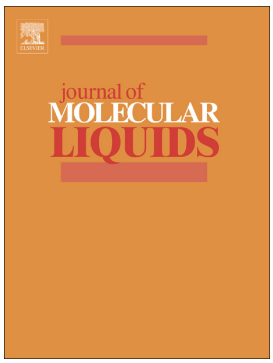

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COSMO-RS Predictions, Hydrogen Bond Basicity Values and Experimental Evaluation of Amino Acid-based Ionic Liquids for Lignocellulosic Biomass Dissolution

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Abstract.

In this study, the bamboo dissolution capability of six amino acid-based ionic liquids (AAILs) with two different cations, i.e. 1-ethyl-3-methylimidazolium (Emim) and Tetrabutylphosphonium (P_{4444}) and three anions derived from amino acids were investigated by Conductor-like screening model for real solvents (COSMO-RS) prediction and hydrogen bond basicity (β) of Kamlet−Taft parameters. COSMO-RS was used for calculating sigma profile, activity coefficients (γ_i) and aqueous base dissociation constant of corresponding acids of the anions (pKa) of AAILs. The trends in sigma profile, γi and pKa for AAILs were compared with β values and the effect of structure moiety of ionic liquids was also discussed. The trend of COSMO-RS prediction for anions was noted similar to the β values of AAILs with the exception of serinate anion. Similarly, the trend predicted by COSMO-RS and β values was also found same while changing the cations of AAILs. To investigate, the correlation of the above-mentioned properties with experimental dissolution ability, tetrabutylphosphonium aminoethanic acid ([P_{4444}]Gly) and 1-ethyl-3-methylimidazolium aminoethanic acid ([Emim]Gly) ionic liquids were synthesized and evaluated. The trend predicted by COSMO-RS and the β values were not correlating with efficiency of AAILs for bamboo dissolution. Both AAILs were able to dissolve the bamboo. However, material of P_{4444}]Gly treated sample was evaluated through XRD analysis where change in crystallinity of cellulose was identified after dissolution and regeneration of bamboo. Scanning Electron microscopy also showed homogenous structure for regenerated materials.