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Introduction

Organic solar cells have received intensive scientific research because of their low-cost, light-weight, mechanical flexibility, roll-to-roll production and the tunable chemical properties of the photovoltaic materials.^{1,2} In the past decades, numbers of scientific researchers have been trying to find an active layer molecule incorporating good solution processability, fine charge carrier mobility, wide optical absorption profile, large absorption coefficient, and appropriate energy band.^{3,4} So far, much of the research effort has been devoted to the design and synthesis of multifused aromatic molecules, such as benzodithiophene (BDT)⁵ and its derivatives, which are excellent building blocks to synthesize organic photovoltaic materials. As shown in Scheme 1, the extended π -conjugation system of naphthodithiophene (NDT)⁶⁻⁹ is expected to afford strong intermolecular orbital overlap and their electron-donating properties have been recently reported for highly efficient solution-processed organic solar cells.¹⁰⁻¹³ Anthradithiophene (ADT), in which two thiophenes are fused to the ends of the anthracene core, have been widely utilized as key building blocks in the development of superior organic semiconductors applicable to organic electronic devices such as organic field effect transistors (OFETs)¹⁴ and displayed high

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Anthradithiophene-benzothiadiazole-based small

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A new A–D–A small molecule involving anthradithiophene as a donor and benzothiadiazole as an acceptor unit has been synthesized by Stille coupling reaction. Its thermal, optical and electronic properties, hole mobility and photovoltaic properties have been fully characterized. The resulting material shows a broad absorption range (300–750 nm), a low band gap (1.59 eV) and a moderate hole mobility (8.81 \times 10⁻⁴ cm² V⁻¹ s⁻¹). We used the new small molecule blended with PC₇₁BM as the

active layer to fabricate solution-processed organic solar cells (OSCs), and employed a variety of post-

treatment methods to optimize the device performance. With the help of polar solvent exposure, the highest power conversion efficiency (PCE) of 0.55% was obtained. These results would supply useful

information to understand the relationship between molecular structure and photovoltaic properties of

molecule donors for organic solar cells

anthradithiophene/benzothiadiazole-based OSCs.

Scheme 1 Chemical structures of acenedithiophene derivatives (BDT, NDT, and ADT).

hole mobility, broad absorption band and large conjugate plane,¹⁵ implying that ADT could be a promising donor building block applied in OSCs. Surprisingly, so far the OSC devices using the ADT-based polymers have only shown power conversion efficiencies (PCE) of less than 1%.¹⁶ Considering the above, we tried to develop small molecules based on ADT to expand its applications in OSCs. We report here on the synthesis, characterization, and photovoltaic properties of a novel small molecule material based on the 5,11-bis(5-alkylthiophen-2-yl)anthra[2,3-b:6,7-b']dithiophene moiety. In order to extend its conjugation and guarantee its good solubility, we introduced 2-(2-ethylhexyl)thiophene in the molecular structure (shown in Scheme 2). The extended π -conjugation system of ADT with alkylthiophene is expected to afford strong intermolecular orbital overlap and electron-donating properties by utilizing a favorable "push-pull" architecture. This could thereby enhance charge separation, transport, and energy level tunability. The thermal, optical and electronic properties were fully characterized. It has been indicated that this small molecule possesses good

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Scheme 2 Synthesis of ADT(DPBT)₂. Reagents and conditions: (a) 1,4-cyclohexanedione–ethanol–15% aq KOH; (b) 2-(2-ethylhexyl)thiophene–*n*-BuLi–THF, -78 °C; (c) *n*-BuLi–trimethylstannylchloride, -78 °C; (d) bis(4-*tert*-butylphenyl)amine–4,7-dibromobenzo[c][1,2,5]thiadiazole–palladiumacetate–tri-*t*-butylphosphine–sodium-*t*-butoxide; (e) anhydrous toluene–DMF–Pd(PPh₃)₄.

solubility, high thermal stability, broad absorption band and moderate hole mobility. Moreover, by adjusting the ratio of small molecules and $PC_{71}BM$, changing the annealing temperature and exposing the active layer to different polar solvents, the highest PCE of 0.55% was achieved. But the result did not show its good properties, so we compared the reported molecules and discussed the possible reasons of the unexpected results.

