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Hydrogen bonding and local structure of imidazolium-based ionic liquids in the water-rich domain

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Since water has a high impact on the chemical-physical characteristics of Ionic Liquids (IL), both as a contaminant or as cosolvent, the detailed knowledge of the intermolecular interactions in IL/water solutions is a crucial step for understanding and predicting the range of properties of these non-conventional solvents for applications in many fields including electrochemistry, biochemistry, and synthesis.
In this work, aqueous solutions of a prototypical set of methyl-imidazolium (MIM) - based ionic liquids is investigated by UV Raman spectroscopy and Small-Angle Neutron Scattering in the water-rich domain. Selected Raman signals in different wavenumber ranges provide insights into the local organization of cation-anion pairs as a function of the increasing amount of water in a wide range of concentrations. The high-frequency range of Raman spectra is analyzed by a differential method to extract from the OH stretching profile of water the solute-correlate (SC) spectra, which emphasize the molecular structuring of the interfacial water present in the hydration shells around the selected anions. The neutron scattering data show the water –IL segregation at nanoscale.
Peculiar solvation behavior is observed for the different MIM-based mixtures in connection with the hydrogen bonding features of the hydrating water molecules. Interestingly, the ionic liquid [MIM][Cl] seems more sensitive to hydration than [MIM][TfO] even in an extremely hydrated regime.

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