

Heteroaromatic-Fused Tetrathiafulvalenes as Organic Semiconductors: Experimental and Theoretical Approaches

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Organic field-effect transistors (OFETs) have attracted current attentions owing to their potential applications. To date, various material classes, e.g. oligoacenes, oligo- and poly- thiophenes, and heteroarenes have been examined as an active material in high performance OFETs^[1]. Tetrathiafulvalene (TTF) derivatives are also reported to be a promising material class in this field: for example, transistors fabricated on single crystals of dibenzo-TTF (DB-TTF) and dithieno-TTF (DT-TTF) showed a field-effect mobility as high as 1.0 cm²/Vs^[2]. We were thus interested in aromatic-fused TTF derivatives, and examined various heteroaromatic-fused TTF derivatives, including thiophene-, selenophene-, and pyrrole-fused TTFs (Figure 1), as an active semiconducting material in thin-film transistors^[3, 4, 5]. In the present contribution, we will present experimental results on the syntheses, physicochemical properties, molecular and crystal structures, and transistor characteristics of chalcogenophene- and pyrrole-fused TTF derivatives.

In addition, with theoretical evaluations of these TTF derivatives in terms of internal reorganization energy (λ) and intermolecular transfer integral (t) in the solid state, we will discuss the relationship from their molecular structure to thin-film transistor characteristics via the molecular packing structure.

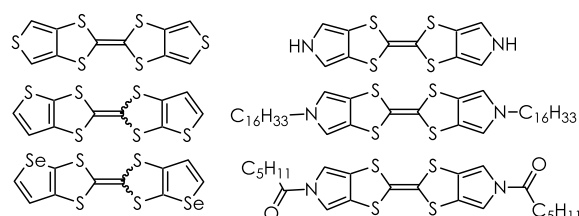


Figure 1. Chalcogenophene- and pyrrole-fused tetrathiafulvalenes examined in this study.

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