

Effect of Hydrogen Bonding on LCST Behavior of Aqueous Ionic Liquid Solutions

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Studies have shown that water consumption and wastewater production might constrain unconventional oil and gas production.¹ Recent studies have proposed using forward osmosis to recover clean water from such wastewater streams.^{2,3} Such a process requires a draw solution that can be easily regenerated once diluted, such as ionic liquids (ILs) showing a lower critical solution temperature (LCST) phase-split with water. Work by other groups has shown that hydrogen bonding between water and the IL anions plays a crucial role in LCST transitions in aqueous IL mixtures.⁴ To study the effects of hydrogen bonding in aqueous IL mixtures, we functionalized tetraalkylphosphonium cations with hydrogen bonding moieties (P_{444m} , $m = -C_3H_6OH$ and $-C_2H_4OCH_3$). We used COSMO-RS to screen for ion pairs that should show LCST behavior when mixed with water. Based on computational results, we synthesized and collected phase diagram using turbidimetry measurements. The cations have been paired with alkylsulfate and alkylsulfonate anions to study the effect of charge localization on the phase behavior of the ILs in aqueous solution. Preliminary results show that either adding alcohol functionality to the cation or using alkylsulfonate as the anion (instead of an alkylsulfate) raises the LCST by approximately 50°C. Current work is focused on determining the osmotic coefficients of aqueous solutions of these ILs to evaluate their performance as draw solutions.

References

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