Accurate Prediction of Deprotonation and pH value of Acids in Aqueous Solutions over the Whole Concentration Range

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Abstract

The pKa of an acid is important for determining the dissociation and thermodynamic properties of solutions containing it. However, the value of pKa is typically determined at dilute limit and cannot be used to describe properties of the solution at high concentrations. In this work, we propose an approach to determine the concentration independent equilibrium constant Keq based on pKa and predicted activity coefficients. The Keq determined is applied to predict the degree of dissociation over whole concentration range for weak to strong acids. The pH of acid aqueous solution is predicted over whole concentration range, showing a good agreement with experiments. Based on this approach, we found that the vapor pressures of acid aqueous solutions strongly depend on the degree of dissociation of acids. The proposed model provides useful insights to link the macroscopic properties of acid aqueous solutions to its microscopic dissociation phenomena over the whole concentration range.

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