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

Chem. Eur. J. 2013, 19, 14573-14580.

## 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 x 10<sup>-2</sup> cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>. Thin films were further characterized by AFM and XRD. Crystal structures were obtained for both compounds and showed multiple S···S contacts.

**SYNFACTS Contributors:** Timothy M. Swager, Georgios Markopoulos Synfacts 2014, 10(1), 0029 Published online: 13.12.2013 **DOI:** 10.1055/s-0033-1340393; **Reg-No.:** \$14913\$F

Synthesis of Materials and Unnatural Products

## **Key words**

fused ring systems

thiepins

heteroacenes