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Supporting Information

Hole Transport Materials based on *β*-cyanodiarylethenes Core Structure for Efficient Inverted Perovskite Solar Cells

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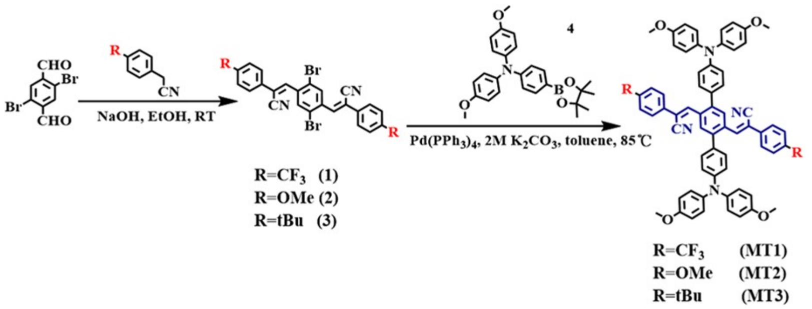
Table of Contents

General information

Unless other wisely stated, all starting materials were purchased from commercial suppliers (Sigma Aldrich, Tansoole, and the Energy Chemical) and used without further purification. The EtOH organic solvent to be used in the reaction was an ultra-dry solvent purchased directly from a pharmaceutical company. The toluene solvent was stirred with calcium hydride one day in advance and used under argon atmosphere after treatment with a distillation unit on the day of the reaction. The nuclear magnetic resonance (NMR) spectra were obtained from a BRUKER AVANCE III 600 MHz NMR Instrument (in $CDCl_3$). The HRMS was measured on Thermo Scientific Q Exactive instrument. UV-vis absorption spectra were measured on a Shimadzu UV-2450 absorption spectrophotometer. Cyclic voltammetry (CV) test was performed on the CorrTest CS 310s in CH_2Cl_2 under a nitrogen atmosphere, using saturated calomel electrode (SCE) as reference electrode and ferrocene as internal standard. Thermal gravimetric analysis (TGA) was performed on a TGA Q50 at a heating rate of 10℃ min^{-1} under a nitrogen atmosphere. Differential scanning calorimetry (DSC) measurement was performed on a DSC Q20 instrument at a heating rate of 10 ℃ min^{-1} under a nitrogen atmosphere. The cross-sectional and surface topography field emission scanning electron microscopy (FE-SEM) image of the device was characterized by FE-SEM images (JSM-7800F). Atomic force microscopy (AFM) were collected in air on a Scanning Probe Microscope (Being Nano-

Instruments, Ltd, CSPM5500) using a tapping mode. The thickness of HTL was measured by a SURFCORDER-ET150. Water contact angles were measured on contact angle measurement apparatus JC2000D, Shanghai Zhongchen Digital Technology Co., Ltd., China. Fluorescence spectra were measured on a Hitachi F-4600 FL Spectrophotometer. The photoluminescence (PL) lifetimes were measured by a single photon counting spectrometer from Edinburgh Instruments (FLS920) with a Picosecond Pulsed UV-LASTER (LASTER377) as the excitation source. Current-voltage curves (J-V) characteristics were measured under 100 mW cm^{-2} (AM 1.5G illumination) using a Newport solar simulator (model 91160) and a Keithley 2400 source/meter. A certified reference solar cell (Fraunhofer ISE) was used to calibrate the light source for an intensity of 100 mW cm^{-2}. The external quantum efficiency (EQE) spectra were recorded using a computer-controlled setup consisting of a Xenon light source (Spectral Products ASB-XE-175), a monochromator (Spectra Products CM110), and a potentiostat (LabJack U6 DAQ board), calibrated by a certified reference solar cell (Fraunhofer ISE). Transient photocurrent (TPC) and transient photovoltage (TPV) were recorded using a ZAHNER®MESSSYSTEME (Instrument model: PP211). For transient photovoltage/photocurrent decay measurements were performed using a light source (LS530).

1. Synthesis procedures



Scheme 1. The synthesis routes of MT1、MT2 and MT3.

Synthesis of Compound 1 (2Z,2'Z)-3,3'-(2,5-dibromo-1,4-phenylene)bis(2-(4-(trifluoromethyl)phenyl)acrylonitrile)

Compound 1 synthesized by Knoevenagel condensation method according to literature.[1] 2,5-dibromoterephthalaldehyde (150.0 mg, 0.5 mmol) and 2-(4-(trifluoromethyl)phenyl)acetonitrile (190.1 mg, 1.0 mmol) were added to a 100 ml round bottom flask with magnets, 20 ml of ethanol was added to make the whole reaction in argon atmosphere, NaOH (303.5 mg, 7.6 mmol) dissolved in super dry anhydrous ethanol (10 ml) was added slowly drop wise to the round bottom flask until it changed color. After 6 h at room temperature a precipitate was formed, filtered under reduced pressure and washed repeatedly with water and ethanol to give a yellow solid product (298.0 mg, 93%).^{1}H NMR (600 MHz, $CDCl_3$) δ 8.39 (s, 2H), 7.86 (s, 2H), 7.85 (d, J = 4.5 Hz, 4H), 7.77 (d, J = 8.3 Hz, 4H). HR-MS, Found: $[M+H]^+$ 623.9277; molecular formula $C_{26}H_{12}Br_2F_6N_2$, requires $[M+H]^+$ 623.9271. FT-IR (KBr): [N≡C], 2222 (s) cm^{-1}; [C-F] 1321 (s) cm^{-1}. Melting Point:249 °C. Compound 1 cannot be characterized by ^{13}C NMR due to its poor solubility.

Synthesis of Compound 2 (2Z,2'Z)-3,3'-(2,5-dibromo-1,4-phenylene)bis(2-

(4-methoxyphenyl)acrylonitrile)

The compound was synthesized by using the same procedure as described above for compound 1. 2,5-dibromoterephthalaldehyde (150.0 mg,0.5 mmol) and 4-Methoxyphenylacetonitrile (151.1 mg, 1.0 mmol) were added to a 100 ml round bottom flask with magnets, 20 ml of ethanol was added to make the whole reaction in argon atmosphere, NaOH (303.2 mg,7.6 mmol) dissolved in super dry anhydrous ethanol (10ml) was added slowly drop wise to the round bottom flask until it changed color. After 6 h at room temperature a precipitate was formed, filtered under reduced pressure and washed repeatedly with water and ethanol to give a yellow solid product (257.1 mg, 92%).^{1}H NMR (600 MHz, $CDCl_3$) δ 8.34 (s, 2H), 7.67 (d, *J* = 8.6 Hz, 4H), 7.63 (s, 2H), 7.00 (d, *J* = 8.6 Hz, 4H), 3.88 (s, 6H). FT-IR (KBr): [N≡C], 2224 (s) cm^{-1}. Melting Point:283 ℃. Compound 2 cannot be characterized by ^{13}C NMR due to its poor solubility.

Synthesis of Compound 3 (2Z,2'Z)-3,3'-(2,5-dibromo-1,4-phenylene)bis(2-(4-(tert-butyl)phenyl)acrylonitrile)

The compound was synthesized by using the same procedure as described above for compound 1. 2,5-dibromoterephthalaldehyde (125.0 mg, 0.5 mmol) and 4-Tert-Butylphenyl-Acetonitrile (148.4 mg, 1.0 mmol) were added to a 100 ml round bottom flask with magnets, 20 ml of ethanol was added to make the whole reaction in argon atmosphere, NaOH (252.9 mg, 6.3 mmol) dissolved in super dry anhydrous ethanol (10 ml) was added slowly drop wise to the round bottom flask until it changed color. After 6 h at room temperature a precipitate was formed, filtered under reduced pressure and washed repeatedly with water and ethanol to give a yellow solid product (243.9 mg, 95%).^{1}H NMR (600 MHz, $CDCl_3$) δ 8.35 (s, 2H), 7.72 (s, 2H), 7.67 (d, *J* = 8.3 Hz, 4H), 7.51 (d, *J* = 8.4 Hz, 4H), 1.36 (s, 18H). HR-MS, Found: $[M+H]^+$ 600.0782; molecular formula $C_{32}H_{30}Br_2N_2$, requires $[M+H]^+$ 600.0776. FT-IR (KBr): [N≡C], 2219 (s) cm^{-1}. Melting Point:243 °C. Compound 3 cannot be characterized by ^{13}C NMR and due to its poor solubility.

