Abstract Submitted
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Structure of Aqueous Organic Nanodroplets from Density Functional Theory[1] G. WILEMSKI, J.-S. LI, University of Missouri-Rolla — Aqueous aerosol droplets play a major, but poorly quantified role in atmospheric radiative forcing. To understand this role better, detailed knowledge of microscopic droplet properties is needed. We use density functional theory to study binary nanodroplets for a model system resembling an aqueous pentanol mixture. The model is a binary mixture of hard spheres with attractive Yukawa forces whose parameters are chosen to give rough agreement with measured vapor pressures, densities, and surface tensions of pure bulk water and pentanol at 250 K. The model properly predicts bulk liquid-liquid phase separation at small pentanol concentrations. Nanodroplet composition, structure, and size (1 nm to 30 nm) were studied by varying the vapor phase composition and pressure. At low pentanol vapor compositions, the nanodroplets have water-rich cores surrounded by a thin pentanol-rich shell. At high pentanol vapor concentrations, the droplets are nearly uniform binary mixtures with an outer layer of pure pentanol. The phase boundary for the core-shell region is not described well by classical thermodynamics. This failure highlights the importance of using nonclassical approaches to investigate the behavior of multicomponent aerosol droplets.

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