
STRUCTURAL AND DYNAMIC FEATURES OF IONIC LIQUIDS SOLUTIONS WITH AROMATIC HYDROCARBONS

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Abstract

Ionic liquids (ILs) have been extensively studied as replacements to sulfolane in the separation of aromatics from alkanes. The employment of ILs could reduce energy requirements and operating costs of the aromatic extraction unit as a result of their nonvolatile character. However, the ILs studied so far have shown mass-based aromatic distribution ratios lower than the sulfolane values, which would increase the solvent-to-feed ratio in the extractor. The performance of hydrophobic ionic liquid (dimethyl-imidazolium chloride) on extraction of aromatic compounds such as benzene, toluene, anisole, phenol and *c*-hexane derivatives from aqueous solution was investigated experimentally.

The MD method was applied using a modified DL_POLY_4.05 with a time step of 2 fs. The long-range electrostatic interaction was taken into account by the Ewald method. In the calculations, the cations, anions, and atoms forming the molecules of the added substance (hydrocarbons: benzene, toluene, phenol, anisole and *c*-hexane) were treated as solid charged model systems with a fixed geometry. The methyl in the dmim⁺ and toluene were treated as a pseudoatom with the total charge. All the studies were conducted for systems composed of 192 dmim⁺ cations, 192 chlorine anions Cl⁻, and one solute molecule at $T = 400$ K. The unit cell volume was calculated from the experimental values of the ionic liquid density at $T = 400$ K. The calculations used periodic boundary conditions. The electrostatic interaction at short distances was described using point charges on each atom. The interaction between dmm⁺ and Cl⁻ molecules in the ionic liquid was described using the Buckingham potential for interactions at short distances. The Berendsen thermostat was used to stabilize the system in the NVT -ensemble.

Analysis of the data allowed to establish: (1) The solvation effect in systems ionic-liquid (dmim⁺/Cl⁻) - non-polar solute molecules (benzene, *c*-hexane) has qualitatively similar to the behavior of the hydrophobic hydration of aromatic solute molecules in liquids like water. The results of the computer experiment for the average total energy of the intermolecular interaction $\langle E_{tot} \rangle$ for the dmim⁺/Cl⁻ non-polar solutions at $T = 400$ K show that the intermolecular interaction $\langle E_{tot} \rangle$ does not depend on the physical characteristics of the structural and non-polar substances dissolved. Therefore, as a possible selection criteria for the data analysis is not appropriate to consider the thermodynamic and structural characteristics of the system. In this case, need to do analysis of its dynamic properties. Based on the data obtained from MSD and VAF the different diffusion mechanisms of nonpolar

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solute molecules in IL were determined. (2) The solvation effect in systems ionic-liquid (dmim⁺/Cl⁻) - polar solute molecules (toluene, phenol, anisole) has qualitatively similar to the behavior of the hydrophobic hydration in liquids like water too. The results of the computer experiment for the average total energy of the intermolecular interaction $\langle E_{tot} \rangle$ for the dmim⁺/Cl⁻-polar hydrocarbons at $T = 400$ K show that the intermolecular interaction $\langle E_{tot} \rangle$ depend on polarity and the physical characteristics of the structural and polar substances dissolved. Based on the data obtained from MSD and VAF the different diffusion mechanisms of polar hydrocarbons solute molecules in IL were determined. (3) Dissolution of hydrocarbons molecules whose size is much higher than the maximum length of the hydrogen bond leads to a radical restructuring of the network of hydrogen bonds in the system up to the loss of its percolation properties.

The results showed that IL had good ability in the extraction. Molecular structure of aromatic compounds was found to have a great influence on the extraction. Due to the increase of the hydrophobicity of solute, the partition coefficient of aromatic compounds was increased.