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Ionic Liquids in Energy and Environmental Science: Properties and Applications

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Abstract

Ionic Liquids (ILs) are salts that include both cations and anions and are generally liquids at temperature below 100°C. At room temperature, salts that are liquids are known as Room-Temperature Ionic Liquids (RTILs). ILs has considerably lower melting points than inorganic salts, owing to the greater sizes of either the cations or the anion, or both. Furthermore, their molecular geometries have a significant degree of asymmetry, which affects ionic packing and, as a result, reduces Coulombic attraction between ions.

Keywords: Ionic liquids; Molecular liquids; Solvents; Electrolytes; Deep eutectic solvents

Introduction

Walden (1914) made the first IL by neutralizing ethylamine with a strong nitric acid solution. The ethyl ammonium nitrate IL $[EtNH^{+3}][NO_3]$ that resulted, had a melting point of 12°C. ILs did not attract much attention from scientists at the time, but they looked to be promising in a variety of electrochemical applications later in the 1980s. ILs, unlike molecular liquids, have a number of distinguishing characteristics that make them ideal solvents for a variety of industrial applications. High polarity, low volatility, strong thermal stability, high ionic conductivity, low melting point, and structural design ability are some of the physicochemical characteristics of ILs. ILs have been regarded as promising solvents with new characteristics in organic synthesis, catalysis, and electrochemistry, metal separation, gas separation, biomass processing, pharmaceuticals, tribology, and energy storage devices such as batteries, super capacitors, and fuel cells for the past two decades.

Deep Eutectic Solvents (DESs) are a novel family of solvents that have many characteristics with ILs, despite the fact that the two systems are quite different. DESs are produced by combining Lewis or Bronsted acids and bases, which may comprise anionic and/or cationic species, in contrast to ILs, which are made up of cations and anions. DES has lately incited a lot of attention as an ecologically friendly alternative for a variety of applications, including synthesis, gas adsorption, biomass processing, electrolytes for energy storage devices, and metal processing.

Hua and Shi have proposed a method for physically adsorbing onto steel-DLC contacts using a non-corrosive green lubricant containing dissolved lignin in ILs (lignin-[Choline][L-Proline]). When compared to commercially available lubricants, this green IL lubricant has a substantial improvement in wear resistance. Tong et al. used a combination of experimental and molecular dynamics modeling to give crucial molecular insight into the influence of lithium salt concentration on IL electrolytes. The study of the physicochemical characteristics, transport properties, and coordination structures of several IL electrolytes at varied lithium salt concentrations revealed changes in structural and physical properties on a micro-scale. Lethesh, et al. synthesized hydroxylcontaining pyridinium-based ILs with various alkyl side chains on the cation, as well as Br and [Tf_2N] anions. The physiochemical and electrochemical characteristics of these ILs were substantially influenced by the various alkyl side chains. The experimentally determined physicochemical characteristics match the expected values. The electrochemical window was found to be between 3.0 and 5.4 V. The 3-methyl/ethyl ILs with $3Tf_2N$ and $10Tf_2N$ had the greatest conductivity values (0.366383κ/S m^{-1}-0.383κ/S m^{-1}) among the synthesized ILs, according to DFT/COSMO-RS calculations.

Data was gathered on CO_2 solubilities and Henry's constant in Deep Eutectic Solvents (DES) from the literature, which they then processed using COSMO-RS-based calculations for enhanced verification and screening. The revised COSMO-RS with changeable universal parameters shows high reliability in predicting CO_2 solubility in DESs, with ARDs of 6.8%, 5.2%, 6.6%, and 4.7% for logarithmic CO_2 solubility in DESs of various HBA and HBD ratios. For efficient deconstruction of wheat straw biomass, Naz et al. propose IL-based catalysts using [BMPy]Cl in combination with a variety of metal chlorides. For [BMPy] +$CoCl_3$, the IL-metal catalytic systems exhibited up to 86% recovery and excellent recycling abilities. These IL-based catalytic systems have been offered as long-term solutions for converting wheat straw into useful goods.