Ion-specific Translational and Rotational Motions in Isotopic Substituted Ionic Liquids by Means of NMR Relaxometry

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Conventional high-field nuclear magnetic resonance (NMR) is used in various fields due to the availability of numerous experiments, including spin-lattice relaxation (SLR) measurements. In contrast, the fast field cycling NMR relaxometry is measuring frequency-dependent SLR rates and is operating at low frequencies, from a few kHz up to several MHz. This leads to a loss of resolution in NMR signals and therefore chemical shifts, but opens the window for the simultaneous determination of self-diffusion coefficients and rotational correlation times. Choosing a suitable system, both dynamical properties can be determined ion-separately. For the ionic liquid (IL) triethylammonium methylsulfonate ([TEA][OMs]) this is not given, due to the fact that the protons are distributed over both ions, cations and anions. Isotopic substitution on either the cation or anion provides access to the ion-separate dynamics. We measured the temperature- and frequency-dependent ^{1}H-SLR rates for the partially deuterated ILs [TEA][OMs-d_3] and [TEA-d_{16}][OMs] as well as for the fully protonated [TEA][OMs] and compare the obtained dynamical properties. The evaluation of the relaxation data involves a numerical fitting algorithm and requires the use of appropriate relaxation models.[1] Apart from this, we provide self-diffusion coefficients directly calculated from the relaxation rates, which are in good agreement.[2]

References

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Lennart Kruse studied chemistry at the university of Rostock and received his B.Sc. degree in 2020. Finishing his M.Sc. three years later, he investigated the low-frequency vibrational motions in amino-acid-based ILs by means of far-infrared spectroscopy. Since 2023 he is member of the Ludwig group at the physical chemistry department of the university of Rostock. In his PhD he is mainly working in the area of fast field cycling NMR relaxometry and infrared spectroscopy. With both methods he is probing structure and dynamics of different classes of ionic liquids and electrolyte solutions.