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Photovoltaic molecules based on vinylene-bridged oligothiophene applied for bulk-heterojunction organic solar cells

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A B S T R A C T

We have synthesized two photovoltaic molecules (HEX-3TVT-ID and EH-3TVT-ID) based on vinylene-bridged oligothiophene applied as donor for the solution-processable bulk-heterojunction organic solar cells (OSCs). Vinylene unit was introduced as π-bridge in the oligothiophenes with 1,3-indenedione as end group and 4,4′-dihexyl-2,2′:5′,2′-terthiophene or 3′,4′-di(octan-3-yl)-2,2′:5′,2′-terthiophene as core, respectively. Due to the different substituent position of the alkyl group relative to the vinylene unit in the terthiophene, HEX-3TVT-ID and EH-3TVT-ID show different optical and electrochemical properties, corresponding to the photovoltaic performance of the OSCs devices. The power conversion efficiency (PCE) of the OSCs based on a blend of HEX-3TVT-ID and $PC_{71}BM$ (1:0.8, w w^{-1}, 0.5% CN) reached 2.3%. In comparison, the OSCs based on the blend of EH-3TVT-ID and $PC_{71}BM$ in the weight ratio of 1:1 without the additive shows a higher PCE of 2.7%, with a typically high V_{OC} of 0.93 V, under the illumination of AM 1.5, 100 mW cm^{-2}.

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1. Introduction

Organic solar cells (OSCs) have attracted exceeding interests and been considered to be one of the prospective alternatives to silicon-based solar cells due to their unique features, such as low processing cost, mechanical flexibility, compatibility with roll-to-roll printing processes and light weight [1–8]. Conventional OSCs are based on the bulk heterojunctions of p-type (electron donor) and n-type (electron acceptor) organic semiconductors. Over the past two decades, fullerene derivatives like PCBM and ICBM have been the major choice of electron acceptors and a power conversion efficiency (PCE) up to 11.7% has been reported for donor-fullerene-based devices [9–13]. On the other hand, rapid progress has been made and the PCE of the devices based on donor and non-fullerene electron acceptors can reach as high as 13.8% [14–20]. For more choices of the n-type organic semiconductors, the demand and the choice of the p-type organic semiconductors increase. So developing new kinds of the p- and n-type organic semiconductors is still vital to enhance the PCE of the OSCs.

Chen et al. have reported a series of small molecules based on oligothiophenes and the OSCs based on them as donor can obtain the PCEs as high as 10%, which illustrate that the simple A-D-A oligothiophenes is a successful design for the donor materials [3, 21–23]. Roncali group have published a review based on oligothienylenevinylenes (nTVs). They demonstrated that the presence of vinylene in the molecule structure can make the molecules possess defined configuration products and a decrease of rotational disorder comparing with the single bond [24, 25].

We have synthesized two molecules (HEX-3TVT-ID and EH-3TVT-ID) based on vinylene-bridged oligothiophene applied for the OSCs. Vinylene unit was introduced as π-bridge instead of single bond with 1,3-indenedione as end group and 4,4′-dihexyl-2,2′:5′,2′-terthiophene or 3′,4′-di(octan-3-yl)–2,2′:5′,2′-terthiophene as core, respectively. Due to the different position of alkyl substituent relative to the vinylene unit in the terthiophene, HEX-3TVT-ID and EH-3TVT-ID show different optical and electrochemical properties, corresponding to the photovoltaic performance of the OSCs devices. The PCE of the OSCs based on a blend of HEX-3TVT-ID and $PC_{71}BM$ (1:0.8, w w^{-1}, 0.5% CN)

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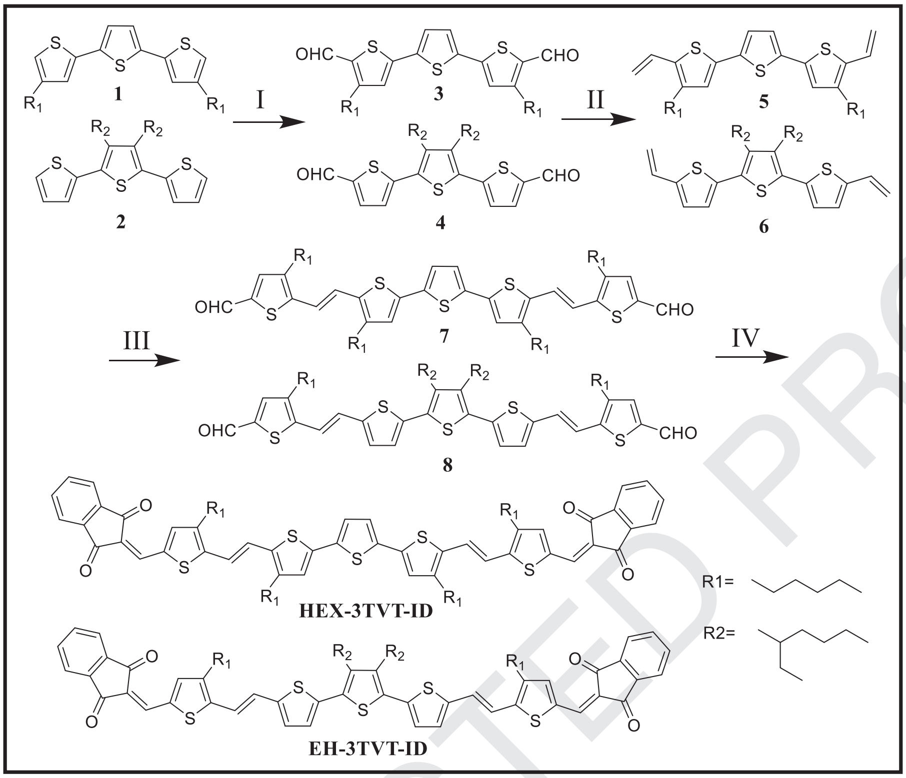

