



A crystalline D- π -A organic small molecule with naphtho[1,2-*b*:5,6-*b'*]dithiophene-core for solution processed organic solar cells

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ABSTRACT

In this work, we have designed and synthesized a new naphtho[1,2-*b*:5,6-*b'*]dithiophene-containing enlarged π -conjugated donor-acceptor (D-A) small molecule, **NDT(TTz)₂**, for use in solution-processed organic photovoltaics. **NDT(TTz)₂**, which contains a thiophene-bridged naphtho[1,2-*b*:5,6-*b'*]dithiophene as the central fused core and triphenylamine-flanked thiophene thiazolothiazole as a spacer, was synthesized via sequential Suzuki and Stille coupling reactions. The thermal, physicochemical, and electrochemical properties of **NDT(TTz)₂** have been evaluated by differential scanning calorimetry, thermogravimetry, UV-Vis spectroscopy, photoluminescence spectroscopy, X-ray diffraction, and cyclic voltammetry. As desired for photovoltaic applications, **NDT(TTz)₂** possesses good solubility, thermal stability, and a well-ordered, π - π stacked, crystallinity. The optical band gap and HOMO level of **NDT(TTz)₂** were determined to be 2.0 eV and -5.23 eV, respectively. In addition to organic thin film transistor studies, application of **NDT(TTz)₂** to preliminary photovoltaic devices has also been investigated by fabricating solution-processed bulk heterojunction solar cells together with PC₇₁BM in a typical layered device structure, ITO/PEDOT:PSS/**NDT(TTz)₂**:PC₇₁BM/LiF/Al. Without extensive optimization of the device, **NDT(TTz)₂** in these devices shows a maximum power conversion efficiency of 1.44% under AM 1.5 illumination at a 100 mW/cm² intensity.

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1. Introduction

Conjugated polymers with alternating donor-acceptor structures have been the subject of continued investigation in recent years as photoactive donor materials in bulk-heterojunction (BHJ) polymer solar cells (PSCs). They have received great attention due to their strong absorption ability, tunable energy levels and good film-forming properties [1–5]. Great progress has recently been seen by thorough structural and device optimization, with power conversion efficiency (PCE) of PSCs reaching as high

as 8.3% for conventional solar cell device structure and 9.2% for an inverted device structure [6].

By virtue of being promising alternative photoactive materials to conjugated polymers due to simple synthesis, monodispersity, and high purity, solution-processable π -conjugated D-A organic small molecules, particularly dendrimers or oligomers, have also concurrently received considerable attention in the recent literature for their applications to BHJ organic solar cells (OSCs) [7–9]. In particular, effort has been dedicated to the development of new small molecules that are solution processable over those that are vacuum-processed because of the promise of the more cost-effective solution-based solar cell device fabrication techniques. Although, D-A conjugated copolymers have proven to be efficient photoactive materials in BHJ

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devices with PCE reaching 8%, the development of solar cells composed of solution processable small molecules are still in their early stages. Typical small molecule solar cell PCEs are much lower than those of polymers, which is the biggest obstacle for their use as alternate photoactive materials in commercial photovoltaic devices. To overcome this, many research endeavors were also devoted along with conjugated polymers to tuning the optical, electrochemical, and electronic properties of the small molecules via the incorporation of electron-donor or -acceptor moieties, including well-known organic dyes such as, merocyanine (MC), squaraine (SQ), borondipyrromethene (BODIPY), quinaclidone (QD), diketopyrrolopyrrole (DPP), and isoindigo (ID) [7–15]. More recently, interest has grown in the incorporation of multicyclic rigidly fused π -conjugated aromatic units into small molecules because it is well-known that fused thiophene rings can stabilize the quinoidal structure and increase the rigidity and coplanarity of the molecular backbone. This can in turn increase absorption, reduce band gap, and improve the charge transport characteristics, which can all contribute to enhanced device efficiency. For instance, Chen and coworkers reported a small molecule including a benzo[1,2-*b*:4,5-*b'*]dithiophene (BDT) fused core unit and an alkyl cyanoacetate-capped oligothiophene as a spacer, which exhibited a high PCE value of 5.44% [16]. Later, the BDT unit was replaced with a dithieno[3,2-*b*:2',3'-*d*]silole (DTS) unit, which improved the PCE value up to 5.84% [17]. Marks and coworkers introduced a naphtho[2,3-*b*:6,7-*b'*]dithiophene fused core in a D–A small molecule using diketopyrrolopyrrole (DPP) as arms [18]. The small molecule derived from the naphtho[2,3-*b*:6,7-*b'*]dithiophene unit demonstrated a high absorption coefficient ($1.1 \times 10^5 \text{ M}^{-1} \text{ cm}^{-1}$), an ideal HOMO energy level (-5.4 eV), and remarkable photovoltaic performance with a PCE of 4.06%. Bazan and coworkers reported synthesis of a small molecule using DTS as the core, which showed broad absorption extending beyond 700 nm [19]. BHJ solar cell devices fabricated by blending this molecule with PC₇₁BM showed a noticeably high short-circuit current (J_{sc}) of 10.9 mA/cm² and a PCE of 3.2%. Later, they reported an analogous small molecule with the same DTS core, in which the acceptor-core linking pattern was changed, which demonstrated outstanding photovoltaic performance with a record PCE of 6.7% [20]. More recently, Seo and coworkers employed the DTS unit as the rigid core and DPP as the acceptor [21]. The solution-processed photovoltaic devices based on this small molecule exhibited a PCE of 2.2%. Along the same lines, we have also recently reported for the first time a novel class of π -conjugated multicyclic rigidly fused building blocks, naphtho[1,2-*b*:5,6-*b'*]dithiophene, with great potential in the development of D- π -A conjugated small molecules in combination with a 2,1,3-benzothiadiazole acceptor unit [22]. Preliminary photovoltaic studies based on one of the small molecule containing the naphtho[1,2-*b*:5,6-*b'*]dithiophene unit, **TBNBT** (Chart 1) exhibited promising photovoltaic properties with a maximum PCE of ~2.20% in preliminary device characterization.

