Thermophysical and Transport Properties of Ammonium-Based Bistriflamide Ionic Liquids and Their Interactions with Molecular Solvents

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One hundred years have elapsed since the publication of the famous ethylammonium nitrate study by Paul Walden, probably one of the most long-known Ionic Liquid (IL). Even so, only recent years witnessed a greater interest on this class of medium, especially when it was realized that they could advantageously replace traditional organic fluids due to their singular properties. Moreover, the possibility of "designing" their structure to achieve the desired properties for a specific application also boosted their use in industrial applications. In this work, we have synthesized three bistriflimide ammonium-based ILs with similar size but with distinctive functional groups in one single alkyl chain, namely $[N_{2\,1\,1\,3OH}][Ntf_2]$, $[N_{2\,1\,1\,2O1}][Ntf_2]$ and $[N_{2\,1\,1\,4}][Ntf_2]$. The aim of this study is to evaluate the impact of these distinctive functional groups on the thermophysical properties of these ILs, such as density, viscosity, conductivity and refractive index and on their fluid phase equilibria behavior with molecular solvents such as ethers, alcohols, diols, and water. Lower critical solution temperatures (LCST) type phase diagrams were observed for the mixtures of these ammonium based ILs with ethers, while upper critical solution temperature (UCST) type phase diagrams were reported for all the other systems. The miscibility behavior of ILs with different solvents strongly depends on the number and position of the functional groups and the size of the alkyl chain of the solvent, as well as, the functional group of the IL. The experimental results also show that for these almost equal sized ammonium based ILs different physical properties can be obtained through a particular exchange of the functional group of one single alkyl chain. Molecular dynamics simulation will be used as a tool to help on the understanding the observed behavior.