

How do different protons contribute to one single NMR dispersion profile? – An isotopic pattern study

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Fast field cycling (FFC) NMR relaxometry is a powerful tool to study rotational and translational motion in ionic liquids (ILs) over broad temperature ranges. In contrast to conventional NMR techniques the spectrometer frequency can be swept between 10 kHz and 40 MHz for ¹H nuclei, yielding to NMR dispersion profiles which allow for the simultaneous observation of several molecular processes at different timescales in one single experiment.

In this joint experimental and molecular dynamics (MD) simulations project we study the decomposition of those NMRD profiles based on the ionic liquid 1-ethyl-3-methylimidazolium dicyanamide [C₂MIm][DCA]. For the fully protonated version overall rotational correlation times, τ_{rot} , as well as translational diffusion coefficients, D_{trans} have been determined. Here, MD simulations are able not only to provide comparable values for both quantities but also to verify the applied relaxation model.[1] In addition to the fully protonated version we now investigate three specially synthesized deuterated analogues. Those different isotopic patterns of the cation allow for a detailed analysis of contributions originating from ¹H nuclei located at different parts of the cation. In general, it can be stated that flexible groups (e.g. ethyl chains) contribute at faster dynamics compared to those of rigid ones (e.g. aromatic rings). To support these results, the FFC experiments are supplemented with temperature-dependant high-field NMR T_1 relaxation time measurements for ¹H as well as for ²H nuclei.

REFERENCES

- [1] P. Honegger, V. Overbeck, A. Strate, A. Appelhagen, M. Sappl, E. Heid, C. Schröder, R. Ludwig, O. Steinhauser, *J. Phys. Chem. Lett.* **2020**, 11, 2165-2170.