Electronic Supplementary Information for:

Pyrene-fused PDI based ternary solar cells: high power conversion efficiency

over 10%, and improved device thermal stability

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1. Materials and Measurements

Toluene for Stille coupling reactions was dried over and freshly distilled from K-Na alloy under an atmosphere of dry nitrogen. Three bis(trimethylstannyl) reagents and other chemicals and reagents were bought from commercial suppliers and used directly without purification. The important intermediates **1** and **2** were synthesized according to our previous work. ¹

¹H NMR spectra were recorded on a Bruker AVANCE III HD 400MHz, using CDCl₃ as solvent and tetramethylsilane (TMS) as an internal standard ($\delta = 0.00$ ppm). ¹³C NMR spectra were recorded on a Bruker AVANCE III HD 400 MHz, using CDCl₃ as a solvent and an internal standard ($\delta = 77.09$ ppm). MS spectra were recorded on a 5800MALDITOF mass spectrometer with *trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene] malononitrile (DCTB) as the matrix. Elemental analysis measurements were recorded on a Vario EL III.

UV-visible absorption spectra were acquired on a Perkin Elmer Lambda 20 UV/VIS Spectrophotometer. Photoluminescence spectra were measured using a Renishaw RM 3000 Micro-Raman/Photoluminescence system with the excitation wavelength at either 514 or 633 nm. All film samples were spin-cast on ITO/ZnO substrates. Optical modeling was conducted using the transfer-matrix optical model. The optical constants, n and k values, for all materials except Al (literature value) were extracted from fitting the variable angle spectroscopic ellipsometry (VASE) result in the wavelength range of 350-893 nm using various mathematical models built in the CompleteEASE software (J. A. Woollam Co.). All samples used for the optical characterizations were fabricated through the same way as the device without top electrode.

Cyclic voltammetry (CV) was carried out on a CHI voltammetric analyzer in a three-electrode cell with a Pt counter electrode, a Ag/AgCl reference electrode, and a glassy carbon working electrode at a scan rate of 100 mVs⁻¹ with 0.1 M tetrabutylammonium perchlorate (purchased from Alfa Aesar) as the supporting electrolyte, in anhydrous CH₃CN solution purged with nitrogen. Thin films of samples were deposited onto the glassy carbon working electrode from a dichloromethane solution. The potential values obtained in reference to the Ag/Ag⁺ electrode were converted to values versus the saturated calomel electrode (SCE) by means of an internal ferrocenium/ferrocene (Fc⁺/Fc) standard.

Geometrical and electronic properties were optimized at B3LYP/6-31G (d) level using Gaussian 09 program. Meanwhile, the molecular orbitals were obtained at the same level of theory.

Device Fabrication: Prepatterned ITO-coated glass substrates (purchased from South China Science & Technology Company Limited) were cleaned by successive sonication in toluene, deionized water, acetone, and isopropyl alcohol for 10 min each. After drying, a 30 min UV-ozone treatment was performed. Then a thin layer of PEDOT: PSS was deposited through spin-coating on the glass from a PEDOT: PSS aqueous solution (Xi'an Polymer Light Technology Corp 4083) at 4,000 rpm and dried subsequently at 150 °C for 15 min in air. Then the device was transferred to a nitrogen glove box, where the active blend layer was spin-coated onto the PEDOT:PSS layer from the chloroform solution of J71, ITIC and each PDI with different ratio. After spin-coating, the active layers were annealed at 150 °C for 10 min. The thickness of the active layers is about 100 nm. Then methanol solution of PDINO at a concentration of 1.0 mg·mL⁻¹ was deposited atop the active layer at 3,000 rpm for 30 s. Finally, top Al electrodes (≈100 nm) were thermally evaporated at a vacuum level of ≤1×10⁻⁵ Pa at rates below 1 Å·s⁻¹.

The current-voltage characteristics of the solar cells were measured under AM 1.5G irradiation on an Enli Solar simulator (100 mW cm⁻²). Before each test, the solar simulator was calibrated with a standard single-crystal Si solar cell (made by Enli Technology Co., Ltd., Taiwan, calibrated by The National Institute of Metrology (NIM) of China). External quantum efficiency (EQE) spectra was measured by Solar Cell Spectral Response Measurement System QE-R3011 (Enlitech Co., Ltd.).

