Ionic liquid as a novel partitioning media

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ABSTRACT

The partition coefficients of large number of organic solute including macrocyclic crown ethers in different water-ionic liquid (IL) bi-phasic systems based on Hartree-Fock (HF) and density functional theory (DFT) are presented here. The structure of imidazolium cation based ILs were optimized at HF-6-31G (d,p) level of theory and then surface charge density were calculated at BP-TZVP level of theory using novel conductor like screening model for real solvents (COSMO-RS) approach. The calculated value of density is decreased with increasing alkyl chain length for all the ILs considered here. The calculated values of partition coefficient for various organic solutes obtained from the first principle based COSMO-RS theory are reasonably in good agreement with the available experimental results. The predicted values of partition coefficient will help in the screening and thus selection and design of suitable ILs prior to solvent extraction experiments.

Keywords: Crown ether; Ionic liquids; Partition coefficients; Extraction; Density functional theory; Molecular modeling

1. Introduction

Chemical reactions are generally carried out in molecular organic solvents. Also, as traditionally practiced, solvent extraction experiments involve water-immiscible organic solvents, many of which are highly volatile, toxic and flammable. These demerits along with their adverse impact on the environment demand the replacement of these molecular organic solvents. Recently, IL has emerged as an alternative to the traditional organic solvents. These solvents composed of entirely of ionic species and some of them even remain liquid in room temperature popularly known as room temperature IL. Both the thermodynamics and kinetics of reactions are different in ILs than those in conventional molecular organic solvents which make them highly fascinating to the users in different field of chemical reactions, catalysis, separation and electrochemical cell. ILs exhibit several remarkable properties that make them highly attractive as a potential solvent medium for efficient extraction processes due to their wide range of liquid density, good thermal stability, and the ability to solubilize a large variety of organic and inorganic molecules, viscosities above those of most common organic solvents, almost zero vapor pressure and high degree of tunability [1,2] (for more details see the nice review by Poole et al. [3]). Advantage of working with ILs is that one can easily functionalize the cations and anions to obtain the properties desired, and when that is insufficient, suitable functional groups can be attached to the ions to meet the desired property. Recently, toxicity has also being considered before its use in practical application [4,5].