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Crystal and Rotator Phases of n-alkanes: a Molecular Dynamics Study NATHANIEL WENTZEL, SCOTT T. MILNER, Pennsylvania State University — The odd n-alkanes exhibit a wide variety of solid phase behavior; experimentally observed phases include an orthorhombic crystal phase, in which the molecules show long range herringbone order, and rotator phases in which the molecules do not diffuse but display various degrees of disorder. The rotator phases are of interest because they are implicated in the nucleation of n-alkane and polyethylene crystals. C_{23} has been found experimentally to have two stable rotator phases, orthorhombic R_I and hexagonal R_{II}, at temperatures between the crystal and melt. The crystal–R_I and R_I–R_{II} phase transitions are observed to be weakly first order. Simulations of C_{23} to date have found the R_I phase but not the R_{II} phase, and have not much characterized the phases or the transitions between them. We report our results for local order and pretransitional fluctuations of rotator phases, from our all-atom molecular dynamics simulations of thin layers of C_{23}. We also comment on how these properties relate to the experimentally observed phase transitions.

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