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Physicochemical Characterization of Chiral Ionic Liquids, Their Applications and Environmental Impact

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The steady interest in ionic liquids (ILs), salts with melting points typically around room temperature and always below 100 °C, comes from their remarkable physicochemical properties, such as a negligible vapor pressure, high thermal stability, high ionic conductivity, non-flammability, wide electrochemical window, task-specificity, and simpler recycling.

Chiral ionic liquids (CILs) are a subclass of ionic liquids; they are prepared from naturally existing building blocks such as amino acids, hydroxyl acids, sugars, alkaloids and other precursors obtained from the chiral pool. CILs provide an essential alternative to transition-metal catalysts in heterogeneous catalysis, especially the stereoselective hydrogenation [1]. To design and optimize efficient applications of CILs [2], the research of properties of these pure substances as well as their mixtures is necessary. Theoretical chemistry provides another way for understanding the relations between the macroscopic properties and the molecular structure. However, the development and prediction of models and computational simulations is not possible without knowledge of basic experimental data [3]. Moreover, the impact of ionic liquids on the environment is becoming increasingly important. Although ILs have a nearly negligible volatility, the potential hazard to the environment is not. A key indicator in the assessment of environmental risk is partition coefficient 1-octanol/water K_{OW} .

This study aims to characterize the thermodynamic properties of a homologous series of 1-[(1*R*, 2*S*, 5*R*)-(-)-menthoxyethyl]-3-alkylimidazolium salts with the bis(trifluoromethyl)sulfonylimide anion where the alkyl chain length ranges from methylene to dodecyl. The present range of CILs has an application potential mainly as reaction media and sources of chirality in asymmetric catalysis, but also as antielectrostatic and antibacterial agents. Basic thermophysical and thermodynamic properties of pure ionic liquids, such as their heat capacity, density, and refractive index are studied for determination of influence of the structure and the length of the alkyl chain on their

properties. To evaluate their hydrophobicity and/or lipophilicity, liquid-liquid equilibria in binary systems CIL + water, CIL + 1-octanol, and their partition coefficient 1-octanol/water K_{OW} are investigated. These parameters may be used as a departure point for the assessment of toxicity, biodegradability and tendency to bioaccumulation [3, 4].

Heat capacities are measured on Setaram μ DSCIIIevo microcalorimeter from 293.15 K to 348.5 K. The results show that the heat capacities of CILs increases both with growing temperature and with the length of the alkyl chain. The liquid-liquid equilibrium in binary system CIL + water is determined by a direct analytical method with spectrophotometer detection. The solubility of studied ionic liquids in water is about 10^{-5} mole fraction units.

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