

Arrhenian Temperature Dependence of the Computational Dielectric Spectra of Ionic Liquids

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Dielectric relaxation spectra of two different neat ionic liquids sharing the same cation, 1-ethyl-3-methylimidazolium dicyanamide and 1-ethyl-3-methylimidazolium triflate have been calculated using polarizable molecular dynamics trajectories at five different temperatures.

DR spectroscopy measures a system's response to an external oscillating electric field of angular frequency ω . The total spectrum can be decomposed into dielectric permittivity ϵ and dielectric conductivity σ , describing the collective dynamics of the rotational and translational dipole moment, respectively.

Results show a blue-shift of peaks in the low-frequency region with increasing temperature, in accordance with experimental data of other ionic liquids reported in literature [1,2]. The high-frequency regime displays a temperature-independent behavior, which is interpreted as the librational motion of ions in their cages.

References:

[1] Johannes Hunger, Thomas Sonnleitner, Liyuan Liu, Richard Buchner, Mischa Bonn and Huib J, Bakker. *The Journal of Physical Chemistry Letters* **3** (2012), 3034-3038.

[2] Johannes Hunger, Alexander Stoppa and Richard Buchner. *The Journal of Physical Chemistry B* **113** (2009) 9527-9537.