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Thermodynamic Properties of Saccharinate-based Ionic Liquids: Comparison of Experimental Data to a Prediction by means of COSMO-RS

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As an overall general aim of this study, thermodynamic properties of hydrophilic 1-alkyl-3-methylimidazolium-based ILs ($n = 4, 6, 8, 10, 16$) with a saccharinate (Sac^-) anion have been investigated. Saccharinate is a natural nontoxic anion, contributing to the application potential of the present ILs series. They were therefore used in a previous study for a laboratory-scale extraction of glaucine from its plant.¹ To design an industrial-scale extraction, it is important to have a good knowledge of the physico-chemical properties in the relevant mixtures of ILs with molecular solvents.

In the present contribution, density of 1-alkyl-3-methylimidazolium saccharinates ($n = 4, 6, 8, 10$) and isobaric heat capacity for 1-butyl-3-methylimidazolium saccharinate were measured in this work for a basic characterization of the studied ionic liquids. Modelling based on the COSMO-RS² model was used to predict density and heat capacity³ for the studied ILs and compared with experimental data. Moreover, a prediction by means of COSMO-RS of liquid-liquid equilibria⁴ for 1-decyl-3-methylimidazolium saccharinate with water was carried out and compared with a preliminary experiment of its limited miscibility.

References

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