

# Ion solvation and diffusion in organic solvents

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Structural and dynamical properties of ions in organic solvents are calculated using molecular dynamics. Coordination numbers, solvation energies and ion diffusivities are considered. It is demonstrated that these properties are defined by the atoms of the organic molecules that are bound to the ion. A theoretical model of the ion solvation and diffusion in organic solvent is developed and tested. It is in a good agreement with results of the molecular dynamics and available experimental data.

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