Supporting information

Modulation of Molecular Geometry on Carbazolebis(thiadiazole)-based Conjugated Polymers for Photovoltaic Applications

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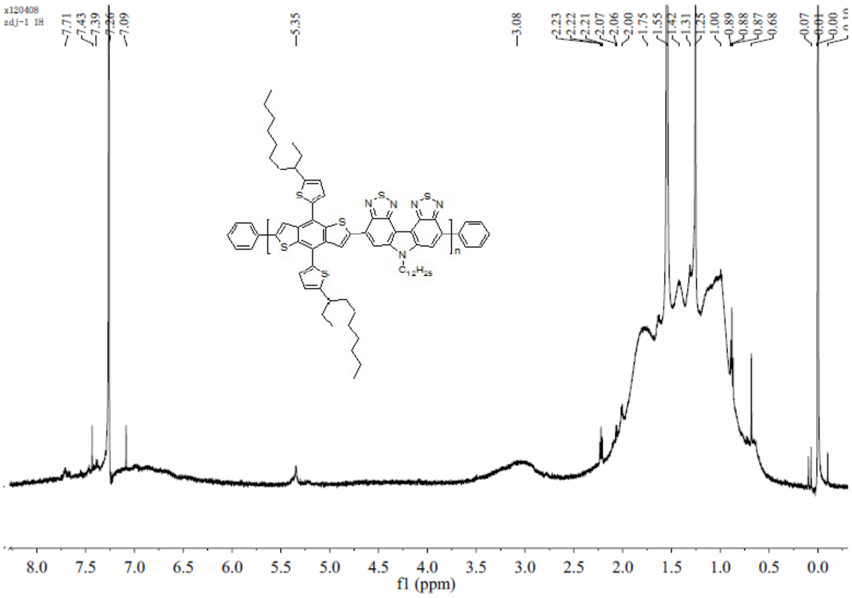

Figure S1 ^{1}H NMR spectra of the copolymer **PTBDTCBT.**

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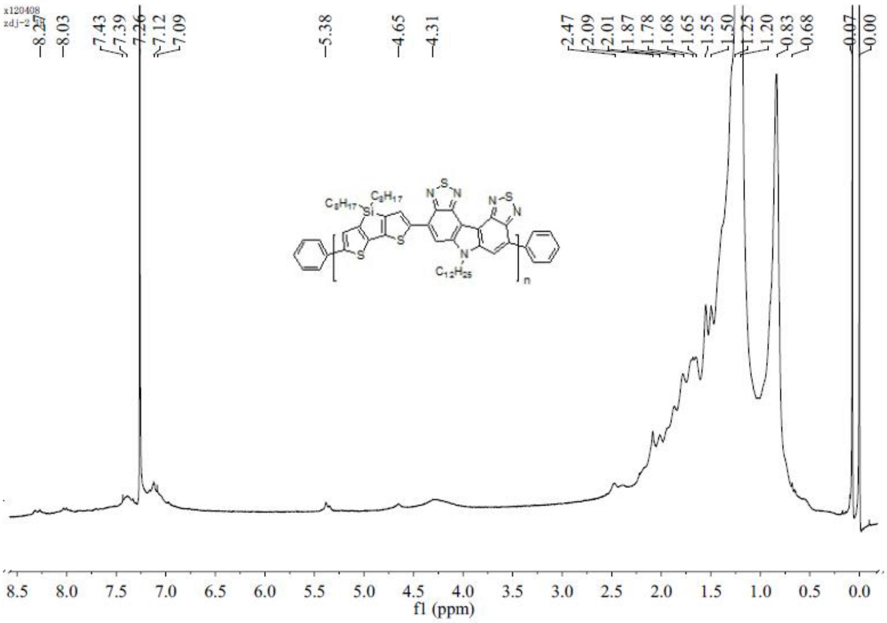

