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Influence of Structure of Ionic Liquids on the Properties of their Mixtures with Water

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Ionic liquids (ILs) represent a group of organic salts with an enormous variability in chemical structure and physico-chemical properties and thus with a broad application potential.¹ However, there is no application without a theoretical base, therefore studies focused on relations between structure and properties are needed.

This contribution reports on a part of the results of a project focused on imidazolium-based ILs with a bis((trifluoromethyl)sulfonyl)imide anion. The choice of the studied ILs is motivated by a study of the influence of the cation structure on the physico-chemical properties of pure ionic liquids and their mixtures with molecular solvents. For this purpose, four isomeric ILs, namely 1-alkyl-3-butylimidazolium bis((trifluoromethyl)sulfonyl)imides (abbreviated $[C_4 \times C_5 \text{im}][\text{Tf}_2\text{N}]$, alkyl = pentyl, isopentyl, 3-pentyl, or cyclopentyl) were selected. In a previous work, fundamental physico-chemical properties such as density, isobaric heat capacity, viscosity, electrical conductivity were measured.² In this part of the study, the properties of the studied range of ILs in systems with water were investigated.

Due to the hydrophobic character of the $[\text{Tf}_2\text{N}]^-$ anion, the studied ILs show limited miscibility with water. The solubilities of ILs in water were measured by means of the direct analytical method using a UV/VIS spectrophotometer (Thermo Scientific Helios γ). Solubilities of water in ILs were measured by the cloud-point method. The determined solubilities of bistriflate-based ILs in water are typically about 10^{-5} in the mole fraction; this concentration range corresponds to the conditions of infinite dilution.³ Therefore, the thermodynamic functions of solubilization of the studied ILs in water could be calculated from these data.

Solubility of water in the studied ILs is on the other hand much higher than that of ILs in water, being as high as approx. 0.15 mole fraction units of water. This enabled us to obtain the excess volumes of mixtures in this part of the concentration interval using a DMA 5000 Anton Paar densitometer.

The data obtained in this study clearly show how a subtle variation in the chemical structure, like isomerisation of one substituent on the cation can affect the physico-chemical properties of pure substances and their mixtures.

References

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