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Alkylammonium-based protic ionic liquids: An *ab initio* investigation

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Protic ionic liquids (PILs) have attracted considerable attention in the search for new materials because of the very rich field of promising applications in various industries. Since the properties of such systems are significantly affected by the presence of hydrogen bonds (H-bonds), the investigation of the structural features of PILs and H-bonding between acid anions (A^-) and base cations (BH^+) at a microscopic level is important for achieving a deeper understanding of these liquids. The present work focuses on the computational study of a series of PILs based on ethyl-, diethyl- or triethylammonium cations with anions of phosphorous (PA), trifluoroacetic (TFA) or p-toluenesulfonic (PTSA) acids. Our study has indicated that not only H-bonded ion pairs ($A^-…BH^+$) but also H-bonded molecular complexes (A-H…B) that form as a result of proton back-transfer from cation to anion exist in these PILs. It has been shown that the strength of H-bonding interactions in these systems considerably depends on the nature of acid and base. The increasing number of ethyl groups attached to the nitrogen atom of alkyl amine causes a stronger H-bonding interaction leading to the formation of ion pairs. In like manner, p-toluenesulfonic acid promotes proton transfer and performs better than the other considered acids. The correlation between our theoretical results and experimental data has been found for PILs based on triethylamine with the aforementioned acids. In particularly, the free energy change associated with the formation of the H-bonded ion pairs increases in the following order: PA<TFA<PTSA. Here, the greater the energy value, the higher is the decomposition temperature.

Biography

Lyubov P Safonova has done scientific research in the area of Physical Chemistry of solutions for many years. She defended PhD thesis in 1981 and Doctorate thesis in 1998. She has held teaching position at Ivanovo State University of Chemistry and Technology. Currently, she is Professor at laboratory of chemistry and physical chemistry of solutions, theoretical foundations of chemical-engineering processes in liquid media, ISC RAS. Her scientific interests mainly concern the study of the structural and energetic characteristics of molecular complexes with hydrogen bonds, ion-molecular equilibrium in solutions, processes of proton transfer in condensed systems. She also teaches and supervises post-graduate students.

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