Figure S2 ^{1}H NMR spectra of the copolymer **PDTSCBT.**

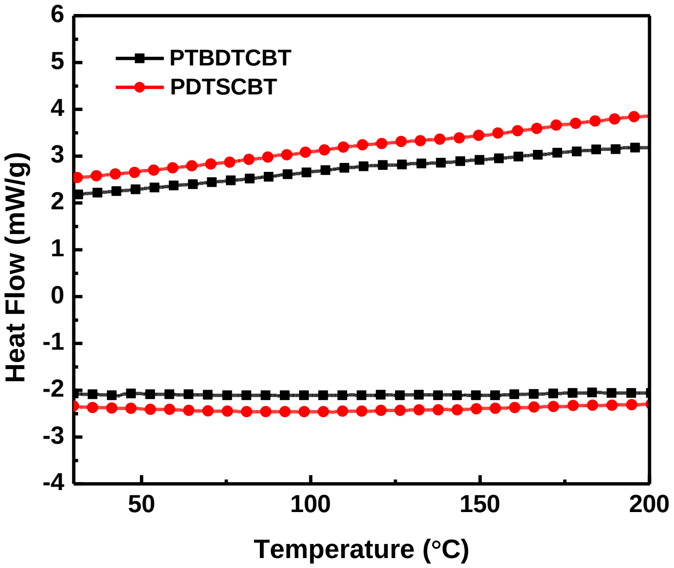

Figure S3 DSC plots of PTBDTCBT and PDTSCBT with a heating rate of 10 °C·min^{-1} under an inert atmosphere.

Electrochemical Cyclic Voltammetry (CV)

Cyclic voltammetry (CV) was performed with a Zahner IM6e electrochemical workstation using glassy carbon discs as the working electrode, Pt wire as the counter electrode, SCE electrode as the reference electrode, and ferrocene/ferrocenium as an internal potential marker. 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) dissolved in THF was employed as the supporting electrolyte. The potential of the saturated calomel reference electrode was internally calibrated using the ferrocene/ferrocenium redox couple (Fc/Fc+), which has a known reduction potential of -4.4 eV. The HOMO and LUMO energy levels were calculated by the following equations, the E_g was obtained from the UV-Vis absorption spectra.

$$\mathrm{HOMO} = -\left(E_{onset}^{ox} + 4.4\ \mathrm{eV} \right)$$

$$\mathrm{LUMO} = \mathrm{HOMO} + E_g^{opt}$$

Device Fabrication

PCEs were measured under an AM1.5G solar simulator (Sciencetech SS-0.5K Solar Simulator) and EQE under dark. The current density-voltage (J-V) characteristics were recorded with a Keithley 2400 source meter. The spectral response was measured with a commercial photo modulation spectroscopic setup (Oriel). A calibrated Si photodiode was used to determine the photosensitivity. Patterned ITO-glass substrates were used as the anode in the polymer solar cells. The ITO coated glass substrates were cleaned by sonication in detergent, deionized water, acetone, and isopropyl alcohol and dried in a nitrogen stream, followed by an oxygen plasma treatment. Then the surface of the ITO substrate was modified by spin-coating the conducting PEDOT:PSS layer, followed by baking at 140 °C for 10 minutes under ambient conditions. The substrates were then transferred into anargon-filled glove box. The polymers were blended with $PC_{61}BM$ and dissolved in chlorobenzene (CB). All blended ratios of polymer/$PC_{61}BM$ were by weight. The solutions were then spin-coated onto the PEDOT:PSS layer at 800-1000 rpm. The thicknesses of the active layer were about 80-90 nm. Then the devices were put on the heater for annealing or not. Subsequently, LiF (0.8 nm) and Al (100 nm) electrodes were deposited via thermal evaporation in vacuum ($<10^{-6}$ Torr) in a thickness of approximately. The thicknesses of all the films were measured by a Dektak profiler.

The effective area was measured to be 0.04 cm^2.