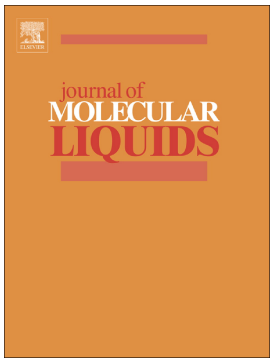

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The structure of aqueous lithium chloride solutions at high concentrations as revealed by a comparison of classical interatomic potential models

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Abstract

Highly concentrated aqueous lithium chloride solutions were investigated by classical molecular dynamics (MD) and reverse Monte Carlo (RMC) simulations. At first MD calculations were carried out applying twenty-nine combinations of ion-water interaction models at four salt concentrations. The structural predictions of the different models were compared, the contributions of different structural motifs to the partial pair correlation functions (PPCF) were determined. Particle configurations obtained from MD simulations were further refined using the RMC method to get better agreement with experimental X-ray and neutron diffraction data. The PPCFs calculated from MD simulations were fitted together with the experimental structure factors to construct structural models that are as consistent as possible with both the experimental results and the results of the MD simulations. The MD models were validated according to the quality of the fits. Although none of the tested MD models can describe the structure perfectly at the highest investigated concentration, their comparison made it possible to determine the main structural properties of that solution as well. It was found that four nearest neighbors (oxygen atoms and chloride ions together) are around a lithium ion at each concentration, while in the surroundings of the chloride ion hydrogen atom pairs are replaced by one lithium ion as the concentration increases. While in pure liquid water four water molecules can be found around a central water molecule, near the solubility limit nearly all water molecules are connected to two chloride ions (via their hydrogen atoms) and one lithium ion (by their oxygen atoms).

Keywords: Molecular dynamics; Reverse Monte Carlo; Aqueous solutions; Lithium chloride; Ion-water potential model; Structure