Experimental

General

¹H and ¹³C NMR spectra were recorded with a Bruker DMX-400 spectrometer. Differential scanning calorimeter (DSC) was measured using a Metler Toledo DSC822 instrument, and thermogravimetric analysis (TGA) was determined by a PerkinElmer Pyris. UV-visible absorption spectra were collected on a PerkinElmer Lambda 950. Cyclic voltammetry (CV) of the polymer film was studied on a CHI650B potentiostat. Surface images were obtained on a Veeco Dimension 3100V atomic force microscope. Solvents for reactions and photophysical measurements were all distilled after dehydration according to conventional methods.

Materials

Compound **1** was synthesized according to the literature.¹⁷ Other compounds were synthesized as following:

Synthesis of compound 2. To a solution of 2-(2-ethylhexyl)thiophene (2.42 g, 10.20 mmol) in 80 mL of dry THF cooled to -78 °C under an argon atmosphere, was added dropwise 4.25 mL of *n*-BuLi (2.4 M in hexane) and the mixture was stirred for 30 min. Then compound 1 (1.0 g, 3.09 mmol) was added in one portion. After another 30 min, the mixture was moved to room temperature and stirred until the complete dissolution of compound 1. Finally, the mixture was protected from the light and SnCl₂·2H₂O (6.3 g, 28 mmol) in HCl (10%, 11.2 mL) was added, and the mixture was stirred for another 3 h. The mixture was quenched with 15 mL ice water and extracted by ethyl acetate three times. The organic phases were dried with anhydrous MgSO₄ and evaporated. The crude product was purified by column chromatography on silica gel (petroleum ether) to give compound 3 as a red solid (1.61 g, 78%). ¹H NMR (CDCl₃, 400 MHz, δ /ppm): 8.45 (s, 2H), 8.40 (s, 2H), 7.42 (d, 2H), 7.28 (d, 2H), 7.10 (s, 2H), 7.04 (s, 2H), 2.96 (m, 4H), 1.76 (m, 2H), 1.56–1.33 (br, 16H), 1.04–0.92 (m, 12H). ¹³C NMR (CDCl₃, 100 MHz, δ /ppm), δ = 154.73, 153.64, 151.56, 145.10, 144.27, 134.90, 127.72, 126.82, 125.20, 124.05, 123.24, 117.52, 117.17, 34.34, 32.40, 29.74, 28.86, 25.63, 23.01, 14.15, 10.82.

Synthesis of compound 3. Under an argon atmosphere, a solution of compound 2 (1.5 g, 2.24 mmol) in 60 mL of dry THF cooled to -78 °C, *n*-BuLi (1.03 mL, 2.46 mmol, 2.4 M in hexane) was added dropwise. After stirring for 1 h, the mixture was brought to room temperature. The stirring was continued for another hour, and then the reaction mixture was cooled to -78 °C again. A solution of trimethylstannyl chloride (0.49 g, 2.46 mmol) was added in one portion. The mixture was slowly warmed up to room temperature and stirred overnight. The reaction mixture was quenched with 30 mL water and extracted by ethyl acetate three times. The organic phases were dried with anhydrous MgSO4 and evaporated to afford a red crude solid. The crude product was purified by recrystallization with ethanol to yield a red solid (1.54 g, 55%). ¹H NMR (CDCl₃, 400 MHz, δ/ppm): 8.45 (s, 2H), 8.39 (s, 2H), 7.19–7.10 (d, 2H), 7.05-7.04 (d, 2H), 3.00-2.95 (t, 4H), 1.79-1.75 (m, 2H), 1.54-1.40 (m, 16H), 1.05–0.96 (m, 12H), 0.51–0.37 (m, 18H). ¹³C NMR (CDCl₃, 100 MHz, δ /ppm), δ = 146.23, 145.20, 141.73, 140.15, 137.28, 131.80, 129.51, 129.35, 129.16, 128.83, 125.18, 119.40, 118.25, 41.57, 34.49, 32.59, 29.02, 26.01, 23.09, 14.26, 11.04.

