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Computer Simulations of Semi-flexible Polymer Chains VENKAT PADMANABHAN, SANAT K. KUMAR, Columbia University, ARUN YETHIRAJ, University of Wisconsin — Monte Carlo Simulations are performed to obtain the isotropic-nematic (IN) transition in systems with semi-flexible polymer chains of different lengths. The chains are modeled as spherical beads that interact via a square-well potential. Bonded beads are connected by strings chosen so that bond length varies between 1.01σ and 1.05σ (where σ is the hard sphere diameter). The stiffness of the molecules is controlled via a potential between beads separated by two bonds; this potential restricts the distance between these beads to be between 2.02σ and 2.1σ. The vapor-liquid coexistence and isotropic-nematic (IN) coexistence curves are obtained using computer simulations. An IN transition is found for $N_b \geq 10$. The density, at which the IN transition occurs, moves to higher values as N_b is increased and then drops on further increase. This is analogous to the initial increase in the critical density for pure alkanes as the chain length is increased.

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