Compound 4 was synthesized according to the literature.[2]

Synthesis of Compound MT1 (2Z,2'Z)-3,3'-(4,4''-bis(bis(4-methoxyphenyl)amino)-[1,1':4',1''-terphenyl]-2',5'-diyl)bis(2-(4-(trifluoromethyl)phenyl)acrylonitrile)

The mixture of compound 1 (129.6 mg, 0.2 mmol), compound 4 (224.0 mg, 0.5 mmol), $Pd(PPh_3)_4$ (24.0 mg, 0.02 mmol), K_2CO_3 (287.2 mg, 2.1 mmol) and ultra-dry tetrahydrofuran (10 mL) was placed in a Schlenk tube and stirred at 85 °C for 12 h in an argon atmosphere. After cooling, the reaction was quenched by adding water, and then was extracted with dichloromethane. The organic layer was washed with brine and dried over anhydrous Na_2SO_4. After solvents were evaporated, the residue was purified by column chromatography over silica gel using petroleum ether:CH_2Cl_2 =2:1 (v/v) as the eluent to give the product (169.0 mg, 75 %) as an orange solid.^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24 (s, 2H), 7.72 (d, *J* = 7.4 Hz, 6H), 7.69 (d, *J* = 8.4 Hz, 4H), 7.26 (d, *J* = 5.8 Hz, 4H), 7.13 (d, *J* = 8.8 Hz, 8H), 6.98 (d, *J* = 8.6 Hz, 4H), 6.86 (d, *J* = 8.9

Hz, 8H), 3.80 (s, 12H).^{13}C NMR (151 MHz, $CDCl_3$) δ 156.47, 149.16, 143.87, 141.09 , 140.17, 137.52, 133.08, 131.24, 130.78, 130.30, 129.48, 127.27, 126.41, 126.15, 119.03, 117.55, 114.89, 111.93, 55.51. HRMS, Found: $[M+H]^+$ 1075.3645; molecular formula $C_{66}H_{48}F_6N_4O_4$, requires $[M+H]^+$ 1075.3652. FT-IR (KBr): [N≡C], 2219 (s) cm^{-1}; [C-F] 1324 (s) cm^{-1}. Melting Point:292 °C.

Synthesis of Compound MT2 (2Z,2'Z)-3,3'-(4,4''-bis(bis(4-methoxyphenyl)amino)-[1,1':4',1''-terphenyl]-2',5'-diyl)bis(2-(4-methoxyphenyl)acrylonitrile)

The mixture of compound 2 (125.0 mg, 0.2 mmol), compound 4 (245.8 mg, 0.7 mmol), $Pd(PPh_3)_4$ (10.5 mg, 0.01 mmol), K_2CO_3 (315 mg, 2.3 mmol) and ultra-dry tetrahydrofuran (10 mL) was placed in a Schlenk tube and stirred at 85 °C for 12 h in an argon atmosphere. The subsequent processing was the same as compound MT1, and ultimately 166.2 mg of orange solid was obtained with a yield of 73%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.17 (s, 2H), 7.54 (d, *J* = 8.7 Hz, 4H), 7.51 (s, 2H), 7.28 (d, *J* = 8.6 Hz, 4H), 7.12 (d, *J* = 8.9 Hz, 8H), 6.97 (d, *J* = 8.6 Hz, 4H), 6.94 (d, *J* = 8.7 Hz, 4H), 6.85 (d, *J* = 8.9 Hz, 8H), 3.85 (s, 6H), 3.80 (s, 12H). HR-MS, Found: $[M+H]^+$ 999.4108; molecular formula $C_{66}H_{54}N_4O_6$, requires $[M+H]^+$ 999.4116. FT-IR (KBr): [N≡C], 2216 (s) cm^{-1}. Melting Point:299 °C. Compound MT2 cannot be characterized by ^{13}C NMR due to its poor solubility.

Synthesis of Compound MT3 (2Z,2'Z)-3,3'-(4,4''-bis(bis(4-methoxyphenyl)amino)-[1,1':4',1''-terphenyl]-2',5'-diyl)bis(2-(4-(tert-butyl)phenyl)acrylonitrile)

The mixture of compound 3 (125.0 mg, 0.2 mmol), compound 4 (224.6 mg, 0.5 mmol), $Pd(PPh_3)_4$ (9.6 mg, 0.01 mmol), K_2CO_3 (287.9 mg, 2.1 mmol) and ultra-dry tetrahydrofuran (10 mL) was placed in a Schlenk tube and stirred at 85 °C for 12 h in an argon atmosphere. The subsequent processing was the same as compound MT1, and ultimately 157.6 mg of orange solid was obtained with a yield of 75%.^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19 (s, 2H), 7.62 (s, 2H), 7.54 (d, *J* = 8.4 Hz, 4H), 7.44 (d, *J* = 8.4 Hz, 4H), 7.29 (d, *J* = 8.6 Hz, 4H), 7.13 (d, *J* = 8.9 Hz, 8H), 6.99 (d, *J* = 8.6 Hz, 4H), 6.86 (d, *J* = 8.9 Hz, 8H), 3.80 (s, 12H), 1.35 (s, 18H).^{13}C NMR (151 MHz, $CDCl_3$) δ 156.53, 150.99, 149.72, 140.85, 139.95, 138.12, 136.27, 133.41, 130.59, 129.84, 127.22, 126.89, 125.54, 125.36, 119.20, 118.45, 114.89, 113.07, 55.51, 34.71, 31.39. HR-MS, found $[M+H]^+$ 1051.5151, molecular formula $C_{72}H_{66}N_4O_4$; requires $[M+H]^+$ 1051.5156. FT-IR (KBr): [N≡C], 2224 (s) cm^{-1}. Melting Point:140 °C.

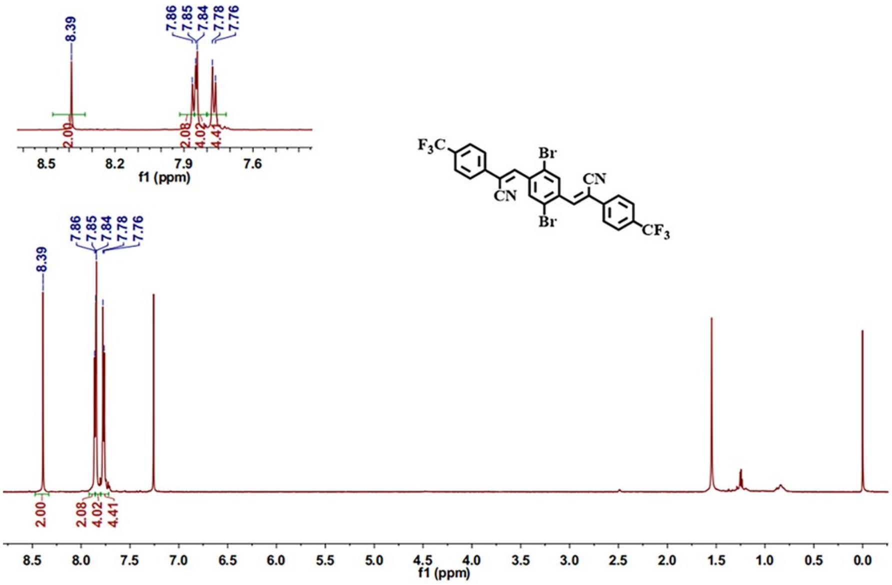


Fig. S1. ^{1}H NMR spectrum of 1 in CDCl$_3$.

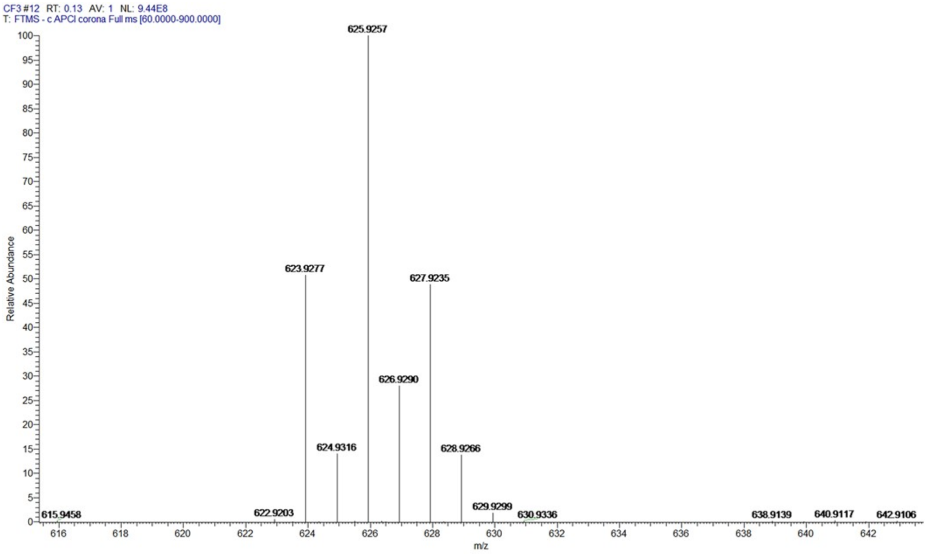


Fig. S2. HRMS of 1.

