167a How to Tailor Ionic Liquids for Separation

Carsten Jork and Wolfgang Arlt

This lecture presents a consequent thermodynamic optimization of ionic liquids (IL) as entrainers in the distillative separation of both an azeotropic aqueous (THF + water) and a close-boiling aromatic test system (methylcyclohexane + toluene) on the basis of COSMO-RS predictions. The use of this method allows for the preselection from the large pool of available IL. Thus, favorable structural variations were identified and used for tailoring IL entrainers. For the prediction of activity coefficients with COSMO-RS, the use of different conformations of the components, derived from conformational analyses, leads to varying results. The simulations showed that the influence of conformations of the volatile components and the ionic liquids depends largely on the type of the phase equilibrium, which is investigated. The approach to tailor ionic liquids as additives for separation science starts with the prediction of the activity coefficients at infinite dilution. The simulation indicated that a higher degree of branching or longer alkyl substituents on the cation, as well as a low nucleophilicity of the anion decreases both selectivity and capacity in the polar test mixture. However, COSMO-RS calculations for the non-polar mixture showed that the selection of an entrainer for this system is more difficult, because -contrarily to (THF + water)- structural variations of the IL entrainer cause converse changes in selectivity and capacity: while the selectivity for toluene increases with a lower degree of branching and a shorter alkyl substituent of the cation as well as with a lower nucleophilicity of the anion, these properties decrease the capacity.