INFLUENCE OF FLEXIBILITY AND CHAIN LENGTH IN THE TRANSPORT PROPERTIES OF IONIC LIQUIDS

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Room temperature ionic liquids (ILs) are currently receiving much attention due to their interesting properties like negligible vapor pressures and extremely wide range of compositions (which allows the tuning of physical properties through design) [1,2]. Transport properties are particularly important in the selection of a given IL for industrial applications. For instance, a low viscosity is desirable, in order to enhance mass transfer in two-phase separation processes with 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.
Equilibrium molecular dynamics simulations (EMD) results for cation/anion self- diffusion coefficients, shear viscosity and electrical conductivity in a rigid model ionic liquid at different temperatures up to 500K were recently reported by Rey-Castro and Vega[3]. When compared with available experimental data, the model showed some discrepancies which could be explained on the basis of the rigidity and lack of polarizability of the molecular model. We present here analogous EMD simulations results in a flexible model ionic liquid[4], in order to see the influence of the model flexibility in the transport properties behaviour. Moreover, the length of the alkyl chain of 1- alky-3-methylimidazolium cations was systematically varied. Thus the influence on the transport properties of the cation volume and the chain length for different temperatures is also analyzed.

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