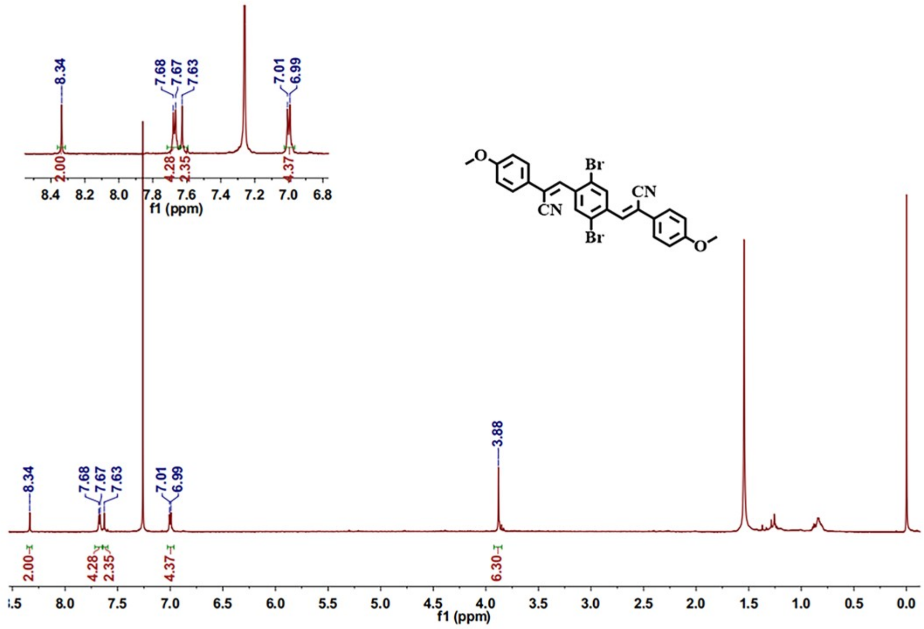


Fig. S3. ^{1}H NMR spectrum of 2 in $CDCl_3$.

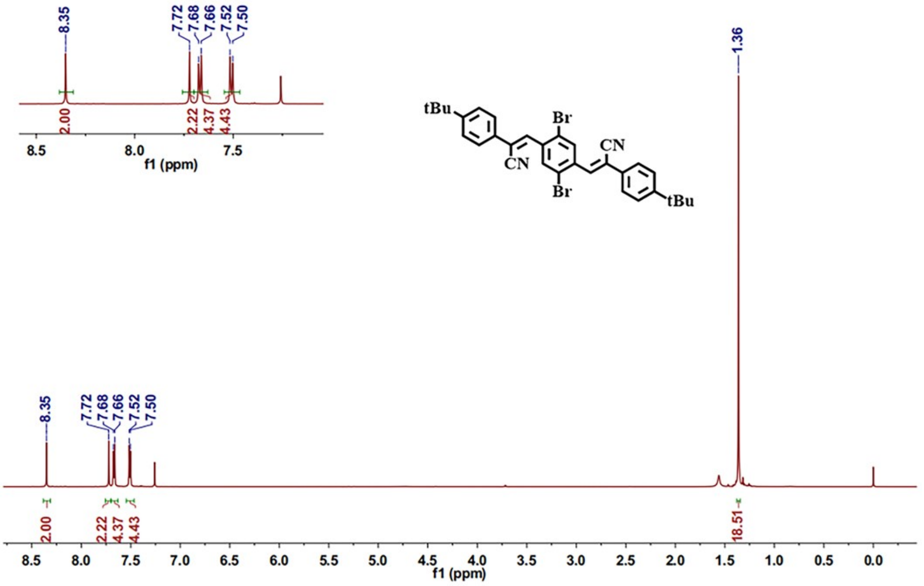


Fig. S4. ^{1}H NMR spectrum of 3 in $CDCl_3$.

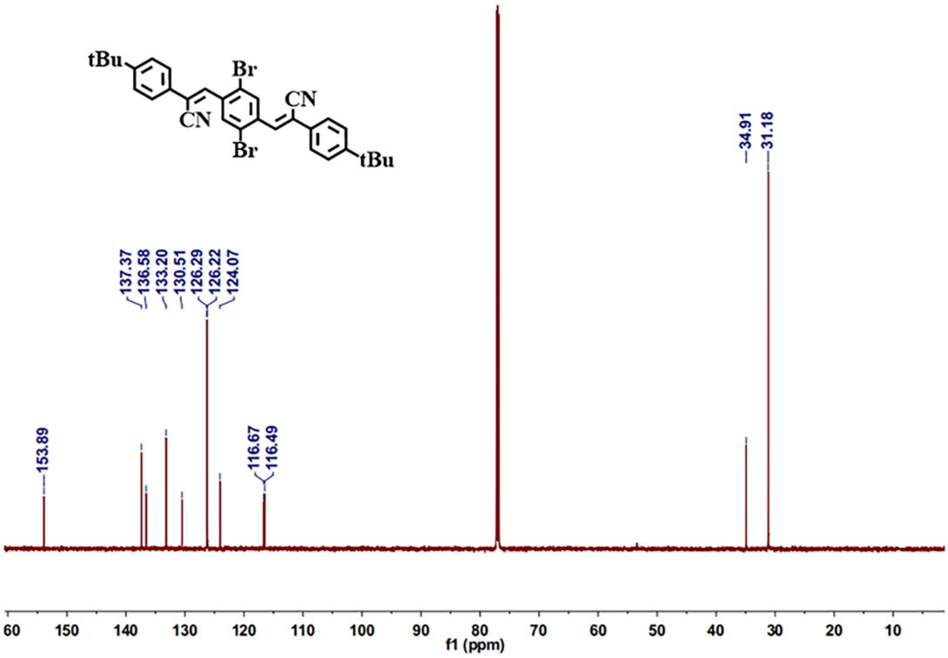


Fig. S5. ^{13}C NMR spectrum of 3 in $CDCl_3$.

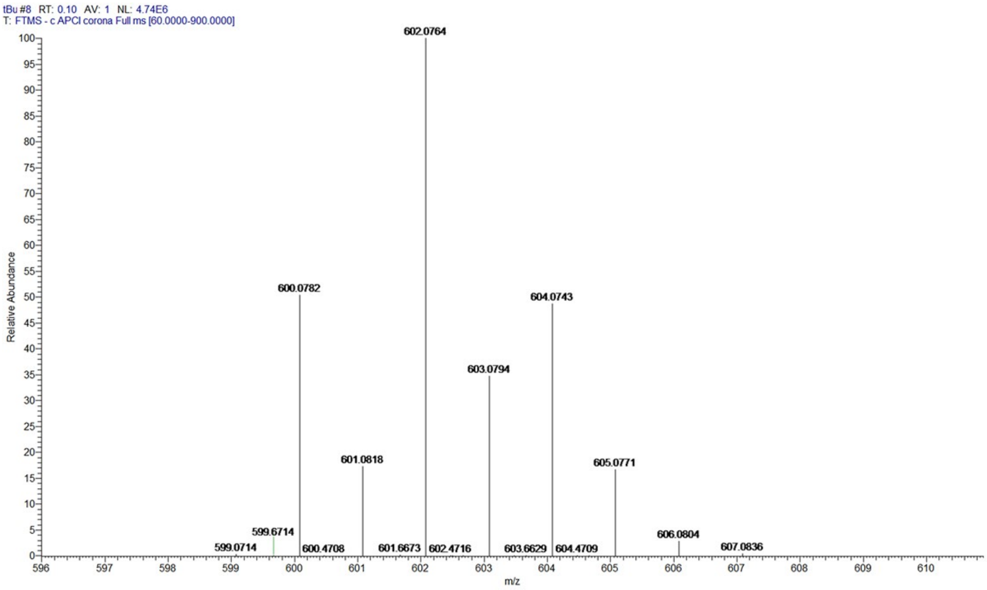


Fig. S6. HRMS of 3.

