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Supporting Information

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Novel Dimethylmethylene-Bridged Triphenylamine-PDI Acceptor for Bulk-Heterojunction Organic Solar Cells

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Materials and Instruments: All chemicals were purchased from commercial suppliers unless otherwise noted and used without further purification. All reactions were performed under a nitrogen atmosphere. Diethyl ether, tetrahydrofuran and toluene were distilled from sodium benzophenone. Intermediate PDI-CC was synthesized according to the reported procedures,[1] and DMTPA-3I was synthesized with slight modification to the reported method.[2]

Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Ultrashield 400 Plus NMR spectrometer. Thermogravimetric analyses (TGA) were conducted on a TA Instruments Q5000IR at a heating rate of 20 °C min^{-1}under nitrogen gas flow. UV-vis spectra were recorded on a PerkinElmer Lambda 20 UV-vis spectrophotometer. Cyclic voltammentry (CV) measurements were carried out in a deoxygenated anhydrous acetonitrile solution on a CHI600 electrochemical workstation. Pt disk was used as the working electrode, $Ag/AgNO_3$ as the reference electrode, Pt wire as the counter electrode, and 0.1 M tetrabutylammonium hexafluorophosphate as the supporting electrolyte, and the measurements were calibrated with ferrocene (Fc) as the internal standard. AFM measurements were performed by using a Scanning Probe Microscope Dimension 3100 in tapping mode. All film samples were spin-casted onto ITO/ZnO substrates. XRD was carried out on a Bruker D8 Discovery with General Area Detector Diffraction System with a Cu Kα radiation excited at 40 kV and 40 mA. The incoming X-ray was scanned at the grazing angle between 0.5-2.5 degree.

***Theoretical Calculation*:** Theoretical calculations for DMTPA-PDI_3 were performed by Gaussian 09 program[3] using Density Functional Theory (DFT). To simplify computations and enhance computational efficiency, the N-hexylheptyl group of DMTPA-PDI_3 was replaced with a simple N-methyl group, and geometric structural optimization was performed at the B3LYP/6-31G* level, yielding optimized geometric structures to obtain the corresponding electron density.

***Hole- and Electron-only Devices*:** The electron and hole mobilities were evaluated using space charge limited current (SCLC) method using electron- and hole-only devices with respective device architectures of ITO/PEDOT:PSS/PTB7-Th:DMTPA-PDI_3 (140 nm) /MoO_3/Ag and ITO/ZnO/PTB7-Th:DMTPA-PDI_3 (140 nm)/ZnO/Ag. The current-voltage curves were obtained and fitted to a space charge limited form described by:

$$J = (8/9)\, \varepsilon_r \varepsilon_0 \mu\, (V^2/L^3) \qquad (1)$$

where ε_0 is the permittivity of free space, ε_r is the relative permittivity of the material, μ is the electron mobility, V is the voltage drop across the device and L is the thickness of the film. For most polymers, ε_r is around 3.

Figure S1. TGA plot of DMTPA-PDI_3 at a heating rate of 20 °C min^{-1} under N_2 atmosphere.

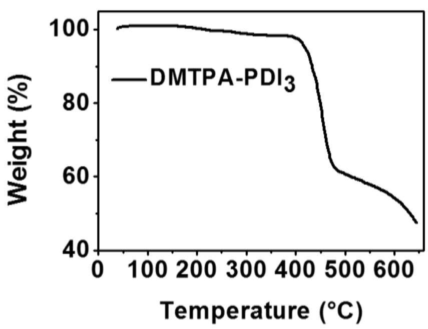


Figure S2. X-ray diffraction pattern of active layer PTB7-Th:DMTPA-PDI_3 (1.5:1 weight ratio, 3% CN).