Mobility Measurements: Hole mobilities and Electron mobilities were measured using the space charge limited current (SCLC) method. The structure of hole only devices was Glass/ITO/PEDOT:PSS/Active Layer/MoOx/Ag. As for electron only devices, the structure was Glass/ITO/ZnO/Active Layer/Ca/Al. The mobilities were obtained by taking current-voltage curves and fitting the results to a space charge limited form.

AFM: Atomic force microscopy (AFM) measurements were performed with a Nano Wizard 4 atomic force microscopy (JPK Inc. Germany) in Qi mode to observe the surface morphologies of the BHJ films deposited on glass substrates.

Contact Angle Measurements: Contact angles were measured with a Contact Angle System OCA20. The solution of each pure organic material was spin-coated on cleaned ITO substrates. Droplets of two different liquids (water and ethylene glycol (EG)) were cast onto the pure organic films with the drop size kept at 10 μ L per drop. Contact angle images were taken at 1 s after the whole droplet was deposited onto the sample surface. At least ten independent measurements were performed for each single liquid. The surface energy of each pure material was calculated directly by instrument using the model of Wu.²

GIWAXS patterns were collected with the highly customized Versatile Advanced X-ray Scattering instrument VAXSTER at the chair for Crystallography and Structural Physics (Universität Erlangen-Nürnberg, Germany). The system is equipped with a MetalJet D2 70 kV X-ray source from EXCILLUM, Sweden. The beam was shaped by a 150 mm Montel optics (INCOATEC, Geesthacht) and 2 of 4 double slit systems with the last slit system equipped with low scattering blades (JJXray/SAXSLAB). Aperture sizes were $(0.7 \times 0.7 \text{ mm}^2, 0.4 \times 0.4 \text{ mm}^2)$ for GIWAXS. The sample was located within the fully evacuated detector tube. The hybrid-pixel 2D Pilatus 300 K detector (Dectris Ltd., Baden, Switzerland) was used to collect the scattered radiation. The measurements were carried out at an energy of 9.28 keV. The collimation line was tilted and shifted with respect to the horizontal plane allowing grazing incidence angles which maximize the scattering volume and enhance the scattered intensity. The incidence angle α for GIWAXS measurements was between 0.183° and 0.189°, which is smaller than the critical angle of total reflection of the glass substrate and PEDOT:PSS layer to limit the penetration depth and the scattering to the thin layer. Grazing incidence geometry of the incident X-ray with respect to the

sample surface is used here to enhance the scattered intensity, to maximize the scattering volume, and to access the 3D structure of the studied thin films (lateral and normal direction). The detector-to-sample distance (SDD) was calibrated with a silver behenate standard to 172.6699 mm for GIWAXS. Data were reduced with dpdak software. The samples have been probed at 3 different positions to check the repeatability and reproducibility of the measurements.

Thermal stability. After cleaning, spin-coating HTL (PEDOT:PSS) and active layer on the ITO-coated glass substrates in the same way, all substrates were put on the hot plate with the temperature of 80 °C for different times (12 hours, 24 hours, 48 hours and 72 hours). Then, the PCE test was performed after spin-coating ETL (PDINO) and vacuum evaporating Al.

2. Synthesis and Characterization



Chart S1. Molecular structure of J71, ITIC and six nonfullerene acceptors (NFAs).

Synthesis of TPDI. Under an atmosphere of dry nitrogen, a mixture of 1 (500 mg, 0.44 mmol), 2,5-bis(trimethylstannyl)thiophene (**3**, 82 mg, 0.20 mmol), and Pd(PPh₃)₄ (30 mg) in anhydrous toluene (25 mL) was stirred at 120 °C for 24 h. After cooling to room temperature. The organic parts are combined and dried over Na₂SO₄. The solution was filtered and concentrated via rotary evaporation. The crude product was purified by column chromatography on silica gel using CH₂Cl₂:petroleum ether (1:1) as eluent to afford dark purple product (91%, 401 mg). ¹H NMR (400 MHz, CDCl₃, 298 K) δ (ppm): 8.67-8.61 (m, 6H), 8.56-8.50 (m, 6H), 8.40-8.38 (d, 2H), 7.45 (s, 2H), 4.12-4.00 (m, 8H), 1.95 (m, 4H), 1.42-1.17 (m, 160H), 0.85-0.80 (m, 24H). ¹³C NMR (100 MHz, CDCl₃, 298 K) δ (ppm): 163.57, 163.41, 163.28, 146.68, 136.23, 134.74, 133.98, 133.54,

132.48, 131.20, 129.77, 128.87, 128.54, 127.94, 127.36, 123.85, 123.36, 122.97, 122.33, 44.76, 36.62, 31.92, 30.07, 29.73, 29.70, 29.67, 29.38, 22.69, 14.13. MS (MALDI-TOF, m/z): 2205.3149 ([M+], calcd for C₁₄₈H₂₁₂N₄O₈S, 2205.6026). Anal. Calcd: for TPDI (C₁₄₈H₂₁₂N₄O₈S): C, 80.53; H, 9.68; N, 2.54. Found C, 80.23; H, 9.77; N, 2.44.