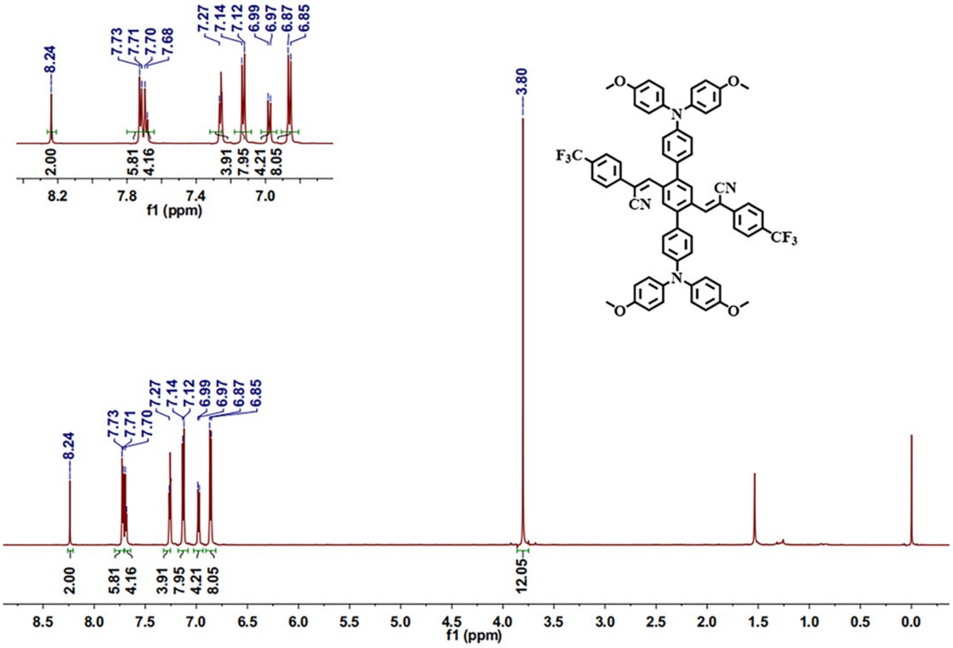


Fig. S7. ^{1}H NMR spectrum of MT1 in $CDCl_3$.

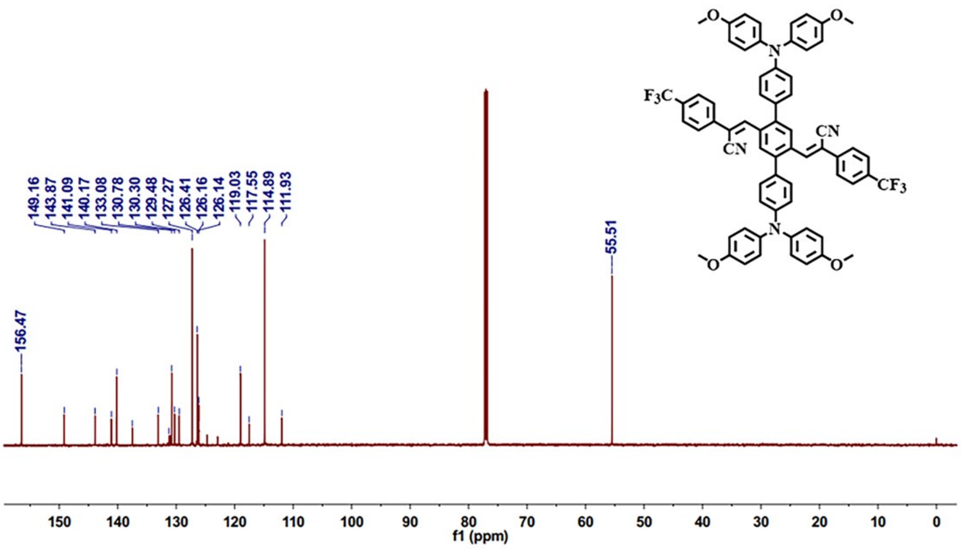


Fig. S8. ^{13}C NMR spectrum of MT1 in $CDCl_3$.

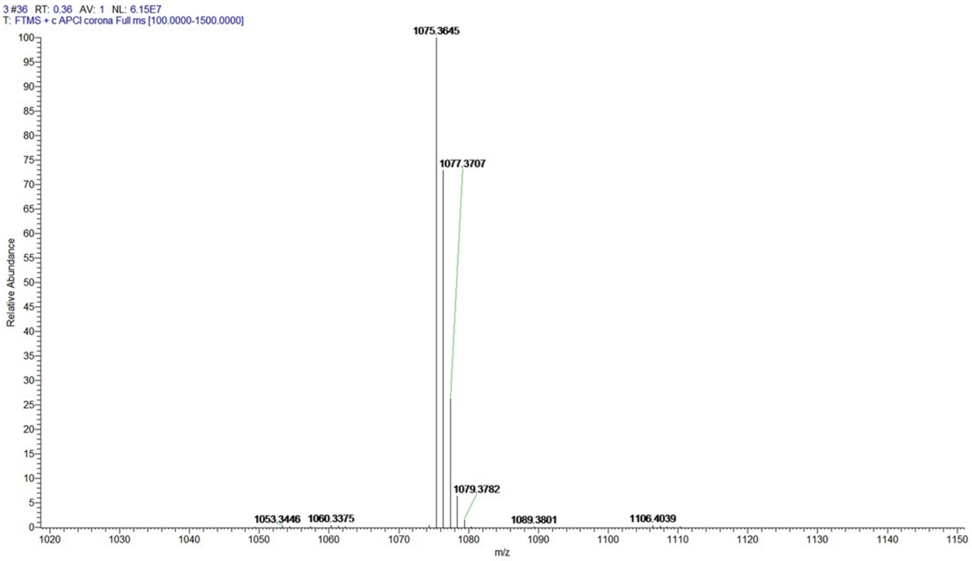


Fig. S9. HRMS of MT1.

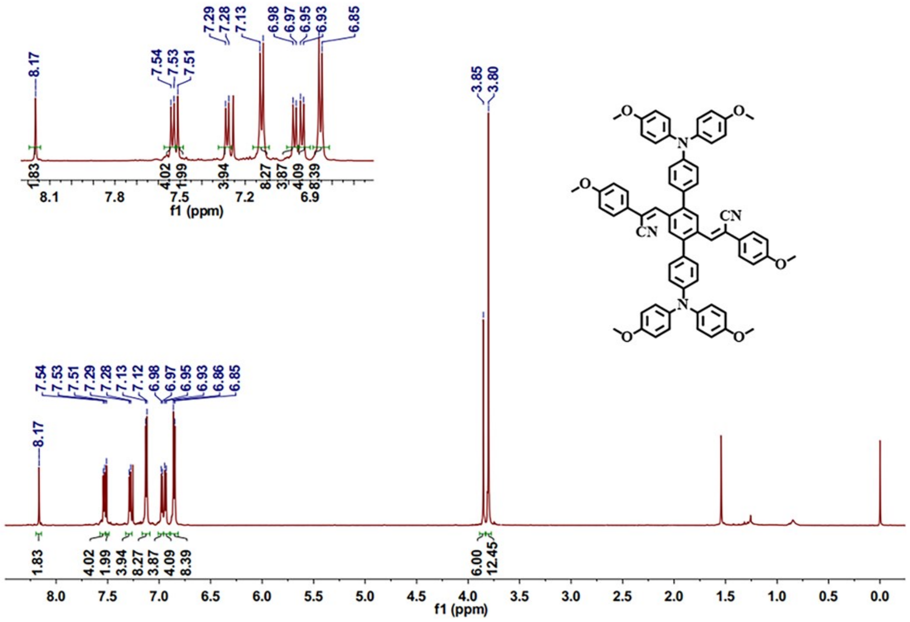


Fig. S10. ^{1}H NMR spectrum of MT2 in $CDCl_3$.

