



Oligothiophene based small molecules with a new end group for solution processed organic photovoltaics



Huijing Zhang, Xuan Yang, Nailiang Qiu, Wang Ni, Qian Zhang, Miaomiao Li, Bin Kan, Xiangjian Wan, Chenxi Li, Yongsheng Chen*

Key Laboratory of Functional Polymer Materials, Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Center for Nanoscale Science and Technology, Institute of Polymer Chemistry, College of Chemistry, Nankai University, Tianjin 300071, China

ARTICLE INFO

Article history:

Received 7 December 2015
Received in revised form
1 March 2016
Accepted 9 March 2016
Available online 16 March 2016

Keywords:

Small molecule
Organic photovoltaic cell
Solvent vapor annealing
Low band gap

ABSTRACT

Two oligothiophene based small molecules (**DINER5T** and **DINER7T**) with a new end group **INER** were synthesized as the donors for organic solar cells, and their photovoltaic performance was studied and compared with the corresponding compounds (**DRHD7T** and **DIN7T**) with the same backbone structure but different end groups. Both of the new molecules exhibit broad and red shift absorption compared with **DRHD7T** and **DIN7T**, with very low band gaps of 1.47 eV and 1.34 eV, respectively. The devices based on **DINER5T**:PC₇₁BM and **DINER7T**:PC₇₁BM blend films gave PCEs of 4.22% and 4.02%, respectively, through a solvent vapor annealing (SVA) process with CH₂Cl₂.

© 2016 Published by Elsevier B.V.

1. Introduction

Organic photovoltaic devices (OPVs) due to their advantages, such as low cost and flexibility, have caught ever growing attention. The power conversion efficiencies (PCEs) of OPVs are increasing quickly and PCEs over 10% have been achieved for both polymer based OPVs (P-OPVs) [1–9] and small molecule based OPVs (SM-OPVs) [10–12]. Based on the equation, $PCE = V_{oc} \times J_{sc} \times FF / P_{in}$, where V_{oc} is the open-circuit voltage, J_{sc} is the short-circuit current density, FF is the fill factor and P_{in} is the incident light intensity, both V_{oc} and FF of the devices have been improved drastically recently, thus one of the current focuses is to enhance J_{sc} for better performance. To get a high J_{sc} , several effective methods have been widely used. For example, morphology control by thermal [13–15] or vapor annealing [16–19], adding additives [20–24], modifying buffer layer [25], introducing metal nano particles [26,27] et al., have been used widely. But the most and fundamental strategy is still to design low band gap molecules to harvest solar light as much as possible, thus more solar energy could be theoretically converted into electric energy.

Oligothiophene based small molecules, due to their relative easy

synthesis and purification, good solubility and outstanding photoelectricity properties, have been widely used in organic solar cells [28–30], dye-sensitized solar cell [31,32], and perovskite solar cells [33]. Besides, their electrochemical properties and crystalline nature could be easily modulated, which makes this kind of molecules catch increasing attention [34,35]. Recent years, we have reported a series of oligothiophene based small molecules with Acceptor-Donor-Acceptor (A-D-A) structures for high efficient organic solar cells [10,12,36,37], and >10% PCE has been achieved [12]. It has been found that the electron withdrawing end groups played a great role on the molecules' absorption, energy levels, solid state packing modes and the final device performance. Among the end groups used for these oligothiophene-like small molecules, the rhodanine unit turns out to be an excellent choice as in the case of DERHD7T which shows excellent absorption in the range from 400 to 800 nm [38]. Thus, device based on DERHD7T gave high J_{sc} over 13 mA/cm². However, the device with DERHD7T as the donor exhibited a low FF of around 47%. On the other hand, the molecule DIN7T with indandione end groups showed broad absorption and a high FF over 0.70. However, its devices gave a lower J_{sc} of 8.21 mA/cm² [39]. Obviously, the big difference on the corresponding devices performance of the two small molecules were caused by the end groups that would lead to different energy levels and morphology of the active layers. Thus, it is rather desirable to design new donor molecules using these different end groups to combine their

* Corresponding author.

E-mail address: yschen99@nankai.edu.cn (Y. Chen).

advantages.

So, herein, a new end group, named **INER**, was designed and two new donor molecules named **DINER5T** and **DINER7T** were synthesized (Scheme 1) using this new end group. Compared with the two previous molecules of DERHD7T and DIN7T, the absorption of the two new molecules were greatly improved with a maximum absorption peak at 664 nm for **DINER7T**, and 680 nm for **DINER5T**, respectively. Devices fabricated using these two molecules as donors and PC₇₁BM as the acceptor were systematically investigated via adding additives and solvent vapor annealing (SVA) optimization. PCEs of 4.02% and 4.22% were achieved for **DINER7T** and **DINER5T** based devices, respectively. The moderate efficiencies are thought to be caused by the unfavorable planarity of the two molecules and unsuitable phase separation scale.

