Monte Carlo Simulations on Model Fluid Electrolyte Solutions

C. Li [C, S], R. Tian, G. Lu and Z. Wang
Department of Chemical Engineering, Beijing University of Chemical Technology, Beijing, P.R. China

A series of radial distribution functions, configuration energies, and pressures for symmetrical electrolyte model fluids of the 1:1 and 2:2 type at various conditions were obtained by Monte Carlo simulations in the NVT canonical ensemble. These results are of great significance for the development of a new reference fluid for electrolyte solutions. The electrolyte solution is represented with a mixture of charged and dipolar hard sphere. The structural order and thermodynamic properties of ion-dipole mixtures as well as their dependence on temperature, concentration and overall density are discussed.