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Mixture Properties of Flexible Chains: Comparisons between Experiment, Simulation and Theory; Contrasts between Lattice and Continuum RONALD WHITE, JANE LIPSON, Dartmouth College — We present new theoretical results for a series of binary chain-molecule mixtures using both the hard-sphere, and the square-well potentials. We compare these results to simulation data, and contrast them to those obtained using the analogous lattice version of the theory. We discuss all of our findings in the context of experimental data for hydrocarbon chain mixtures. In the course of these studies we consider mixtures of components with varied chain lengths and energetics, and examine the effects of changing composition, temperature, and density. In addition, by calculating the free energy over a wide range of the P,V,T and composition space, we are able to characterize coexistence, both liquid-vapor as well as liquid-liquid partial miscibility.

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