Synthesis of Th-PDI. The synthetic procedure was similar to that of TPDI. **1** (500 mg, 0.44 mmol), (4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene-2,6-diyl)bis(trimethylstanna ne) (**4**, 181 mg, 0.20 mmol), and Pd(PPh₃)₄ (30 mg). Dark purple product (87%, 470 mg). ¹H NMR (400 MHz, CDCl₃, 298K) δ (ppm): 8.70-8.47 (m, 14H), 8.30 (s, 2H), 7.96 (m, 2H), 6.88-6.87 (d, 2H), 4.10-4.00 (m, 8H), 2.74-2.73 (d, 4H), 1.98 (m, 4H), 1.62-1.61 (s, 2H), 1.32-1.19 (m, 170H), 0.85-0.70 (m, 42H). ¹³C NMR (100 MHz, CDCl₃, 298K) δ (ppm): 163.67, 163.38, 146.40, 146.03, 140.25, 137.70, 136.72, 136.18, 134.92, 134.05, 133.71, 133.53, 131.38, 131.02, 130.74, 130.20, 128.80, 128.21, 127.81, 127.25, 125.52, 125.30, 123.64, 123.37, 122.96, 122.89, 122.12, 44.77, 41.20, 32.37, 31.93, 31.77, 31.64, 30.06, 29.72, 29.68, 29.37, 28.76, 26.45, 25.53, 22.90, 22.60, 14.13, 14.02, 10.70. MS (MALDI-TOF, m/z): 2699.3901 ([M+], calcd for C₁₇₈H₂₅₀N₄O₈S₄, 2699.8162). Anal. Calcd: for Th-PDI (C₁₇₈H₂₅₀N₄O₈S₄): C, 79.12; H, 9.33; N, 2.07. Found C, 78.85; H, 9.60; N, 1.98.

Synthesis of O-PDI. The synthetic procedure was similar to that of TPDI. **1** (500 mg, 0.44 mmol), (4,8-bis((2-octyldodecyl)oxy)benzo[1,2-b:4,5-b']dithiophene-2,6-diyl)bis(trimethylstannae) (5, 222 mg, 0.20 mmol), and Pd(PPh₃)₄ (30 mg). Dark purple product (89%, 517 mg). ¹H NMR (400 MHz, CDCl₃, 298 K) δ (ppm): 8.83 (s, 2H), 8.74-8.65 (m, 8H), 8.40 (m, 2H), 8.31 (m, 2H), 7.76 (s, 2H), 4.24-4.08 (m, 12H), 2.03 (m, 4H), 1.77-1.76 (m, 2H), 1.42-1.04 (m, 222H), 0.87-0.68 (m, 38H). ¹³C NMR (100 MHz, CDCl₃, 298 K) δ (ppm): 163.46, 145.61, 144.29, 136.47, 133.35, 132.64, 131.24, 130.51, 130.23, 128.81, 128.68, 127.69, 127.08, 123.32, 122.85, 122.16, 120.33, 44.60, 39.19, 38.74, 36.68, 36.59, 31.95, 31.81, 30.12, 29.74, 29.70, 29.40, 22.70, 22.67, 22.61, 14.13, 14.12, 14.06, 14.01, 10.98. MS (MALDI-TOF, m/z): 2904.9187 ([M+], calcd for C₁₉₄H₂₉₄N₄O₁₀S₂, 2904.2061). Anal. Calcd: for O-PDI (C₁₉₄H₂₉₄N₄O₁₀S₂): C, 80.17; H, 10.20; N, 1.93. Found C, 79.83; H, 10.45; N, 1.87.