2. Experimental section

2.1. Materials and synthesis

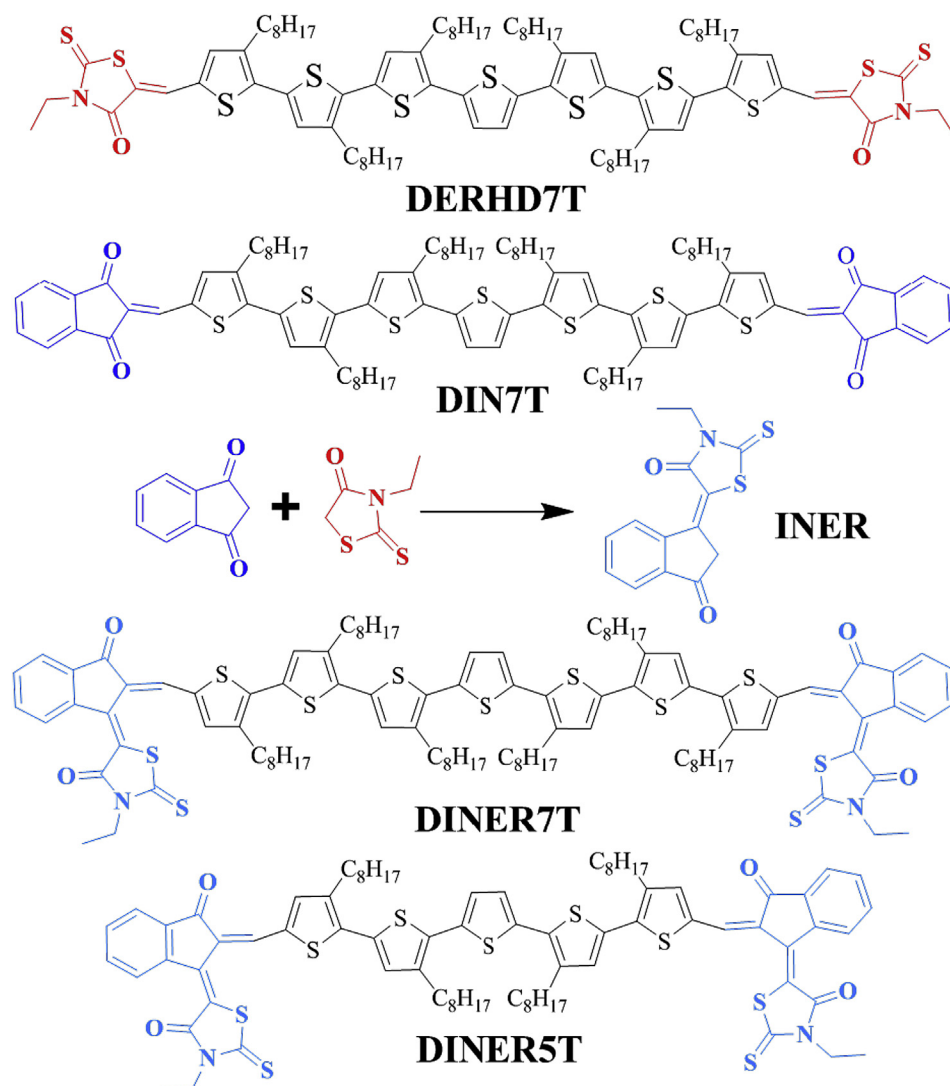
All reactions and manipulations were carried out under argon atmosphere with the use of standard Schlenk techniques. Unless otherwise specified, all the starting materials were purchased from

commercial suppliers and used directly without any purification. Compounds DF5T and DF7T were synthesized according to the literature [30]. The procedure of synthesis of **INER**, **DINER5T** and **DINER7T** is outlined in Scheme 2.

2.2. Synthesis of compound **INER**, **DINER5T** and **DINER7T**

2.2.1. Synthesis of compound **INER**

Indandione (146 mg, 1 mmol) and 3-ethylrhodanine (161 mg, 1 mmol) were dissolved in absolute ethanol (50 mL), then 30 mg CH₃COONa was added and the resulted solution were stirred for 30 h at 65–70 °C under argon. After removal of the solvent, the crude product was dissolved with chloroform and separated by chromatography using silica gel and a mixture of dichloromethane and petroleum ether (2: 1) as eluent to afford **INER** as a yellow solid (145 mg, 50% yield). ¹H NMR (400 MHz, CDCl₃): δ 7.95 (d, 1H), 7.85 (t, 1H), 7.80 (d, 1H), 7.68 (t, 1H), 4.22 (m, 2H), 3.95 (s, 2H), 1.31 (t, 3H). ¹³C NMR (100 MHz, CDCl₃): δ 200.54, 191.64, 166.71, 146.28, 139.10, 139.03, 135.47, 131.98, 126.19, 124.49, 118.27, 43.35, 39.82, 12.27. MS (EI) *m/z* calcd. for C₁₄H₁₁NO₂S₂ [M⁺], 289.37, Found, 288.0.



Scheme 1. The chemical structures of DERHD7T, DIN7T, **INER**, **DINER7T** and **DINER5T**.

Download English Version:

<https://daneshyari.com/en/article/1264214>

Download Persian Version:

<https://daneshyari.com/article/1264214>

[Daneshyari.com](https://daneshyari.com)