

CHIRAL RECOGNITION OF NEUTRAL ALANINE: A LASER ABLATION ROTATIONAL STUDY

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The chiral-tagging method based on rotational spectroscopy is gaining relevance for investigating chirality in the gas phase ^{a,b} Enantiomers of chiral molecules of interest can be complexed with a well-characterized chiral molecule of known handedness, the chiral tag. This results in the formation of diastereomeric complexes, which can be differentiated by their rotational spectra and establishes the absolute configuration of the molecule of interest. However, up to date, this methodology has been limited to molecular specimens having an appreciable vapor pressure. Thus, the study of the whole series of relevant chiral biomolecules, like amino acids, escapes from chiral-tagging studies due to its intrinsically high melting points and associated low vapor pressures.

Laser ablation rotational spectroscopic techniques made the transfer of bare neutral amino acids into the gas phase possible to probe their most stable conformers in a supersonic expansion. However, severe experimental difficulties arise when they are applied to the formation of complexes due to the hot plasma created by the laser ablation process. In the last years, we have made some technical and experimental advances allowing a precise control of the experimental conditions and, therefore, of the complexation process. We report the first chiral determination of the simplest chiral proteogenic amino acid alanine. A broadband, chirped-pulse LA-CP-FTMW spectrometer has been used to perform structural characterization of the complexes formed between racemic alanine (R/S alanine) and S-propylene oxide (S-PO) as a chiral tag. The observation of two different complexes for each alanine enantiomer, characterized by their values of rotational and quadrupole coupling constants, allows the conclusive determination of the absolute configurations of R- and S- enantiomeric forms.

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