Mathematical model describing solubility of hydrophobic ionic liquids in hydrochloric acid media

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A mathematical model to explain cations' solubility of both protic (betainium-) and aprotic (pyrrolidinium- and imidazolium-based) ionic liquids with common *bis*(trifluoromethanesulfonyl)imide anion in a wide range of hydrochloric acid solutions has been developed. The concept of this model is based on an assumption of the mineral acid extraction into the organic phase [1], formation of a chloride-containing salt there due to ionic liquid and extracted acid ions recombination and partial salt back-extraction [2]. The proposed approach allows for estimating corresponding extraction constants. Comparison of calculated and experimentally measured solubility product constants shows that they are in good agreement. It was found also that the lower the hydrophilicity of the ionic liquids' cation the more hydrochloric acid is extracted. Fig. 1 shows some results of this work. It can be seen that experimentally measured solubility product constants and the calculated constant of hydrochloric acid extraction into a series of imidazolium based ionic liquid ([$C_n$mim][Tf_2N], where n = 2, 4, 6, and 8) decreases with

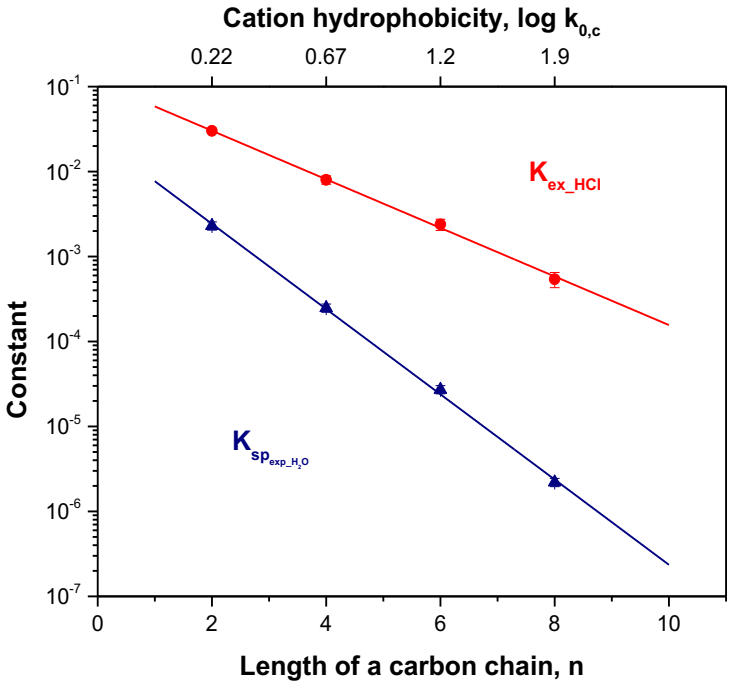

Fig. 1. Influence of the carbon chain length on the solubility and HCl extraction into imidazolium-based ionic liquids [$C_n$mim][Tf_2N], where n = 2, 4, 6, and 8. The imidazolium-based cations hydrophobicity data are taken from [3].

increasing cation hydrophobicity. These are preliminary data submitted to a peer reviewed journal.

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