Aggregation Volume Bias Monte Carlo Simulations of Alkanoic Acids

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Aggregation volume bias Monte Carlo simulations in the isobaric-isothermal and Gibbs ensembles are used to explore the vapor-phase compressibilities and structures and the vapor-liquid coexistence curves of alkanoic acids. Particular emphasis is placed on a sampling protocol that allows for reliable sampling of the aggregate distribution in the vapor phase. Simulation results for the united atom versions of the OPLS (optimized potentials for liquid simulations), TraPPE (transferable potentials for phase equilibria), and SPEADMD (step potential equilibria discontinuous molecular dynamics) force fields are extensively compared to experimental data.