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Fluctuating confinement of water in aqueous organic nanodroplets[1] GERALD WILEMSKI, FAWAZ HRAHSHEH, Missouri University of Science and Technology — Supercooled and nano-confined water occurs frequently as nanometer-sized aqueous-organic aerosol droplets that are ubiquitous in the atmosphere and in many industrial processes. Nanodroplet structure is important because it influences droplet growth and evaporation rates, heterogeneous reaction rates, and radiative properties. We use classical molecular dynamic simulations to study the structure of ternary water-butanol-nonane nanodroplets for several temperatures and droplet sizes. We study the effects of butanol on the wetting of the water/butanol core-shell droplet by the nonane lens. At low concentrations, butanol acts as a surfactant to significantly enhance the wetability of the water droplet by nonane. At 250 K, with sufficient butanol and nonane, perfect wetting (thin film formation by nonane) occurs. Perfect wetting also occurs at higher temperatures, 270 K to 300 K, but this wetting state is progressively destabilized at higher temperature. All of the nanodroplets studied undergo distinct transitions between partial dewetting and perfect wetting states due to isothermal fluctuations in the local distribution of butanol on the surface of the water core. These fluctuations favor the wetted state at lower temperatures and the dewetted state at higher temperatures.

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