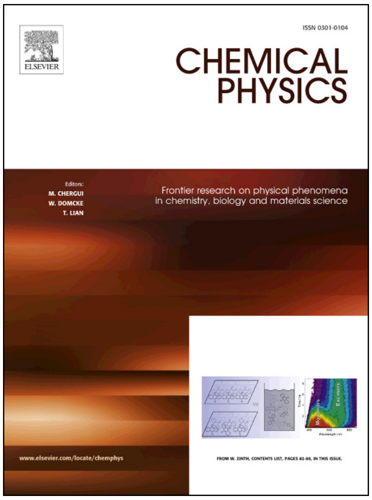

Determination of Hansen Solubility Parameters of Ionic Liquids Using Double-Sphere Type of Hansen Solubility Sphere Method

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Data Article

Title: [Determination of Hansen Solubility Parameters of Ionic Liquids Using Double-Sphere Type of Hansen Solubility Sphere Method]

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Abstract

The Hansen solubility parameters (HSPs) of eight ionic liquids with different combinations of cations and anions were calculated. The Hansen solubility sphere method was used to calculate the HSPs from experimental data on the solubility of the ionic liquids in organic solvents. The double-sphere method rather than the typical single-sphere method was used. In the double-sphere method, the high-polarity side represents an ionic domain and the nonpolar side represents a neutral domain. The value of the center of each sphere is assumed to be the HSP of each domain. Our calculation results confirmed the positions of the double-spheres for each ionic liquid and revealed a dependence on the types of cation and anion.

Keywords: Ionic liquid, Hansen solubility parameter, Hansen solubility sphere method, Domain structure, Double sphere

1. Introduction

Ionic liquids are salts that are generally liquids below 100 °C [1]. Such salts have attracted attention for applications in various fields. Ionic liquids have features of salts, such as high polarity, nonvolatility, flame resistance, and high ionic conductivity at room temperature. Because of these properties, ionic liquids are used in secondary-ion batteries [2], electric double-layer capacitors [3], and extraction solvents. Ionic liquids with appropriate physical properties for a specific use can be designed by changing the type and combinations of the constituent cations and anions.

Compatibility with solvents strongly depends on the solubility of the solute in the solvent. The values of physical properties that are used to evaluate and control the compatibility between a solute and an ionic liquid used as a solvent are important.

The Hildebrand solubility parameters [4] [5] and Kamlet–Taft parameters [6] have been widely reported. However, there are few other indexes describing solute compatibility with ionic liquids. Problems are associated with the Hildebrand solubility parameters in that the solubility may differ even if the values of the parameters are the same because they reflect interactions based on