Synthesis of compound 4. Bis(4-tert-butylphenyl)amine (1.5 g, 5.34 mmol), 4,7-dibromobenzo[c][1,2,5]thiadiazole (1.57 g, 5.34 mmol), palladium acetate (0.03 g, 0.13 mmol), and tri-tbutylphosphine (0.55 g, 2.67 mmol), sodium-t-butoxide (0.65 g, 6.68 mmol) were dissolved in a flask with anhydrous toluene under a nitrogen atmosphere. The reaction mixture was stirred for 12 h at 100 °C. The mixture were extracted with dichloromethane and washed with distilled water three times. The organic laver was dried over anhydrous MgSO4 and evaporated to give the crude product, and the crude product was purified by column chromatography to yield a light-red powdery product (1.43 g, 54%). ¹H NMR (acetone, 400 MHz, δ /ppm): 7.86–7.84 (d, 1H), 7.35-7.33 (d, 4H), 7.03-7.01 (d, 1H), 6.99-6.97 (d, 4H), 1.3 (s, 18H). ¹³C NMR (CDCl₃, 100 MHz, δ /ppm): δ = 154.59, 150.56, 146.52, 144.86, 140.28, 132.58, 126.09, 123.74, 122.54, 106.53, 53.43, 34.35, 31.41.

Synthesis of the ADT(DPBT)₂. Compound 3 (1.00 g, 0.80 mmol) and compound 4 (0.82 g, 1.65 mmol), $Pd(PPh_3)_4$ (0.10 mg, 8.0 \times 10⁻⁵ mmol) were dissolved in a flask with anhydrous toluene (20 mL) and DMF (5 mL). The flask was evacuated and refilled with argon three times. Then the mixture was heated to 120 °C and stirred for 48 h under an argon atmosphere. Then, the reactant was cooled to room temperature and poured slowly into methanol (150 mL). The precipitate was filtered to obtain a purple solid and further purified by column chromatography and recrystallized with methanol to yield a purple-dark powdery product (0.56 g, 46.8%). ¹H NMR (CDCl₃, 400 MHz, δ /ppm): 8.56 (s, 2H), 8.43–8.42 (d, 2H), 8.37 (s, 2H), 7.75-7.73 (s, 2H), 7.31-7.29 (d, 8H), 7.15-7.14 (t, 2H), 7.12 (s, 2H), 7.08-7.06 (m, 2H), 7.03-7.00 (d, 8H), 3.03-2.99 (m, 4H), 1.83-1.79 (m, 2H), 1.35 (d, 36H), 1.57-1.43 (m, 16), 1.07–0.98 (m, 12H). ¹³C NMR (CDCl₃, 100 MHz, δ /ppm): δ = 153.84, 151.00, 146.70, 146.37, 144.89, 141.62, 141.48, 140.61, 136.99, 129.90, 129.76, 129.46, 129.10, 126.08, 125.21, 124.10, 123.64, 121.41, 121.01, 118.41, 41.56, 34.56, 34.38, 32.62, 31.42, 29.69, 29.01, 26.07, 23.08, 14.25, 11.04. Elemental analysis (%) calcd for C₉₄H₁₀₀N₆S₆: C, 74.94; H, 6.69; N, 5.58. Found: C, 75.18; H, 6.55; N, 5.37.

Device fabrication

OSCs were fabricated on the basis of ITO/PEDOT:PSS/ ADT(DPBT)₂:PC₇₁BM/Ca/Al configuration and their performances were measured in an argon glovebox (200B, MBraun) under an AM 1.5 Solar Constant 575 PV simulator (Steuernagel Lichttecknik, equipped with a metal halogenide lamp). The ITO electrodes (10 Ω per square, Kintec Company) were cleaned in ultrasonic baths and then modified by a 40 nm thick spin-cast layer of PEDOT/PSS "Clevios P VP AI 4083" (HC Stark), which was dried at 130 °C for 20 min. The Clevios suspension was stirred and filtered through a 0.45 mm membrane (Minisart RC 15, Sartorius) just prior to casting. Active layer ADT(DPBT)₂/PC₇₁BM was spin-coated on top of the PEDOT/PSS layer at 1000 rpm. A 20 nm thick layer of Ca and 100 nm Al were thermally evaporated through a shadow mask, at a pressure of about 10⁻⁶ mbar. The mask geometry defined a device area of 0.1257 cm².

