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Orientational Pair Correlation Functions Modelling of the LiCl6H2O by the Hybrid Reverse Monte Carlo: Using an Environment Dependence Interaction Potential

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Abstract : On the basis of four partial correlation functions and some geometric constraints obtained from neutron scattering experiments, a Reverse Monte Carlo (RMC) simulation has been performed in the study of the aqueous electrolyte LiCl6H2O at the glassy state. The obtained 3-dimensional model allows computing pair radial and orientational distribution functions in order to explore the structural features of the system. Unrealistic features appeared in some coordination peaks. To remedy to this, we use the Hybrid Reverse Monte Carlo (HRMC), incorporating an additional energy constraint in addition to the usual constraints derived from experiments. The energy of the system is calculated using an Environment Dependence Interaction Potential (EDIP). Ions effects is studied by comparing correlations between water molecules in the solution and in pure water at room temperature Our results show a good agreement between experimental and computed partial distribution functions (PDFs) as well as a significant improvement in orientational distribution curves.

Keywords : LiCl6H2O, glassy state, RMC, HRMC
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