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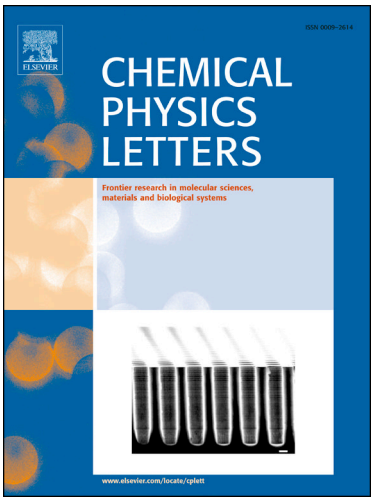

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Direction-dependent secondary bonds and their stepwise melting in a uracil-based molecular crystal studied by infrared spectroscopy and theoretical modeling

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Abstract

Three types of supramolecular interactions are identified in the three crystallographic directions in crystals of 1,4-bis[(1-hexylurac-6-yl)ethynyl]benzene, a uracil-based molecule with a linear backbone. These three interactions, characterized by their strongest component, are: intermolecular double H-bonds along the molecular axis, London dispersion interaction of hexyl chains connecting these linear assemblies, and π–π stacking of the aromatic rings perpendicular to the molecular planes. On heating, two transitions happen, disordering of hexyl chains at 473 K, followed by H-bond melting at 534 K. The nature of the bonds and transitions was established by matrix-isolation and temperature-dependent infrared spectroscopy and supported by theoretical computations.

Keywords: H-bond, DFT computations, self-assembly

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