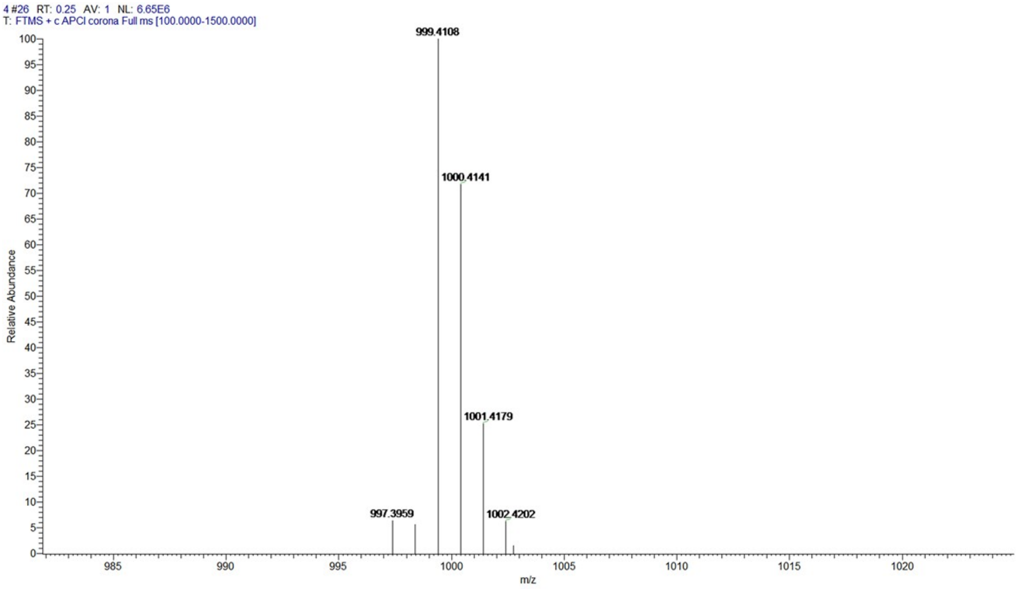


Fig. S11. HRMS of MT2.

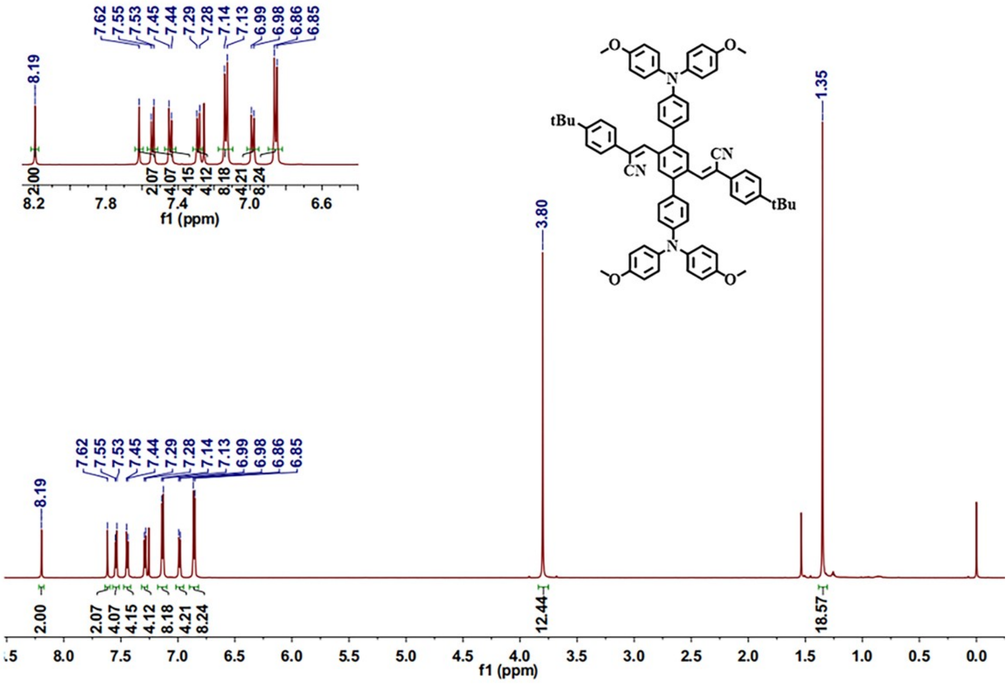


Fig. S12. ^{1}H NMR spectrum of MT3 in $CDCl_3$.

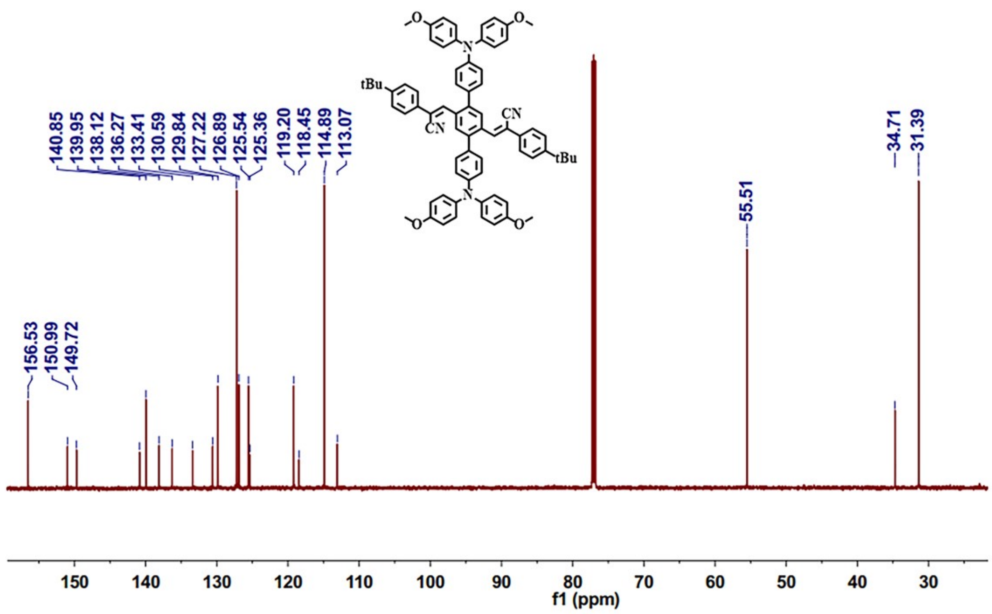


Fig. S13. ^{13}C NMR spectrum of MT3 in CDCl$_3$.

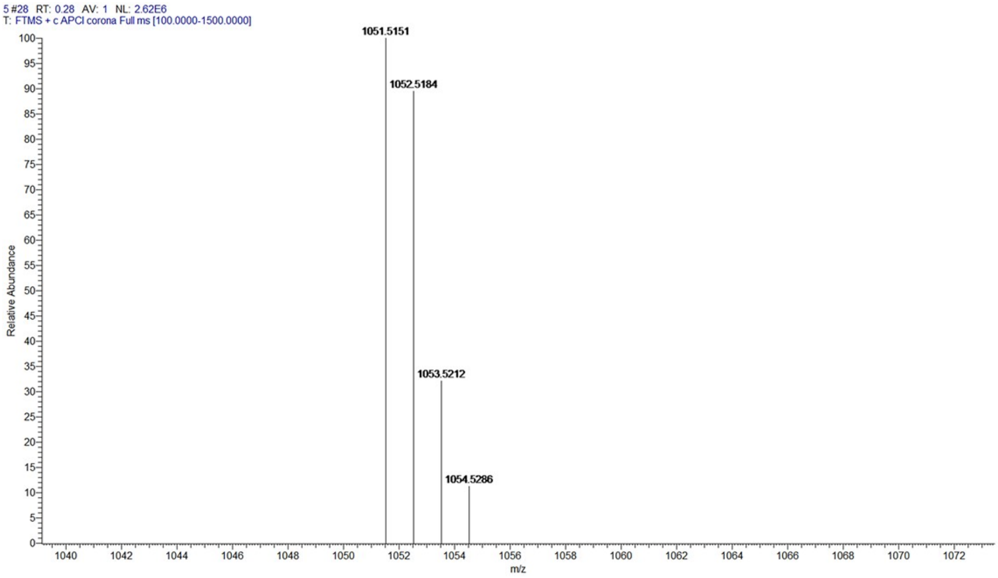


Fig. S14. HRMS of MT3.

