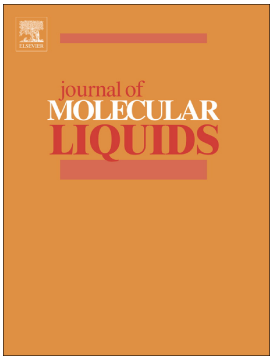

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Prediction of dielectric constant of ionic liquids

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Abstract

Ionic liquids are compounds commonly used as solvents in many fields of chemistry such as electrochemistry or separation techniques. One of the crucial properties for accommodation of the appropriate solvent to the specific process, is the solvation power of the solvent. It is usually expressed by the polarity and could be measured by the dielectric constant value (ε). Unfortunately, in case of ionic liquids there is a lack of available experimental data for dielectric constant. For that reason, this work presents a new approach that allows to find relationship between structural features and dielectric constant value. Our approach is based on the quantitative structure–property relationship (QSPR) method, therefore no additional experimental data is required. In this study, we found that both the ions have impact on the modeled value. Structural features like size, branching and polarizability play the main role in case of cation. However, the mass and shape of the anion are also important. Additionally, predictive ability of our approach was tested by using external data set. Moreover, the developed QSPR model have been additionally applied for estimating dielectric constant for new computationally designed 15 000 ionic liquids.

Keywords

Ionic liquids, dielectric constant, QSPR

1 Introduction

The dynamic progress in the pharmaceutical and medicinal chemistry as well as material science, especially in the area of semiconductors, caused necessity of finding new chemicals with preferable properties. A class of compounds that could be easily modified to obtain expected properties includes ionic liquids (ILs). Ionic liquids are usually defined as a subset of molten salts with the melting point (T_m) below 373.15 K, usually built by a large