Z. CAI, H. ZHANG, H. GENG, Z. LIU,* S. YANG, H. LUO, L. JIANG, Q. PENG, G. ZHANG, J. CHEN, Y. YI, W. HU, D. ZHANG* (BEIJING NATIONAL LABORATORY FOR MOLECULAR SCIENCES, P. R. CHINA)

Thiepin-Fused Heteroacenes: Simple Synthesis, Unusual Structure, and Semiconductors with Less Anisotropic Behavior

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Category

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One-Pot Synthesis of Thiepin-Fused Heteroacenes

Significance: Polycyclic aromatic hydrocarbons with heteroatom substitution are attractive materials for semiconductor applications. The authors present the efficient installation of a thiepin unit onto easily accessible DIDT (C.-H. Chen, Y.-J. Cheng, M. Dubosc, C.-H. Hsieh, C.-C. Chu, C.-S. Hsu *Chem. Asian J.* **2010**, *5*, 2483). In this one-pot synthesis, DIDT was deprotonated with potassium *tert*-butoxide, reacted with carbon disulfide, and quenched with methyl iodide or hexyl bromide. The fused thiepins were obtained in 90% and 80% yield.

Comment: HOMO and LUMO energies were determined by cyclic voltammetry (−5.35 eV and −3.26 eV, respectively, regardless of the alkyl chain). Both compounds exhibited typical p-type semiconducting behavior with hole mobilities up to $1.0 \times 10^{-2} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. Thin films were further characterized by AFM and XRD. Crystal structures were obtained for both compounds and showed multiple S⋯S contacts.

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