



High-performance organic solar cells based on a small molecule with thieno [3,2-*b*]thiophene as π -bridge

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ABSTRACT

Herein, we synthesized a new acceptor- π -donor- π -acceptor (A- π -D- π -A) type small molecule donor material **BTTR** based on thienyl-substituted benzo[1,2-*b*:4,5-*b'*]dithiophene (BDT-T) as the electron-donating core, thieno [3,2-*b*]thiophene (TT) along with two thiophene units as the π -bridge, and 3-ethylrhodanine (TR) as the electron-deficient end group. The optical, electrical, thermal properties and photovoltaic performance were investigated. **BTTR** shows strong absorption in the range of 300–700 nm, deep-lying HOMO energy level of -5.32 eV and high hole mobility of 1.01×10^{-3} cm² V⁻¹ s⁻¹. The organic solar cells (OSCs) based on **BTTR**:PC₇₁BM (1:0.8, w/w) blend with tetrahydrofuran (THF) solvent vapor annealing (SVA) exhibited an optimized power conversion efficiency (PCE) of 8.0% with an open circuit voltage (V_{oc}) of 0.93 V, a short circuit current density (J_{sc}) of 13.2 mA cm⁻², and a fill factor (FF) of 65.4% under the illumination of AM 1.5G, 100 mW cm⁻². The good photovoltaic performance indicates **BTTR** could be a promising donor material in solution-processed OSCs.

1. Introduction

As a competitive technology of green energy, solution-processed bulk-heterojunction (BHJ) organic solar cells (OSCs) have attracted great attention due to their unique advantages of low cost, light weight, large-area fabrication, solution processability and mechanical flexibility [1–11]. Compared to the polymer counterparts, small-molecule (SM) donor materials have many unique characters including versatile molecular structures, well-defined molecular weight, tunable molecular energy level and less batch-to-batch variation [11–15], so the SM-OSCs are an attractive alternative to polymer-based solar cells (PSCs). Recently, the SM-OSCs have made a breakthrough [16–22], and the corresponding power conversion efficiencies (PCEs) over 10% have been achieved [19–24]. Although the SM-OSCs have made great progress, further efforts would be required to achieve higher photovoltaic performance for commercial applications. As the key component of the active layer, the rational design of SM donor materials will play a crucial role in improving the photovoltaic performance of the devices.

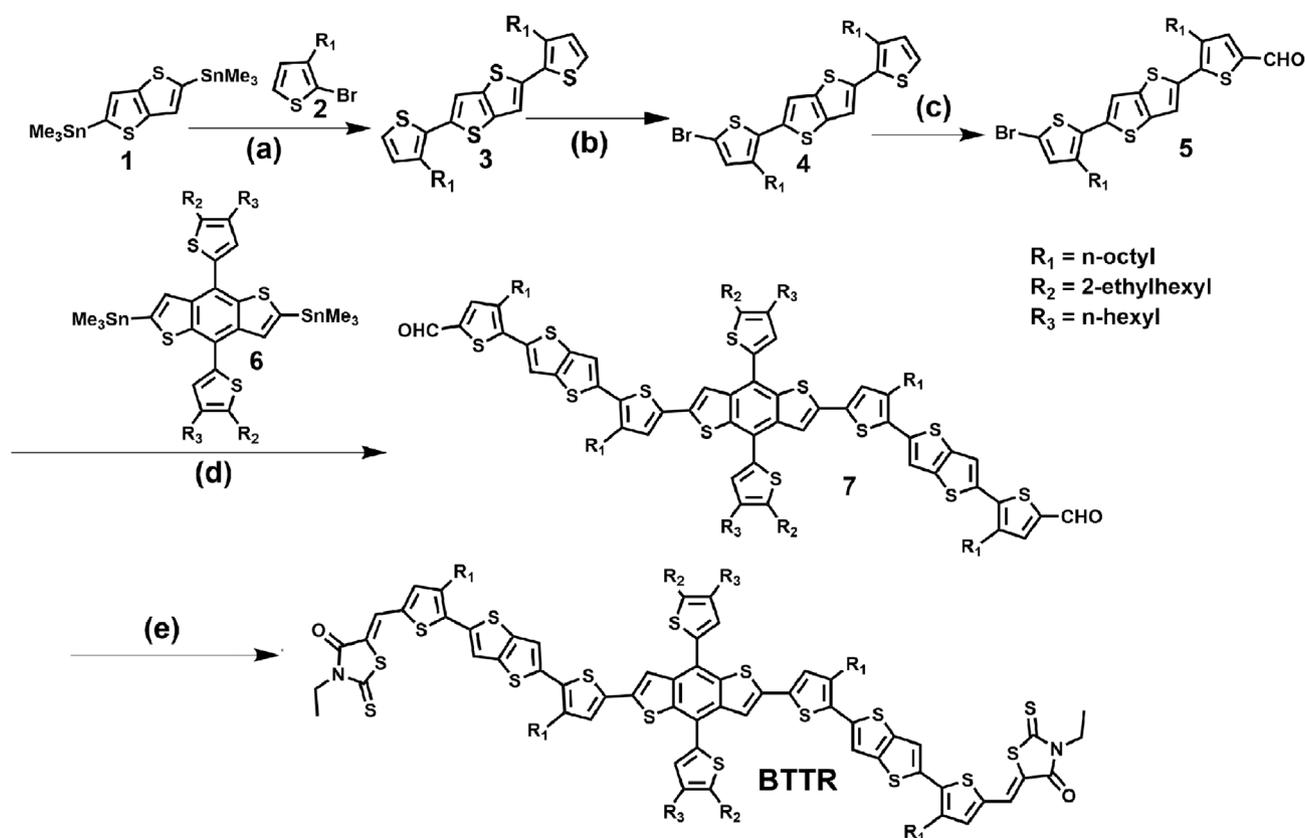
For the design of donor materials, it is essential to consider several issues altogether and maintain a delicate balance: good solubility, wide

