Simple Prediction of Some Physical Properties of Ionic Liquids: The Residual Volume Approach

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Dedicated to Professor Mariana Palamareva on the occasion of her retirement from the University of Sofia

A new method for prediction of fundamental physical properties of ionic liquids (ILs) is proposed. The Residual Volume Approach (RVA) allows the estimation of density and viscosity of unknown ILs, using a simple linear correlation between a given property and a newly defined substituent parameter β^X. The proposed method has been developed for the density estimation of 50 *n*-alkyl-substituted imidazolium and tetraalkylammonium salts in a homologous series of ILs and has been extended for the estimation of viscosity, which also correlates linearly with the corresponding β^X. In addition, the parameters β^X are temperature and pressure independent, which allows the prediction of these values at any temperature and pressure.

Key words: Ionic Liquids, Predictive Methods, Physical Properties, Structure-Property Relationships, Residual Volume Approach

Introduction

Ionic liquids (ILs) are organic salts with melting points near r. t. (or by agreement below 100 °C). Recently, the unique material and solvent properties of such salts have led to an extraordinary increase of interest in them [1f]. Their fascinating properties favor application in diverse fields, such as synthesis [1d], catalysis [1a], electrochemistry [1b], separation technology, analytical chemistry, and nanotechnology [1e]. Nowadays, an immense number of possible ILs ($> 10^{14}$) [1c] can be easily obtained, but since the experimental study of such a huge number of potential cation-anion combinations together with their many substitution patterns is impossible, the fine-tuning of a certain property to fit a specific task is rather difficult. Therefore, understanding the behavior of ILs at molecular level and further implementing this knowledge in different property-predicting models is a great challenge for the research community, and any success in this field would facilitate their rational design. In this direction, several attempts at quantitative prediction of density [2a – h], viscosity [3a – f], surface tension [4a, b], conductivity [3b, 5] and melting points [2a, 6a – d] have been reported. The significance of these efforts is clear: on the one hand, to diminish the time- and money-consuming experimental work and, on the other, to promote the synthesis of the targeted IL.

Inspired by this work, we report here a facile and rapid method for the estimation of fundamental physical properties of room-temperature ionic liquids (RTILs) using a simple linear correlation between the given IL property and the residual volume of the *n*-alkyl substituents. Thus, we will show that the prediction of density and viscosity is an "easy game", and that this procedure can be carried out even by a non-specialist. Moreover, the application of this approach to a selected anion-cation combination allows both fine-tuning the desired property by a slight variation of *n*-alkyl substituents and predictions for different temperatures and pressures. This is of great importance from a practical point of view.