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Nonspherical structure of aqueous organic nanodroplets[1] BARBARA E. WYSLOUZIL, HARSHAD PATHAK, Ohio State University, FAWAZ HRAHSHEH, GERALD WILEMSKI, Missouri University of Science and Technology — The structure of nanodroplets plays a critical role in many natural phenomena involving atmospheric nucleation and aerosol formation. Here, we review our experimental and theoretical work on the structure of nonane/water nanodroplets. The experiments involve small angle x-ray scattering (SAXS) of nanodroplets formed in supersonic nozzles. Classical density functional theory (DFT) calculations of species density profiles are made in cylindrical coordinates, which allows for the possibilty of non-spherical droplets under appropriate conditions. One key theoretical result is the occurrence of a nonspherical Russian-Doll (RD) structure at low temperatures that is confirmed by molecular dynamics (MD) simulations. Some, but not all, of the measured SAXS spectra can be well-fit by a simple RD model, but the poor x-ray contrast between nonane and deuterated water generally makes it difficult to distinguish among well-mixed, core-shell, and RD structural models.

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