ROTATIONAL SPECTRA AND STRUCTURE OF PROLINE: A JET-COOLED LASER ABLATION STUDY

ALBERTO LESARRI, SANTIAGO MATA, EMILIO J. COCINERO, JUAN C. LÓPEZ and JOSÉ L. ALONSO, *Grupo de Espectroscopía Molecular, Departamento de Química Física, Facultad de Ciencias, Universidad de Valladolid, 47005 Valladolid, Spain*.

The conformational behaviour of aminoacids is of critical interest to understand the dynamical role of these molecules in protein or polypeptide formation. Consequently, extensive structural research has been conducted in their natural condensed phases. This point is worth noting since solid or diluted aminoacids present a zwitterionic structure i.e., a bipolar ionized form of the type $^{+}H_3N$-CH(R)-COO^{-}, which does not occur in the polypetide chain. In order to obtain the structure of the neutral form of aminoacids research should be conducted in an environment essentially free of intermolecular interactions with other partners, either the solvent or other atoms of the molecule itself. In particular, the collisionless environment of a supersonic jet seems particularly well adapted for such studies. The obvious difficulties for the experimental studies in gas phase are due to the high melting points and associated low vapour pressures of aminoacids. For these species laser ablation can be an effective way of vaporizing neutral sample molecules, preventing the thermal decomposition of the heating methods. A laser vaporization source combined with Fourier transform microwave spectroscopy in a supersonic jet has been applied to the structural investigation of the essential aminoacid proline in gas phase. Analysis of the rotational spectrum has revealed the presence of two conformers of neutral proline in gas-phase, both exhibiting an intramolecular hydrogen bond between the hydrogen atom of the carboxylic
group and the nitrogen atom of the ring (OH···N), the carboxyl moiety being in trans position with respect to the imino group. The five membered-ring of the molecule adopts in both conformers a bent-like structure, with near symmetrical endo or exo conformations respect to the carboxyl group. The endo form is the most stable species, as evidenced from a conformational relaxation from the exo to the endo form. The rotational spectra of the parent, ^{15}N, ^{13}C (in natural abundance), N-D and O-D isotopic species have been anlyzed and r_0-like structures have been derived for both conformers.