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Contrasting Nonaqueous against Aqueous Solvation on the Basis of Scaled-Particle Theory HENRY S. ASHBAUGH, Tulane University

Normal hexane is adopted as a typical organic solvent for comparison with liquid water in modern theories of hydrophobic hydration, and detailed results are worked-out here for the C-atom density in contact with a hard-sphere solute, $rho^*G(R)$, for the full range of solute radii. The intramolecular structure of an n-hexane molecule introduces qualitative changes in G(R) compared to scaled-particle models for liquid water. Also worked-out is a revised scaled-particle model implemented with molecular simulation results for liquid n-hexane. The classic scaled-particle model, acknowledging the intramolecular structure of an n-hexane molecule, is in qualitative agreement with the revised scaled-particle model results, and is consistent in sizing the methyl/methylene sites which compose n-hexane in the simulation model. The classic and revised scaled-particle models disagree for length scales greater than the radius of a methyl group, however. The liquid-vapor surface tension of n-hexane predicted by the classic scaled-particle model is too large, though the temperature variation is reasonable; this contrasts with the classic scaled-particle theory for water which predicts a reasonable magnitude of the water liquid-vapor surface tension, but an incorrect sign for the temperature derivative at moderate temperatures. Judging on the basis of the arbitrary condition that drying is indicated when G(R) < 1, hard spheres dry at smaller sizes in n-hexane than in liquid water.