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β -NMR studies of Ionic Liquids

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Nuclear Magnetic Resonance (NMR) analysis of vacuum-compatible solvents, such as Ionic Liquids (ILs) is crucial to understand their inter- and intramolecular arrangement in the pure liquid environment. This knowledge is useful to increase the electrochemical properties of ILs, resulting directly from their structure. Recent studies revealed that small aggregations of water molecules can become well isolated and vacuum-stable in specific types of ILs. One of the most studied examples are imidazolium salts able to form networks based on the cation-anion interactions and trap water molecules in between. This behaviour of ILs is especially important for their electrochemical properties, such as conductivity which can be significantly increased by the presence of the defined number of water molecules with a special arrangement in the solvent.

Due to the high hygroscopicity of Ionic Liquids, precise analysis of water-ILs interaction is often not possible. In comparison to conventional NMR, liquid-state β -NMR spectroscopy can provide a qualitative knowledge about such interactions, because it allows to implant short-lived isotopes of alkali metals directly into a liquid host in high vacuum environment. The change in the detected beta-decay asymmetry represents the on- and off-resonance response of the implanted atoms to an applied rf field and can be used to obtain detailed information about the chemical environment of the implanted short-lived isotope.

This contribution will present the results of β -NMR measurements performed with the short-lived ^{26}Na in imidazolium-based Ionic Liquids with short side alkyl chains, such as BMIM-HCOO and EMIM-DCA, together with complementary 1D and 2D NMR measurements and Molecular Dynamics simulations.

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