## Colorimetric Cyanide Detection Using an Azobenzene Acid in Aqueous Solutions

Xiaoding Lou, Jingui Qin and Zhen Li\*

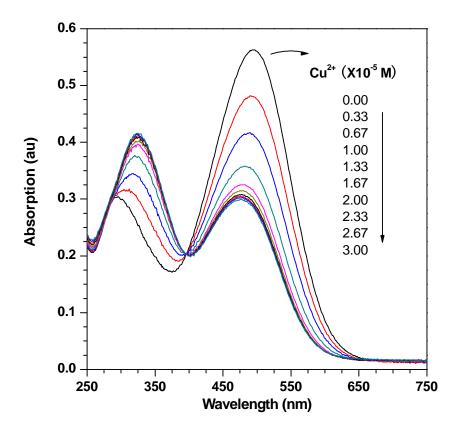
Department of Chemistry, Hubei Key Laboratory on Organic and Polymeric Optoelectronic Materials, Wuhan University, Wuhan, 430072, China. Fax: +86-27-6875-6757; Phone: +86-27-6225-4108; E-mail: <a href="mailto:lizhen@whu.edu.cn">lizhen@whu.edu.cn</a>.

**Equation S1**: the reaction between Cu<sup>2+</sup> and CN<sup>-</sup>

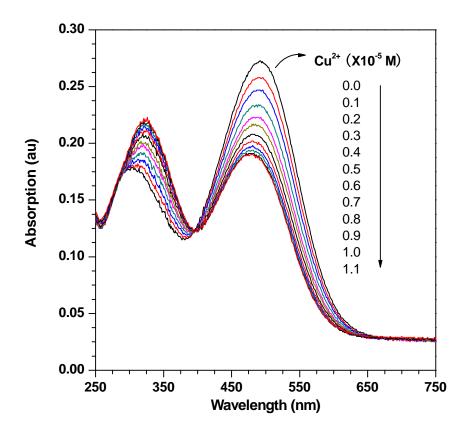
$$2Cu^{2+} + 4CN^{-} = 2CuCN + (CN)_{2}$$
 (CuCN is white precipitant).

**Equation S2**: the reaction between CuCN and CN<sup>-</sup>

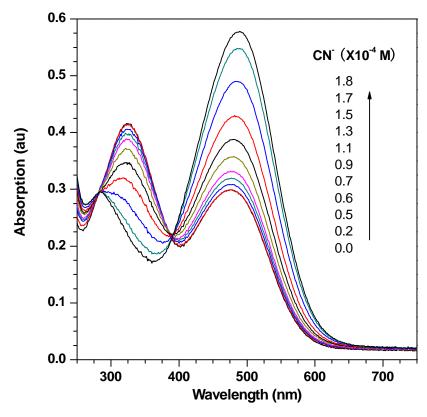
CuCN + (x-1)CN<sup>-</sup> = 
$$[Cu(CN)_x]^{1-x}$$
, (x = 2, 3, or 4)  
The stability constants (K),  $[Cu(CN)_2]^-$ :  $K = 1.00 \times 10^{24}$ ;  $[Cu(CN)_4]^{3-}$ :  $K = 2.00 \times 10^{30}$ .



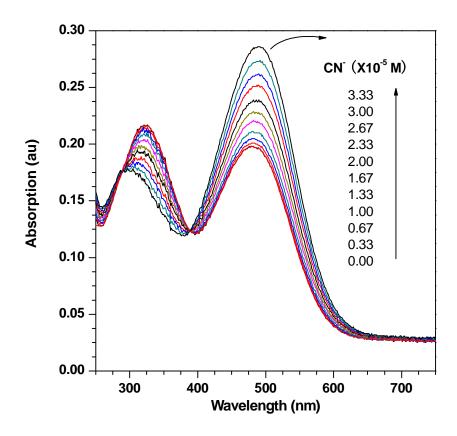
**Figure S1.** UV-vis spectra of compound **I** with increasing amounts of  $Cu^{2+}$  in water at pH 6.7. The concentration of **I** was  $3.0 \times 10^{-5}$  mol/L.



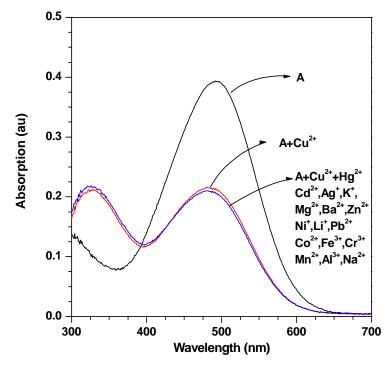
**Figure S2.** UV-vis spectra of compound **I** with increasing amounts of  $Cu^{2+}$  in water at pH 6.7. The concentration of **I** was  $1.5 \times 10^{-5}$  mol/L.



