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# Detailed Overview about Hydrogen-Bonding Motifs in Hydroxy-Functionalized Ionic Liquids

Anne Strate,[a]* Dietmar Paschek[a] and Ralf Ludwig[abc]

[a] *University of Rostock, Institute of Chemistry, Albert-Einstein-Str. 27, 18059 Rostock, Germany*
[b] *Department LL&M, University of Rostock, Albert-Einstein-Str. 25, 18059 Rostock, Germany*
[c] *Leibniz Institute for Catalysis at the University of Rostock, Albert-Einstein-Str. 29a, 18059 Rostock, Germany*
**anne.strate@uni-rostock.de*

Hydroxy-functionalized ionic liquids (ILs) exhibit a fascinating interplay of Coulomb interactions, hydrogen bonding, and dispersion forces, leading to the formation of not only classical cation–anion (c-a) hydrogen bonds but also the more elusive and counterintuitive cation-cation (c-c) hydrogen bonds. In this contribution, we summarize recent advances in characterizing these hydrogen-bonding motifs both in the bulk liquid and the gas phase,[1] providing a comprehensive understanding of their structure, dynamics, and energetics. In the bulk phase, a combination of IR spectroscopy, NMR relaxometry and deuteron quadrupole coupling constant (DQCC) measurements as well as neutron diffraction[2] (ND) has revealed the coexistence and competition of c-a and c-c hydrogen bonds. Molecular dynamics (MD) simulations complement these experimental observations by quantifying cluster distributions, hydrogen bond lifetimes, and providing detailed insights into the local structure and dynamic properties of these clusters. The studies highlight that c-c hydrogen bonds, despite their formation between like-charged species, can exhibit comparable or even shorter H-bond distances and longer lifetimes than their c–a counterparts, particularly in ILs with weakly coordinating anions, polarizable cations and extended cation alkyl chains. To gain a clear picture about the specific contacts within isolated H-bonded cationic clusters formed in the gas phase, cryogenic ion vibrational predissociation (CIVP) spectroscopy[3] of mass-selected gas-phase clusters has been employed in combination with density functional theory (DFT) calculations. Taken together, these multi-technique investigations bridge the gap between bulk and gas phase studies and offer fundamental and detailed insights into the nature of hydrogen bonding in ILs.

## References

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A. Strate obtained her PhD in 2017 from the University of Rostock (Germany), focusing on cationic cluster formation in ILs. In 2017, she had a research stay at Yale University (USA) in Mark Johnson's group applying CIVP spectroscopy on IL clusters in the gas phase. Since 2019 A. Strate has been a Research Associate at the University of Rostock, responsible for FFC NMR Relaxometry. Over the past three years, she has led an independent research project on the dynamics of ILs funded by the German Research Foundation (DFG).