

Influence of Water on Diffusion in Imidazolium-Based Ionic Liquids by NMR

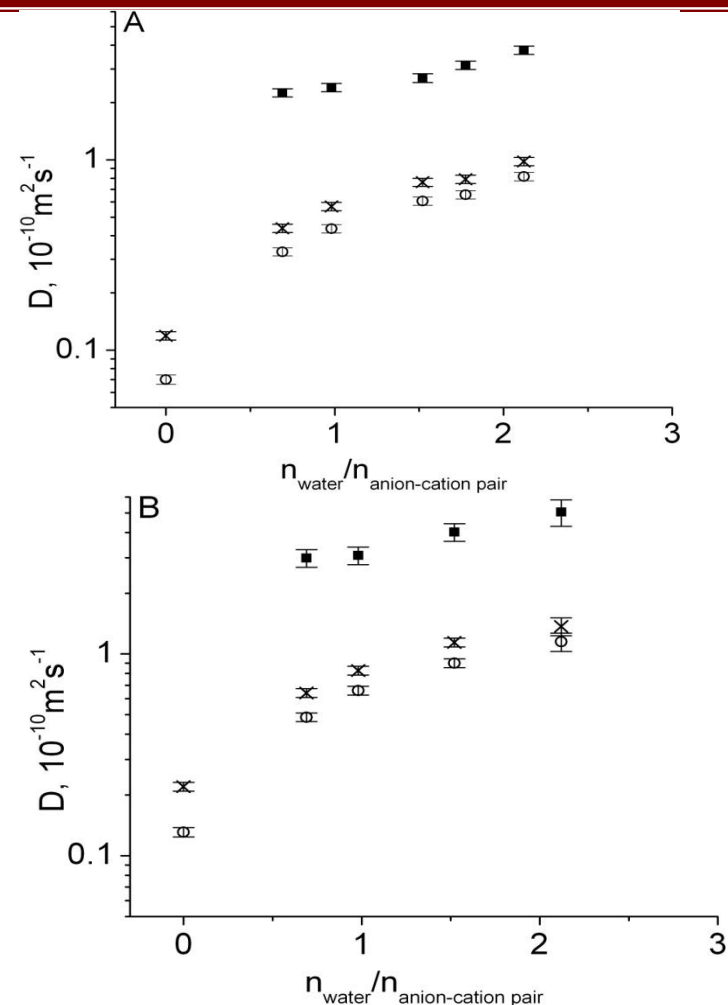
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In this work we applied a novel pulsed field gradient (PFG) NMR option developed at AMRIS, University of Florida to study diffusion of anions, cations and water in two 1-ethyl-3-methylimidazolium-based ionic liquids. This technique combines advantages of high field (17.6 T) NMR and high magnetic field gradients (up to 30 T/m). Application of high field allows for an easy recording of an NMR signal from small amounts of water added to the ionic liquids. Using high gradients is advantageous because under conditions of such gradients any susceptibility-induced inhomogeneities in the local magnetic field are expected to be negligibly small in comparison with the applied gradients.

Our data show that the anomalous relationship between the ion diffusivities, i.e. larger self-diffusion coefficient of the bulkier cation than that of the less bulky anion, becomes much less pronounced due to addition of water into the ionic liquid. This observation is explained by the distortion of the local structure in the ionic liquid by water molecules leading to a possible loss of the diffusion anisotropy for the cation diffusion.

Menjoge, A.; Dixon, J.; Brennecke, J.F.; Maginn, E.J.; Vasenkov, S., *Influence of Water on Diffusion in Imidazolium-Based Ionic Liquids: A Pulsed Field Gradient NMR study*, J. Phys. Chem. B, 113 (18), 6353-6359 (2009)



Diffusivities of the cation (x), anion (o), and water (■) measured by proton PFG NMR in [Emim][ETSO4] ionic liquid as a function of the number of water molecules per anion-cation pair ($n_{\text{water}} / n_{\text{anion-cation pair}}$): (A) at 298 K, (B) at 308 K.