

## Effect of Positional Isomerism of Picenodithiophene Derivatives on Semiconducting Properties

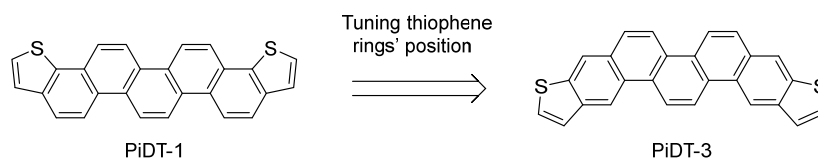
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A number of  $\pi$ -conjugated semiconducting materials have been developed for application in organic field-effect transistor (OFETs).<sup>1</sup> In particular, thienoacenes have received much attention due to their excellent organic semiconducting properties.<sup>2</sup> However, the introduction of thiophene rings into the acene backbone poses new problems due to the formation of various isomers such as stereoisomers and regioisomers, *etc.*<sup>3</sup> Recently, our research group has reported the synthesis of piceno[4,3-*b*:9,10-*b'*]dithiophene (PiDT-1) with seven fused rings and a  $\pi$ -extended conjugated system and its transistor properties, which exhibited high hole mobility but relatively larger threshold voltage.<sup>4</sup> In order to achieve higher mobility and low-voltage operation, we report the design, synthesis, physicochemical and FET properties of piceno[3,2-*b*:10,11-*b'*]dithiophene PiDT-3, an isomer of PiDT-1.

Initially, PiDT-3 was synthesized by Suzuki-Miyaura coupling reaction of 1,4-phenylenediboronic acid with 5-bromobenzo[*b*]thiophene-6-carbaldehyde as a key step. Subsequently, epoxidation and Lewis acid-catalyzed intramolecular cycloaromatization reactions were carried out to yield PiDT-3. The HOMO level of PiDT-3 increased from  $-5.6$  eV to  $-5.5$  eV with the change in the position of the thiophene rings. Additionally, the UV-vis absorption spectra of the obtained PiDT-3 showed a clear red-shift behavior due to the extended  $\pi$ -conjugation compared to PiDT-1. The OFETs based on PiDT-3 fabricated on FOTS-treated substrates exhibited hole mobility of  $1.8 \times 10^{-2} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ . However, the hole mobility of PiDT-3 was found to be lower than that of PiDT-1 despite the surface modification with different types of SAMs. These results highlight the importance of regioisomeric effects on intrinsic electronic and charge transport properties, and indicate the importance of further rationalization of molecular design.



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