Electronic Supplementary Information

Benzo[5]helicene-based conjugated polymers: synthesis, photophysical properties, and application for the detection of nitroaromatic explosives

Li-Li Zhou,^a Meng Li,^b Hai-Yan Lu,^{*,a} and Chuan-Feng Chen^{*,b}

^aUniversity of Chinese Academy of Sciences, Beijing 100049, China. E-mail: haiyanlu@ucas.ac.cn.

^bBeijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Molecular Recognition and Function, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China. E-mail: cchen@iccas.ac.cn.

Contents

- S1. Copies of ¹H NMR and ¹³C NMR spectra
- S2. TGA thermogram of the polymers
- S3. IR spectra of the polymers
- S4. AFM topography image of the spin-coated film of P2
- S5. Fluorescence spectra of the polymers in presence of different concentrations of the analytes in CDCl₃ and their corresponding Stern-Volmer plots
- S6. Fluorescence spectra of the film of P2 upon exposure to the saturated vapor of the analytes at diffident time interval and their corresponding quenching efficiency against time
- S7. Absorption spectra of compound 2 and the polymers



S1. Copies of the ¹H NMR and ¹³C NMR spectra

Fig. S2 ¹³C NMR spectrum (125 MHz, CDCl₃) of 2.



Fig. S4 ¹³C NMR spectrum (75 MHz, CDCl₃) of 3.





Fig. S6 13 C NMR spectrum (125 MHz, CDCl₃) of 4.

160



Fig. S8 ¹H NMR spectrum (500 MHz, CDCl₃) of P2.





Fig. S10 ¹H NMR spectrum (500 MHz, CDCl₃) of P4.



Fig. S11 ¹H NMR spectrum (500 MHz, CDCl₃) of P5.

S2. TGA thermogram of the polymers



Fig. S12 TGA plots of the polymers with a heating rate of 10°C/min under nitrogen.

S3. IR spectra of the polymers



Fig. S13 IR spectrum of P1.



Fig. S14 IR spectrum of P2.



Fig. S15 IR spectrum of P3.



Fig. S16 IR spectrum of P4.



Fig. S17 IR spectrum of P5.

S4. AFM topography image of the spin-coated film of P2



Fig. S18 AFM topography image of the spin-coated film of P2 and the thickness of the film.

S5. Fluorescence spectra of the polymers in presence of different concentrations of the analytes in CDCl₃ and their corresponding Stern-Volmer plots



Fig. S19 Fluorescence spectra of **P1** in presence of different concentrations of TNT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S20 Fluorescence spectra of **P1** in presence of different concentrations of DNT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S21 Fluorescence spectra of **P1** in presence of different concentrations of PA in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S22 Fluorescence spectra of **P1** in presence of different concentrations of NT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S23 Fluorescence spectra of **P1** in presence of different concentrations of BP in CDCl₃.



Fig. S24 Fluorescence spectra of **P2** in presence of different concentrations of TNT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S25 Fluorescence spectra of **P2** in presence of different concentrations of DNT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S26 Fluorescence spectra of **P2** in presence of different concentrations of PA in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S27 Fluorescence spectra of **P2** in presence of different concentrations of NT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S28 Fluorescence spectra of **P2** in presence of different concentrations of BP in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S29 Fluorescence spectra of **P3** in presence of different concentrations of TNT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S30 Fluorescence spectra of **P3** in presence of different concentrations of DNT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S31 Fluorescence spectra of **P3** in presence of different concentrations of PA in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S32 Fluorescence spectra of **P3** in presence of different concentrations of NT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S33 Fluorescence spectra of **P3** in presence of different concentrations of BP in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S34 Fluorescence spectra of **P4** in presence of different concentrations of TNT in CDCl₃.



Fig. S35 Fluorescence spectra of **P4** in presence of different concentrations of DNT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S36 Fluorescence spectra of **P4** in presence of different concentrations of PA in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S37 Fluorescence spectra of **P4** in presence of different concentrations of NT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right)



Fig. S38 Fluorescence spectra of **P4** in presence of different concentrations of BP in CDCl₃.



Fig. S39 Fluorescence spectra of **P5** in presence of different concentrations of TNT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S40 Fluorescence spectra of **P5** in presence of different concentrations of DNT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S41 Fluorescence spectra of **P5** in presence of different concentrations of PA in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S42 Fluorescence spectra of **P5** in presence of different concentrations of NT in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).



Fig. S43 Fluorescence spectra of **P5** in presence of different concentrations of BP in CDCl₃ (left) and its corresponding Stern-Volmer plot (right).

S6. Fluorescence spectra of the film of P2 upon exposure to the saturated vapor of the analytes at diffident time interval and their corresponding quenching efficiency against time



Fig. S44 Fluorescence spectra of the film of **P2** upon exposure to the saturated vapor of TNT at diffident time interval (left) and quenching efficiency against time (right).



Fig. S45 Fluorescence spectra of the film of P2 upon exposure to the saturated vapor of DNT at diffident time interval (left) and quenching efficiency against time (right). S19



Fig. S46 Fluorescence spectra of the film of **P2** upon exposure to the saturated vapor of PA at diffident time interval (left) and quenching efficiency against time (right).



Fig. S47 Fluorescence spectra of the film of **P2** upon exposure to the saturated vapor of NT at diffident time interval (left) and quenching efficiency against time (right).



Fig. S48 Fluorescence spectra of the film of **P2** upon exposure to the saturated vapor of BP at diffident time interval (left) and quenching efficiency against time (right).

S7. Absorption spectra of compound 2 and the polymers



Fig. S49 The absorption spectra of compound 2 and the polymers in CHCl₃ at 1.0×10^{-6} M.