

Abstract Submitted
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Enantiotropic Polymorphism in Di-Indenoperylene¹ THEO SIEGRIST, Bell Laboratories, Murray Hill, NJ, USA, MICHAEL HEINRICH, Bell Laboratories, Murray Hill, NJ, USA, JENS PFLAUM, ASHUTOSH TRIPATHI, WOLFGANG FREY, University of Stuttgart, Stuttgart, Germany, MICHAEL STEIGERWALD, Columbia University, New York, NY, USA — The enantiotropic polymorphic phase transformation of di-indenoperylene (DIP), an organic semiconductor material, with transition temperature of 403 K, has been structurally characterized using single crystal X-ray diffraction. Both the low temperature α - and the high temperature β -phase have a herringbone-type structure, with the α -phase being triclinic with doubled unit cell volume compared to the monoclinic β -phase. In the latter, the molecules have a more upright orientation in the herringbone plane. The epitactic transformation from the β - to the α -phase involves strong shearing displacements as well as bending and torsional deformations of the DIP molecules. The β -phase of DIP is equivalent to the thin film phase.

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