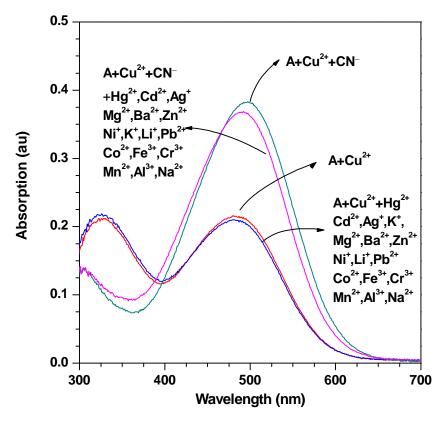
**Figure S3.** UV-vis spectra of the solution of compound **I**  $(3.0 \times 10^{-5} \text{ mol/L})$  and  $\text{Cu}^{2+}$   $(3.0 \times 10^{-5} \text{ mol/L})$  with increasing amounts of CN<sup>-</sup> in water at pH 6.7.



**Figure S4.** UV-vis spectra of the solution of compound **I**  $(1.5 \times 10^{-5} \text{ mol/L})$  and  $\text{Cu}^{2+} (7.0 \times 10^{-6} \text{ mol/L})$  with increasing amounts of CN<sup>-</sup> in water at pH 6.7.



**Figure S5.** UV-vis spectra of complex **I** (A) at the presence of different cations mixture  $(1.0 \times 10^{-5} \text{ mol/L})$  in water at pH 7.4 (20 mM HEPES, 135 mM NaCl). The concentration of compound **I** was  $6.0 \times 10^{-5}$  mol/L, and that of Cu<sup>2+</sup> was  $1.0 \times 10^{-5}$  mol/L.



**Figure S6.** UV-vis spectra of complex **I** (A) at the presence of different cations mixture  $(1.0 \times 10^{-5} \text{ mol/L})$  in water at pH 7.4 (20 mM HEPES, 135 mM NaCl). The concentration of compound **I** was  $6.0 \times 10^{-5} \text{ mol/L}$  (Cu<sup>2+</sup>:  $1.0 \times 10^{-5} \text{ mol/L}$ ; CN<sup>-</sup>:  $6.0 \times 10^{-5} \text{ mol/L}$ ).



**Figure S7.** Different solutions of compound **I** and copper ions  $(1.0 \times 10^{-4} \text{ and } 5.0 \times 10^{-5} \text{ mol/L}$ , respectively) in water at pH 7.4 (20 mM HEPES, 135 mM NaCl) in the presence of different concentrations of CN<sup>-</sup>. From left to right (×10<sup>-5</sup> mol/L): no copper ions and no cyanide, 0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0 and 9.0.



**Figure S8.** From left to right: compound **I**  $(1.0\times10^{-4} \text{ mol/L})$ , compound **I**  $(1.0\times10^{-4} \text{ mol/L})$ +  $Cu^{2+}(5.0\times10^{-5} \text{ mol/L})$ , compound **I**  $(1.0\times10^{-4} \text{ mol/L})$ +  $Cu^{2+}(5.0\times10^{-5} \text{ mol/L})$ +  $CN^{-}(6.0\times10^{-5} \text{ mol/L})$  at pH 7.4 (20 mM HEPES, 135 mM NaCl).



**Figure S9.** Different solutions of compound **I** and copper ions in water at pH 7.4[20 mM HEPES, 135 mM NaCl]  $(1.0\times10^{-4} \text{ and } 5.0\times10^{-5} \text{ mol/L}, \text{ respectively})$  in the presence of anion  $(6.0\times10^{-5} \text{ mol/L})$ . From left to right: no copper ions and no anion; no anion, CN<sup>-</sup>, SCN<sup>-</sup>, F<sup>-</sup>, ClO<sub>4</sub><sup>-</sup>, HSO<sub>4</sub><sup>-</sup>, Br<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, NO<sub>2</sub><sup>-</sup>, SO<sub>4</sub><sup>2-</sup>, I<sup>-</sup>, Cl<sup>-</sup>, IO<sub>3</sub><sup>-</sup>, the mixture.