

Peripheral group effects on the photophysical and photovoltaic properties of bulk-heterojunction type solar cells based on star-shaped conjugate molecules with triphenylamine core



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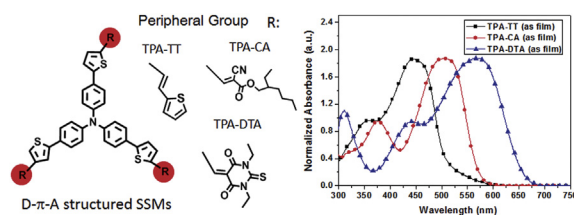
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HIGHLIGHTS

- A series of novel star-shaped molecules (SSMs) have been synthesized for OSCs.
- Excellent charge transfer between the triphenylamine core and branches resulted in a high mobility for SSMs.
- The SSM with higher mobility led to a larger photoenergy conversion efficiency (1.43%) of OSC.

GRAPHICAL ABSTRACT



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ABSTRACT

In this study we prepared three star-shaped, triphenylamine-cored conjugated molecules, possessing thienylenevinylene units as conjugated π bridges and thienyl, 2-ethylhexyl cyanoacetate, and 1,3-diethyl-2-thiobarbituric acid moieties, respectively, as peripheral groups—for use as donor materials in small molecule/fullerene bulk heterojunction-type organic photovoltaic cells (OPVs). The peripheral groups affected the UV–Vis absorption behavior and electrochemical properties of star-shaped molecules, and photovoltaic performance of the star-shaped molecules based OPVs. The wavelength of maximum absorption for star-shaped molecule with 1,3-diethyl-2-thiobarbituric acid moiety was red-shifted relative to those of molecules with thienyl and 2-ethylhexyl cyanoacetate groups, while molecule with thienyl moiety exhibited the largest hole mobility. The photovoltaic properties of cells incorporating molecule with thienyl group and a fullerene derivative were better than those containing corresponding molecule with 2-ethylhexyl cyanoacetate/fullerene or molecule with 1,3-diethyl-2-thiobarbituric acid/fullerene blends. An OPV featuring molecule with thienyl group/fullerene derivative (1:3, w/w) as the active layer exhibited a power conversion efficiency of 1.43%, a short-circuit current density of 5.23 mA/cm², an open-circuit voltage of 0.73 V, and a fill factor of 0.37.

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1. Introduction

Organic photovoltaic cells (OPVs) with light-weight, low cost, and flexibility advantages are a promising cost effective alternative for utility of solar energy [1]. Bulk heterojunction (BHJ)-type OPVs based on small conjugated organic molecules and fullerene

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derivatives are attractive for many reasons, including well-defined structures, simple purification, defined molecular weights, ready production on large scales, and good batch-to-batch reproducibility [2,3]. Such conjugated small molecules have included linear molecules [4,5], star-shaped molecules (SSMs) [6,7], X-shaped molecules [8,9], and dendritic molecules [10]. Among the many soluble organic conjugated molecules, SSMs have emerged as particularly attractive photo-energy conversion materials for OPVs [6,7]. By tailoring and substituting their functional groups, including their donor units, acceptor units, and conjugated bridges, SSMs can exhibit good solution processability, high charge mobility, low band gaps, and broad absorption in the visible region, resulting in high photo-energy conversion efficiencies (PCEs) for their OPVs [6,7]. SSMs featuring strong electron-donating triphenylamine (TPA) units at their cores and three-dimensional structures can display high hole-donating ability and good solution-processability. Several TPA-cored SSMs have been investigated featuring various types of conjugated branches, including electron donor/ π -conjugate/acceptor (D- π -A), electron donor/acceptor/donor (D-A-D), and donor/acceptor/acceptor (D-A-A) arms [11–13]. In addition, the triazine-cored SSMs featuring A- π -D conjugated branches also have been studied for the OPV applications [14–17].