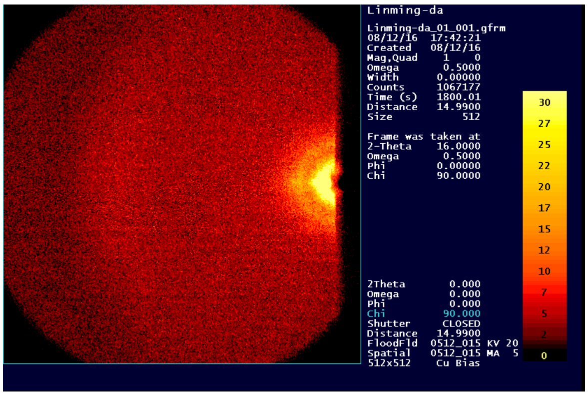


Figure S3. X-ray diffraction pattern of acceptor DMTPA-PDI_3.

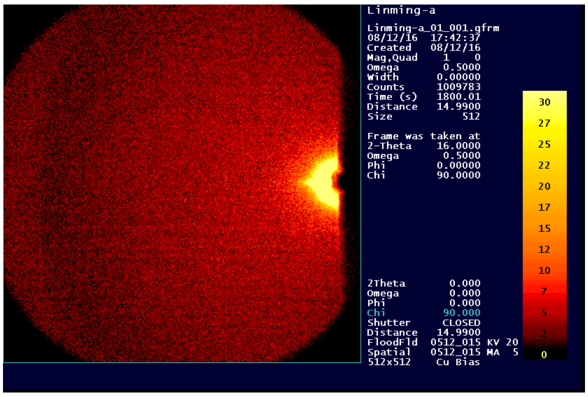


Figure S4. X-ray diffraction pattern of donor PTB7-Th.

