Prediction of Dissociation and pH value of Acids in Aqueous Solutions

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The pKa of an acid is important for determining the dissociation and thermodynamic properties of solutions containing it. However, the value of pKa is not concentration independent and cannot be used to describe properties of high concentration solutions. In this work, we propose an approach to determine the concentration independent equilibrium constant Keq based on pKa and predicted activity coefficients. The equilibrium constant thus determined is applied to predict the degree of dissociation over whole concentration range for weak to strong acids. The proposed method is capable of capturing the redissociation phenomenon observed in sulfuric acid aqueous solutions. Furthermore, 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.