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Study of Impurities and their Effect on the Physico-Chemical Properties of Ionic Liquids

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The primary aim of the present study is to characterize thermophysically three novel ionic liquids 1-(2-(2-ethoxyethoxy)ethyl)-3-alkylimidazolium with the bistriflate anion, where the alkyl stands for pentyl, isopentyl or neopentyl. For this purpose thermodynamic and transport properties such as density, heat capacity, electrical conductivity, and viscosity are studied.

The purity of an IL follows from the quality of the precursors used in synthesis. To get an IL of highest purity, *e. g.* for spectrocopic use, extreme care must be taken to control purity in each step of the synthesis, which leads to an elevated cost of the product. For most of the applications, however, a less demanding synthesis protocol is sufficient. Different synthesis approaches typically lead to ILs with diverse levels of impurities and intensity of colouring. However, the origin of the colour is not well known. It is assumed that the concentration of these species is in the ppb range and they have no impact on physicochemical properties [1].

If a colourless IL is required, a simple purification method is recomended [1]. The IL is diluted with dichloromethane (1:1 per volume in this study) to decrease the viscosity. The solution is stirred with active carbon for a given time and afterwards passed through a column with aluminium oxide. The solvent is then easily entirely removed under vacuum [2].

This purification method was used in this study. As colouring was not always removed in a single step, the procedure was repeated several times, leading to significant changes in the measured properties in each of the steps.

Even though it is widely accepted that the colouring of ILs has negligible influence on the properties [1], our new results seem to be in contradiction with such findings. Therefore it was necessary to identify the impurities and their quantity and link them with observed changes in measured properties. Ion chromatography was used to analyze inorganic residues. To analyze the organic compounds, NMR spectroscopy was used. Because the original concentration of impurities in ILs was lower than the detection limit of NMR, the impurities

were first concentrated using aluminium oxide in a solid phase extraction.

A comprehensive characterization of the impurities will require more experiments tailored to the specific character of ILs. On the other hand, the outcome will be useful in further applications of ILs.

References

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2. Stark, A.; Behrend, P.; Braun, O.; Müller, A.; Ranke, J.; Ondruschka, B.; Jastorff, B. *Green Chem.* **2008**, *10*, 1152–1161.