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Volumetric, Viscometric and molecular simulation studies of glycine in aqueous sodium sulphate solutions at different temperatures

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Abstract

The densities and viscosities of Glycine in five aqueous solutions of Sodium Sulphate, were measured in the temperature range from 283.15 to 308.15 K at intervals of 5 K, using a vibrating U-tube densimeter Anton Paar DMA 5000 and the Automatic Microviscosimeter AMVn, respectively. The measured densities were used to calculate the limit-apparent molar volume (V_{ϕ}^0), limit-transfer molar volume ($\Delta_{tr}V_{\phi}^0$) and hydration number (n_h). The partial volumes at infinite dilution of the glycine in aqueous solution of sodium sulfate were evaluated through extrapolation at each temperature. The behavior of $\Delta_{tr}V_{\phi}^0$ was interpreted in terms of solute–solvent interactions on the basis of the cosphere-overlap model. The hydration numbers were positive and interpreted in terms of dehydration and electrostriction effects. The relative viscosity data were adjusted by least-squares for obtain the Jones-Dole equation coefficients A , B and D . To accompany the experimental results, a series of small molecular complexes simulating the interactions present in the glycine + water/sodium sulfate systems were modeled by the Density Functional Theory with the basis function 6-31G(d). From viscosity dates, the activation parameters of the viscous flow (free molar energy of Gibbs ΔG^{\ddagger} , enthalpy ΔH^{\ddagger} , and entropy ΔS^{\ddagger}) were evaluated. The temperature dependence of the partial molar volume at infinite dilution and the viscosity B coefficient were discussed in terms of the dominant interactions in solution; it was found that the glycine has a making effect in the structure of the solvent, and at infinite dilution ion-solvent interactions are dominant between NH_3^+ and COO^- groups of the amino acid with Na^+ and SO_4^{2-} ions. From the theoretical point of view, the complexes studied turned out to be stable and represent a good approximation to rationalize the intermolecular interactions that occur in glycine + water / sodium sulphate mixtures.

Keywords: Aqueous solution; density; viscosity; partial molar volume of transfer; hydration number.

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