Thin Films of Decane and its Branched Isomers Adsorbed on a Metal Substrate

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Hydrocarbons are important components of lubricant systems, and there is much interest in their interactions with solid surfaces. Prior research has shown longer alkanes are preferentially adsorbed and form a solid monolayer close to the surface[1]. This research has been extended to observe the effect of branching on adsorption. Using the Metropolis Monte Carlo method, molecular thin films containing decane and its isomers are simulated near a solid surface. The isomers are 2,2-dimethyloctane and 4-propylheptane. There are three binary mixtures and one ternary mixture all containing equal mole fractions of each isomer. Each mixture was simulated at three temperatures: 300 K, 350 K, and 400 K. Simulation results were in good agreement with experimental findings. Molecules close to the surface are characterized by fewer conformational defects and are more densely packed than molecules in the bulk region of the film. The linear alkane, decane, was preferentially adsorbed over the branched isomers at 4 and 8 Angstroms from the surface. The branched isomers are oriented into a few specific positions closer to the interface. Additional analyses include density and orientation profiles, conformational defect analysis, and an examination of the end-to-end length of the molecule as a function of distance from the surface.

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[1] Castro, M. A.; Clarke, S. M.; Inaba, A.; Arnold, T.; Thomas, R. K. *J. Phys. Chem.* **1998,** 102, 10528