To shed more light on the potential of the naphtho[1,2-*b*:5,6-*b'*]dithiophene building block in solution-processed small molecule organic solar cells, we designed a novel and elongated naphtho[1,2-*b*:5,6-*b'*]dithiophene-based conju-

gated D- π -A small molecule, **NDT(TTz)₂** (Chart 1) consisting of a naphtho[1,2-*b*:5,6-*b'*]dithiophene as both donor and core, thiazolothiazole as acceptor, and triphenyl amine as auxiliary donor and hole transporting material. As an electron acceptor, thiazolothiazole has attracted a great deal of attention in the recent literature in the construction of D–A conjugated polymers for application to PSCs because of its rigid coplanar structure, which facilitates favorable intermolecular π - π interaction interactions, thus facilitating charge transport through intermolecular hopping [23–30]. Although the electron-withdrawing ability of thiazolothiazole unit is weaker than that of benzothiadiazole, the low-lying HOMO of molecules containing thiazolothiazole lends a better oxidative stability to the corresponding molecule and a higher open circuit voltage (V_{oc}) in the final solar cell devices [27–30]. Because of the higher V_{oc} in the related solar cell devices, encouraging photovoltaic device performances have also recently been extracted from the small molecules containing the thiazolothiazole unit with very simple molecular architectures [31,32]. Additionally, we have incorporated decylthiophene into the conjugated backbone of **NDT(TTz)₂**, expecting to simultaneously increase the effective π -conjugation and improve the solution-processability of the resultant molecule. **NDT(TTz)₂** was synthesized by sequential palladium(0)-catalyzed Suzuki and Stille coupling reactions and its physical properties have been carefully investigated. Organic thin film transistor devices (OTFT) have been constructed to evaluate the charge transport ability of **NDT(TTz)₂**. Finally, solution-processed bulk-heterojunction photovoltaic devices were fabricated using **NDT(TTz)₂** as donor and (6,6)-phenyl C₇₁-butyric acid methyl ester (PC₇₁BM) as acceptor to explore its potential in OSCs.

2. Experimental section

2.1. Materials

2,6-Dihydroxy naphthalene, 4-(diphenylamino)phenylboronic acid (14), anhydrous chlorobenzene (99.8%), and tri(*o*-tolyl)phosphine [P(*o*-tol)₃] and were purchased from Aldrich. Palladium(II)acetate [Pd(OAc)₂], tris(dibenzylideneacetone)dipalladium(0) [Pd₂(dba)₃], tetrakis(triphenylphosphine)palladium(0) [Pd(PPh₃)₄] were obtained from Strem Chemicals. Tetrahydrofuran was distilled over sodium/benzophenone immediately before use to maintain the anhydrous conditions. Chloroform was purified by refluxing with calcium hydride and then distilled. All other chemicals were reagent grade and obtained from commercial sources (Fluka, Across, and TCI) and used as-received without further purification unless stated otherwise. 2-Bromo-3-decylthiophene [33], naphtho[1,2-*b*:5,6-*b'*]dithiophene (**5**) [34], and 2,5-bis(5-bromo-3-decylthiophen-2-yl)thiazolo[5,4-*d*]thiazole (**13**) [32] were synthesized according to literature procedures.

2.2. Synthesis

2.2.1. 2,7-Bis(trimethylstannyl)naphtho[1,2-*b*:5,6-*b'*]dithiophene (**6**)

To a solution of naphtho[1,2-*b*:5,6-*b'*]dithiophene (0.5 g, 2.08 mmol) in THF (20 mL), TMEDA (0.68 mL, 4.57 mmol)

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