

# Explaining Nonmonotonic Ionic Conductivity in Binary Ionic Liquid-Solvent Mixtures

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Binary mixtures consisting of ionic and molecular solvents are known to exhibit composition dependent non-monotonic transport properties. These deviations from ideality are more pronounced in some mixtures and may be highly beneficial for specific applications. For example, ionic conductivity of binary mixtures can be increased by suitable choice of solvents, providing a powerful approach for electrolyte design in electrochemical systems and energy storage applications. This nonideality has often been attributed to changes in the solvation of ions, clustering of the ions, and the number of charge carriers. In this work, we implement molecular dynamics simulations to examine the ionic liquid 1-ethyl-3-methylimidazolium dicyanamide and its mixtures with ethylene glycol, the system which exhibits non-monotonic behavior for ionic conductivity as the composition of the mixture is varied. We estimate ionic conductivities of these mixtures at different ionic liquid mole fractions and compare them with experimental values. By analyzing the solvation structures of cations and anions through radial distribution functions and three dimensional spatial distribution functions, we will attempt to identify structural changes in an effort to explain the ionic conductivity maximum. We will also demonstrate the accuracy of the commonly used force fields in quantitatively predicting the ionic conductivity of ionic liquid-solvent mixtures and our efforts to improve predictive power of force fields for systems involving electrolytes and organic solvents.