Results and discussion

Synthesis

The synthetic routes of ADT(DPBT)₂ are outlined in Scheme 2. *n*-BuLi was added to a solution of 2-(2-ethylhexyl)thiophene in THF, then compound **1** and SnCl₂·2H₂O in HCl(aq) was added, finally the target product (compound 2) can be gained with extraction and purification by column chromatography in 78% yield. *n*-BuLi was added to a solution of compound **2** in THF, then trimethylstannyl chloride was added in one portion, and compound **3** can be got with extraction and purification by column chromatography in 55% yield. Compound **4** was synthesized by Buchwald–Hartwig cross-coupling reaction with a 54% yield, and ADT(DPBT)₂ was synthesized by Stille coupling reaction between compound **3** and compound **4** in 46.8% yield. All the compounds were verified by ¹H NMR and ¹³C NMR. ADT(DPBT)₂ is readily soluble in common organic solvents such as chloroform, chlorobenzene and dichlorobenzene.

Thermal properties

The thermal properties of ADT(DPBT)₂ were analyzed by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) under a nitrogen atmosphere at a heating rate of 10 °C min⁻¹. The TGA analysis reveals that the 5% weight-loss temperature (T_d) of ADT(DPBT)₂ is 414 °C (Fig. 1a). This indicates that ADT(DPBT)₂ has good thermal stability, which is very important in the device fabrication process and other kinds of applications. DSC analysis (Fig. 1b) reveals that ADT(DPBT)₂ possesses a prominent melting temperature (T_m) at 247.4 °C and a distinct glass transition temperature (T_g) at 172.0 °C, though no obvious crystallization point was observed.

Optical properties

The UV-Vis absorption spectra of $ADT(DPBT)_2$ in diluted chloroform solution and in thin film are shown in Fig. 2. It exhibits relatively broad and strong absorption between 300 and 650 nm for the solution. The absorption maximum at 527 nm should result from an intramolecular charge transfer (ICT) between the electron-rich unit (ADT) and the electron-deficient unit (BT). The absorption in the thin film state showed a similar absorption trend with a red shift of about 3 nm, and exhibited broader absorptions than its corresponding absorption in solution. The optical band gap calculated from the film absorption edge is 1.69 eV.



Fig. 1 Thermogravimetric analysis (TGA) of ADT(DPBT)₂ performed at a heating rate of 10 $^{\circ}$ C min⁻¹ under a nitrogen atmosphere.



Fig. 2 UV-Vis absorption spectra of $ADT(DPBT)_2$ in diluted chloroform solution and in thin film.

Electrochemical properties

Cyclic voltammetry (CV) was employed to examine the electrochemical properties and evaluate HOMO and LUMO energy levels of the polymers. Fig. 3 shows the CV curves of ADT(DPBT)₂ with a platinum plate as working electrode and Ag/Ag⁺ as reference electrode in acetonitrile with a 0.1 M solution of Bu₄NPF₆ at room temperature with a scanning rate of 50 mV s⁻¹. For calibration, the redox potential of ferrocene/ ferrocenium (Fc/Fc⁺) was measured under the same conditions, and it is located at 0.40 eV to the Ag/AgCl electrode. It is assumed that the redox potential of Fc/Fc⁺ has an absolute energy level of -4.80 eV under vacuum.¹⁸ The HOMO and LUMO energy levels were calculated according to the following equations:¹⁹

$$E_{\rm HOMO} = -(E_{\rm on}^{\rm ox} + 4.4) \, {\rm eV}$$
 (1)

$$E_{\rm LUMO} = -(E_{\rm on}^{\rm red} + 4.4) \,\,\mathrm{eV} \tag{2}$$

$$E_{g}^{ec} = -(E_{HOMO} - E_{LUMO}) eV$$
(3)

The oxidation and reduction onset potentials of $ADT(DPBT)_2$ are 0.81 and -0.78 eV, respectively. The HOMO and LUMO energy levels can be calculated as -5.21 eV and -3.62 eV, respectively. The relatively deep HOMO level of $ADT(DPBT)_2$ indicates its relatively high stability against oxidation and is beneficial for obtaining high V_{OC} when using PCBM as the acceptor. The corresponding electrochemical bandgap is 1.59 eV, which is similar to the optical band gap. The HOMO and LUMO energy levels of the ADT(DPBT)_2 are illustrated in Fig. 4.



Fig. 3 CV of ADT(DPBT)_2 films cast on platinum wire in 0.1 M Bu_4NPF_6/CH_3CN at a scan rate of 100 mV s $^{-1}$.



Fig. 4 Energy diagram of the HOMO–LUMO energy levels for ADT(DPBT)₂ and $PC_{71}BM$.