2. Cyclic voltammetry

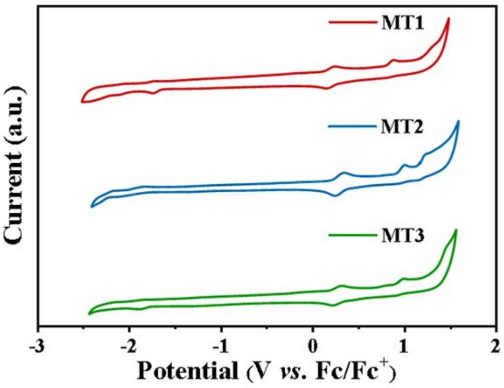


Fig. S15. CV with ferrocene as the reference for MT1, MT2 and MT3.

3. Thermal properties

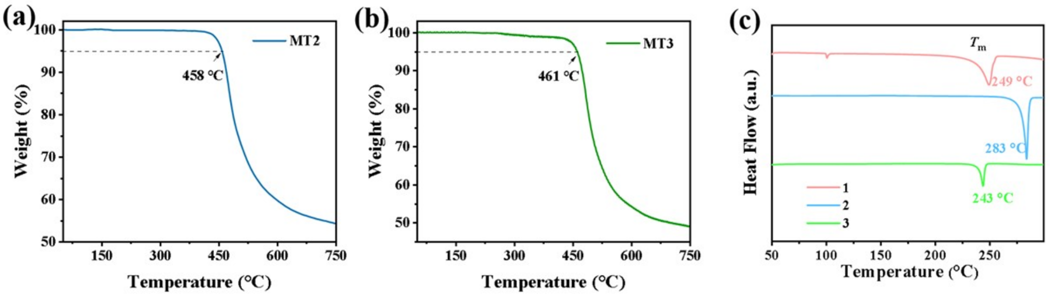


Fig. S16. Thermogravimetric analysis (TGA) of the a) MT2, b) MT3 under N_2 atmosphere; c) DSC curves of the intermediates 1, 2, and 3.

5. Transmittance spectroscopy, hole mobility, conductivity spectrum

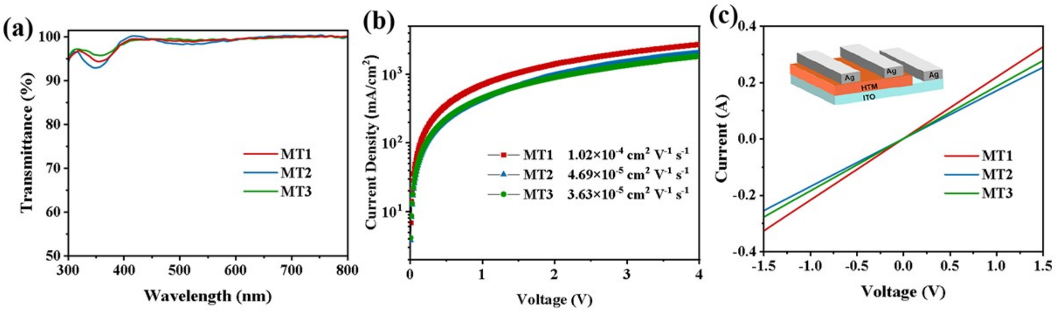


Fig. S17. (a) Transmittance spectroscopy of the HTMs. (b) Space-charge-limited-current (SCLC) *J*-*V* characteristics of MT1, MT2 and MT3 based hole-only devices. (c) The conductivity measurement (the inset shows the device structure).

6. FT-IR spectral

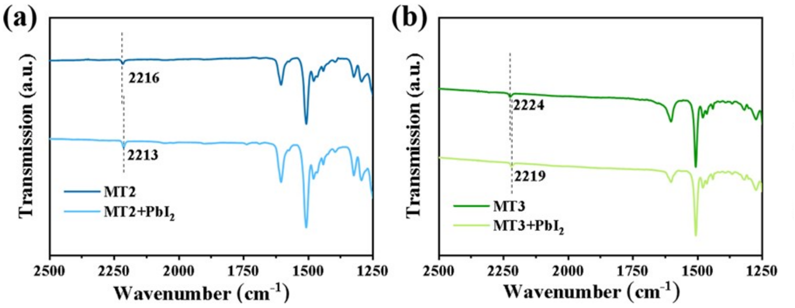


Fig. S18. FT-IR spectra of a) MT2 and b) MT3 with and without PbI_2.

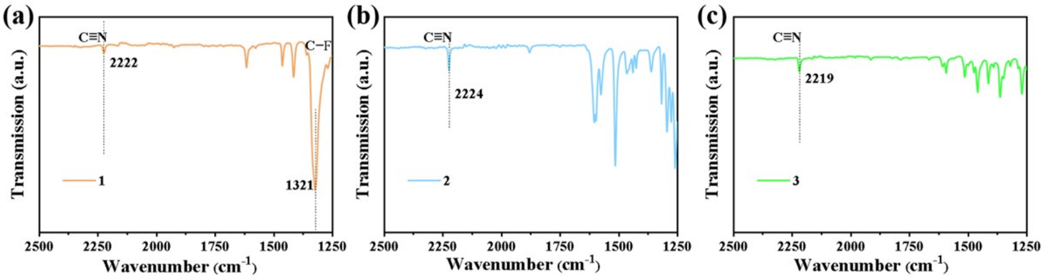


Fig. S19. FT-IR spectra of the intermediates 1, 2, and 3.

7. The Space-charge-limited current (SCLC) hole mobility measurements

Hole mobility tests were conducted using a diode configuration of ITO/PEDOT:PSS/HTM/Ag by taking current-voltage current in the range of 0-4 V and fitting the results to a space charge limited form, based on the following equation:

$$J = 9\varepsilon_{\theta}\varepsilon_{\gamma}\mu_{h}V^{2}/ 8L^{3} \quad (1)$$

J is the current density, L is the film thickness of the active layer, μ_h is the hole mobility, ε_γ is the relative dielectric constant of the transport medium, ε_θ is the permittivity of free space (8.85×10^{-12} F m^{-1}), V is the internal voltage of the device.

8. Trap density tests

Trap density (n_{trap}) was measured with the "hole only device":

ITO/HTM/perovskite(500nm)/Spiro-OMeTAD/Ag. Three different regions were identified by the different values of the exponent n ($J \propto V^n$): the ohmic region for n=1, the trap-filled limited (TFL) region for n=2, and Child region for n > 3. The voltage of the crossover point between the ohmic and TFL regions is the trap-filled limit voltage (V_{TFL}) and can be used to determine the trap density. The V_{TFL} of the hole-only devices based on MT1, MT2 and MT3 HTLs were 0.165 V, 0.232 V and 0.313 V, respectively. The n_{trap} was estimated using the following equation:

$$n_{trap} = \frac{2 \varepsilon_0 V_{TFL}}{eL^2} \qquad (2)$$

where, V_{TFL} is the trap-filled limit (TFL) voltage, ε is the dielectric constant of the perovskite layer. ε_0 is the vacuum permittivity. e is the charge. L is the thickness of the perovskite layer.

9. Device Fabrication and characterization

We fabricated the device based on the methods reported in the literature[3]. Glass/ITO substrates (15 Ω sq^{-1}) were sequentially cleaned by sonication with detergent, deionized water, acetone and ethanol for 20 min, respectively. Then, the glass/ITO substrates were dried at 100 °C in oven, and then were treated with oxygen plasma for 10 min and finally transferred into a N_2-filled glovebox before use. MT1, MT2 or MT3 solutions were prepared with a concentration of 1 mg mL^{-1} in CB, and stirred at 25 °C for 1 hours. The thicknesses of HTLs are about 5 nm. PTAA solution (2 mg mL^{-1} in CB) was used as a control experiment. The MT1, MT2, MT3 or PTAA solutions were spin-coated onto the ITO substrates at 6000 rpm for 30 s. For a perovskite layer, a perovskite precursor solution was prepared by dissolving 226.6 mg of formamidine iodide (FAI), 750.3 mg of lead iodide (PbI_2), 17.3 mg of methyl ammonium bromide (MABr), 20.9 mg of methyl ammonium chloride (MACl), and 20.1 mg of cesium iodide (CsI) in1ml of N, N-dimethyl formamide (DMF)/dimethyl sulfoxide (DMSO) (4:1 v/v) mixed solvent. The perovskite solution was deposited by two-step spin-coating process of 2000 rpm for 10 s and 6000 rpm for 30 s. During the second step, 150 μL of CB as antisolvent was quickly dripped onto the center of perovskite film 15 s before the end of spin-coating process and then annealed at 120 °C for 20 min. PEAI with concentration of 2.5 mg/ml in isopropyl alcohol solution (35 μL) was dynamically spin-coated on top (3000 rpm, 20 s) and annealed at 100 °C for 5 min. After that, the PCBM and C_{60} mixed solution[3,4] (25 mg mL^{-1}, 4/1, w/w, 1mL CB) was spin-coated on the PEAI at speed of 4000 rpm for 30 s. The thickness of the ETL is approximately 45 nm. Next, BCP was spin coated on it at 4000 rpm for 30 s. Finally, an Ag electrode (90 nm) was thermal evaporated (under a vacuum condition of <10^{-5} Pa) using a shadow mask to complete the fabrication. When measuring, a 0.0625 cm^2 non-reflective mask was used to define the accurate active cell area.

