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Self-diffusion and interactions in mixtures of imidazolium bis(mandelato)borate ionic liquids with polyethylene glycol: 1H NMR study

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Abstract

© 2015 John Wiley & Sons, Ltd. We used 1H nuclear magnetic resonance pulsed-field gradient to study the self-diffusion of polyethylene glycol (PEG) and ions in a mixture of PEG and imidazolium bis(mandelato)borate ionic liquids (ILs) at IL concentrations from 0 to 10wt% and temperatures from 295 to 370K. PEG behaves as a solvent for these ILs, allowing observation of separate lines in 1H NMR spectra assigned to the cation and anion as well as to PEG. The diffusion coefficients of PEG, as well as the imidazolium cation and bis(mandelato)borate (BMB) anion, differ under all experimental conditions tested. This demonstrates that the IL in the mixture is present in at least a partially dissociated state, while the lifetimes of the associated states of the ions and ions with PEG are less than ~30ms. Generally, increasing the concentration of the IL leads to a decrease in the diffusion coefficients of PEG and both ions. The diffusion coefficient of the anion is less than that of the cation; the molecular mass dependence of diffusion of ions can be described by the Stokes-Einstein model. NMR chemical shift alteration analysis showed that the presence of PEG changes mainly the chemical shifts of protons belonging to imidazole ring of the cation, while chemical shifts of protons of anions and PEG remain unchanged. This demonstrated that the imidazolium cation interacts mainly with PEG, which most probably occurs through the oxygen of PEG and the imidazole ring. The BMB anion does not strongly interact with PEG, but it may be indirectly affected by PEG through interaction with the cation, which directly interacts with PEG.

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Keywords

Chemical shift alteration, Ionic liquids, NMR diffusometry, Nuclear magnetic resonance, PEG, Pulsed-field gradient