Corresponding-States Correlations for Estimating Partial Molar Volumes at Infinite Dilution of Nonelectrolytes in Water over Extended Temperature and Pressure Ranges

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Corresponding-state correlations, based on a universality of properly reduced properties, provide an extremely valuable tool for physical property estimation. We have previously shown that the infinite dilution solute–solvent direct correlation function for the simple fluids argon and methane in water at 298-700 K at different pressures can be universally scaled as a function of water density. This correlation has now been extended to aqueous alcohols from 298 to 600 K with the remarkable characteristic that the hydrocarbon backbone (aliphatic, aromatic, cyclic) is unimportant; the density dependence of the reduced correlation function integral for aqueous alcohols is determined chiefly by the hydroxyl group. Similar universalities have also been found for the aqueous nitrogen-containing compounds of ammonia, aliphatic and aromatic amines, and pyridine.

Additionally, values of the scaled solute–solvent direct correlation function integrals systematically decrease with the strength of solute-solvent attractions from simple fluids through carbon dioxide, phenol, boric acid, etc., at water densities below 900 $kg \cdot m^{-3}$. On the other hand, at higher water densities all correlation function integrals, even for pure water, appear insensitive to the detailed nature of the solute. Both of these results suggest a corresponding states method for estimating the infinite dilution properties of aqueous solutes over wide ranges of water densities.