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Structure and Stereo-Specific Infrared Features of Proton-Bound Diastereomeric Complexes of Amino Acids Studied with IRMPD Spectroscopy at CLIO Free Electron Laser

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Stereospecific molecular interaction is one of the means used in nature to maximize the specificity of biochemical reactions. Most biomolecules are chiral, i.e. exist in two enantiomeric forms that are non-superimposable mirror images of each other. Different enantiomers of a compound may differ substantially in their biochemical activities and result in different biological response. The large number of today's pharmaceuticals are chiral and consequently, the demand in optically pure pharmaceuticals increases and drives the need for efficient enantioselective, qualitative and quantitative analytical methods. The origin of homochirality in nature has been debated, yet its significance is undoubtful and believed to be a probable precondition for life. The role of different astrophysical mechanisms in formation of interstellar chiral compounds and enantiomeric excess generation is are important contemporary questions.
Utilizing free electron lasers for IRMPD spectroscopy allows to study structure and properties of biomolecules in a unique spectral region. We have been employing CLIO FEL (Orsay, France) and OPO laser in combination with FT-ICR mass spectrometer (Bruker Esquire) to study protonated homo- and hetero-chiral dimers of Tryptophan, Methionine and Tryptophan-Methionine. The vibrational modes have been investigated in the spectral regions of 800-2000 cm-1 and 2700-3750 cm-1. The structure of complexes has been elucidated. Observed vibrational modes have been assigned using density functional theory (DFT) calculations. The conformational analysis has shown several conformers present for each diastereomer at room temperature. This result is in a good agreement with our experimental data. Specific chirality dependent features have been found and analyzed. The applicability of found stereo-dependent vibrational features for routine optical purity analysis of the sample.

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