Conjugated Thiophene-Containing Oligoacenes Through Photocyclization: Bent Acenedithiophenes and a Thiahelicene

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General Experimental

All photochemical reactions were carried out in a photoreactor equipped with 16 RPR-3000 Å (300 nm, 21 W) lamps. $^1$H NMR spectra (300 or 400 MHz) are referenced to the residual protonated solvent at $\delta$ 5.32 for deuterated dichloromethane (CD$_2$Cl$_2$) and $\delta$ 7.24 for deuterated chloroform (CDCl$_3$). All $^{13}$C NMR experiments were carried out in CD$_2$Cl$_2$ and referenced at $\delta$ 54.00. Solution absorption spectra were obtained in dichloromethane (DCM, CH$_2$Cl$_2$) on a UV-vis-near-IR spectrophotometer using a 1 cm quartz cuvette. IR spectra were obtained on powder samples (neat) or from KBr dispersions. Powder X-ray diffraction measurements were carried out using a diffractometer with graphite monochromated Cu-Kα radiation. Fluorescence spectra were obtained in DCM using a 1 cm quartz cuvette. Quantum yields were referenced to a solution of anthracene in EtOH ($\Phi_f = 0.3$).$^1$ Electron ionization (EI) mass spectra were obtained at the UBC Mass Spectrometry facility. Elemental analyses were obtained at the UBC Microanalytical facility.

Films of BADTs 5a-d were prepared by vacuum evaporation onto cover glass substrates at temperatures between 150 and 200 °C at a pressure of ~0.1 to 1 Torr. The substrate temperature was not controlled but was ca. 25 °C. All glass substrates were cleaned with a sulfuric acid/hydrogen peroxide mixture (4:1) prior to use in order to remove surface organic contaminants. Solid-state absorption spectra of 5a-d were obtained from drop-cast films deposited from DCM solutions onto cover glass substrates.
Supplemental Spectra

**Figure S1.** $^1$H NMR Spectrum (400 MHz, CD$_2$Cl$_2$) of compound 3e.

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Figure S3. $^1H$ NMR Spectrum (400 MHz, CD$_2$Cl$_2$) of compound 4e.

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Figure S6. $^1$H NMR Spectrum (400 MHz, CD$_2$Cl$_2$) of compound 6.
Figure S7. $^1$H NMR Spectrum (400 MHz, CD$_2$Cl$_2$) of compound 7.

Figure S8. $^1$H NMR Spectrum (400 MHz, CD$_2$Cl$_2$) of compound 8.
Figure S9. $^{13}$C NMR Spectrum (100 MHz, CD$_2$Cl$_2$) of compound 8.

Figure S10. $^1$H-$^1$H COSY NMR Spectrum (400 MHz, CD$_2$Cl$_2$) of compound 8.
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References