absorption spectrum with high extinction coefficient, suitable energy levels, and high mobility [19,25]. Previous works have revealed that combining two electron-deficient end groups (acceptor) and an electron-rich central core (donor) to form acceptor-donor-acceptor (A-D-A) type of SM is one of the effective strategies to broaden absorption spectrum, tune energy levels and achieve high performance [26–28]. Among the various SM donor materials, the linear A-D-A-type SMs based on thienyl-substituted benzo[1,2-*b*:4,5-*b'*]dithiophene (BDT-T) as the electron-donating core [29–32], and alkyl-substituted terthiophene as π -bridge [24,26,32] with different end groups such as cyanoacetate (CA) [29–31], rhodanine (TR) [14–18,33], 1H-indene-1,3(2H)-dione [24,31,32] et al. have exhibited excellent photovoltaic performance. As is well known, the π -bridge plays an important role to enhance conjugation length and π - π stacking of SM materials, which leads to red-shifted absorption spectrum, good coplanarity, strong crystallinity and high charge carrier mobility [29,34,35]. Moreover, introducing thieno [3,2-*b*]thiophene (TT) unit as π -bridge has been proved to be an effective strategy to improve photovoltaic performance of conjugated polymers, resulting from the extended conjugated backbone and minus influence on the molecular energy levels [36,37]. However, it has been

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Scheme 1. Synthetic routes for the **BTTR**: (a) Pd(PPh₃)₄, toluene, 110 °C, 24 h; (b) NBS, CHCl₃/CH₃COOH (1:1), 0 °C then room temperature, 12 h; (c) POCl₃, DMF, 0 °C, 1 h, then 65 °C, 12 h; (d) Pd(PPh₃)₄, toluene, 110 °C, 24 h; (e) 3-ethylrhodanine, piperidine, CHCl₃, 75 °C, 12 h.

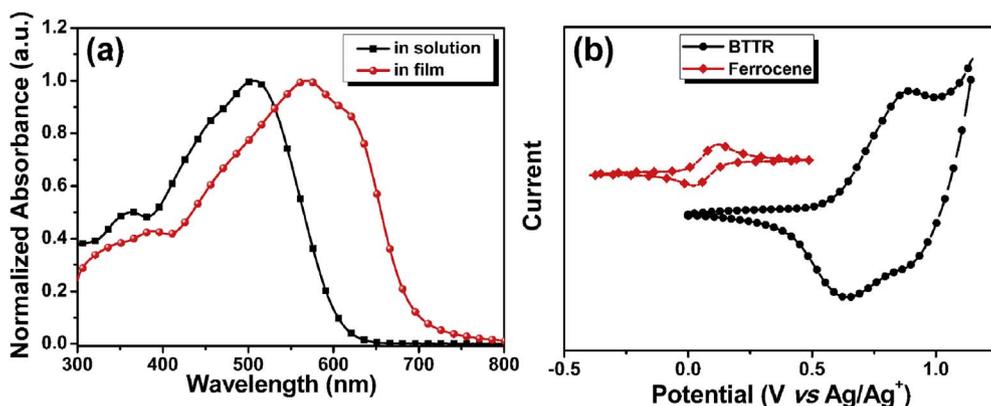


Fig. 1. (a) UV-vis absorption spectra of **BTTR** in CF solution and thin film and (b) cyclic voltammogram of **BTTR** film on a glassy carbon electrode measured in 0.1 mol L⁻¹ Bu₄NPF₆ acetonitrile solution at a scan rate of 50 mV s⁻¹.

seldom used in the design of SM donor materials [28,38,39].

Based on the above considerations, in this work, we synthesized a new two-dimensional (2D)-conjugated SM donor material **BTTR** (see [Scheme 1](#)) based on BDT-T as the electron-donating core, fused ring TT along with two thiophene units as the π -bridge, and TR as the electron-deficient end group. **BTTR** shows a superior solubility in common halogenated solvents such as chloroform (CF) and chlorobenzene (CB), strong absorption in the range of 300–700 nm, deep-lying the highest occupied molecular orbital (HOMO) energy level of -5.32 eV and high hole mobility of 1.01×10^{-3} cm² V⁻¹ s⁻¹. Moreover, the OSCs based on **BTTR** [6,6]-phenyl-C₇₁-butyric acid methyl ester (PC₇₁BM) (1:0.8, w/w) blend with tetrahydrofuran (THF) solvent vapor annealing (SVA) exhibited an optimized power conversion efficiency (PCE) of 8.0%, with an open circuit voltage (V_{oc}) of 0.93 V, a short circuit current density (J_{sc}) of 13.2 mA cm⁻², and a fill factor (FF) of 65.4% under the illumination of AM 1.5G, 100 mW cm⁻².

2. Results and discussion

The synthetic routes and molecular structure of **BTTR** are shown in [Scheme 1](#). The detailed synthesis and characterization data are provided in [Supporting Information \(SI\)](#). **BTTR** exhibits good solubility in general halogenated solvents such as CF and CB. Thermogravimetric analysis (TGA) was carried out to study the thermal stability of **BTTR**, and a high decomposition temperature (T_d) of 394 °C with 5% weight-loss was achieved as shown in [Fig. S1a](#). Differential scanning calorimetry (DSC) thermogram of **BTTR** (see [Fig. S1b](#)) exhibits three endothermic peaks at 203 °C, 226 °C and 236 °C, and three corresponding exothermic peaks at 189 °C, 218 °C and 232 °C, indicating the existence of crystalline structure.

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