



# A new small molecule with indolone chromophore as the electron accepting unit for efficient organic solar cells



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## ABSTRACT

A new small molecule (TIBDT) with indolone chromophore as the electron acceptor unit and benzodithiophene as electron donor unit was synthesized and first applied in organic solar cells (OSCs). TIBDT was characterized by NMR, TGA, UV–Vis absorption spectroscopy and cyclic voltammetry measurements. Results show that TIBDT possesses excellent thermal stability, appropriate absorption spectra, low-lying highest occupied molecular orbital (HOMO) level and high hole mobility. The OSCs based on TIBDT: PC<sub>71</sub>BM (1:1, w/w) showed a power conversion efficiency (PCE) up to 3.94% with an open circuit voltage ( $V_{oc}$ ) of 0.89 V, short circuit current ( $J_{sc}$ ) of 7.36 mA cm<sup>-2</sup>, fill factor (FF) of 60.2% under the illumination of AM 1.5 G, 100 mW cm<sup>-2</sup> without solvent additives and thermal annealing treatment. These preliminary investigations show that indolone chromophore can probably be an excellent electron accepting unit for constructing high performance optoelectronic materials.

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## 1. Introduction

Bulk heterojunction (BHJ) organic solar cells (OSCs) have drawn broad attentions over the past decade because of their advantages in lightweight, flexibility and simple manufacturing process [1]. In the past few years, we have witnessed a significant progress of BHJ OSCs with a PCE up to 9% [2] for single-layer BHJ and 10% [3] for tandem solar cells. Though higher PCEs have been obtained in polymer solar cells (PSCs), the imperfections of broad molecular weight distribution, tedious purification and difficult reproducibility restrict their wide applications [4]. Meanwhile, small molecule photovoltaic materials are drawing increasing attentions due to their certain molecular structure, definite molecular weight, high purity and excellent repeatability [5]. Lately, considerable efforts on small molecule donor materials are dedicated to design new molecular structures. To further increase the efficiency of small molecule OSCs (SM-OSCs), the new donor materials should exhibit: 1) good solubility for solution processing; 2) a broad absorption to harvesting photons; 3) a relatively low HOMO energy level to enhance the  $V_{oc}$  and 4) high hole mobility [6] Up to date, acceptor–donor–acceptor (A–D–A) small

molecular structure is one of the most successful structure to satisfy these requirements [7]. For instance, the small molecule *p*-DTS(FBTTh<sub>2</sub>)<sub>2</sub> [8] and *p*-SIDT-(FBTTh<sub>2</sub>)<sub>2</sub> [9], both of them exhibited a broad absorption, a low-lying HOMO energy level, a moderate mobility and a fairly high PCE.

Recently, the isoindigo unit has attracted great interest as an acceptor building block for conjugated polymers due to its large coplanar and strong electron-withdrawing character. To date, conjugated polymers based on isoindigo unit have led to PCEs over 7% [10]. However, the twist of isoindigo unit could reduce donor–acceptor interactions and adversely affect the inter-chain stacking [11]. Thus, the expanded isoindigo with two indolone unit was introduced into organic photovoltaics. This structure could expand the conjugated core effectively, and avoid the steric repulsion between the protons on the phenyl rings and the carbonyl oxygens of the oxindoles successfully. Up to now, PCE of 6.4% [11] has been obtained in PSC with expanded isoindigo as acceptor unit. Nevertheless, to our knowledge, small molecules based on the indolone unit for OSCs have rarely been reported.

Simultaneously, benzodithiophene (BDT) and BDT derivatives as the core of donor materials are widely used in organic photovoltaics, mostly due to its superior extended conjugation and planar structure, which probably can enhance the FF and  $J_{sc}$ . Furthermore, BDT-containing molecules usually have a low HOMO level [12], which can provide a relatively high  $V_{oc}$ .

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In this work, we designed and synthesized a new molecule TIBDT based on BDT unit as electron donor core, indolone as the electron acceptor and terminated with hexyl-substituted bithiophene. This small molecule exhibits broad absorption in visible range, a low-lying HOMO energy level and a high mobility. All of the OSC devices based on TIBDT blend with PC<sub>71</sub>BM exhibited a high FF of above 50% and  $V_{oc}$  nearly of 0.9 V. Especially when the weight ratio of TIBDT and PC<sub>71</sub>BM was 1:1, a highest PCE of 3.94% was achieved with a  $V_{oc}$  of 0.89 V,  $J_{sc}$  of 7.36 mA cm<sup>-2</sup> and a FF of 60.2% (see Scheme 1).

## 2. Experimental

### 2.1. Materials

Palladium(0)tetrakis(triphenylphosphine) (Pd(PPh<sub>3</sub>)<sub>4</sub>), 5-formylthiophen-2-ylboronic acid (3) and 6-bromoindolin-2-one (5) were obtained from Acros Organics, and they were used as received. Other starting materials and reagents were purchased commercially as analytically pure and used without further purification unless stated otherwise.

