Research Colloquium Seminar

Application of Imidazolium based Ionic Liquids for Desulfurization of Fuel and Preparation of Inclusion Complexes with Cyclodextrin

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Ionic liquids (ILs), organic salts having melting point at or below 100 °C, have received appeal across various fields due to their unique physico chemical properties such as appreciable thermal stability, low volatility, tunability as per their application etc. Environmental impact of pollution has attracted significant attention of ILs for removal of Sulphur and nitrogenic impurity from fuel. When fossil fuel burns, SO_x and NO_x particulate (SPM) matters are emitted. Hydro desulfurization (HDS) is the conventionally used method of desulfurization in industries. In this method, operating temperature ranges from 300-500 °C and H₂ pressure of 3.0 - 5.0 MPa. To overcome these disadvantages, extractive desulfurization (EDS) method has been developed where increasing use of ILs have been observed.¹

Host guest chemistry as a fascinating area has invited ILs as their guest components for the preparation of host guest or inclusion complexes (ICs). ICs have enormous potential in pharmaceutical industries in controlled release of drugs, removal of pollutants from industrial effluents and anti microbial activity. Cyclodextrin is a well-known host to accommodate variety of guests due to its extended hydrogen bonding and hydrophobic cavity. In recent years ILs are being studied for their activity as a guest for the preparation of host guest inclusion complexes.

In this work, Benzyl substituted imidazolium based isomeric aprotic ionic liquids have been synthesized and used to understand their on extraction efficiency (EE). Various parameters such as duration of rotation, temperature, concentration of IL, equilibration time were optimized to make the process more economical. Density functional theory (DFT) was employed to optimize the synthesized ILs using B3LYP method and 6-311G (++) (d, p) using Gaussian 09 software.³ Later on the same ILs were converted to their eutectic mixture by incorporating metal halide and their EE was found to improve to a greater extent. Due to structural and functional similarity of these ILs with a potent drug as an inhibitor of aldosterone synthase, they were used to prepare ICs with β -cyclodextrin and the same were characterized using various spectroscopic and conductometric techniques. The binding constants were estimated from UV-Vis spectra and conductometric experiment. Meta isomer proved to be best for removal of Sulphur content from fuel whereas the para isomer showed highest binding constant among all synthesized ICs.

References:

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