Synthesis and Photophysical Properties of Small Molecule Donor Materials Based on Indacenodithieno[3, 2-b]Thiophene Core for Organic Solar Cells

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Abstract. We synthesized a small molecule donor material based on IDTT for solar cells, named C6S2ThBSeIDTT, which was obtained by IDTT-2SnMe3 and a capping fragment by a simple Stiller coupling reaction. Its structure and properties were HNMR. C6S2ThBSeIDTT was confirmed that it exhibited good solubility in conventional organic solvent. It can be found that strong intermolecular charge transfer (ICT) exists in the D-A-D-A-D conformation. It has been found to have broad and strong absorption by absorption spectroscopy with a medium wide band gap of 1.70 eV, and will well agree with fullerene acceptors such as PC60BM and PC71BM for efficient bulk heterojunction solar cells.

1. Introduction

Due to its wide distribution, abundant reserves, clean and pollution-free, and easy storage, solar energy has received wide attention from scientists in various countries in recent years. Solar cells convert solar energy into electricity, which is the most direct and effective way to use solar energy. At present, the highest conversion efficiency based on organic solar cells has exceeded 17%, which indicates that there is a promising future for realizing the commercialization of organic solar cells and using this as an opportunity to solve energy problems.1-9 Organic solar cell materials are mainly composed of donors and acceptors. Currently, the development of acceptor materials is rapid, but the study of donor materials is relatively rare. Because donors and acceptors are equally important, the study of donors is also very meaningful.

For the donor material of organic solar cells, the structurally determined nature is the most basic common sense. The formation of available materials by the combination of electron donating parts and electron deficient units is an access to current research. The IDTT unit has been reported to be a very good fused ring electron donating unit because of its strong electron delocalization ability and good molecular planarity. However, there are currently relatively few reports based on its use for donor materials (As shown in Figure 1).10 We used it as a core unit to construct a small molecule donor of D-A-D-A-D type, which showed good spectral absorption due to charge transfer in the molecule.
Figure 1. Some typical small molecule donor materials based on the core of IDTT.

2. Synthesis

Scheme 1. Synthetic routes of C6S2ThBSeIDTT

The synthetic ways of C6S2ThBSeIDTT was displayed in Scheme 1. C6S2ThBSeIDTT was coupled to synthesize by compounds 1 and 2 and yields 54%. Compound 1 (0.15 g, 0.09 mmol) and compound 2 (0.15 g, 0.27 mmol) were putted into a 50 ml small single-neck round bottom glass flask, and metal catalysts of the Pd3(dba)3 (0.003 g, 0.004 mmol) and the ligand of P(o-tol)3 (0.003 g, 0.010 mmol) were putted into a 50 ml glass flask, too. Then, under the dissolution of toluene, IDTT-2SnMe3 and compound 2 was transferred to Shrek tube, respectively. After that, those were evacuation and filling inert gas 5 times. Heat to reflux, and the tube was kept this state for overnight under the N2 atmosphere. When the temperature cooled slowly to r.t., toluene was removed under low pressure and high temperature, the dark crude was purified through detailed flash column chromatography carefully. The solution of PE and CH2Cl2 was added to 2:1 very slowly, and GPC was used to further purification, finally, recrystallized to give a purple solid (0.10 g) with a yielding of 54%.
$^1$H NMR was used to affirm the final molecular C6S2ThBSeIDTT, and shown in Figure 2. The data is above: $^1$H NMR (CDCl$_3$, 400 MHz, ppm): δ 9.14-9.20 (m, 4H, Ph-H), 7.77-7.78 (d, J = 4.0 Hz, 2H, Th-H), 7.47-7.49 (d, J = 4.0 Hz, 2H, Th-H), 7.31-7.35 (t, J = 8.0 Hz, 2H, Ph-H), 7.15-7.16 (d, J = 4.0 Hz, 2H, Th-H), 7.02-7.06 (t, J = 8.0 Hz, 2H, Ph-H), 6.91-6.92 (d, J = 4.0 Hz, 2H, Ph-H), 6.87-6.88 (d, J = 4.0 Hz, 2H, Th-H), 6.76-6.78 (d, J = 8.0 Hz, 2H, Ph-H), 6.67 (s, 2H, Ph-H), 3.65-3.74 (m, 8H, CH$_2$), 2.90-2.98 (m, 4H, CH$_2$), 2.81-2.83 (m, 4H, CH$_2$), 1.86-1.96 (m, 4H, CH), 1.62-1.75 (m, 4H, CH), 1.31-1.42 (m, 66H, CH$_2$), 0.89-1.02 (m, 48H, CH$_3$).

![Figure 2. $^1$H NMR spectra of C6S2ThBSeIDTT](image_url)

3. Results and discussion.
We found in experiments that C6S2ThBSeIDTT has good solubility in most solvents, which is very conducive to the subsequent device processing of materials, and we studied its spectral absorption capacity through its UV absorption test in the solid state, and detailed data of C6S2ThBSeIDTT were summarized in Table 1.
From the Figure 3 we can find that C6S2ThBSeIDTT in the film state has very strong absorption, and the absorption range covers 400-760 nm. The wavelength value of C6S2ThBSeIDTT at the maximum absorption peak is 673 nm, and the wavelength value of C6S2ThBSeIDTT at the beginning of absorption is 729 nm, and the calculated band gap of C6S2ThBSeIDTT is 1.70 eV. The intermolecular forces of C6S2ThBSeIDTT play a significant role at 550-700 nm. The electron rich core IDTT we took was a great choice, it has a very good ability to donate electrons, and IDTT’s extended seven-membered ring plane has good skeleton rigidity, which will have a positive impact on all aspects of its photoelectric properties. Since C6S2ThBSeIDTT is a D-A-D-A-D-type molecule, this is very beneficial for spectral absorption. Considering the delicate relationship between the spectrum and the energy level, we can also boldly predict that C6S2ThBSeIDTT will be a very good donor material. At the same time, it is necessary to improve the end of the material C6S2ThBSeIDTT.

Table 1. The detailed photophysical properties of C6S2ThBSeIDTT.

| Molecule       | $\lambda_{\text{max}}^{\text{film}}$ [nm] | $\lambda_{\text{onset}}^{\text{film}}$ [nm] | $E_{\text{g}}^{\text{opt}}$ [eV] |
|----------------|----------------------------------------|----------------------------------------|---------------------------------|
| C6S2ThBSeIDTT  | 673                                    | 730                                    | 1.70                            |

4. Conclusion

To sum up, based on the seven-number ring fused core (IDTT), a D-A-D-A-D small molecule donor material C6S2ThBSeIDTT was designed and obtained. We carefully described its synthetic route, and confirmed its structural properties by $^1$H NMR, and studied its photophysical properties. We found it to be a very good donor alternative for traditional polymer donor due to the good solubility and strong and broad spectral response. Our experiments provide some reliable advice for the development of small molecule donor materials.

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