### 2.2. Characterization

All <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were recorded using an AVANCE III 500 MHz spectrometer in Chloroform-d solution at 298 K with tetramethylsilane (TMS) as internal reference (0 ppm). MALDI-TOF was performed on a Bruker Autoex III instrument. Elemental analyses were performed on a Flash EA112 instrument. UV–Vis absorption spectra were recorded on a SHIMADZU UV-2700 spectrophotometer. The film on quartz used for UV–Vis measurements were prepared from spin-coating chloroform solution. Thermogravimetric analysis (TGA) measurements were conducted on a Perkin–Elmer TGA-7 with a heating rate of 10 K min<sup>-1</sup> under inert atmosphere. The electrochemical cyclic voltammetry (CV) curve was recorded with a computer controlled Zahner IM6e electrochemical workstation with platinum electrode (1.0 cm<sup>2</sup>), a platinum wire and Ag/Ag<sup>+</sup> (0.1 M) as the working electrode, counter electrode and reference electrode respectively in an anhydrous and argon-saturated solution of 0.1 M tetrabutylammonium hexafluorophosphate (Bu<sub>4</sub>NPF<sub>6</sub>) acetonitrile solution with a scanning rate of 50 mV s<sup>-1</sup>. X-ray diffraction (XRD) was used to investigate the crystallinity of spin-coated TIBDT thin films prepared on silicon substrates, XRD measurements of the polymer thin film were carried out with a 2 kW Rigaku X-ray diffraction

system. XRD patterns were obtained using Bragg–Brentano Geometry ( $\theta$ – $2\theta$ ) with Cu K $\alpha$  radiation as an X-ray source in the reflection mode at 45 kV and 300 mA. The morphologies of the TIBDT/PC<sub>71</sub>BM blend films were investigated by a SPI 3800 N atomic force microscope (AFM).

### 2.3. Fabrication and characterization of organic solar cells

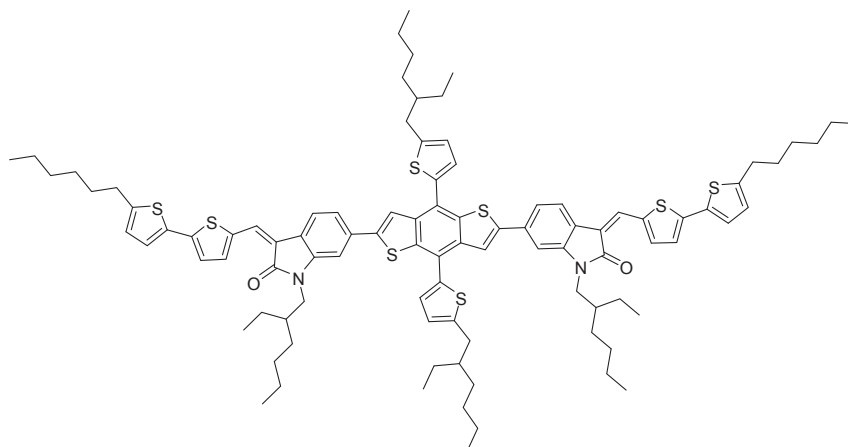
The SM-OSC devices were fabricated on cleaned and UV/ozone treated patterned ITO glasses. PEDOT:PSS (poly(3,4-ethylene dioxithiophene): poly(styrene sulfonate)) (Baytron PVP Al 4083, Germany) was filtered through a 0.45  $\mu$ m poly(tetrafluoroethylene) (PTFE) filter and spin coated at 3000 rpm for 40 s on the ITO substrate as the first layer and was dried at 150 °C for 15 min under ambient atmosphere. The active layers were dissolved in chloroform (CHCl<sub>3</sub>) for half an hour, and then spin-cast at 2000 rpm for 60 s above the PEDOT:PSS layer. Films were allowed to dry for 30 min under inert atmosphere at the room temperature. Cathodes were deposited by sequential thermal evaporation of 20 nm of calcium followed by 80 nm of aluminum under a shadow mask with a base pressure of ca. 10<sup>-5</sup> Pa. The active area of the devices is 4 mm<sup>2</sup>. Device characterization was carried out under AM 1.5 G irradiation with the intensity of 100 mW cm<sup>-2</sup> (Oriel 67005, 500 W), calibrated by a standard silicon cell.  $J$ – $V$  curves were recorded with a Keithley 236 digital source meter.

### 2.4. Synthesis

Reagents and conditions:(a) DMF, NBS, rt, 24 h; (b) 5-formylthiophen-2-ylboronic acid, potassium carbonate, Pd(PPh<sub>3</sub>)<sub>4</sub>, 90 °C, 14 h; (c) 6-bromoindolin-2-one, piperidine, methanol, 70 °C, 24 h; (d) DMF (40 mL), potassium carbonate, 2-ethylhexyl bromide, 100 °C, 24 h; (e) toluene, Pd(PPh<sub>3</sub>)<sub>4</sub>, 110 °C, 24 h.

#### 2.4.1. 2-bromo-5-hexylthiophene (1)

A solution of 2-hexylthiophene (6.72 g, 40 mmol) in CHCl<sub>3</sub> (100 mL) was placed in a 250 mL three-necked flask at 0 °C, and then DMF (40 mL) with NBS (7.12 g, 40 mmol) mixture was added dropwisely. The reaction mixture was warmed up to room temperature and stirred for overnight absent from light, after this the mixture was poured into water, extracted by CH<sub>2</sub>Cl<sub>2</sub>, organic phase was washed several times with sodium hydrogen carbonate aqueous solution, and dried by a rotary evaporator to give a crude product. Further purification was carried out by column chromatography on the silica gel using petroleum ether as the eluent to



Scheme 1. Structure of TIBDT.

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