Prediction of Individual Ionic Activity Coefficients for Some Aqueous Chloride Salt Solutions

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Theoretical calculations of individual ionic activity coefficients (IIAC) for four chlorine salts in aqueous solutions are presented. The IIAC are predicted first by using Debye-Hückel theory with different ion radii, and the results show a significant deviation from experimental data. IIAC are also predicted by using Debye-Hückel theory plus the Born equation, and the results show that the Debye-Hückel theory plus Born equation can accurately predict the IIAC (for example, the average relative deviations between predicted values and experimental data for the activity coefficients of Na⁺, Cl⁻ and NaCl are 0.6%, 1.7%, and 0.9%, respectively). In calculations, experimental liquid densities and relative static permittivity are used, and the ion-ion interaction and ion-water interaction contributions of the activity coefficients are analysed and discussed. The effects of ion size on electrostatic interaction calculations are further discussed.

Keywords: Individual Ionic Activity Coefficients; Aqueous Electrolyte Solution; Classical Solution Theory; Ion Radius

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