10. Photovoltaic performances.

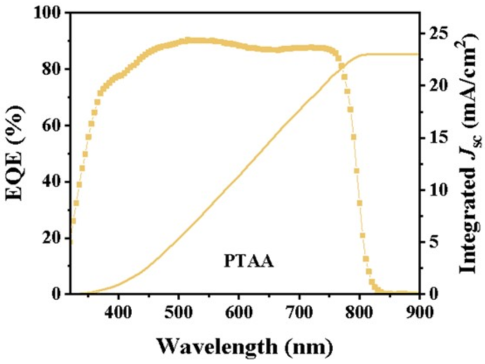


Fig. S20. EQE spectra of PTAA device and the integrated J_{sc} curve.

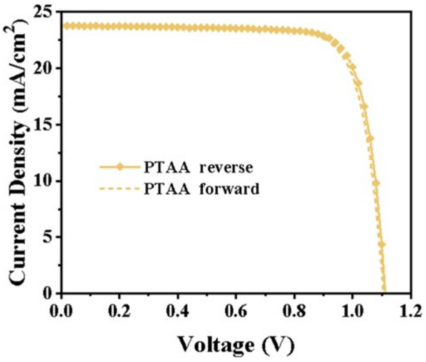


Fig. S21. *J-V* curve of forward scan and reverse scan of the device with PTAA as HTL.

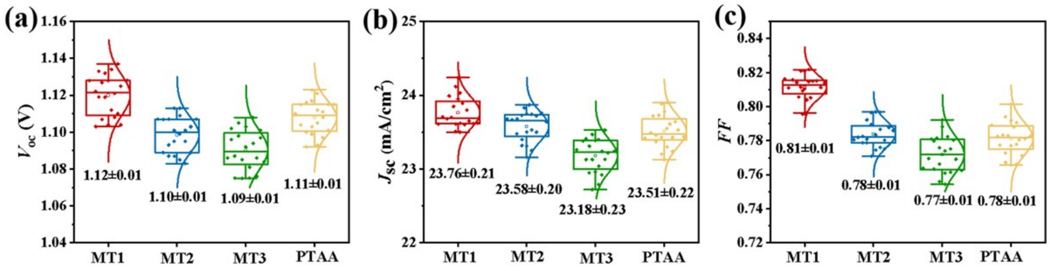


Fig. S22. Statistical distribution of a) V_{oc}, b) J_{sc}, and c) *FF* based on 20 independent devices.

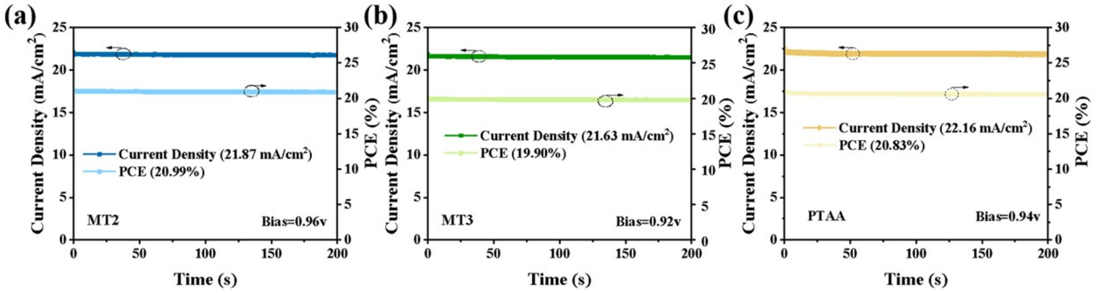
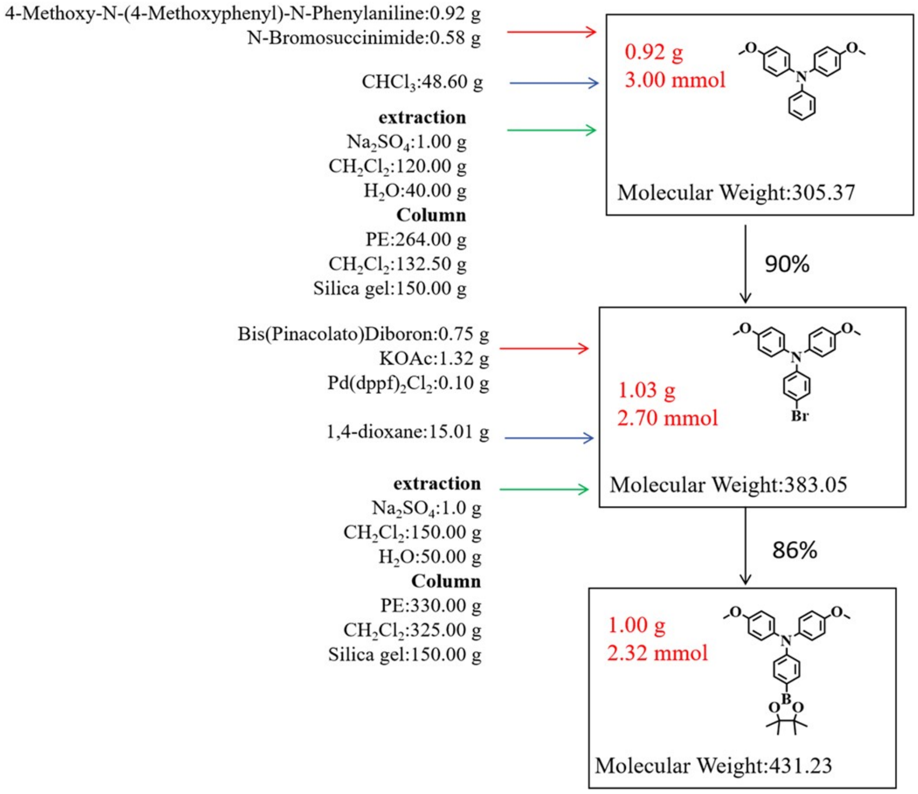


Fig. S23. Stable PCE and current density based on a) MT2, b) MT3 and c) PTAA device.

11. Cost analysis.

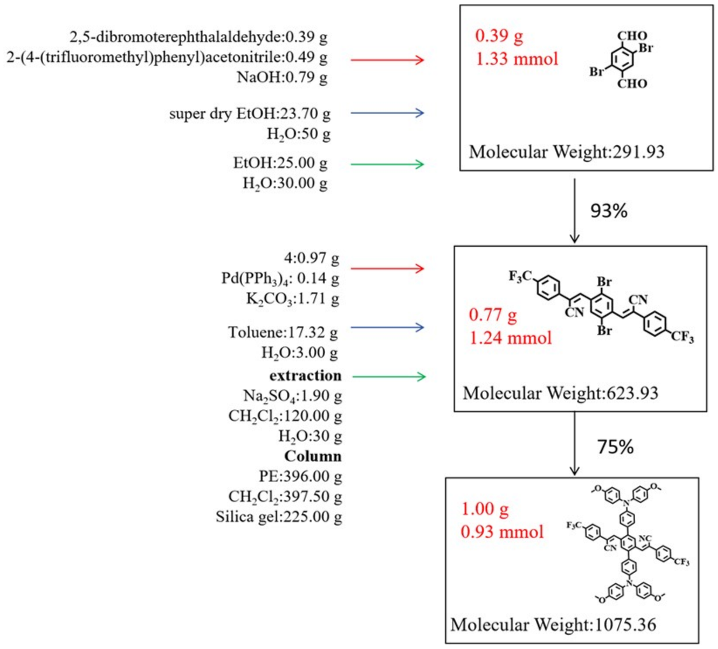
We have roughly estimated the synthesis costs of 1 gram of MT1, MT2, and MT3 based on the cost model that were reported previously[5,6]. The estimated synthesis costs of MT1, MT2, and MT3 are approximately ¥133.08, ¥147.87, and ¥138.82 per gram, equivalent to \$18.33, \$20.37, \$19.12 per gram, respectively.



