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Mutual solubilities of ammonium-based ionic liquids with water and with water/methanol mixture

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Over the last two decades, ionic liquids have gained importance as alternative solvents to conventional VOCs in the field of homogeneous catalysis. This success is not only due to their ability to dissolve a large amount of metal catalysts, but it is also due to their potential to enhance yields of enantiopure products. The art of preparation of a specific enantiomer is a highly desired one and searched for in pharmaceutical industry.

This work presents a study on solubility in water and in water/methanol mixture of a set of ILs composed of the bis(trifluoromethylsulfonyl)imide anion and of the N-alkyl-triethyl-ammonium cation (abbrev. [NR₂₂₂][NTf₂]) with the alkyl chain *R* ranging from 6 to 14 carbons. These ILs were successfully tested for enantioselective hydrogenation of β -ketoesters catalyzed by the chiral complex Ru-BINAP in presence of methanol [1]. From which, it appears that these ILs immobilise the catalyst in the mixture for easier recycling and further re-use and protect it from air/oxygen. The final separation of the product is carried out by rinsing the solution with water, which may also wash out the ILs with catalyst. For this reason, mutual solubilities between ILs and water, as well as between ILs and methanol/water mixture need to be investigated in detail.

These solubilities were measured using two well-known and accurate experimental techniques based on a volumetric, [2] and a cloud-point, [3] methods. Both methods enabled us to measure the *T_x* diagrams reflecting the mutual solubilities between water (or water/methanol) and selected ILs in the temperature range from 293.15 to 338.15 K.

The data were fitted by the modified Flory-Huggins equation proposed by de Sousa and Rebelo [4] and compared with the prediction carried out by Cosmo-RS [5].

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