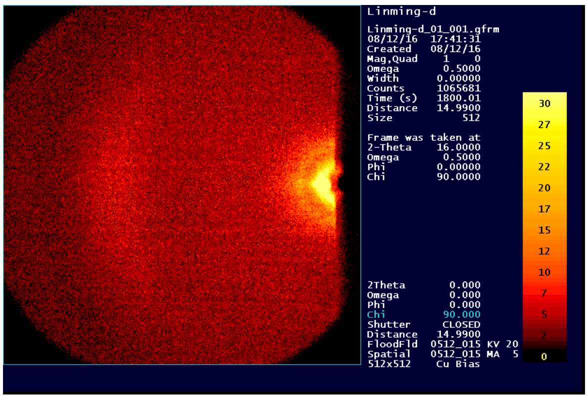


Figure S5. $J_{1/2}$-V characteristics of the hole and electron-only devices

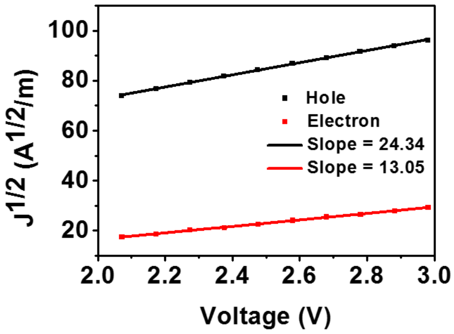


Figure S6. ^{1}H NMR of compound **DMTPA-PDI$_3$**

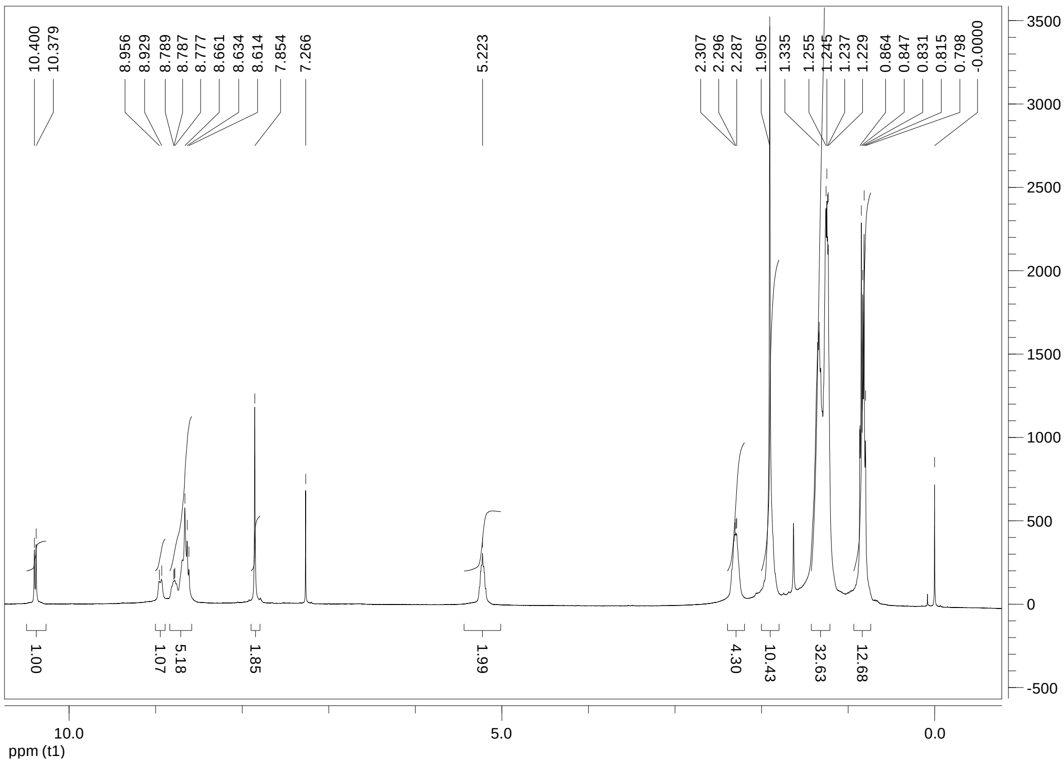


