

Supporting Information

Visible and Near-Infrared Chemosensor for Colorimetric and Ratiometric Detection of Cyanide

Gang Qian,^{a,b} Xianzhen Li,^c and Zhi Yuan Wang^{*a,c}

^a State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, ^b Graduate School of Chinese Academy of Sciences, Changchun 130022, China, and ^c Department of Chemistry, Carleton University, 1125 Colonel By Drive, Ottawa, Ontario, Canada K1S 5B6

* To whom all the correspondence should be addressed. E-mail: wayne_wang@carleton.ca



Figure S1. Color changes of **2** ($20\ \mu\text{M}$ in $\text{DMF}/\text{H}_2\text{O} = 99/1\ \text{v/v}$) in the presence of 5.0 molequiv. of anions after 1 hour at $60\ ^\circ\text{C}$. From left: no anion, CN^- , F^- , AcO^- , H_2PO_4^- , Cl^- , Br^- , I^- , NO_3^- and HSO_4^- .

(a)



(b)



Figure S2. (a) Color changes of **3** ($10\ \mu\text{M}$) in $\text{DMF}/\text{H}_2\text{O}$ solution ($99/1\ \text{v/v}$) in the presence of 2 equivalents of anions. From left: CN^- , F^- , Cl^- , Br^- , I^- , H_2PO_4^- , HSO_4^- , NO_3^- , and no anion. (b) Color contrast of **3** in $\text{DMF}/\text{H}_2\text{O}$ solution ($99/1\ \text{v/v}$) in the presence of 2 equivalents of CN^- ($0.5\ \mu\text{M}$, $1\ \mu\text{M}$, $5\ \mu\text{M}$, $10\ \mu\text{M}$, $50\ \mu\text{M}$ and $100\ \mu\text{M}$). Left is the blank solution of **3**.

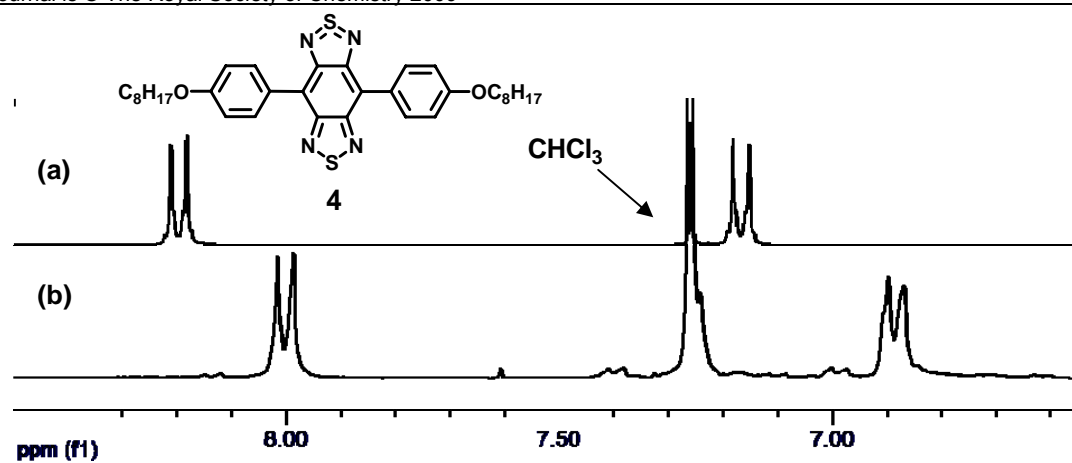


Figure S3. Partial ¹H NMR spectral change (300 MHz, 10 mM, CDCl₃, 25 °C) of model compound **4**: (a) before and (b) after addition of 4 molequiv. of tetrabutylammonium cyanide.

