

Abstract Submitted  
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**Enantiotropic Polymorphs in Pentacene**<sup>1</sup> THEO SIEGRIST, Bell Laboratories, Murray Hill, NJ 07974, CELINE BESNARD, EPFL, Lausanne, Switzerland, SIMON HAAS, ETHZ, Zurich, Switzerland, MARK SCHILTZ, PHILIP PATTISON, EPFL, Lausanne, Switzerland, DMITRY CHERNYSHOV, SNBL, ESRF, Grenoble, France, BERTRAM BATLOGG, ETHZ, Zurich, Switzerland, CHRISTIAN KLOC, Bell Laboratories — The high temperature structural phase transformation in bulk pentacene has been characterized by X-ray single crystal and powder diffraction. A well-defined transition temperature of 463K was observed in single crystals. In contrast, pentacene powders heated above the phase transformation temperature do not always fully convert, and upon cooling, coexistence of the two polymorphs in varying concentrations is observed down to room temperature. The 1<sup>st</sup> order phase transformation is isostructural, whereby the close packed herringbone-type layers shift against each other, keeping the same symmetry. The present results demonstrate that the structure of pentacene first reported in 1961 is actually stable only at high temperatures, and thus metastable at room temperature.

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