Hole mobility

As an important parameter of small molecules for photovoltaic applications, the hole mobility of ADT(DPBT)₂ was investigated by the space-charge-limited current (SCLC) model with a device structure of ITO/PEDOT:PSS/ADT(DPBT)₂:PC₇₁BM (90 nm)/Au.²⁰ For the hole-only devices, SCLC is described by modified Mott–Gurney's law:

$$J = (9/8)\varepsilon_0\varepsilon_r \mu(V^2/d^3) \exp[0.89\beta\sqrt{V/d}]$$

$$\ln(Jd^3/V^2) \cong 0.89\beta(V/d)^{1/2} + \ln(9\varepsilon_0\varepsilon_r\mu/8)$$

The results are plotted as $\ln(Jd^3/V^2)$ versus $(V/d)^{1/2}$, as shown in Fig. 5. *J* stands for current density, *d* is the thickness of the active layer, *V* is the applied potential, ε_0 is the relative dielectric constant of the blend (assuming that 3.5), ε_r is the permittivity of free space (8.85×10^{-12} C V⁻¹ s⁻¹), β is the field activation factor and μ is the hole mobility. The hole mobility of ADT(DPBT)₂ is evaluated to be 8.81×10^{-4} cm² V⁻¹ s⁻¹. Obviously, the hole mobility of ADT(DPBT)₂ is moderate as the photovoltaic donor material in small-molecule BHJ solar cells.²¹

Theoretical calculations

To gain more insight into the geometrical and electronic properties of the ADT(DPBT)₂, density functional calculations were conducted using the B3LYP/6-31G* basis and Gaussian 03 program package. To simplify the calculations, the two 2-ethylhexyl substituents on the thiophene unit and the four 1-*tert*-butyl substituent on the benzene unit were replaced by methyl groups. The frontier molecular orbitals of the ADT(DPBT)₂ are shown in



Fig. 5 $\ln(ld^3/V^2)$ versus $(V/d)^{1/2}$ plots of ADT(DPBT)₂ for the measurement of hole mobility by the SCLC method for the device ITO/PEDOT:PSS/ADT(DPBT)₂: PC₇₁BM/Au.



Fig. 6 Frontier molecular orbitals of the ADT(DPBT)₂. LUMO (top) and HOMO (bottom).

Fig. 6. The dihedral twist angle between the central ADT core and the benzothiadiazole bridge unit obtained from the optimized geometry of the small molecule is 13°, illustrating that the A–D–A π -conjugated system is a quasi-planar conjugated system. The molecular orbitals show that the HOMO is essentially localized on the ADT core, in contrast, as the LUMO is distributed over the entire A–D–A π -conjugated system. The calculated energy levels (HOMO = -4.40 eV, LUMO = -2.48 eV) are considerably higher than experimental data, but it should be underlined that solvent effects are neglected in calculation.²²

Photovoltaic properties

The photovoltaic properties were investigated with the conventional device structure as follows: ITO/PEDOT:PSS/ADT(DPBT)2:PC71BM/ Ca/Al. Herein we selected PC71BM instead of PC61BM as the electron acceptor to get better absorption in the visible range, and fabricated a large number of devices under various conditions, such as different weight ratios of ADT(DPBT)₂/PC71BM, changing the annealing temperature and employing a variety of polar solvent, etc. The I-V curves and I-V parameters of the OSCs based on ADT(DPBT)₂/PC₇₁BM under the illumination of AM 1.5G, 100 mW cm^{-2} are shown in Fig. 7 and Table 1. As shown in Table 1, a 1:1 ratio of ADT(DPBT)₂-PC₇₁BM gave a performance of the OSCs with a $J_{\rm SC}$ of 1.55 mA cm⁻², a $V_{\rm OC}$ of 0.69 V and a PCE of 0.26% and after 10 min of the thermal treatment at 150 °C, approximately 1.5 times higher PCE (0.39%) was obtained. In order to further improve the performance of the OSCs, three different polar solvents were used to optimize the morphology of the active layer.²³ The procedure was as follows: after the active layer was spin-coated, 0.2 mL polar solvent was added dropwise on the active layer and removed by spin coating. With the help of polar solvent treatment, a large increase of J_{SC} and V_{OC} were obtained and we got the highest PCE of 0.55% after the ethanol treatment.

