Thermophysical Properties of Ionic Liquids: Contribution of the -CN Group

Mara G. Freire [C]
Universidade Nova de Lisboa, Instituto de Tecnologia Química e Biológica, Oeiras, Portugal
maragfreire@ua.pt

Catarina M. S. S. Neves and João A. P. Coutinho
Universidade de Aveiro, Departamento de Química, CICECO, Aveiro, Portugal

Isabel M. Marrucho
Universidade Nova de Lisboa, Instituto de Tecnologia Química e Biológica, Oeiras, Portugal

José N. Canongia Lopes [S]
Instituto Superior Técnico, Centro de Química Estrutural, Lisboa, Portugal

Luís Paulo N. Rebelo
Universidade Nova de Lisboa, Instituto de Tecnologia Química e Biológica, Oeiras, Portugal

Most of the known ionic liquids present remarkable physicochemical properties, a fact that has led to a growing area of research concerning their possible applications. An important feature of ionic liquids is based on the possibility of tuning their physical/chemical properties by varying the nature of the cation and/or the anion, and at least, theoretically, it should always be possible to tailor a given ionic liquid for a specific application. Therefore, the current search for novel ionic liquids is largely driven by the need to develop materials with special properties and functions. Cyano-based ionic liquids have been recently explored as potential candidates for the desulfurization of fuels, in the selective separation of aromatic/aliphatic hydrocarbons, and in extractive distillation approaches. Nevertheless, the complete characterization of this series of ionic liquids is still far from being accomplished. The aim of this work is to characterize cyano-based ionic liquids *via* their thermophysical properties — density, viscosity, refractive index, and conductivity. These properties were determined for several imidazolium-based ionic liquids containing anions substituted with the cyano group (–CN) in a large temperature range (from 278.15 K to 363.15 K) and at atmospheric pressure. The selected ionic liquids include the 1-ethyl-3-methylimidazolium, 1-butyl-3-methylimidazolium, and 1-hexyl-3-methylimidazolium cations combined with the $[SCN]^-$, $[N(CN)_2]^-$, $[C(CN)_3]^-$ and $[B(CN)_4]^-$ anions. The results along the homologous series were analyzed and will be presented taking into account the effect of the –CN group on their thermophysical properties. In particular, group contribution methods for the description of the experimental data will be shown in what concerns the addition of consecutive –CN groups.