Evaluation of the effect of the charges model in the OPLS-AA force field for ionic liquids, which best reproduces its properties in liquid phase conditions

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Abstract

Nowadays, ionic liquids have a great importance because they exhibit properties that replace volatile solvents and properties such as electrically conductive fluids. [1] In the present investigation, six physical properties (density, viscosity, dielectric constant, diffusion coefficient, enthalpy of vaporization and surface tension) of 14 ionic liquids were evaluated. For this purpose, the density functional theory was used within DeMon 2K program with the functional CAM B3LYP and the TZVP base to optimize the gas phase structures and obtain the atomic partial charges. Six types of population analysis were carried out (NBO, Hirshfeld, Voronoi, Becke, Mulliken and Bader) to obtain the aforementioned properties in liquid phase. The program Gromacs 5.0.7 was used using the OPLS force field modifying the charges obtained. [2] [3] The results showed that for the experimental densities found, the charges of Voronoi and Becke are closer to these data.

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