In general, the light absorption, charge mobility, and photovoltaic (PV) performance of OPVs are closely related to the chemical structures of their conjugated molecules. The conjugated branches of TPA-cored SSMs terminated with strong electron-acceptor units can improve the degrees of light absorption and intramolecular charge transfer (ICT) and decrease the band gap energy, resulting in OPVs exhibiting improved PCEs [18–28]. TPA-cored SSMs featuring electron-accepting 3-ethylrhodanine, dicyanovinyl (DCN), alkyl cyanoacetate, and benzothiadiazole units as peripheral groups have been studied extensively [18–28]. Hu et al. reported that an SSM presenting 3-ethylrhodanine groups exhibited a broader solar spectral coverage, a lower energy level for its highest occupied molecular orbital (HOMO), higher hole mobility, and better PV performance relative to that of the corresponding SSM presenting alkyl cyanoacetate groups [13]. In addition, the photo-physical properties of such SSMs terminated with strongly electron-accepting units are closely related to the number of branches. Zhang et al. reported a series of D-A-D-structured SSMs featuring benzothiadiazole units as electron-acceptor groups [29]. They found that an SSM containing three conjugated branches displayed better PV performance than those of corresponding SSMs having one or two conjugated branches. In addition, TPA-cored SSMs having unsymmetrical structures can display broad absorptions, high absorption coefficients, and low-lying HOMO energy levels, resulting in their OPVs functioning with high open-circuit voltages (V_{OC}) [19,22]. TPA-cored SSMs having longer π -conjugation lengths induce shifts in their absorption onsets toward longer wavelengths and corresponding higher PCEs for their OPVs, relative to those based on SSMs having shorter conjugation lengths [23,25,29,30]. Ripaud et al. synthesized extended star-shaped conjugated systems presenting DCN termini connected to TPA cores through thiophene (T), thienylenevinylene (TV), and bithiophene (BT) conjugated bridges [23]. The maximum absorption wavelength of the SSM incorporating the TV bridging unit was longer than those of the SSMs featuring T and BT units. Zhang et al. reported that an OPV based on an SSM incorporating 4,4'-dihexyl-2,2'-bithiophene vinylene bridges exhibited a broader absorption band and a higher PCE than that of the corresponding device based on the SSM incorporating 4,4'-dihexyl-2,2'-bithiophene bridges [25]. The electron-acceptors benzothiadiazole and dialkylated diketopyrrolopyrrole (DPP) have been incorporated as bridging units for SSMs having D-A-D conjugated branches [29,31–34]. The incorporation of the bulky DPP groups as acceptor units in the conjugated

branches prevents the formation of ordered, long-range, coplanar π -stacking, potentially enhancing charge transport across thin film-based OPVs [32–34]. Although TPA-cored SSMs having various conjugated branches have been reported [35], only few papers reported the optoelectronic properties of TPA-cored SSMs with different peripheral groups [21,36]. Therefore, it is important to investigate the influence of the peripheral groups on their photophysical properties and PV performance.

Accordingly, in this study we synthesized three TPA-cored SSMs (TPA-TT, TPA-CA, TPA-DTA), possessing different peripheral groups, as donor materials for OPVs. The structural features of these SSMs include TPA units as cores; TV moieties as conjugated π bridges; and thienyl (TT), 2-ethylhexyl cyanoacetate (CA), and 1,3-diethyl-2-thiobarbituric acid (DTA) units as peripheral groups. The CA and DTA groups with different electron-withdrawing capacities were incorporated as the peripheral groups of SSMs. The SSM with TT as peripheral groups was synthesized and used as the reference sample as we discussed the effect of electron-withdrawing CA and DTA on the PV performance of these SSMs based OPVs. The incorporation of the strong electron acceptor CA or DTA was expected to enhance the ICT effect and decrease the band gap energy, resulting in OPVs exhibiting improved PCEs. These D- π -D- and D- π -A-structured SSMs exhibited different absorption behaviors in the visible region, hole-transporting capacities, and PV performances. Herein, we describe the correlations between the chemical structures, photophysical properties, and PV performances of these SSMs-based OPVs.

2. Experimental details

2.1. Chemicals

Tetrakis(triphenylphosphine)palladium(0) [Pd(PPh₃)₄], potassium carbonate (K₂CO₃), *n*-butyllithium (*n*-BuLi, 2.5 M in hexane), *N*-bromosuccinimide (NBS), and other reagents and chemicals were purchased from Aldrich, Alfa, Acros, and TCI Chemical and used as received. Dichloromethane (DCM), tetrahydrofuran (THF), dimethylformamide (DMF), toluene, CHCl₃, and *o*-dichlorobenzene (*o*-DCB) were freshly distilled over appropriate drying agents; prior to use as solvents, they were purged with N₂. Tris[4-(5-formyl-2-thienyl)phenyl]amine (**3**) and diethoxyphosphino(2-thienylmethyl)-1-one (**5**) were synthesized as displayed in Scheme 1. 4,4',4''-Tribromotriphenylamine (**1**) was synthesized according to the literature [37]. Tris[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]amine (**2**) was obtained from the reaction of **1** with 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane. Compound **3** was synthesized through Suzuki coupling of **2** and 5-bromothiophene-2-carbaldehyde. 2-(Chloromethyl)thiophene (**4**) was synthesized through the reaction of 2-thiophenemethanol with thionyl chloride (SOCl₂). The straightforward reaction of **4** with triethyl phosphite afforded **5**. Detail synthesis routes of compounds 2–5 have been shown in Supporting information. TPA-TT, TPA-CA, and TPA-DTA were synthesized through Knoevenagel condensations of **3** with **5**, CA, and DTA, respectively (Scheme 2). Indium tin oxide (ITO)-coated glass (sheet resistance: 20 Ω square⁻¹) was purchased from Applied Film. PC₆₁BM and PC₇₁BM were purchased from American Dye Source and used as received.

2.1.1. TPA-TT

A mixture of **3** (5.75 g, 10 mmol) and **5** (6.6 mL, 33 mmol) in THF (35 mL) was stirred in an ice-water bath for several minutes and then potassium *tert*-butoxide in THF (1 M, 20.0 mL) was added dropwise. The solution was maintained at 0 °C and stirred continuously for a further 8 h. After evaporating the solvent under

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