Conformational properties of oxazole-amino acids: effect of the intramolecular N-H···N hydrogen bond.

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Streszczenie

Oxazole ring occurs in numerous natural peptides, but conformational properties of the amino acid residue containing the oxazole ring in place of the C-terminal amide bond are poorly recognized. A series of model compounds constituted by the oxazole-amino acids occurring in nature, that is, oxazole-alanine (L-Ala-Ozl), oxazole-dehydroalanine (ΔAla-Ozl), and oxazole-dehydrobutyrine ((Z)-ΔAbu-Ozl), was investigated using theoretical calculations supported by FTIR and NMR spectra and single-crystal X-ray diffraction. It was found that the main feature of the studied oxazole-amino acids is the stable conformation β2 with the torsion angles φ and ψ of -150°, -10° for L-Ala-Ozl, -180°, 0° for ΔAla-Ozl, and -120°, 0° for (Z)-ΔAbu-Ozl, respectively. The conformation β2 is stabilized by the intramolecular N-H···N hydrogen bond and predominates in the low polar environment. In the case of the oxazole-dehydroamino acids, the π-electron conjugation that is spread on the oxazole ring and C(α)═C(β) double bond is an additional stabilizing interaction. The tendency to adopt the conformation β2 clearly decreases with increasing the polarity of environment, but still the oxazole-dehydroamino acids are considered to be more rigid and resistant to conformational changes.

Adres publiczny

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https://www.acs.org/content/acs/en.html