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Molecular Aggregation in Binary Mixtures of Pyrrolidine, N-Methylpyrrolidine, Piperidine, and N-Methylpiperidine with Water: Thermodynamic, SANS, and Theoretical Studies

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Abstract

© 2017 American Chemical Society. Piperidine and N-methylpiperidine hydrates aggregate in liquid aqueous solutions due to hydrogen bonds between hydration water molecules. No such effects occur in the mixtures of the amines with methanol, that supports the idea of active role of water solvent in the aggregation. However, the question of contributions in thermodynamic functions due to specific interactions, van der Waals forces, and the size and shape of the molecules remains open. In the present study, limiting partial molar enthalpies of solution of pyrrolidine, N-methylpyrrolidine, piperidine, and N-methylpiperidine in water and methanol and vice versa were measured and compared with those assessed from theoretically calculated molecular interaction energies using a simple "chemical reaction" model. Nearly quantitative agreement of the enthalpies was achieved for the systems studied, except the amines in water. The latter required an empirical hydrophobic hydration term to be considered. The hydrogen bonds formation and breaking which accompany the mixtures formation leads to considerable excess volumes, while the size of the solute molecules is manifested rather in the compressibility of aqueous solutions. SANS evidenced that aqueous solutions are microheterogeneous on the nanometer-order length scale. The propensity to promote phase separation increases in the order: N-methylpiperidine < N-methylpyrrolidine < piperidine < pyrrolidine.

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