Scheme 1. Synthetic route of HEX-3TVT-ID and EH-3TVT-ID: (I) $POCl_3$, DMF, $ClCH_2CH_2Cl$, under N_2, 45 °C for 2 h; (II) $MePh_3PBr$, *n*-butyllithium, THF, under N_2, −78 °C; (III) 5–bromo–4-hexylthiophene-2-carbaldehyde, $Pd(OAc)_2$, NaOAc, *n*-Bu_4NBr, DMF, under N_2, 100 °C for 24 h; (IV) 1,3-indanedione, toluene, under N_2, 90 °C for 12 h.

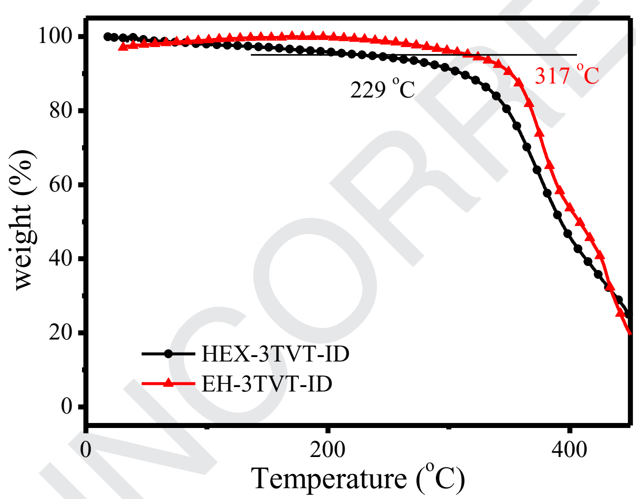

Fig. 1. TGA plots of HEX-3TVT-ID and EH-3TVT-ID.

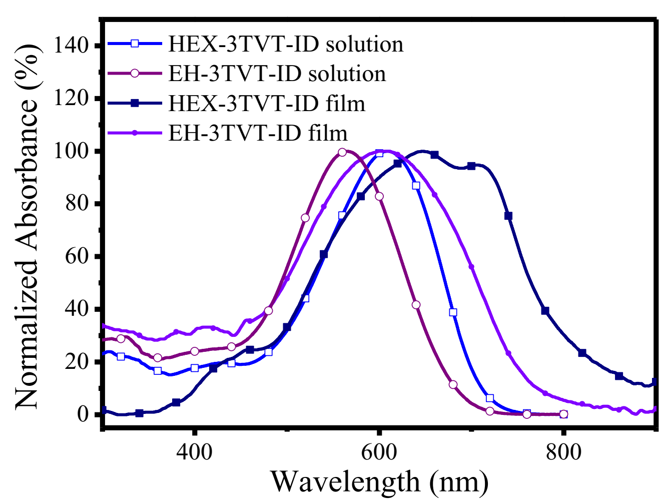

Fig. 2. UV–vis absorption of HEX-3TVT-ID and EH-3TVT-ID in $CHCl_3$ solution and in film state.

reached to 2.3%. In comparison, the PCE of the OSCs based on the blend of EH-3TVT-ID and $PC_{71}BM$ in the weight ratio of 1:1 without the additive shows a higher PCE of 2.7%, with a typically high V_{OC} of 0.93 V, under the illumination of AM 1.5, 100 mW cm^{-2}.

2. Experimental

2.1. Chemicals

All of the chemicals were obtained from Acros Organics including methyltriphenylphosphonium bromide, *n*-butyllithium (2.88 mol L^{-1} in hexane), tetrabutylammonium bromide, sodium acetate, palladium acetate and so on.

2.2. Measurements

MALDI-TOF spectra, nuclear magnetic resonance (NMR) spectra, absorption spectra, the TGA measurement and the electrochemical cyclic voltammogram were recorded by Bruker BIFLEXIII, Bruker DMX-400 spectrometer, Hitachi U-3010 UV–vis spectrophotometer, Perkin-Elmer TGA-7 apparatus and Zahner IM6e, respectively, according to the method of the ref. [26]. OSCs devices

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