On the Properties of 1-Butyl-3-Methylimidazolium Octylsulfate Ionic Liquid

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In the framework of green chemistry, Ionic Liquids constitute quite an attractive alternative to a number of volatile organic solvents used in many industrial settings. This class of solvents can be cleverly designed and their properties finely tuned for any particular sophisticated application by adequately selecting the proper combinations of ions that they consist of. So far, the growing interest in these fluids, both in industry and academia, has rested on the uncountable number of possible combinations of cations and anions. To this end, prior to attaining the technological development stage, sistematic measurements on the thermophysical and structural properties for different families of ions must be performed over wide ranges of pressure and temperature. In this work, a theoretical and experimental study on the ionic liquid 1-Butyl-3-methylimidazolium octylsulfate ([BMIM]OS) is presented. [BMIM]OS is a halogen–free ionic liquid, stable regarding hydrolysis reactions, whose availability, toxicologically favorable profile and well documented biodegradability turns it into a suitable alternative for different applications in an industrial multi-ton scale. The pressure-volume–temperature (PVT) behavior of this fluid was accurately evaluated over wide temperature and pressure ranges and correlated successfully with the empirical TRIDEN equation. From the measured PVT data, the important derived coefficients isothermal compressibility, isobaric expansibility and internal pressure have been calculated. Other relevant physical properties such as isobaric heat capacity, speed of sound and refractive index were all measured at atmospheric pressure and several temperatures. The molecular structure of the fluid was looked into through both quantum computations at the B3LYP/6-31 g(d) level and classical molecular dynamics simulations in the NPT ensemble with the OPLS–AA forcefield. The macroscopic and microscopic studies both fully concur on a complex structure of the fluid. The aggregation of the non–polar anionic chains gives rise to microheterogeneities with well defined polar and non polar domains.