The Computational and Experimental Study of Cellulose in Ionic Liquids and Water for Finding an Optimal Solvent for Biofuel Production

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Cellulosic ethanol is a renewable, alternative fuel that could reduce the reliance on fossil fuels. However, cellulose is resistant to breaking down into glucose because its crystalline structures make it inaccessible to catalysts in solution and this has prevented the widespread use of cellulosic ethanol. Ionic liquids have the potential for dissolving cellulose effectively to allow for catalysts to hydrolyze it for biofuels. This research investigated the solubility of cellotriose and cellopentaose in ionic liquids and water to determine what solvent can best promote dissolution of cellulose. Molecular dynamics simulations were performed on ionic liquid solutions of 1-ethyl-3-methylimidazolium chloride ([EMIM]Cl), 1-butyl-3-methylimidazolium chloride ([BMIM]Cl), 1-ethyl-3-methylimidazolium acetate ([EMIM]OAc), and 1-butyl-3-methylimidazolium acetate ([BMIM]OAc). The methods for analyzing the efficacy of the solvents include center of mass distance between cellulose molecules, number of hydrogen bonds, number of interactions by solvent, rotational entropy, nonpolar hydrogen interactions, dihedral angles plot, ring angles, orientation of the solvent molecules with cellulose, and radial distribution of the solvents. In addition, solvent shell models were made with two cellotriose molecules with a solvent shell and were minimized in energy to optimize the positions of molecules. The findings from these models suggest that ionic liquids are a superior solvent for dissolving cellulose. In particular, [BMIM]Cl appears to be the most effective solvent in dissolving cellulose based on the results from these models and experimental data. The results from this research could lead to more efficient hydrolysis of cellulose for biofuel production.

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