

Formation and Analysis of Deep Eutectic Solvents in p-Toluenesulfonic Acid Monohydrate - Tetrabutylammonium Salt Systems

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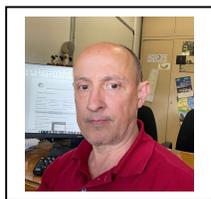
In recent years, Deep Eutectic Solvents (DESS) have emerged as promising alternatives to traditional solvents, owing to their lower environmental impact and reduced cost. Among the systems explored for potential use in solvometallurgical processes, those based on p-toluenesulfonic acid monohydrate (PTSA) have shown particular promise due to their ability to improve the dissolution of metal oxides [1]. In parallel, tetrabutylammonium (TBA) salts have been successfully implemented in the design of eutectic systems with tailored properties [2].

This study investigates a series of binary mixtures combining PTSA with various TBA salts, differing in anionic species such as bromide, chloride, tetrafluoroborate, triflate, and bis(trifluoromethylsulfonyl)imide. The selected anions vary in terms of size, structural complexity, and acid-base behavior. The thermal behavior and phase transitions of these mixtures were analyzed using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). DES formation was observed only in specific anion-composition combinations.

To elucidate the molecular interactions underpinning eutectic behavior, the systems were characterized through infrared spectroscopy across the mid- and far-IR regions. These measurements provided insights into the key intermolecular forces driving DES formation. Additionally, density functional theory (DFT) calculations were employed to model the interaction patterns at the molecular level, enhancing the interpretation of the experimental findings and offering a coherent picture of the coordination mechanisms within the studied systems.

References

1. N. Rodriguez Rodriguez, L. Machiels, and Koen Binnemans, *ACS Sustainable Chem. Eng.* 2019, 7, 3940–3948
2. S. Di Muzio, F. Trequattrini, O. Palumbo, P. Roy, J.-B. Brubach, A. Paolone, *ChemPhysChem* 2024, 25(16), e202400219.



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