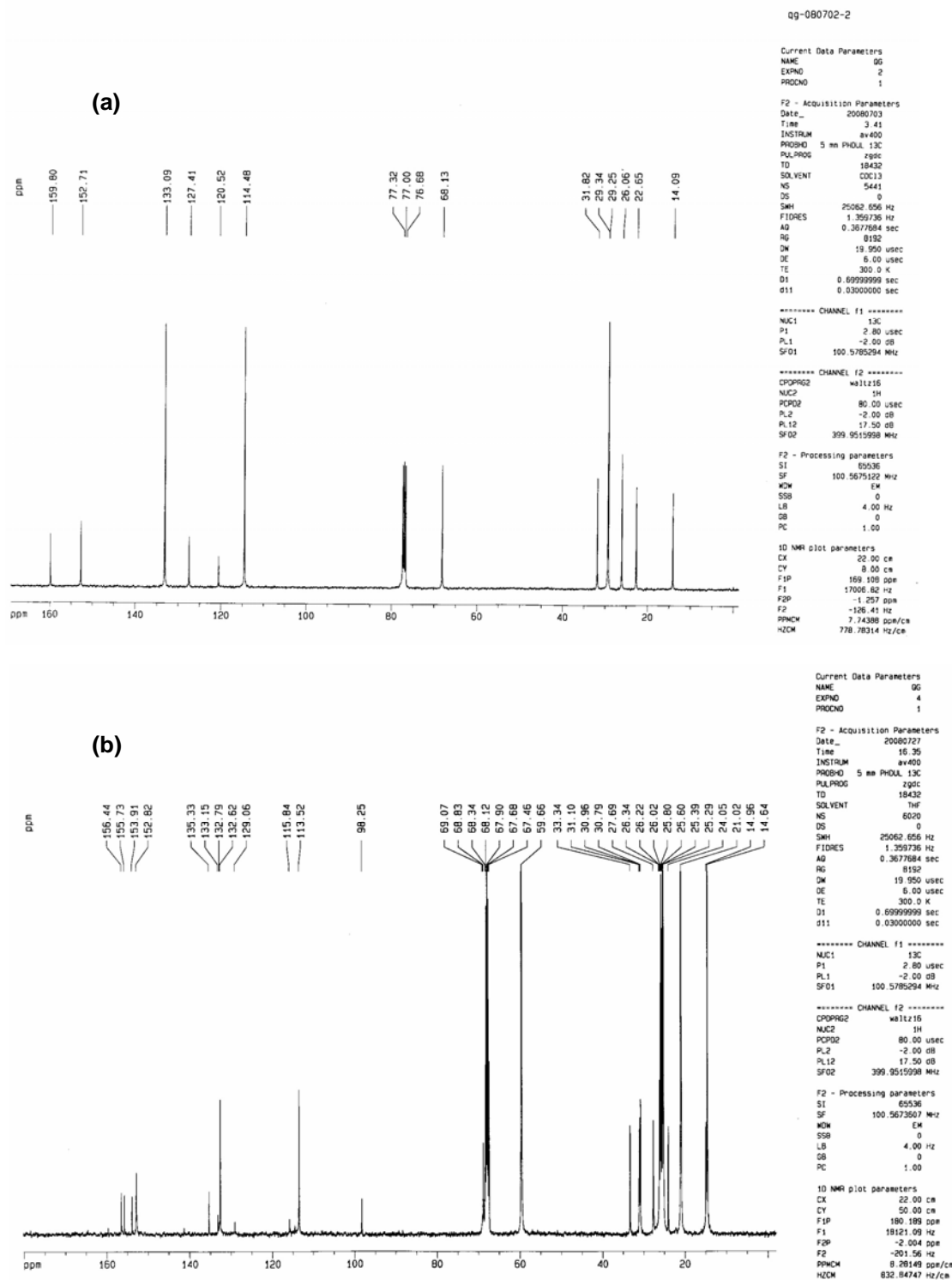


Figure S4. ^{13}C NMR spectral change (100 MHz, a: CDCl_3 , b: d_8 -THF, 25 °C) of model compound **4** (a) before and (b) after addition of 4 molequiv. of tetrabutylammonium cyanide.

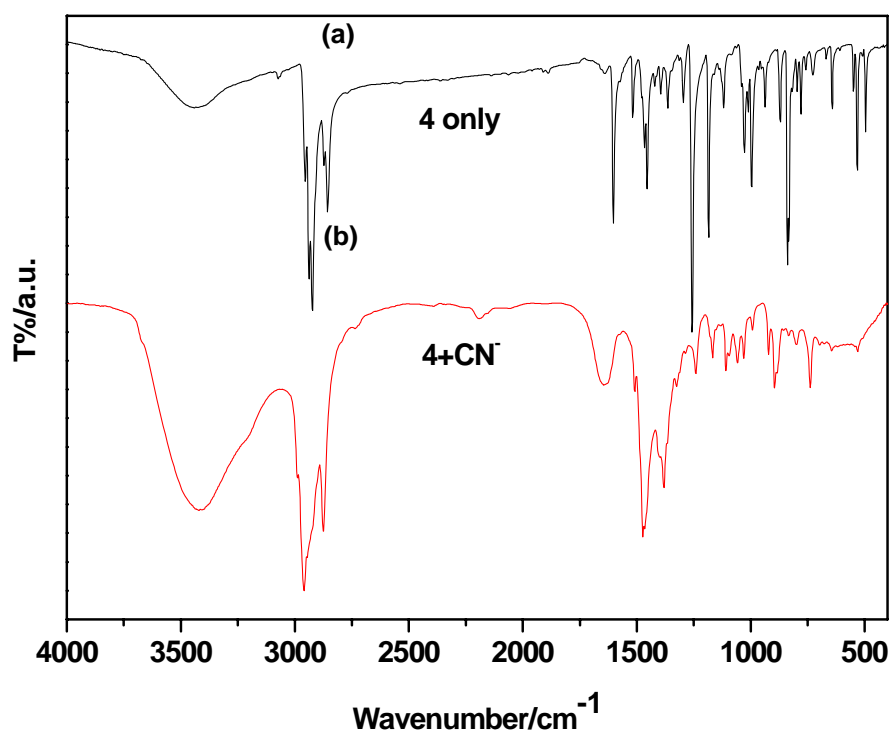


Figure S5. FTIR spectral change of model compound **4** (a) before and (b) after addition of 4 molequiv. of tetrabutylammonium cyanide.