Synthesis of TPYPDI. The synthetic procedure was similar to that of TPDI. **2** (300 mg, 0.21 mmol), **3** (39 mg, 0.09 mmol), and Pd(PPh₃)₄ (20 mg). Black product (90%, 238 mg). ¹H NMR (400 MHz, CDCl₃, 298 K) *δ* (ppm): 10.45 (s, 4H), 9.33 (s, 2H), 9.13 (s, 4H), 9.04 (s, 2H), 8.82 (s, 2H), 8.34 (m,

4H), 8.12 (m, 4H), 7.65 (m, 2H), 4.18 (m, 8H), 2.08 (m, 4H), 1.69-1.67 (d, 36H), 1.28-1.12 (m, 160 H), 0.81-0.75 (m, 24H). ¹³C NMR (100 MHz, CDCl₃, 298 K) δ (ppm): 164.10, 149.40, 147.52, 134.86, 134.29, 133.10, 132.49, 131.07, 129.80, 129.05, 127.66, 127.28, 127.04, 126.71, 126.12, 124.50, 123.56, 122.43, 121.88, 121.01, 44.78, 36.72, 35.55, 35.52, 31.89, 29.77, 29.74, 29.72, 29.67, 22.67, 14.11, 14.09. MS (MALDI-TOF, m/z): 2825.5053 ([M+], calcd for C₁₉₆H₂₅₆N₄O₈S, 2825.9469). Anal. Calcd: for TPYPDI (C₁₉₆H₂₅₆N₄O₈S): C, 83.24; H, 9.12; N, 1.98. Found C, 82.85; H, 9.21; N, 1.94.

Synthesis of Th-PYPDI. The synthetic procedure was similar to that of TPDI. **2** (300 mg, 0.21 mmol), **4** (85 mg, 0.09 mmol), and Pd(PPh₃)₄ (20 mg). Black product (86%, 267 mg). ¹H NMR (400 MHz, CDCl₃, 298 K) δ (ppm): 10.49 (s, 4H), 9.31-9.25 (m, 4H), 9.05 (s, 4H), 8.84 (m, 2H), 8.37 (m, 4H), 8.26 (m, 2H), 8.17 (m, 4H), 7.49 (s, 2H), 6.84 s, 2H), 4.27 (m, 8H), 2.78-2.77 (m, 4H), 2.11 (m, 4H), 1.87 (m, 2H), 1.69-1.64 (d, 36H), 1.26-1.16 (m, 170 H), 0.88-0.71 (m, 42H). ¹³C NMR (100 MHz, CDCl₃, 298 K) δ (ppm): 164.27, 149.34, 147.12, 146.30, 140.61, 137.88, 136.55, 134.36, 133.39, 133.10, 132.68, 131.08, 129.66, 129.14, 128.36, 127.68, 127.19, 127.01, 126.79, 126.04, 125.61, 125.39, 124.75, 123.85, 123.52, 122.86, 121.74, 121.31, 120.97, 41.25, 31.92, 31.89, 31.87, 30.15, 30.11, 29.73, 29.67, 29.39, 28.78, 26.70, 26.59, 22.94, 22.60, 14.13, 14.06, 10.74. MS (MALDI-TOF, m/z): 3320.7036 ([M+], calcd for C₂₂₆H₂₉₄N₄O₈S₄, 3320.1605). Anal. Calcd: for Th-PYPDI (C₂₂₆H₂₉₄N₄O₈S₄): C, 81.69; H, 8.92; N, 1.69. Found C, 81.37; H, 8.97; N, 1.66.

Synthesis of O-PYPDI. The synthetic procedure was similar to that of TPDI. **2** (300 mg, 0.21 mmol), **5** (104 mg, 0.09 mmol), and Pd(PPh₃)₄ (20 mg). Black product (87%, 287 mg). ¹H NMR (400 MHz, CDCl₃, 298 K) δ (ppm): 10.48 (s, 4H), 9.33 (s, 2H), 9.25 (m, 2H), 9.13 (m, 2H), 9.04 (m, 2H), 8.84-8.77 (m, 2H), 8.34 (m, 4H), 8.15 (m, 4H), 8.08 (m, 2H), 4.41-4.27 (m, 12H), 2.14 (m, 4H), 1.89 (m, 4H), 1.69 (m, 38), 1.29-0.93 (m, 222H), 0.87-0.78 (m, 24H), 0.64-0.57 (m, 14H). ¹³C NMR (100 MHz, CDCl₃, 298 K) δ (ppm): 164.21, 149.33, 145.70, 145.50, 134.87, 134.26, 133.19, 133.05, 132.86, 131.08, 129.71, 127.69, 127.42, 127.07, 126.67, 126.08, 125.54, 124.74, 124.58, 123.84, 123.53, 122.58, 121.94, 121.05, 120.28, 44.86, 31.95, 31.88, 31.76, 30.20, 30.17, 30.07, 29.78, 29.70, 29.42, 29.40, 22.71, 22.56, 22.53, 14.15, 13.97. MS (MALDI-TOF, m/z): 3524.0624 ([M+], calcd for C₂₄₂H₃₃₈N₄O₈S₂, 3524.5504). Anal. Calcd: for O-PYPDI (C₂₄₂H₃₃₈N₄O₁₀S₂): C, 82.40; H, 9.66; N, 1.59. Found C, 82.09; H, 9.75; N, 1.54.

