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Negative Thermal Expansion in Pentacene S. HAAS, ETH Zurich, T. SIEGRIST, Bell Labs, Murray Hill, NJ, P. PATTISON, EPF Lausanne, Switzerland, B. BATLOGG, ETH Zurich, Switzerland — The molecules in organic semiconductors, such as the oligoacenes, are held together by weak van-der-Waals (v-d-W) forces. As a result, one observes low dissociation temperatures, and large thermal expansion coefficients. Surprisingly, we have found a negative expansion coefficient in particular crystal directions. We have performed a complete X-ray structure analysis of pentacene and tetracene single crystals in a temperature range from 100–380 K. The anisotropic thermal parameters are analyzed in terms of librations and translations of the rigid molecules. Interestingly, we find upon increasing temperature a near-zero thermal expansion along a in tetracene, and a distinct contraction in pentacene. Upon close inspection of the full expansivity tensor and the thermal parameters we find a consistent explanation assuming that the v-d-W forces tend to minimize the relative shift along the long axis of adjacent molecules. This is further supported by the observation of an unusually large thermal expansion perpendicular to the layers, and the indications in our data of a distinctly anharmonic potential for the sliding motion along the long axis. These v-d-W forces leading to negative thermal expansion are expected to be larger in longer molecules and also to be the driving force behind the well known polymorphism of pentacene.

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