A Flexible 1,8-Naphthyridyl Derivative and Its Zn(II) Complexes:

Synthesis, Structures, Spectroscopic Properties

and Recognition of Cd(II)

Hui-Miao Zhang, Wen-Fu Fu*, Xin Gan, Yan-Qing Xu, Jun Wang, Quan-Qing Xu
and Shao-Ming Chi

Key Laboratory of Photochemical Conversion and Optoelectronic Materials, TIPC CAS,
Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing, 100190, P.R.
China.

College of Chemistry and Chemical Engineering, Yunnan Normal University, Kunming, 650092,
P.R. China.

The Institute for Chemical Physics, and Department of Chemistry, Beijing Institute of Technology,
Beijing 100081, P.R. China.

wf_fu@yahoo.com.cn

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**Fig. S1** UV-Vis spectra changes of 1 in CH$_2$Cl$_2$ upon addition of CH$_3$OH.

**Fig. S2** UV-vis spectra changes of 1 in CH$_2$Cl$_2$ upon addition of CH$_3$CN.

**Fig. S3** Crystal packing diagram of 1.
Calculation of the binding constant of L-Cd

\[ \frac{I_0}{I - I_0} = \frac{I_0}{[L]} + \frac{I_0}{[L] \cdot Ks} \frac{1}{[Cd]} \]  

(1)

Ks = Binding constant

I_0 = The fluorescence intensity of L

I = The observed fluorescence intensity of L in the presence of Cd(II)

Due to the fluorescence intensity of L-Cd at 402 nm was four times more than that of L, I-I_0 can be approximate to I. Plot of 1/I against 1/[Cd] was shown in Fig. S4.

**Fig. S4** Fitting analysis of L-Cd at different Cd(II) concentrations.

Emission was recorded at 402 nm.

Linear Regression for Data1_B:

\[ Y = A + B \times X \]

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<td>B</td>
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R SD N P

| 0.99426 | 2.12622E-5 | 7 | <0.0001 |

Ks = A/B = (4.83087/1.7856) \times 10^5 = 2.71 \times 10^5

\[ \Delta Ks = \frac{|\Delta A/A - \Delta B/B|}{Ks} \times Ks = 5.60 \times 10^3 \]

K = Ks + \Delta Ks = (2.71 \pm 0.056) \times 10^5
Calculation of the binding constant of $\text{L-Zn } (\text{I})$

$$\frac{A_0}{A_0 - A} = \frac{A_0}{[L]} + \frac{A_0}{[L]*K_s} * \frac{1}{[Zn]} \quad (2)^{ii}$$

$m = \text{Binding constant; }$
$m \text{ } A_0 = \text{The observed absorbance at the absence of cation; }$
$m \text{ } A = \text{The observed absorbance in the presence of cation.}$

**Fig. S5** Fitting analysis of $\text{L-Zn } (\text{I})$ at different Zn(II) concentrations.
Absorptions were recorded at 332 nm.

Linear Regression for Data6_B:
$Y = A + B \times X$

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$m = \text{A/B = (-3.93859/-9.19632) \times 10^5 = 4.28 \times 10^4}$
$m \Delta K_s = |\Delta A/A - \Delta B/B| \times K_s = 80$
$mK = K_s + \Delta K_s = (4.28 \pm 0.008) \times 10^4$
**Fig. S6** Comparison of IR spectra of L-Cd and L-Zn (1).
Top: L-Zn (1); Bottom: L-Cd.

**Fig. S7** Fluorescence response of L (1.0×10^{-5} M, CH₃OH) to different ions (1.0×10^{-4} M), \( \lambda_{ex}=340 \) nm.
**Fig. S8** Fluorescence response of L (1.0×10⁻⁵ M, CH₃OH) to Cd(II) in the presence of competing metal ions (1.0×10⁻⁵ M), λₑₓ=340 nm.

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