Thiourea-Functionalized Poly(phenyleneethynylene): Fluorescent

Chemosensors for Anions and Cations

Xue Yong, Wen Wan, Mingjian Su, Wenwei You, Xinwei Lu, Yichen Yan, Jinqing Qu, Ruiyuan Liu, Toshio Masuda

Contents

Figure S1. ¹H NMR spectrum of 1 in CDCl_{3.}

Figure S2. ¹³C NMR spectrum of 1 in CDCl₃.

Figure S3. IR spectrum of 1

Figure S4. ¹HNMR spectrum of poly(1) in DMSO- d_6 . * indicates H₂O,** indicates solvent.

Figure S5. IR spectrum of poly(1).

Figure S6. Relative intensity (I/I₀) of fluorescence at 452 nm of poly(1) in DMF/water ([PRU] = 23.8μ M). Excitation at 380 nm.

Figure S7. UV-vis spectra of poly(1) in DMF/H₂O (99:1 v/v) ([PRU] = 23.8μ M) upon titration with F⁻ (0–50 equivalents).

Figure S8. Stern-Volmer plots of poly(1) emission quenching by different anions in DMF.

Figure S9. Schematic map of the interaction between poly(1) and fluoride ion.

Figure S10. Relative energy alignments about PET between poly(1) and fluoride ion.

Figure S11. UV-vis spectra of poly(1) in DMF/H₂O (99:1 v/v) ([PRU] = 23.8 μ M) upon titration with Ag⁺ (0–10 equivalents).

Figure S12. Schematic map of the interaction between poly(1) and silver ion.

Figure S13. Relative energy alignments about ET between poly(1) and silver ion.

Figure S14. Absorption spectra of poly(1) in DMF/H₂O (99:1 v/v) ([PRU] = 23.8 μ M) upon the addition of various cations ([cation]/[PRU] = 2).

Figure S15. Fluorescence quenching (I/I₀) by different cations at the maximum emission wavelength (I: fluorescence intensity upon addition of a cation; I₀: initial fluorescence intensity). [PRU] = 23.8 μ M, [cation]/[PRU] =2. 1: Mn²⁺, 2: Na⁺. 3: Pb²⁺, 4: Cu²⁺, 5: K⁺, 6:Zn²⁺, 7: Co²⁺, 8: Ag⁺.

Figure S16. Stern-Volmer plots of poly(1) emission quenching by different cations in DMF/H₂O (99:1 v/v).

Figure S17. *ksv* values for different cations. 1: Co^{2+} , 2: Na⁺, 3: Pb²⁺, 4: K⁺, 5: Mn²⁺, 6:Zn²⁺, 7: Cu²⁺, 8: Ag⁺.



Figure S1. ¹H NMR spectrum of 1 in CDCl_{3.}



Figure S2. ¹³C NMR spectrum of 1 in CDCl₃.



Figure S3. IR spectrum of 1



Figure S4. ¹HNMR spectrum of poly(1) in DMSO- d_6 . * indicates H₂O, ** indicates solvent.



Figure S5. IR spectrum of poly(1).



Figure S6. Relative intensity (I/I_0) of fluorescence at 452 nm of poly(1) in DMF/water ([PRU] =

23.8 μ M). Excitation at 380 nm.



Figure S7. UV-vis spectra of poly(1) in DMF/H₂O (99:1 v/v) ([PRU] = 23.8μ M) upon titration

with F^{-} (0–50 equivalents).



Figure S8. Stern-Volmer plots of poly(1) emission quenching by different anions in DMF.



Figure S9. Schematic map of the interaction between poly(1) and fluoride ion.



Figure S10. Relative energy alignments about PET between poly(1) and fluoride ion.



Figure S11. UV-vis spectra of poly(1) in DMF/H₂O (99:1 v/v) ([PRU] = 23.8 μ M) upon titration

with Ag^+ (0–10 equivalents).



Strong Fluorescent

Weak Fluorescent

Figure S12. Schematic map of the interaction between poly(1) and silver ion.



Figure S13. Relative energy alignments about ET between poly(1) and silver ion.



Figure S14. Absorption spectra of poly(1) in DMF/H₂O (99:1 v/v) ([PRU] = 23.8 μ M) upon the addition of various cations ([cation]/[PRU] = 2).



Figure S15. Fluorescence quenching (I/I₀) by different cations at the maximum emission wavelength (I: fluorescence intensity upon addition of a cation; I₀: initial fluorescence intensity). $[PRU] = 23.8 \mu M$, [cation]/[PRU] = 2.1: Mn²⁺, 2: Na⁺. 3: Pb²⁺, 4: Cu²⁺, 5: K⁺, 6:Zn²⁺, 7: Co²⁺, 8: Ag⁺.



Figure S16. Stern-Volmer plots of poly(1) emission quenching by different cations in DMF/H₂O

(99:1 v/v).



Figure S17. *ksv* values for different cations. 1: Co^{2+} , 2: Na^+ , 3: Pb^{2+} , 4: K^+ , 5: Mn^{2+} , 6: Zn^{2+} , 7:

Cu²⁺, 8: Ag⁺.