Development of Fused Polycyclic Electron-Accepting Molecules Composed of Dithienothiophenes and Benzothiadiazole

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Electron-deficient fused polycyclic π-conjugated compounds are attracting attention as acceptor materials for organic solar cells (OSCs) because their material properties can be tuned through chemical structure design. We have developed sulfanyl substituted naphthobisthiadiazole-based acceptor materials[1] by nucleophilic substitution of fluorine atoms.[2,3] In this work, we synthesized new fused-ring **TTTBTz** by the ring-closure reaction of thienothiophenes and sulfinyl substituted benzothiadiazole, and developed **TTTBTz**-based acceptors (**TTTBTz-DCI**, **TTTBTz-Rhd**).

On UV-vis absorption spectra in chloroform, **TTTBTz-DCI** and **TTTBTz-Rhd** showed the maximum absorbance peak at 648 nm and 569 nm, respectively. From the onset wavelength, the optical energy gaps of **TTTBTz-DCI** and **TTTBTz-Rhd** were estimated to be 1.78 and 2.04 eV, respectively. Cyclic voltammetry measurements showed reduction waves with the half-wave reduction potentials ($E_{red}^{1/2}$) of –0.94 and –1.44 V vs. Fc/Fc^+, respectively. Based on $E_{red}^{1/2}$, the lowest unoccupied molecular orbital energy levels of **TTTBTz-DCI** and **TTTBTz-Rhd** were estimated to be –3.86 and –3.36 eV, respectively. The OSC devices using **TTTBTz-DCI** and **TTTBTz-Rhd** as acceptor materials, and PBDB-T (CAS No. 1415929-80-4) and P3HT as donor materials showed photovoltaic characteristics.

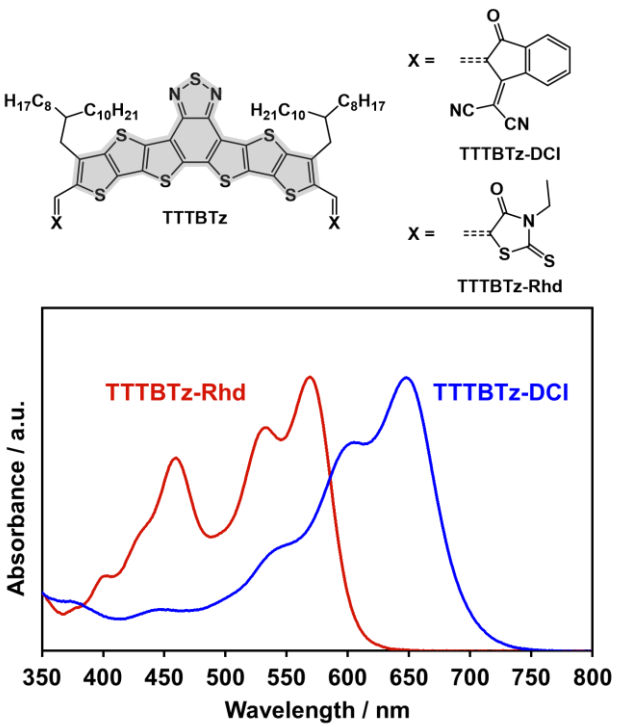

Fig. 1 Chemical structures and UV-vis absorption spectra of **TTTBTz-DCI** and **TTTBTz-Rhd**.

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2) K. Iguchi, Y. Ie, I. Osaka et al., *Chem. Mater.* **2021**, *33*, 2218.
3) S. Jinnai, A. Oi, T. Moriyama, Y. Ie et al., *Synthesis* **2021**, *53*, 3390.