Figure S7. ^{13}C NMR of compound **DMTPA-PDI$_3$**

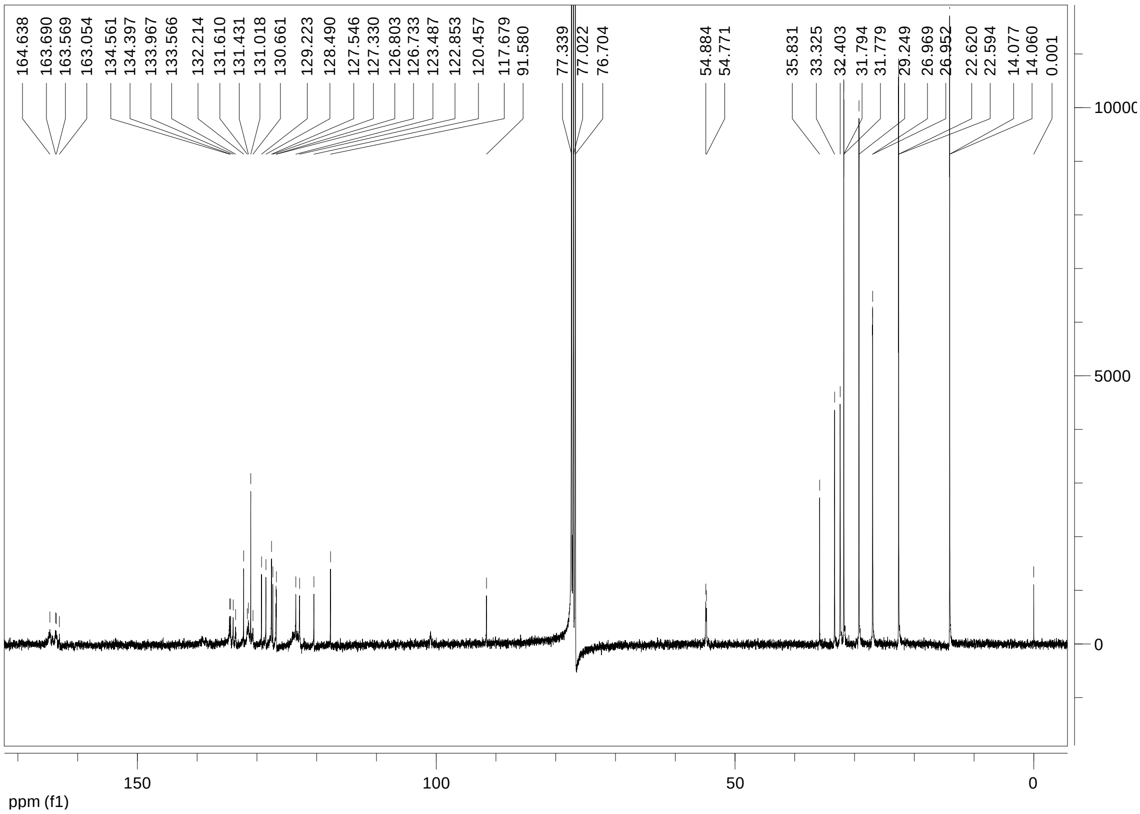
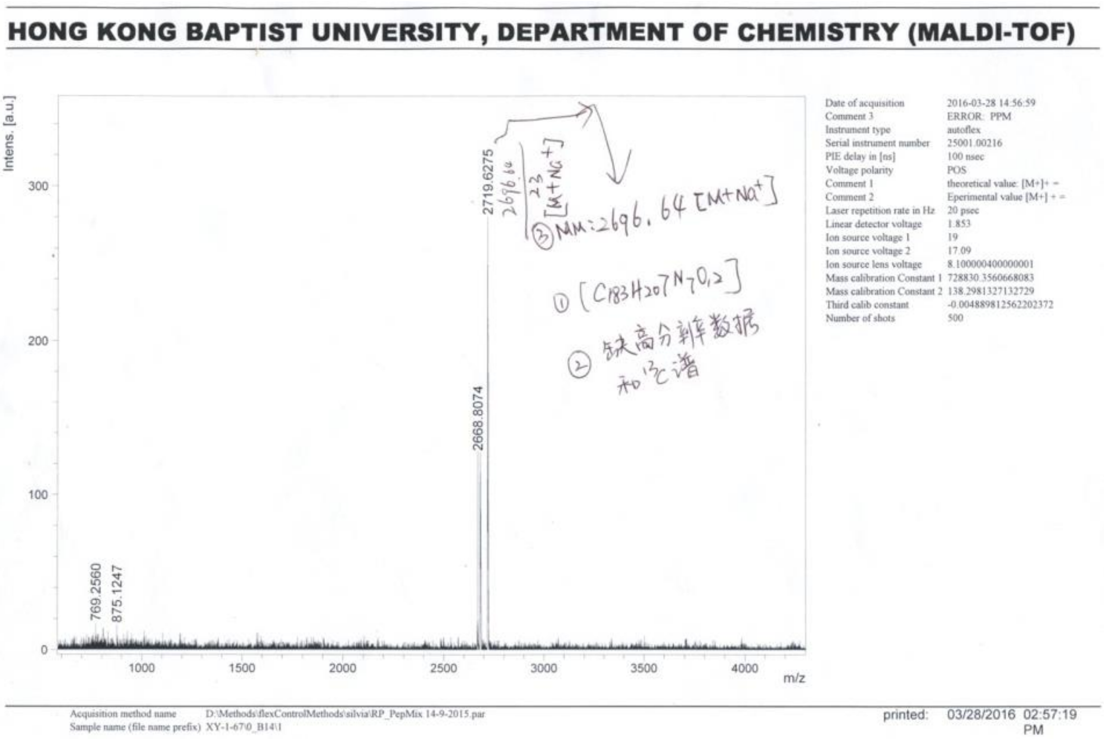


Figure S8. HR-MS (MALDI-TOF) mass spectrum of **DMTPA-PDI$_3$**



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