Supporting Information

Synthesis, Characterization, and Transistor and Solar Cell Applications of A Naphthobisthiadiazole-Based Semiconducting Polymer

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Single crystal X-ray analysis of NTz2T-Me and BTz2T-Me.
Single crystals of NTz2T-Me and BTz2T-Me for X-ray structural analysis were obtained by sublimation and recrystallization from ethyl acetate, respectively. The X-ray crystal structural analysis was performed on a Rigaku CCD Mercury (Mo Ka radiation, l = 0.71070 Å, graphite monochromator, T = 293 K, 2qmax = 55.0°). The structure was solved by the direct method using SHELXS-97.51 Non-hydrogen atoms were refined anisotropically, and all hydrogen atoms were included in the calculations but not refined. All calculations were performed using the crystallographic software of SHELXL-97.51
Crystal data for NTz2T-Me: C20H12N4S4, M=436.60, red plate, 0.8 × 0.5 × 0.1 mm3, monoclinic, space group C2/c, a = 11.7955(15), b = 8.5619(9), c = 18.814(2) Å, b = 106.7224 (13) °, V=1819.7(4) Å3, T =
293 K, $Z=4$, $D_{\text{calc}}=1.594$ g/cm$^3$, GOF = 0.745, reflections measured 6722, 2068 unique ($R_{\text{int}} = 0.0448$) which were used in all calculations. The final $R_1$ was 0.0398, and the final $wR$ on $F_2$ was 0.1123 (all data).

Crystal data for BTz2T-Me: C$_{16}$H$_{12}$N$_2$S$_3$, $M=328.47$, red needle, 0.8 x 0.1 x 0.1 mm$^3$, orthorhombic, space group $Pbca$, $a = 19.562(12)$, $b = 20.298(13)$, $c = 7.523(5)$ Å, $V=2987(3)$ Å$^3$, $T = 293$ K, $Z = 8$, $D_{\text{calc}} = 1.461$ g/cm$^3$, GOF = 0.946, reflections measured 20831, 3294 unique ($R_{\text{int}} = 0.0731$) which were used in all calculations. The final $R_1$ was 0.0599, and the final $wR$ on $F_2$ was 0.1656 (all data).

Reference

Figure S1. GPC chromatograms of the polymers.

Figure S2. Calculated HOMOs and LUMOs of the model compounds of PNTz4T and PBTz4T.
Figure S3. Transistor properties of the polymer-based devices with the HMDS-modified substrate: (a) transfer and (b) output curves of PNTz4T-device, (c) transfer and (b) output curves of PBTz4T-device.
Figure S4. Changes in mobility ($\mu$) and on/off ratio ($I_{on}/I_{off}$) with time.

Figure S5. J–V curves of (a) PNTz4T- and (b) PBTz4T-based solar cells with different p:n ratios.
Figure S6. AFM topographic images of the polymer thin films on FDTS-modified OFET devices; (a) PNTz4T, (b) PBTz4T.

Figure S7. AFM topographic images of the polymer/PC_{61}BM thin films on solar cells; (a) PNTz4T, (b) PBTz4T.