GAS PHASE STRUCTURE OF AMINO ACIDS: LASER ABLATION JET-COOLED ROTATIONAL STUDIES

J. L. ALONSO, A. LESARRI, S. BLANCO, M. E. SANZ, E. J. COCINERO and J. C. LÓPEZ, *Grupo de Espectroscopía Molecular (GEM), Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, 47005 Valladolid, Spain*.

The structural analysis of natural amino acids using rotational spectroscopy was hindered in the past by the high melting points and thermal fragility of these compounds. Recently, these studies have received an important impulse with the introduction of a technique which combines laser ablation with Fourier transform microwave spectroscopy in supersonic jets[a] (Laser-ablation molecular-beam Fourier transform microwave spectroscopy, LA-MB-FTMW). Using this technique we have studied under isolation conditions in gas phase more than 15 amino acids[b] to date. Several conformers (up to six for serine, cysteine, and aspartic acid and five for γ-aminobutyric acid) have been detected in the jet-cooled rotational spectrum and their rotational and ^{14}N-nuclear quadrupole coupling constants determined; the latter are crucial to distinguish unequivocally between conformations with similar rotational constants. The observed conformers present different intramolecular hydrogen bonds involving the –COOH, –NH_2, –OH and –SH groups which influence their stability.
The first observation of the 1:1 complex of glycine-water[c] is also presented. The water molecule has been reliably located in the complex from the analysis of several isotopomers. The complex is stabilized by two intermolecular hydrogen bonds formed between the carbonyl group and one of the hydrogen atoms of water (Ow–H$\cdots$O=C) and between the hydroxyl group and the electron lone pair at the oxygen atom of water (Ow$\cdots$H–O–C)).

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