

Quantifying Hydrogen Bonding Interactions in Gas Phase Model Systems Using Ion Vibrational Spectroscopy

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Recent advances in the gas phase vibrational spectroscopy of hydrogen-bonded ion-molecule complexes in the context of (i) anion microsolvation[1-3] as well as (ii) enantiomeric excess determination[4] are described. The use of cryogenic ion traps in combination with widely wavelength-tunable IR lasers in the context of vibrational action spectroscopy has allowed for detailed molecular-level insights into the nature of hydrogen bond interactions, in particular, when combined with electronic structure calculations.[5] Advances and challenges in the interpretation of infrared photodissociation spectra, in particular, the importance of considering anharmonic as well as entropic effects, correlating vibrational frequency shifts with molecular properties (e.g. hydrogen-bond acceptor/donor strengths) as well as quantifying solution phase properties through gas phase measurements will be discussed.

References

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Keywords

gas phase ion vibrational spectroscopy, ionic hydrogen bonds, vibrational red-shifts, chirality recognition, enantiomeric excess determination

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