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H-bond Driven Diastereomer Formation in Chiral Selector Ion Vibrational Spectroscopy of Protonated Amino Acids

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Molecular chirality plays a central role in how the building blocks of life, like amino acids, sugars, or nucleotides, interact. The stereochemistry and conformational flexibility of chiral molecules have a strong impact on their biological, biochemical, and pharmacological properties. A central analytical challenge is the generally applicable differentiation of enantiomers, as well as the fast and accurate determination of the enantiomeric excess of a chiral sample. Gas phase Chiral Selector Ion Vibrational Spectroscopy is a highly sensitive, selective, and fast tool for this purpose.

Chiral protonated amino acids are transferred into the gas phase, where they interact with volatile chiral selector molecules in a gas-filled ion guide under the formation of diastereomeric complexes. These are then mass-selected, cryogenically cooled, messenger-tagged and an infrared photodissociation (IRPD) spectrum is measured. The spectra of the vibrationally cold diastereomers exhibit sufficiently different IR fingerprints, such that they can be spectrally distinguished and quantified.

We study how to maximize the differences in the IRPD spectra of the diastereomers and gain insights into the chiral recognition process. For this purpose, a set of chiral selectors and chiral amino acids with different structural motifs and different number of stereocenters is investigated. We identify the intermolecular noncovalent interactions at work, with H-bonds being the most decisive for diastereomer formation.

Keywords

gas phase, chiral, enantiomeric excess, action spectroscopy

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