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MOLECULAR DYNAMICS SIMULATIONS OF 1-BUTYL-3-METHYLIMIDAZOLIUM TETRAFLUOROBORATE IONIC LIQUID

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Ionic liquids are compounds that are made entirely of ions and have a melting point below 100°C. In the last two decades, ionic liquids became a major scientific area on account of applications in organic chemistry, solar energy, and pharmaceutical manufacturing where it is used in many chemical reactions as solvents, catalysts, reagents, or combinations of these [1].

Experimental, theoretical, and molecular modeling research methods must be applied to describe the application of ionic liquids for specific applications. One of the most common nanostructure analysis mechanisms used in this research is molecular dynamics simulations.

In this work, MD simulations were applied to simulate 1-butyl-3-methylimidazolium tetrafluoroborate [C4mim][BF_4] ionic liquid and to analyze its intermolecular structure.

The parameters of the force field potential, which were taken from B. Doherty's research article, were determined, and 1-butyl-3-methylimidazolium tetrafluoroborate was modeled using "GaussView" software before running the simulations [2,3]. Thereafter, the MD simulations were carried out in an NPT ensemble where the density of the simulated ionic liquid was registered until its fluctuation became negligible with a value of 1,15 g/ml. Afterwards, the simulations were run in an NVT ensemble where the trajectories of molecules were noted.

Here we focus on radial distribution functions, which were calculated between cations' C10 atoms as well as between cations' imidazolium rings' H2, H4, H5, and anions' B atoms. The coordination numbers were also calculated between the pairs mentioned. In both RDFs clear peak points are visible therefore the formation of polar and nonpolar regions takes place. The calculated values of coordination numbers show us that the strongest interaction between cations' imidazolium rings and anions appears in the H2-B atom pair.

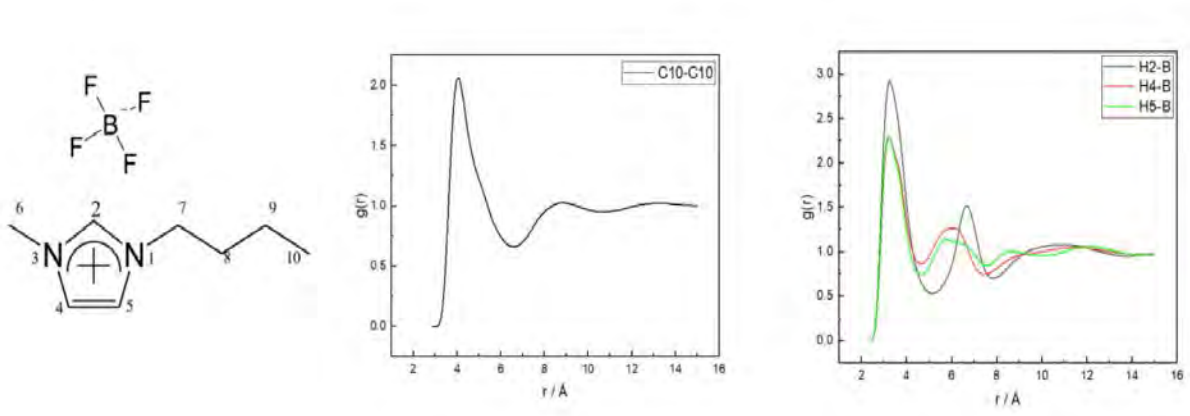

Fig. 1. [C4mim][BF_4] structure with main atom numbers [4] and calculated RDFs between cations' C10 atoms as well as between cations' imidazolium rings' H2, H4, H5 and anions' B atoms.

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