PRES17.0225

Study on the Structure of Potassium Chloride Aqueous Solution by Molecular Dynamics and Raman Spectroscopy Methods

F. Li¹, S. Li¹, X. Zhuang¹, J. Yuan*¹

¹Hebei University of Technology, China

Abstract

Study of aqueous solution micro structure is conducive to the development of water treatment materials. In this paper, molecular dynamics simulation of structure of dilute KCl aqueous solutions at 298 K was systematically carried out using the COMPASS force field. Based on simulation results, when the concentrations of KCl are 0.01 M, 0.05 M, 0.10 M, 0.50 M, 0.75 M, 1.00 M and 2.00 M, the coordination numbers of $\text{K}^+$ are 6.43, 6.41, 6.41, 6.36, 6.27, 6.24, and 5.73. Raman spectrum has been performed on this series of solutions. It revealed that the hydrogen bonds between water molecules were almost the same as that in pure water when the concentrations were below 0.10M. While at 0.50 M, 0.75 M, 1.00 M, and 2.00 M, the hydrogen bonds were obviously disturbed. The results obtained by Raman spectrum can directly support the simulation results. In general, it was speculated that the structure tends to be steady in dilute KCl solutions when the concentration is lower than 0.10 M.