

Vapor-Liquid Equilibria of Linear Molecules with a Center Shifted Point Dipole

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We are presenting results for models of linear rods with a point dipole embedded in the geometric center. Previously, we have obtained results for the vapor-liquid equilibrium (VLE) of similar systems with centered point dipoles. Our results included models [1] as well as real systems [2]. More recently, we have obtained structural properties for a system with a shifted dipole respect to the geometric center, and have found relevant results relating to the appearance of dimmers [3]. Now, we present systematic simulations for linear systems with a shifted point dipole in order to calculate the VLE of models with different aspect ratios, shifts, and dipole strengths. Our simulations using the Gibbs ensemble Monte Carlo (GEMC) method allow us to calculate equilibrium densities, as well as vapor pressures at each temperature. Moreover, from our results for models, we have found intermolecular parameters for some important substances including 1-alcohols and 1-amines. The results obtained fit the experimental data very well.

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