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Article

A carbon-oxygen-bridged ladder-type building block for efficient donor and acceptor materials used in organic solar cells

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ABSTRACT

A carbon-oxygen-bridged ladder-type donor unit (CO5) was invented and prepared via an "intramolecular demethanolization cyclization" approach. Its single crystal structure indicates enhanced planarity compared with the carbon-bridged analogue indacenodithiophene (IDT). Owing to the stronger electron-donating capability of CO5 than IDT, CO5-based donor and acceptor materials show narrower bandgaps. A donor-acceptor (D-A) copolymer donor (PCO5TPD) and an A-D-A nonfullerene acceptor (CO5IC) demonstrated higher performance than IDT-based counterparts, PIDTTPD and IDTIC, respectively. The better performance of CO5-based materials results from their stronger light-harvesting capability and higher charge-carrier mobilities.

1. Introduction

Ladder-type conjugated molecules with linearly fused aromatic or heterocyclic rings are important building blocks for developing donor and acceptor materials used in organic solar cells [1]. Prominent merits of ladder-type units are as follows: (1) the extended π systems reduce the bandgaps of donor-acceptor (D-A) copolymers or small molecules, enhancing the light-harvesting capability of the materials; (2) the rigid coplanar structures facilitate π-π stacking, improving the charge-transporting property [1–9]. Last three years, carbon-bridged (C-bridged) ladder-type electron-donating units functioned well in constructing efficient donor and acceptor materials for solar cells [10–24]. Copolymer donors and nonfullerene acceptors based on C-bridged units, such as indacenodithiophene (IDT) and indacenodithienothiophene (IDTT), gave 9.1% and 12.1% power conversion efficiencies (PCEs), respectively [11,19]. However, the medium electron-donating capability of the C-bridged units is unfavorable for making materials with stronger light-harvesting capability [25]. In this regard, we use "carbon-oxygen (CO) bridge" to replace the carbon bridge to develop new ladder-type units with stronger electron-donating capability. The rationale is that the electron-rich oxygen atoms can significantly improve the electron-donating capability via the conjugation effect. Meanwhile, the inserted oxygen atoms expand backbone planarity, which can facilitate π-π stacking and further improve the charge-transporting property of the materials. Here, we report the synthesis of a pentacyclic CO-bridged unit, CO5 (Fig. 1), and its application in the development of donor and acceptor materials for solar cells. Compared with the C-bridged analogue IDT, CO5 exhibits stronger electron-donating capability and enhanced planarity. The CO5-based D-A copolymer donor, PCO5TPD, and the CO5-based A-D-A nonfullerene acceptor, CO5IC, possess narrower bandgaps, stronger light-harvesting capability, higher charge-carrier mobilities and better photovoltaic performance than the IDT-based counterparts.

2. Experimental

2.1. Inverted solar cells

The ZnO precursor solution was prepared according to literature [26]. It was spin-coated onto indium tin oxide (ITO) glass

