Influence of hydrophobic properties of dissolved substance to the local structure of the ionic liquid dmim+/Cl- at 400K

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Ionic liquids (IL) are a new class of solvents that find their application in various sectors of the chemical industry, which in the future may become alternative substances to replace volatile organic solvents in hazardous chemical plants. Spectroscopic and neutron research confirm the existence of hydrogen bonds between cations and anions of ionic liquids. Most specific interaction between the ions and cations leads to the formation of hydrogen bonds between ions and cations, which hardly sensitive to adding polar or non-polar substances. Experimentally shown that the addition of non-polar compounds to ionic liquids leads to anomalous temperature dependence of the solubility of nonpolar substances in ionic solutions at different concentrations. In this case, decrease the solubility of nonpolar substances in IL with increasing temperature. The dependence of the anomalous behavior of the solubility of nonpolar substances in IL correlates with the size of molecules soluble substances.

Determine the impact of the structure and size of molecules nonpolar substance on the process of local structure and dynamic properties of ILs allows the use of molecular modeling, which allows to analyze the interaction of solvent molecules (dimetylimidazolium chloride (dmim+ /Cl-) and solute (argon, methane benzene) at the micro level. This, in turn, helps to explain the behavior of macro-characteristics of the liquid systems.

Given that one of the classic lines of research in physical chemistry is the study of movement and interaction in solution at infinite dilution and their properties depending on the size dissolved in the IL solute molecules (argon, methane benzene). The method of molecular dynamics (MD) was used to investigate the effect of non-polar molecules to form the local structure of dmim+ /Cl- at T = 400K. It is found that that the amount of non-polar molecules, what dissolved in dmim+ /Cl- and affect the nature of its size in a solvent. Increasing the size of nonpolar molecules leads to the rupture of hydrogen bonds between the components of ionic liquids and the loss of grid percolation properties of hydrogen bonds in the studied systems. Obtained, in the case of infinite dilution in the absence of interaction between the nonpolar solute molecules there are various mechanisms restructuring local structure of IL.