3. Photophysical properties



Figure S1. The absorption spectra of six NFAs in toluene solution.



Figure S2. CV curves of the six NFAs in thin film.

4. Theoretical calculations



Figure S3. The HOMO/LUMO distribution and optimal geometrics of six NFAs (the alkyl groups are simplified to the methyl one) calculated by the Gaussian 09 program at the B3LYP/6-31G* level.

5. Photovoltaic properties



Figure S4. (a) Device architecture of organic solar cells. (b) The energy level of J71 and ITIC.



Figure S5. J-V curve and EQE spectra of these binary OSC devices based on J71:ITIC.

mass ratio	$V_{\rm oc}({ m V})$	$J_{\rm sc}$ (mA/cm ²)	FF	PCE _{max} (average)
J71:ITIC:TPDI (1:0.95:0.05)	0.916	13.77	63.41	8.00 (7.88)
J71:ITIC:TPDI (1:0.9:0.1)	0.913	13.55	62.03	7.67 (7.34)
J71:ITIC:TPDI (1:0.8:0.2)	0.905	13.68	61.25	7.59 (7.44)
J71:ITIC:TPDI (1:0.5:0.5)	0.872	11.28	51.68	5.10 (5.01)
J71:TPDI (1:1)	0.703	1.41	48.8	0.47 (0.43)
J71:ITIC:TPYPDI (1:0.95:0.05)	0.948	14.39	64.85	8.85 (8.56)
J71:ITIC:TPYPDI (1:0.9:0.1)	0.951	15.54	66.27	9.80 (9.52)
J71:ITIC:TPYPDI (1:0.8:0.2)	0.958	15.11	64.95	9.41 (9.38)
J71:ITIC:TPYPDI (1:0.5:0.5)	0.965	13.06	47.59	6.00 (5.91)
J71:TPYPDI (1:1)	1.047	3.19	29.73	0.99 (0.91)
J71:ITIC:Th-PDI (1:0.95:0.05)	0.927	13.66	65.73	8.33 (7.96)
J71:ITIC:Th-PDI (1:0.9:0.1)	0.93	15.23	62.82	8.91 (8.71)
J71:ITIC:Th-PDI (1:0.8:0.2)	0.927	15.35	59.69	8.50 (8.46)
J71:ITIC:Th-PDI (1:0.5:0.5)	0.918	13.19	42.97	5.19 (5.00)
J71:Th-PDI (1:1)	0.833	1.33	33.01	0.36 (0.32)
J71:ITIC:Th-PYPDI (1:0.95:0.05)	0.953	16.42	68.42	10.71 (10.57)
J71:ITIC:Th-PYPDI (1:0.9:0.1)	0.955	16.66	65.34	10.63 (10.42)
J71:ITIC:Th-PYPDI (1:0.8:0.2)	0.958	14.58	69.41	9.70 (9.30)
J71:ITIC:Th-PYPDI (1:0.5:0.5)	0.965	13.93	52.12	7.01 (6.94)
J71:Th-PYPDI (1:1)	1.023	1.26	28.71	0.37 (0.33)
J71:ITIC:O-PDI (1:0.95:0.05)	0.918	12.34	61.18	6.94 (6.49)
J71:ITIC:O-PDI (1:0.9:0.1)	0.916	11.96	59.46	6.46 (6.33)
J71:ITIC:O-PDI (1:0.8:0.2)	0.907	9.83	58.81	5.25 (5.07)
J71:ITIC:O-PDI (1:0.5:0.5)	0.892	9.17	54.81	4.48 (4.17)
J71:O-PDI (1:1)	0.652	1.52	40.88	0.40 (0.39)
J71:ITIC:O-PYPDI (1:0.95:0.05)	0.938	15.88	68.06	10.14 (9.81)
J71:ITIC:O-PYPDI (1:0.9:0.1)	0.945	16.59	69.92	10.96 (10.71)
J71:ITIC:O-PYPDI (1:0.8:0.2)	0.962	14.45	70.63	9.82 (9.73)
J71:ITIC:O-PYPDI (1:0.5:0.5)	0.971	11.58	59.53	6.67 (6.46)
J71:O-PYPDI (1:1)	1.013	4.22	34.42	1.47 (1.45)
J71:ITIC (1:1)	0.939	17.55	67.28	11.08 (10.83)

