Chapter 8
The Importance of Ionic Liquids and Applications on Their Molecular Modeling

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ABSTRACT

Ionic liquids are salts with melting points generally below 100 °C made of entirely ions by the combination of a large cation and a group of anions. Some ionic liquids are found to have therapeutic properties due to their toxic effects (e.g., anticancer, antibacterial, and antifungal properties). The determination of the most stable molecular structures, that is, the lowest energy conformer of these ionic liquids with versatile biological activities, is of particular importance. Density function theory (DFT) based on quantum mechanical calculation method, one of the molecular modeling methods, is widely used in physics and chemistry to determine the electronic structures of these stable geometries and molecules. With the theory, the energy of the molecule is determined by using the electron density instead of the wave function. It is observed that the theoretical models developed on the ionic liquids in the literature are in agreement with the experimental results because of electron correlations included in the calculation.

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INTRODUCTION

The first ionic liquid was synthesized by Paul Walden 104 years ago. Ionic liquids are eutectic salt mixtures that consist completely of ions and their melting point is normally below 100 °C. Ionic liquids have been of interest by reason of their many unique features such as superior capacity to dissolve organic and inorganic substances, enormously low volatility, adjustable nature, high thermal stability, high chemical inertness, adjustable viscosity, high conductivity, high heat capacity, wide electrochemical range. Ionic liquids have outstanding handling advantages like nearly zero probability of explosion in high-temperature chemical reactions on account of their low volatilities and non-flammability, their use over a broad range of reaction temperatures owing to their high thermal stabilities (ie thermal decay generally above 350 °C) and high boiling points, dissolution of several organic and inorganic materials in this liquids and usage of polar aprotic ionic liquids to replace harmful and flammable polar aprotic solvents such as dimethylsulfoxide, acetonitrile and dimethylformamide. As long as the synthesis routes and purification methods are more complicated, the costs of ionic liquids become even higher (Ozokwelu et al., 2017; Dupont et al., 2015).

General Synthesis Methods of Ionic Liquids

Lately, more ionic liquids have been synthesized by different methods. The reactions of the processes are commonly neutralization, quaternization and ion exchange reactions.

1. Acid-Base Neutralization

The exothermic neutralization reaction between equimolar Brönsted acid and Brönsted base that is performed either in a vessel equipped with a cooling jacket or in a flask immersed into a water bath, or an ice bath brings about the formation of ionic liquids through proton transfer, which is among the easiest synthesis routes. Following the reaction, remaining unreacted starting materials in ionic liquid can be readily removed from the formed product by washing with water, and the final product is dried in a vacuum oven (Wasserscheid and Welton, 2002). When carboxylic acids are treated with some amines at high temperatures, amides can form in place of ionic liquid.

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