This relatively low PCE did not reflect its superior properties, which were out of our expectation. The related research of Jiang *et al.*²⁴ also presented a similar phenomenon in which polymers with a high hole mobility did not show high efficiency.





Fig. 7 *J–V* characteristics of the OSCs based on ADT(DPBT)₂/PC₇₁BM under the illumination of AM 1.5G, 100 mW cm⁻². (a) Prepared with different weight ratios of ADT(DPBT)₂/PC₇₁BM; (b) treated with different annealing temperature; (c) exposed with different polar solvents. *J–V* characteristics of the OSCs in the dark.

 Table 1
 J--V parameters for the ADT(DPBT)₂:PC71BM OSCs with different weight ratio or treatments

Weight ratio (wt%)	Treatment	$V_{\rm OC}$ (V)	$J_{ m SC} \ ({ m mA~cm^{-2}})$	FF (%)	PCE (%)
2:1	None	0.67	0.93	25.22	0.18
1:2	None	0.75	0.94	24.93	0.19
1:1	None	0.69	1.55	24.38	0.26
1:1	120 °C annealed	0.64	1.54	25.04	0.25
	150 °C annealed	0.66	2.26	26.23	0.39
	180 °C annealed	0.61	1.69	26.94	0.28
1:1	MeOH exposed	0.80	2.38	25.52	0.49
	EtOH exposed	0.80	2.58	26.43	0.55
	i-PrOH exposed	0.73	2.38	26.53	0.46

Zhong *et al.*²⁵ had proved that a mixture of *syn* and *anti* isomers in the active layer led to a lower PCE than pure *syn* isomers; they held the opinion that *anti* isomers behave essentially as inactive impurities, forming poorly-functioning crystalline domains that hinder charge transport. We believe that the traditional synthesis of



Fig. 8 Tapping-mode AFM topography images (left) and 3D surface plots (right) of the blend film of ADT(DPBT)₂–PC₇₁BM (1:1, w/w): (a) without any treatment; (b) annealed at 150 °C; (c) exposed to ethanol (all images: 5.0 μ m × 5.0 μ m).

the ADT inevitably afforded an inseparable mixture of *syn* and *anti* isomers resulting in undefined molecular conformation,²⁶ and the existence of the two isomers led to the irregular state of aggregation and invalid phase separation so as to affect the electron and hole transfer which may be the main reason for the low power conversion efficiency.

Morphology

As a very important factor to affect the performance of OSCs, the morphological features of the photoactive layer were studied by tapping-mode atomic force microscopy (AFM). The AFM topography and 3d surface plots are shown in Fig. 8. It could be observed that the blend films exhibited uneven surfaces with a lot of peak-like spikes with a root-mean-square (RMS) roughness of 0.332 nm, which could have a side effect on the exciton separation, thus leading to a lower J_{SC} and PCE. When the blend films were annealed at 150 °C or exposed with ethanol, the root-mean-square (RMS) roughness decreases to 0.276 nm for ADT(DPBT)₂: PC71BM (1:1, w/w, annealed at 150 °C) and 0.251 nm for ADT(DPBT)2:PC71BM (1:1, w/w, exposed with ethanol), and led to a 1.5-3 times increase in I_{SC} and PCE compared with the devices without any treatment. As shown in the images, morphologies of the blend films were moderately homogenous and there was no large phase separation, indicating that both of the small molecules possessed good miscibility with PC₇₁BM,²⁷ which is not favorable for electron and hole transfer and may be another reason for the low power conversion efficiency.

Conclusions

We have successfully synthesized a new A–D–A small molecule $ADT(DPBT)_2$ involving anthradithiophene as donor block and

benzothiadiazole as acceptor unit by Stille coupling reaction, and its thermal, optical and electronic properties, hole mobility and photovoltaic properties have been fully characterized. We used $ADT(DPBT)_2$ blending with $PC_{71}BM$ as the active layer to fabricate solution-processed OSCs and employed thermal annealing and polar solvent treatment to optimize the device performance. After exposure to polar solvents, the highest PCE of 0.55% was obtained due to the optimized morphology of the active layer, and the relatively low efficiency may be caused by the existence of the two isomers. Though the device parameters were not ideal, these results would supply useful information to design, optimize and understand the relationship between molecular structure and photovoltaic properties of anthradithiophene/benzothiadiazole-based OSCs.

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