Identification of Serine Conformers by Matrix-Isolation IR Spectroscopy Aided by Near-Infrared Laser-Induced Conformational Change, 2D Correlation Analysis, and Quantum Mechanical Anharmonic Computations

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Streszczenie

The conformers of α-serine were investigated by matrix-isolation IR spectroscopy combined with NIR laser irradiation. This method, aided by 2D correlation analysis, enabled unambiguously grouping the spectral lines to individual conformers. On the basis of comparison of at least nine experimentally observed vibrational transitions of each conformer with empirically scaled (SQM) and anharmonic (GVPT2) computed IR spectra, six conformers were identified. In addition, the presence of at least one more conformer in Ar matrix was proved, and a short-lived conformer with a half-life of $(3.7 \pm 0.5) \times 10^3$ s in N_2 matrix was generated by NIR irradiation. The analysis of the NIR laser-induced conversions revealed that the excitation of the stretching overtone of both the side chain and the carboxylic OH groups can effectively promote conformational changes, but remarkably different paths were observed for the two kinds of excitations.

Słowa kluczowe

Irradiation, Mathematical methods, Molecular structure, Monomers, Peptides and proteins

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