Transport Properties of Room Temperature Ionic Liquids by Molecular Dynamics Simulations

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Room temperature ionic liquids (ILs) are currently receiving much attention due to their interesting physicochemical properties: negligible vapor pressure, extremely wide range of compositions (which allows the tuning of physical properties through design), etc. For these reasons, ILs are thought to be promising alternative solvents for a number of technological applications in the context of green processes [1, 2].

Among all of the physical properties of ILs, viscosity, self diffusion, and electric conductivity are particularly important in the selection of a given IL for an industrial application. For instance, a low viscosity is desirable, in order to enhance mass transfer, in two-phase separation processes using ILs. Due to their high variability in composition, the systematic and exhaustive characterization of ILs is not affordable from an experimental point of view. Therefore, there is a great need for accurate predictions of thermophysical properties using theoretical models. Indeed, molecular modeling tools can provide an insight into the relationship between the molecular structure and the macroscopic behavior of ILs [3].

This work summarizes some results obtained through equilibrium molecular dynamic simulations (MD) regarding the transport properties of simple models of ILs. In particular, the cation/anion diffusion coefficients, electrical conductivity, and shear viscosity at different temperatures up to 500 K have been calculated, in good agreement with other simulation results, although the viscosity and conductivity are somewhat higher and lower, respectively, than experimental values, when available. The comparison of the calculated diffusion coefficients and conductivities on one side (Nernst-Einstein relation), and the viscosities and conductivities on the other (Walden product) reflects the importance of cross-correlation among ions, which is further investigated through space-time correlation analysis.

The long-term objective of this work is the development of a methodology that allows for the systematic search of ILs tailor-made for desired specific applications. This will be done with a combination of molecular modeling tools and experimental data.

[1] R.D. Rogers and K.R. Seddon (Eds.) “Ionic liquids as green solvents. Progress and prospects,” ACS Symposium series, 856 (2003).
[2] P. Wasserscheid and T. Welton (Eds.) “Ionic liquids in synthesis,” Wiley-VCH (2003).
[3] J.K. Shah and E.J. Maginn, *J.Phys.Chem.B.* **109**, 10395 (2005).