GAS PHASE CONFORMATIONAL BEHAVIOUR OF β-ALANINE, PHENYLGLYCINE AND γ-AMINOBUTYRIC ACID (GABA)

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The rotational spectrum of β-alanine (NH_2–$(CH_2)_2$–COOH, m.p. 205 °C), phenylglycine (C_6H_5–CH(NH_2)–COOH, m.p.> 300 °C) and γ-Aminobutyric acid (GABA, NH_2–$(CH_2)_3$–COOH, m.p.> 190 °C), have been investigated using our Laser-Ablation Molecular Beam Fourier Transform Microwave Spectrometer (LA-MB-FTMW)[a].

For β-alanine a new conformer has been detected together with the two conformers previously identified[b]. Fully-resolved quadrupole hyperfine structure has been analyzed for the three conformers. Their configurations have been established on the basis of the rotational and N-nuclear quadrupole coupling constants. Two of them are stabilized by a NH$\cdots$O interaction (type I of glycine), and the other presents a OH$\cdots$N interaction (type II). Partial conformational relaxation has been observed between the two conformers bearing a type I hydrogen bond.

For phenylglycine, the simplest aromatic analog of glycine, two conformers have been detected. These conformers are stabilized by either type I or type II intramolecular hydrogen bonds. The conformer bearing type I interaction is the global minimum.

For GABA, quantitatively one of the most important inhibitory transmitters of the central nervous system, one conformer has been observed up to the present. In this form the molecule closes a cicle by means of a n-π^* interaction between the amino group nitrogen atom and the carboxyl group carbon atom.

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[a] A. Lesarri, S. Mata, J. C. López and J. L. Alonso, *Rev. Sci. Instrum.*, 74 (2003) 4799.

[b] S. J. McGlone and P. D. Godfrey, *J. Am. Chem. Soc.*, 117 (1995) 1043.