

Abstract

In this work, 13 surface active ionic liquids, SAILs, were synthesized and their micellization properties were examined by isothermal titration calorimetry, ITC. An improved mass-action model, which describes micellization as the equilibrium between micelles and monomers with the constant aggregation number, was used for interpretation of the obtained data. Additionally, molecular dynamics, MD, simulations were performed for all the systems confirming the experimentally obtained results. Finally, the toxicity of studied systems towards wheat culture was tested in order to study the impact of the structural change of SAILs on the level of toxicity.

From the thermodynamic study, it was found that the investigated systems behave mainly like common ionic surfactants and already investigated SAILs: the micellization process is entropically driven at low temperatures (due to the hydrophobic effect), while at high temperatures the enthalpy contribution becomes equally important (possibly due to counterion binding). Moreover, it was confirmed that the counterion isomerism influences the micellization process the most, followed by the prolongation of the shorter alkyl chain length on the imidazolium ring and isomerism of cation. MD simulations have revealed that, in addition to hydration and ion-ion interactions, steric hindrance plays a very important role in the process of self-aggregation. Additionally, toxicity tests with wheat culture showed that the prolongation of the shorter alkyl chain on cation, as well as the anion/cation isomerism, do not play an important role in increasing or decreasing the germination level. Therefore, the hydrophobicity of the compound is a key property dictating the degree of toxicity, so it can be concluded that the longest substituent on the cation has the biggest influence on the overall toxicity of SAILs.

Keywords: thermodynamics, surface active ionic liquids, micellization