Synthetic routes of 1 gram of molecule 4

Materials quantities and cost for the synthesis of molecule 4

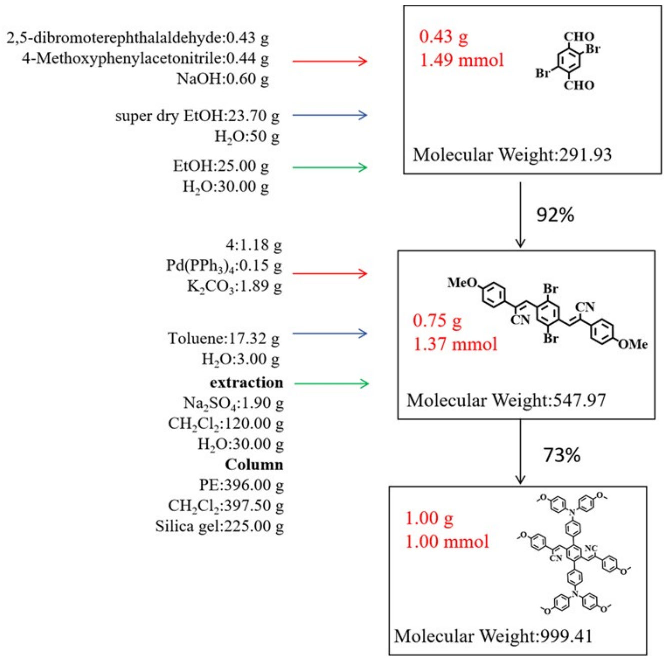
Chemical name	**Weight reagent (g/g)**	**Weight solvent (g/g)**	**Weight workup (g/g)**	**Price of Chemical (¥/kg)**	**Material cost (¥/g product)**	**Cost per step (¥/step)**
4-Methoxy-N-(4-Methoxyphenyl)-N-Phenylaniline	0.92			10040.00	9.24	25.19
N-Bromosuccinimide	0.58			66.00	0.04	
Trichloromethane		48.60		32.00	1.55	
Na_2SO_4			1.00	44.28	0.04	
Dichloromethane			120.00	11.00	1.32	
Water			40.00	-	-	
Petroleum ether			264.00	15.30	4.04	
Dichloromethane			132.50	11.00	1.46	
Silica gel			150.00	50.00	7.5	
Bis(Pinacolato)Diboron	0.75			700.00	0.53	36.65
KOAc	1.32			100.00	0.13	
$Pd(dppf)_2Cl_2$	0.10			164065.00	16.40	
1,4-dioxane		15.01		118.00	1.77	
Na_2SO_4			1.00	44.28	0.04	
Dichloromethane			150.00	11.00	1.65	
Water			50.00	-	-	
Petroleum ether			330.00	15.30	5.05	
Dichloromethane			325.00	11.00	3.58	
Silica gel			150.00	50.00	7.5	
Total	**3.67**	**63.61**	**1713.5**			**61.84**



Synthetic route of 1 gram MT1

Materials quantities and cost for the synthesis of MT1

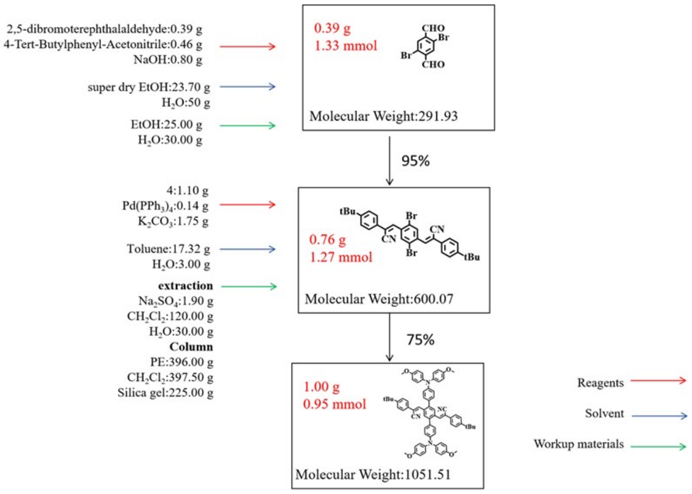
Chemical name	**Weight reagent (g/g)**	**Weight solvent (g/g)**	**Weight workup (g/g)**	**Price of Chemical (¥/kg)**	**Material cost (¥/g product)**	**Cost per step (¥/step)**
2,5-dibromoterephthalaldehyde	0.39			99760.00	38.91	44.68
2-(4-(trifluoromethyl)phenyl) acetonitrile	0.49			5680.00	2.78	
NaOH	0.79			38.25	0.03	
super dry EtOH		23.70		104.00	2.46	
Water		50.00		-	-	
EtOH			25.00	20.00	0.50	
Water			30.00	-	-	
4	0.97			61840.00	59.98	88.40
$Pd(PPh_3)_4$	0.14			34950.00	4.89	
K_2CO_3	1.71			40.00	0.07	
Toluene		17.32		27.00	0.47	
Water		3.00		-	-	
Na_2SO_4			1.90	44.28	0.08	
Dichloromethane			120.00	11.00	1.32	
Water			30.00	-	-	
Petroleum ether			390.00	15.30	5.97	
Dichloromethane			397.50	11.00	4.37	
Silica gel			225.00	50.00	11.25	
Total	**4.49**	**91.02**	**1219.40**			**133.08**



Synthetic route of 1 gram MT2

Materials quantities and cost for the synthesis of MT2

Chemical name	**Weight reagent (g/g)**	**Weight solvent (g/g)**	**Weight workup (g/g)**	**Price of Chemical (¥/kg)**	**Material cost (¥/g product)**	**Cost per step (¥/step)**
2,5-dibromoterephthalaldehyde	0.43			99760.00	42.90	46.03
4-Methoxyphenylacetonitrile	0.44			344.00	0.15	
NaOH	0.60			38.25	0.02	
super dry EtOH		23.70		104.00	2.46	
Water		50.00		-	-	
EtOH			25	20.00	0.5	
Water			30	-	-	
4	1.18			61840.00	72.97	101.84
$Pd(PPh_3)_4$	0.15			34950.00	5.24	
K_2CO_3	1.89			40.00	0.08	
Toluene		17.32		27.00	0.47	
Water		3.00		-	-	
Na_2SO_4			1.90	44.28	0.08	
Dichloromethane			120.00	11.00	1.32	
Water			30.00	-	-	
Petroleum ether			396.00	15.30	6.06	
Dichloromethane			397.50	11.00	4.37	
Silica gel			225.00	50.00	11.25	
Total	**4.69**	**91.02**	**1225.40**			**147.87**



Synthetic route of 1 gram MT3

Materials quantities and cost for the synthesis of MT3

Chemical name	**Weight reagent (g/g)**	**Weight solvent (g/g)**	**Weight workup (g/g)**	**Price of Chemical (¥/kg)**	**Material cost (¥/g product)**	**Cost per step (¥/step)**
2,5-dibromoterephthalaldehyde	0.39			99760.00	38.91	42.29
4-Tert-Butylphenyl-Acetonitrile	0.46			850	0.39	
NaOH	0.80			38.25	0.03	
super dry EtOH		23.70		104.00	2.46	
Water		50		-	-	
EtOH			25	20.00	0.5	
Water			30	-	-	
4	1.10			61840.00	68.02	96.53
$Pd(PPh_3)_4$	0.14			34950.00	4.89	
K_2CO_3	1.75			40.00	0.07	
Toluene		17.32		27.00	0.47	
Water		3.00		-	-	
Na_2SO_4			1.90	44.28	0.08	
Dichloromethane			120.00	11.00	1.32	
Water			30.00	-	-	
Petroleum ether			396.00	15.30	6.06	
Dichloromethane			397.50	11.00	4.37	
Silica gel			225.00	50.00	11.25	
Total	**4.64**	**94.02**	**1225.40**			**138.82**

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