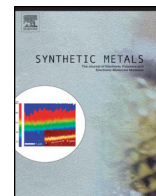




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Short communication

Novel conjugated polymer for organic photovoltaics: Synthesis and device optimization

Bong-Gi Kim ^{a,*}, Hui Joon Park ^{b,**}^a Dongjin Semichem Co., Ltd., 613, Sampyung-Dong, Bundang-Gu, Seongnam-Si, Gyeonggi-Do 463-400, South Korea^b Division of Energy Systems Research, Ajou University, Suwon 443-749, South Korea

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ABSTRACT

A novel conjugated polymer, TdTB, having an alternating configuration of electron donor and acceptor was synthesized for organic photovoltaic (OPV) application. Intramolecular charge transfer made TdTB exhibit bimodal-shaped absorption in visible region, which secured about 4% power conversion efficiency (PCE) via enhanced absorption efficiency. OPV cells could be further optimized by means of additive-assisted annealing or additional super critical CO₂ liquid treatment after additive annealing, and more developed TdTB aggregation was achieved. Consequently, their performances were dramatically improved about 17% and 33%, compared to the non-annealed PV cell, giving 4.65 and 5.27% PCEs, respectively.

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1. Introduction

Organic photovoltaic (OPV) cells adopting conjugated polymers (CPs) have drawn great attention as a cost-effective alternative to silicon-based solar cells. The power conversion efficiency (PCE) of OPV cell has been rapidly enhanced during the last couple of years and currently exceeds 6% [1–6]. This dramatic improvement of OPV performance could be ascribed to the development of new materials, mostly CPs, and to the growing understanding of OPV operation principles [1–11]. One of the fundamental requirements for photovoltaic energy conversion is the collection of photon as much as possible. In this regard, there have been lots of efforts to match the absorption range of CP to the high photon flux region of the solar spectrum, including the energy level modulation of CP by means of computational calculations. The most promising strategy for tailoring the CP band-gap involves introducing donor (D) and acceptor (A) monomers together into the polymer framework [12,13]. The underlying concept is that the interaction between alternating electron-rich donors and electron deficient acceptors results in a compressed band-gap via molecular orbital hybridization and intra-molecular charge transfer.

Moreover, it is also well known that the film morphology, mostly induced by the aggregation of CP, decisively determines

OPV performance, because the aggregation facilitates intermolecular charge transfer via strong π – π interaction, which results in outperforming electrical mobility. To enhance the crystallinity of CP, several film-forming techniques have been reported, such as thermal treatment [14], additive-assisted annealing [15], and super-critical liquid treatment [16].

In order to address these points, in this contribution, we designed and synthesized a novel low band-gap CP that could secure considerable absorption efficiency. Furthermore, the performances of OPV cells, prepared by several film fabrication techniques, were characterized to verify the effects of those fabrication process on the performances.

2. Experimental

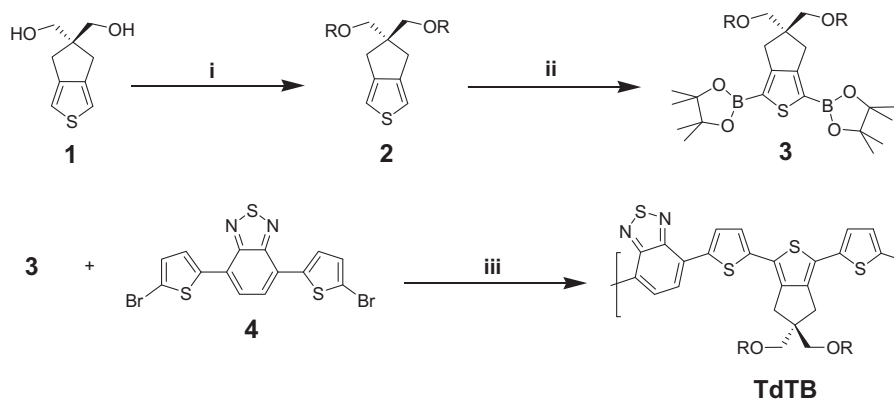
2.1. Compound 2

Under Ar condition, compound 1 (1 g, 5.43 mmol) and NaH (0.65 g, 3.0 eq) were stirred in anhydrous DMF at 60 °C for 30 min. After adding 2-ethylhexyl bromide (3.86 ml, 21.7 mmol) slowly at room temperature, the mixture was stirred for 24 h at 60 °C. Then, water was added to quench the mixture, and the mixture was extracted with diethyl ether. The extracted organic solution was dried with MgSO₄, and solvent was evaporated *in vacuo*. Compound 2 (73%) was obtained from column chromatography using an eluent of dichloromethane. Compound 1, 2, 3 and 4 are denoted in Scheme 1. ¹H-NMR (400 MHz, CDCl₃) δ 6.73 (s, 2H), 3.38 (s, 4H), 2.28 (d, 4H), 2.71 (s, 4H), 1.49 (m, 2H), 1.2–1.35 (m, 16H), 0.8–0.9 (m, 12H), and *m/z* EIMS 409.

* Corresponding author. Tel.: +82 31 627 3536.

** Corresponding author. Tel.: +82 31 219 2577.

E-mail addresses: bgkim@dongjin.com (B.-G. Kim), huijoon@ajou.ac.kr (H.J. Park).



