Synthesis and characterization of liquid crystalline organic semiconductor materials with benzothiophene skeleton

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[Introduction] Organic thin-film transistors are made with organic compounds with semiconductor characteristics and can be fabricated in a large area on thin substrates at low temperatures. However, the field-effect mobility indicative of transistor performance is low. One of the factors related to the low field-effect mobility is the crystal grain boundaries created during the fabrication of thin films for semiconductor devices. It has been reported that the self-organization of liquid crystal (LC) molecules can be used to improve this problem by suppressing the crystal grain boundaries¹. In this study, we focused on benzodithiophene (BDT) which has a planar conjugated structure expected to show high field-effect mobility². The objective of this study is to synthesize LC organic semiconducting polymers with high field-effect mobility at low temperatures by introducing polymerizable parts into organic semiconducting molecules with BDT cores and polymerizing them while retaining an LC order.

[Experiment] The target compound, 6-(6-(thiophen-3-yl-ethynyl)benzo[1,2-b:4,5-b']dithiophen-2-yl)hexa-5-yn-1-yl acrylate (PE-BDT-AA), was synthesized through the synthetic routes as shown in Figure 1 and was subjected to ¹H NMR (JEOL ECS-400) measurements to identify its structure.



Figure 1 Synthetic pathway of PE-BDT-AA.

[Results and Discussion] The results of differential scanning calorimetry (DSC) and powder X-ray diffraction (XRD) measurements of the obtained PE-BDT-AA are shown in Figures 2 and 3, respectively. As shown in Figure 2, an endothermic peak was observed at around 170 °C in the heating process. A fan-shaped texture was observed under a polarizing optical microscope around this temperature, suggesting the presence of the LC phase. Based on the results of XRD measurement at 160 °C as shown in Figure 3, this phase was determined to be a smectic E phase which is a higher-order LC phase.



[Reference]

1) W. Pisula, M. Zorn, and J. Y. Chang, Macromol. Rapid Commun., 2009, 30, 1179.

2) H. Wu, H. Iino, and J. Hanna, Chem. Lett., 2018, 47, 510.