Structure of Ionic Liquids and their Mixtures with Molecular Solvents

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Student: Ing. Jan Rotrekl
Supervisor: Ing. Magdalena Bendová, Ph. D.

Even after three decades of intensive research the properties and behaviour of ionic liquids (ILs) are still not described exhaustively. From the variability of ILs structure originates the idea of task-specific ionic liquids (TSILs); by modifying their chemical structure, the properties of ILs can be tailored to a concrete application [1, 2, 3]. The rational design of TSILs requires to have a sufficiently comprehensive thermodynamic description of pure substances and industrially important mixtures. In this way, a starting point and a benchmark for the theoretical description of the studied systems and the base for group contribution method developement is provided [4]. Consequently, the theoretical and group contribution methods will enable us to predict properties of new ILs from their chemical structure.

This work adresses an experimental study of novel imidazolium-based ILs synthesized with the aim to expand the knowledge on physico-chemical properties of ILs. Three isomeric ILs, 1-alkyl-3-butylimidazolium bis{(trifluoromethyl)sulfonyl}imide (abbrev. $[C_4yC_5im][Tf_2N]$), where alkyl stands for pentyl, isopentyl, and cyclopentyl, are studied. Density, viscosity and electrical conductivity of these ILs as function of temperature was already measured in previous work [5]. In this work, isobaric heat capacities from 293.15 K to 348.15 K and the temperatures of decomposition of these ILs were acquired.

In addition to the basic thermodynamic characterization of pure compounds, emphasis is placed on the description of mixtures. Due to its enviromental importance, the solubility of ILs in water is measured. Because of the hydrophobicity of the $[Tf_2N]^-$ the solubilities of the studied ILs in water are low, typically between 10^{-4} and 10^{-5} in mole fraction. By measuring the properties of homogeneous mixtures it is possible to obtain the excess thermodynamic quantities, i. e. the deviations from ideal behaviour of the mixture as defined by the Amagat law. Excess thermodynamic quantities as function of composition are of a fundamental importance, as they can provide information about

the behaviour of the mixture at the molecular level [6]. For this reason, the excess molar volume and excess isobaric heat capacity will be measured with methanol and acetonitrile.

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References

1. Plechkova, N. V.; Seddon, K. R. Applications of ionic liquids in the chemical industry. *Chem. Soc. Rev.* **2008**, *37*, 123–150.
2. Davis Jr., J. H. Task-Specific Ionic Liquids. *Chem. Lett.* **2004**, *33* (9), 1072–1077.
3. Ranu, B. C.; Banerjee, S. Ionic Liquid as Catalyst and Reaction Medium. The Dramatic Influence of a Task-Specific Ionic Liquid, [bmIm]OH, in Michael Addition of Active Methylene Compounds to Conjugated Ketones, Carboxylic Esters, and Nitriles. *Org. Lett.* **2005**, *7* (14), 3049–3052.
4. Lei, Z.; Zhang, J.; Li, Q.; Chem, B. UNIFAC Model for Ionic Liquids. *Ind. Eng. Chem. Res.* **2009**, *48*, 2697–2704.
5. Andresová, A.; Storch, J.; Traïkia, M.; Wagner, Z.; Bendová, M.; Husson, P. Branched and cyclic alkyl groups in imidazolium-based ionic liquids:Molecular organization and physico-chemical properties. *Fluid Phase Equilib.* **2014**, *371*, 41–49.
6. García-Miaja, G.; Trocoso, J.; Romaní, L. Excess properties for binary systems ionic liquid + ethanol: Experimental results and theoretical description using the ERAS model. *Fluid Phase Equilib.* **2008**, *274*, 59–67.