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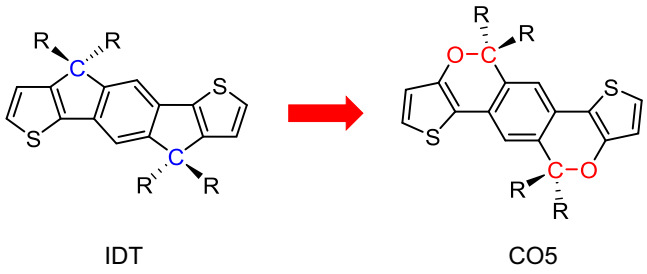
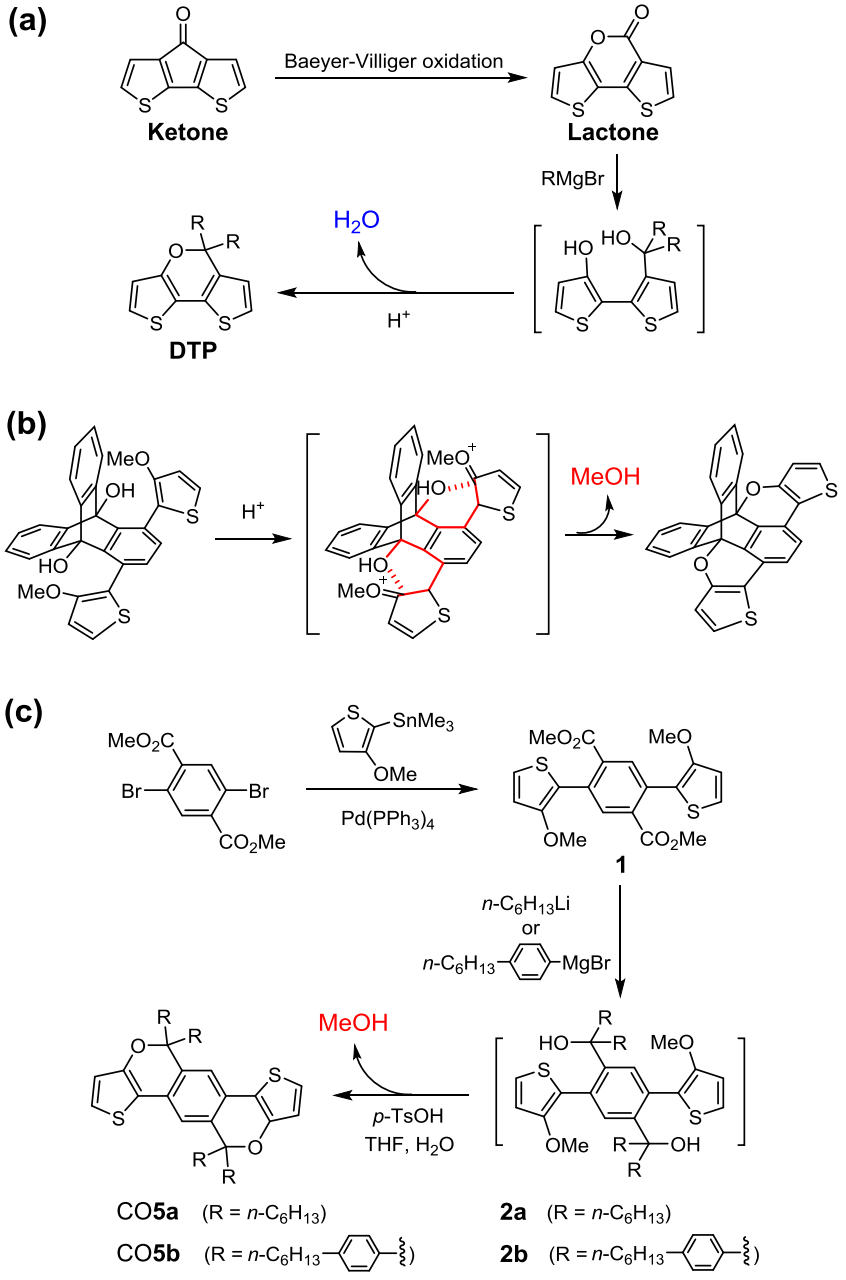


Fig. 1. (Color online) The structures of IDT and CO5.

(4,000 r/min for 30 s). The films were annealed at 200 °C in air for 30 min. ZnO film thickness is ~30 nm. A donor-acceptor blend in chlorobenzene (CB) with DIO additive was spin-coated onto ZnO layer. MoO_3 (~6 nm) and Ag (~80 nm) was successively evaporated onto the active layer through a shadow mask (pressure ca. 10^{-4} Pa). The effective area for the devices is 4 mm^2. The thicknesses of the active layers were measured by using a KLA Tencor D-120 profilometer. *J-V* curves were measured by using a computerized Keithley 2400 SourceMeter and a Xenon-lamp-based solar simulator (Enli Tech, AM 1.5 G, 100 mW/cm^2). The illumination intensity of solar simulator was determined by using a monocrystalline silicon solar cell (Enli SRC2020, 2 cm × 2 cm) calibrated by NIM. The external quantum efficiency (EQE) spectra were measured by using a QE-R3011 measurement system (Enli Tech).

2.2. Hole-only devices

The structure for hole-only devices is ITO/PEDOT:PSS/active layer/MoO_3/Al (PEDOT: poly(3,4-ethylenedioxythiophene); PSS: polystyrene sulfonate). A 30 nm thick PEDOT:PSS layer was made by spin coating an aqueous dispersion onto ITO glass



Scheme 1. (Color online) The synthetic methods for CO-bridged conjugated molecules. (a) The "intramolecular dehydration cyclization" route for DTP [26]; (b) the acid-promoted annulation for preparing a triptycene-containing polycyclic molecule [27]; (c) the "intramolecular demethanolization cyclization" route for CO5.