

Computer Simulation of Ionic Diffusion and Mobility in Molten Chlorides

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The transport properties of different ions dissolved in a potassium chloride melt are studied using Nosè-Hoover molecular dynamics and the new fast method of evaluation of Coulombic forces in ionic liquids [1]. The diffusion coefficients, external mobilities, and structure characteristics are determined in the whole range of Li concentrations, from pure LiCl to a dilute solution of Li in KCl, using the ionic model and Fumi-Tosi potentials. In strongly non-ideal LiCl-KCl melts, the diffusion coefficients and mobility of all of the ions strongly depend on the temperature, density, and concentration of Li. Estimated diffusion coefficients are reasonably well reproduced by the Stokes-Einstein formula with an effective ionic radius as the only parameter. Ionic mobility is largely affected by the electrophoretic drift of solvation shells, and cannot be described within the conventional Nernst-Einstein approximation. The dependency of the apparent charge, which is less sensitive to variations in density and temperature, and depends mainly on the concentration of Li ions, was determined at constant temperature and density of molten LiCl-KCl as a function of concentration. For some ions, negative values of apparent charge at low concentrations are found, and a possible explanation for this effect is proposed.

[1] E. Yakub and C. Ronchi, *Journ. Chem. Phys.* **119**, 11556 (2003).