Scheme 1. Synthetic procedures of TdTB. R indicates 2-ethylhexyl group. (i) 2-Ethylhexyl bromide, NaH, DMF, 60 °C, 24 h, (ii) bis(pinacolato) diboron, DBP, Ir(I), heptanes/hexane, 50 °C, 16 h, (iii) Pd(0), tetraethyl ammonium hydroxide, water, 90 °C, 36 h.

2.2. Compound 3

Under Ar condition, compound 2 (1 g, 2.45 mmol), 4,4'-di-tert-butyl-2,2'-bipyridine (DBP) (19.845 mg, 3.0 mol%) and bis(pinacolato) diboron (0.497 g, 1.96 mmol) were added to heptanes. After adding bis(1,5-cyclooctadiene) di- μ -methoxydiiridium(I) (Ir(I)) (24.01 mg, 0.04 mmol), the mixture was stirred at 50 °C for 16 h and poured into cold water. Then, the mixture was extracted with chloroform and dried with MgSO₄. Compound 3 (65%) was obtained from column chromatography after elution of chloroform/hexane (1:5). ¹H-NMR (400 MHz, CDCl₃) δ 3.40 (s, 4H), 2.28 (d, 4H), 2.71 (s, 4H), 1.49 (m, 2H), 1.2–1.35 (m, 40H), 0.8–0.9 (m, 12H), and *m/z* EIMS 661.

2.3. TdTB

Under inert conditions (Ar), compound 3 was dissolved into toluene, and the equivalent amount of corresponding monomer (compound 4) was mixed. After adding 5 mol% of tetrakis (triphenylphosphine) palladium(0) (Pd(0)) and 1.8 ml of tetraethyl ammonium hydroxide (20% solution), the mixture was stirred at 90 °C for 36 h. Bromobenzene (24 μ m) and benzene boronic acid (26 mg) were added respectively to the mixture for chain end modification. The final polymer was collected via reprecipitation into methanol. The solid was collected through 0.45 μ m nylon filter and washed with methanol and acetone in a soxhlet apparatus to remove the oligomers and catalyst residue. After dissolving obtained polymer into chloroform, the polymer solution was eluted through a column, packed with Cellite and Florosil.

Then, the solution was concentrated and reprecipitated from methanol again (Mn:21500, Mw: 35470, and PDI: 1.65).

2.4. Film preparation for OPV device

PCBM[70] was purchased from SES research and used without further purification. After dissolving obtained TdTB (10 mg) and PCBM[70] (15 mg) into *o*-dichlorobenzene (1.0 mL), the mixture was filtered with a syringe filter (0.45 μ m pore diameter) and used to form an active layer by means of spin-casting. In case of additive-assisted annealing, 1,8-octanedithiol (8.0 μ L) was added to the TdTB:PCBM[70] blend solution, and the same procedure was utilized to obtain an active layer. To additionally treat the active layer with super critical CO₂ liquid, the film that contains the additive was left into the closed chamber filled with CO₂ gas under 1500 psi at 35 °C for 30 min.

2.5. OPV device fabrication

ITO-coated glass was cleaned with acetone and IPA followed by UV ozone treatment for 10 min. PEDOT:PSS (Baytron PH 1000) was spin-cast on the substrate and baked at 140 °C for 15 min. TdTB:PCBM[70] blend solution was spin-cast at 700 rpm for 30 s and the blend film was used for metal electrode evaporation without further treatment. Final devices were fabricated by depositing 1 nm-thick LiF and 70 nm Al layer (9.6 mm²) sequentially under 5×10^{-7} Torr (1 Torr = 133.32 Pa). All devices were characterized under nitrogen and the typical illumination intensity was 100 mW/cm² (AM 1.5G Oriel solar simulator).

3. Results and discussion

As illustrated in Scheme 1, terthiophene and 2,1,3-benzothiadiazole were adopted as electron donating and accepting moieties, respectively for D-A type alternating configuration. All starting materials were purchased from the commercial suppliers (Aldrich and Fisher Sci.), and the detailed synthetic procedures are summarized in Section 2. Monomers, compound 3 and compound 4, were prepared as previously described [17,18], and their

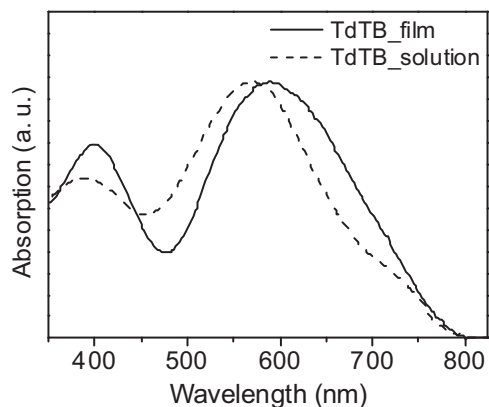


Fig. 1. UV-vis absorption of obtained TdTB both in solution (chloroform) and film.

Table 1
Summary of OPV device performance obtained with TdTB and additional processes.

Process	None	Additive	Additive + CO ₂
V _{oc} (V)	0.88	0.85	0.8
J _{sc} (mA)	9.95	10.93	12.29
FF (%)	45.4	50	53.7
PCE (%)	3.97	4.65	5.27

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