GAS PHASE STRUCTURE OF AMINO ACIDS: LA-MB-FTMW STUDIES

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Recent improvements in our laser ablation molecular beam Fourier transform microwave (LA-MB-FTMW)[a] spectrometer such as using Laval-type nozzles[b] and picoseconds Nd:YAG lasers (30 to 150 ps) have allowed a major step forward in the capabilities of this experimental technique as demonstrated by the last results in serine[c] cysteine[d] and threonine[a] for which seven, six and seven conformers have been respectively identified. Taking advantage of these improvements we have investigated the natural amino acids metionine, aspartic and glutamic acids and the γ-aminobutyric acid (GABA) with the aim of identify and characterize their lower energy conformers. Searches in the rotational spectra have lead to the identification of seven conformers of metionine, six and five of aspartic and glutamic acids, respectively, and seven for the γ-aminobutyric. These conformers have been unambiguously identified by their spectroscopic constants. In particular the ^{14}N nuclear quadrupole coupling constants, that depend heavily on the orientation of the amino group with respect to the principal inertial axes of the molecule, prove to be a unique tool to distinguish unambigously between conformations with similar rotational constants. For the γ-aminobutyric acid two of the seven observed structures are stablized by an intramolecular interaction n-π*. Two new conformers of proline have been identified together with the two previously observed.[e]

[a] J. L. Alonso, C. Pérez, M. E. Sanz, J. C. López, S. Blanco, *Phys.Chem.Chem.Phys.*, 2009, 11, 617.
[b] D. B. Atkinson, M. A. Smith, *Rev. Sci. Instrum.* 1995, 66, 4434.
[c] S. Blanco, M. E. Sanz, J. C. López, J. L. Alonso, *Proc. Natl. Acad. Sci. USA*2007, 104, 20183.
[d] M. E. Sanz, S. Blanco, J. C. López, J. L. Alonso, *Angew. Chem. Int. Ed.,*2008, 120, 6312.
[e] A. Lesarri, S. Mata, E. J. Cocinero, S. Blanco, J.C. López, J. L. Alonso, *Angew. Chem. Int. Ed.* , 2002, 41, 4673