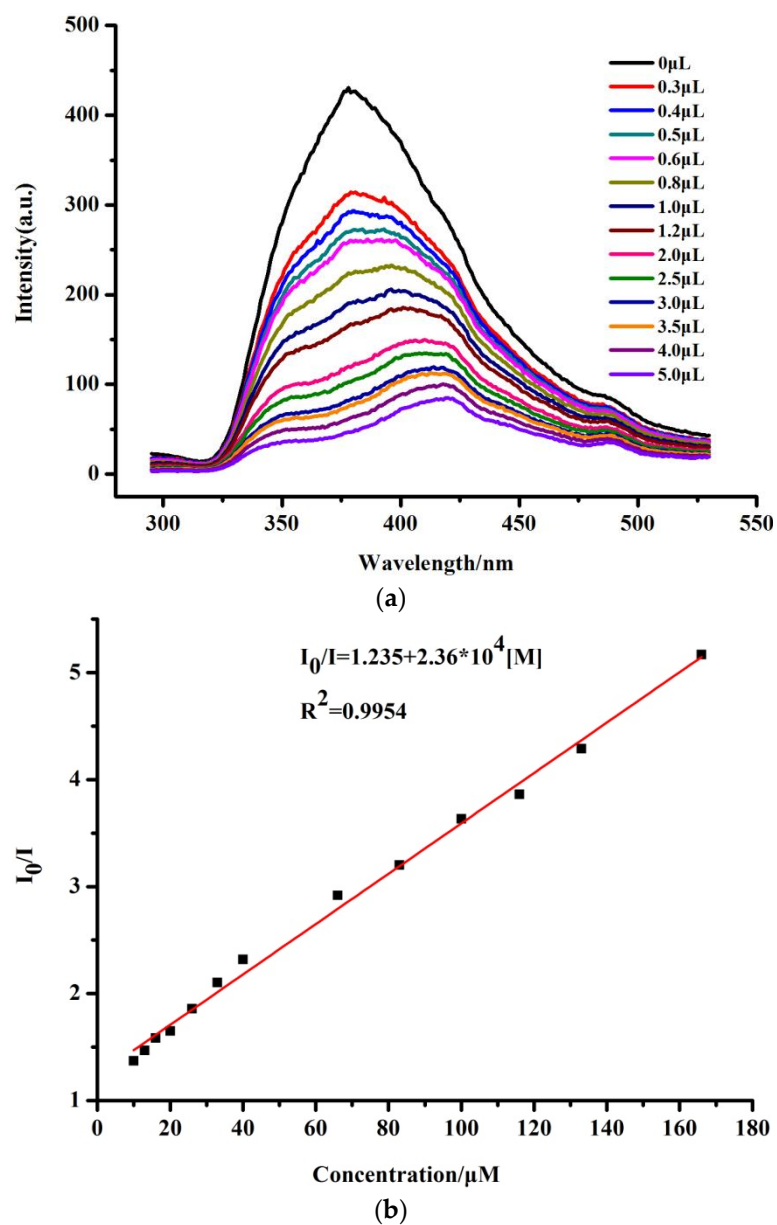


Figure S5. (a) Fluorescence spectra of complex 1 dispersed in aqueous suspension upon incremental addition of $\text{Cr}_2\text{O}_7^{2-}$ ions. (b) The linear correlation for the plot of I_0/I vs concentration of $\text{Cr}_2\text{O}_7^{2-}$.

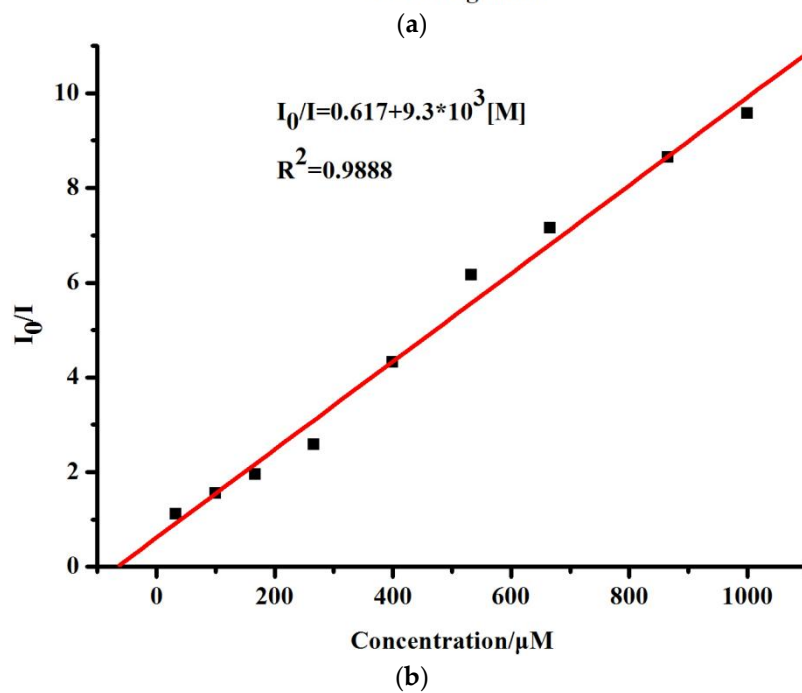
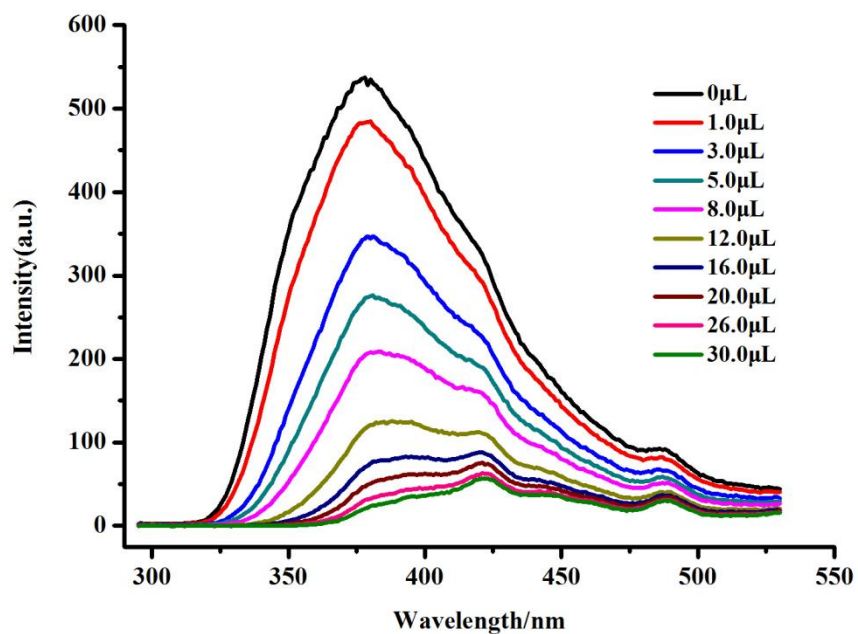


Figure S6. (a) Fluorescence spectra of complex **1** dispersed in aqueous suspension upon incremental addition of p-Nitrophenol. (b) The linear correlation for the plot of I_0/I vs concentration of p-Nitrophenol.