 Table S1. Summary of device parameters of J71:ITIC:NFAs ternary OSCs devices with different

 NFAs content.



Figure S6. Photoluminescence spectra of neat films of pure J71 and ITIC and binary film of J71:ITIC.

 Table S2. Charge mobility of six J71:ITIC:NFAs (1:0.9:0.1) ternary films.

Devices	$\mu_{\rm h} [{\rm cm}^2 {\rm V}^{-1} {\rm s}^{-1}]$	$\mu_{\rm e} [{\rm cm}^2 {\rm V}^{-1}{\rm s}^{-1}]$	$\mu_{ m h}/\mu_{ m e}$
J71:ITIC:TPDI (1:0.9:0.1)	0.92×10 ⁻³	1.89×10 ⁻³	0.49
J71:ITIC:TPyPDI (1:0.9:0.1)	1.30×10 ⁻³	1.02×10 ⁻³	1.27
J71:ITIC:Th-PDI (1:0.9:0.1)	2.52×10-3	1.50×10 ⁻³	1.68
J71:ITIC:Th-PyPDI (1:0.9:0.1)	1.10×10 ⁻³	1.38×10 ⁻³	0.80
J71:ITIC:O-PDI (1:0.9:0.1)	1.97×10 ⁻³	1.23×10 ⁻³	1.60
J71:ITIC:O-PyPDI (1:0.9:0.1)	2.84×10 ⁻³	2.39×10 ⁻³	1.19
J71:ITIC (1:1)	1.75×10-3	1.96×10 ⁻³	0.89

6. Film morphology



Figure S7. Atomic force microscopy (AFM) profiles of binary J71:ITIC film and J71:ITIC:NFAs (1:0.9:0.1) ternary films.



Figure S8. GIWAXS patterns of J71:ITIC binary film (a), J71:ITIC:Th-PYPDI (1:0.9:0.1) ternary film (b) and J71:ITIC:Th-PDI (1:0.9:0.1) ternary film (c). Scattering profiles (horizontal and vertical) of J71:ITIC binary film (d), J71:ITIC:Th-PYPDI (1:0.9:0.1) ternary film (e), J71:ITIC:Th-PDI (1:0.9:0.1) ternary film (f)



Figure S9. GIWAXS patterns of J71:ITIC binary film (a), J71:ITIC:TPYPDI (1:0.9:0.1) ternary film (b) and J71:ITIC:TPDI (1:0.9:0.1) ternary film (c). Scattering profiles (horizontal and vertical) of J71:ITIC binary film (d), J71:ITIC:TPYPDI (1:0.9:0.1) ternary film (e), J71:ITIC:TPDI (1:0.9:0.1) ternary film (f).



Figure S10. GIWAXS patterns (a) and scattering profiles (b, horizontal and vertical) of each pure materials used in ternary OSCs devices.

7. NMR spectra



Figure S12. The ¹³C NMR spectrum of TPDI recorded in CDCl₃.





Figure S14. The ¹³C NMR spectrum of Th-PDI recorded in CDCl₃.



Figure S15. The ¹H NMR spectrum of O-PDI recorded in CDCl₃.



Figure S16. The ¹³C NMR spectrum of O-PDI recorded in CDCl₃.



Figure S17. The ¹H NMR spectrum of TPYPDI recorded in CDCl₃.



Figure S18. The ¹³C NMR spectrum of TPYPDI recorded in CDCl₃.



Figure S19. The ¹H NMR spectrum of Th-PYPDI recorded in CDCl₃.



Figure S20. The ¹³C NMR spectrum of Th-PYPDI recorded in CDCl₃.



Figure S21. The ¹H NMR spectrum of O-PYPDI recorded in CDCl₃.



Figure S22. The ¹³C NMR spectrum of O-PYPDI recorded in CDCl₃.

8. References

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