

A Molecular Dynamics Study of the Electrostatics of
Solute-Solvent Interactions in Ionic Liquids - M. Kobrak
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The recent emergence of room-temperature molten salts (“ionic liquids”) as solvents for synthetic chemistry has created the need for an understanding of the interactions between a molecular solute and an ionic solvent. Such interactions are qualitatively different than for molecular solvents, and properties such as solvent dipole moment and dielectric constant are no longer simply related to the solvation behavior of the liquid. We present the results of molecular dynamics simulations characterizing energetic and dynamic aspects of the electrostatics of solute-solvent interactions for molecular solutes in molten salts, and discuss how ionic structure influences these interactions.