

Effect of branching on the fluid phase behavior of alkane monolayers

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Abstract

Configurational-bias Monte Carlo simulations in the grand canonical ensemble with histogram reweighting were used to obtain the vapor-liquid coexistence curves of three hexane isomers physisorbed on a flat gold substrate. Examination of the critical ordering operator distributions confirms that these systems exhibit critical behavior consistent with the 2D Ising universality class. The critical temperatures for 2,2-dimethylbutane, 2,3-dimethylbutane and *n*-hexane were determined as $T_c^{2D} = 195.0, 161.2$ and 152.4 K, respectively. This is qualitatively different from the behavior observed for bulk (3D) fluids where branched alkanes typically exhibit lower critical temperatures than their linear counterparts.

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