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# Structural Design of Ionic Liquids for Biomass Processing

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Ionic liquids (ILs) are molten salts at room temperature. ILs possess remarkable physio-chemical properties including high solubility of compounds that are otherwise insoluble in molecular solvents. One important application is the dissolution of lignin during pretreatment of biomass. Previous studies have shown low-cost and biocompatible ILs containing cholinium as the cation and an amino acid as the anion. Cholinium lysinate (ChLys) demonstrates the highest potential as a lignin processing solvent, with low viscosity and high selectivity at ambient temperature. The treatment is effective with up to 20% water.

Time-of-flight neutron diffraction directly measures the structure of ILs and its mixtures. Using isotopic substitution of hydrogen by deuterium, we simultaneously fit a series of diffraction patterns into a simulation method called Empirical Potential Structure Refinement (EPSR). This method experimentally refines a simulation box to describe liquid structure at the nano- and atomic scale. Our study investigates the structure of amino-acid ILs, with and without the presence of water. We use guaiacol (2-methoxy-phenol) as a model aromatic residue of lignin to identify key solvent-solute interactions. Bio-based ILs can be nanostructured. Results show pronounced nanostructure of ChLys before and after the addition of water. The added water molecules form domains at the nanoscale, without disrupting the amphiphilic nanostructure of ILs. Based on key intermolecular interactions, we present a framework for the design of IL structure to minimize competition and to enhance driving forces for aromatic extraction.

## Topic

Chemistry

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