Ferroelectric Organic Semiconductor: Structural and Physical Properties of Alkylamide Substituted BTBT Derivatives

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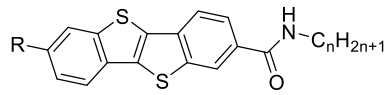
[1]Benzothieno[3,2-*b*][1]-benzothiophene (BTBT) derivatives can form the 2D electronic structure and organic field-effect transistors (OFET) with high hole mobility.[1] On the other hand, alkylamide-substituted π-electronic molecules can show ferroelectric behavior accompanying by the dipole inversion at hydrogen bonding (HB) sites of alkylamide units.[2] Such polarization change has a potential to affect the semiconducting behavior. Herein, we synthesized alkylamide-substituted R-BTBT-CONHC$_n$H$_{2n+1}$ (**Fig. 1**), which semiconducting behavior, ferroelectricity, and molecular assembly structures were examined. Single-crystal X-ray structural analyses of **1** and **3** revealed the formation of herringbone arrangement of BTBT skeleton and the 1D HB chains of alkylamide groups (**Fig. 2**). The thin-films of **2** were fabricated for channel layer of a top-contact type OFET device and its μ_{FET} and V_{Th} values were observed at 0.021 cm^2 V^{-1} s^{-1} and −9.7 V, respectively (**Fig. 3**). Based on the DSC and XRD measurements, **2** formed the SmE phase above 369 K followed by the melting at 469 K. The ferroelectric hysteresis behavior of **2** was observed in the *P*-*E* curve at the SmE phase with E_c = 5.65 V μm^{-1} and P_r = 2.21 μC cm^{-2} at 413 K and 0.1 Hz, respectively (**Fig. 4**).



1 : R = C_8H_{17} n = 3
2 : R = C_8H_{17} n = 14
3 : R = H n = 3
4 : R = H n = 14

Fig. 1. R-BTBT-CONHC$_n$H$_{2n+1}$

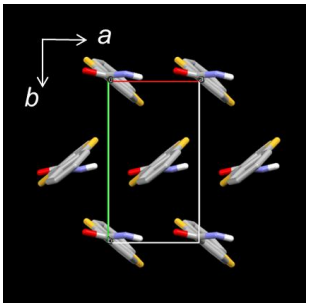


Fig. 2. Crystal structure of **1**.

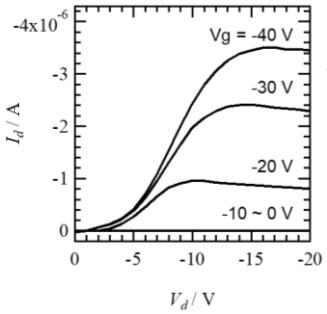


Fig. 3. Output curves of **2**.

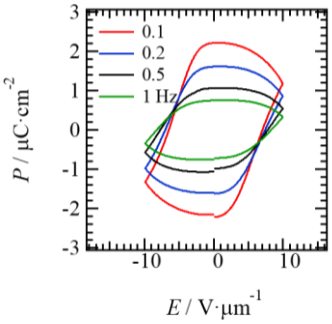


Fig. 4. *P*-*E* curves of **2**.

1) K. Takimiya, I. Osaka, T. Mori, M. Nakano, *Acc. Chem. Res*. **2014**, *47*, 1493.
2) H. Anetai, T. Takeda, N. Hoshino, H. Kobayashi, N. Saito, M. Shigeno, M. Yamaguchi, T. Akutagawa, *J. Am. Chem. Soc.* **2019**, *141*, 2391.