CONFORMATIONAL LANDSCAPE OF ASPARTIC ACID IN GAS PHASE

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The neutral form of the aspartic acid (COOH–CH(NH_2)–CH_2–COOH) has been observed for the first time in gas phase using our Laser-Ablation Molecular Beam Fourier Transform Microwave Spectrometer (LA-MB-FTMW).[a] A solid rod of aspartic acid (m.p.> 300 °C) was impinged by the second harmonic of the fundamental emission of a Nd:YAG laser, and vaporized aspartic acid molecules were dragged by a flow of Ne or Ar at 5.5 bar into the Fabry-Pérot resonator. Four different conformers of the aspartic acid have been identified through the observation and analysis of their rotational spectra, and their spectroscopic constants have been determined. Ab initio calculations at high level of theory predicted rotational and quadrupole coupling constants which helped us to identify the different conformations unequivocally. These four conformers possess diverse intramolecular hydrogen bonds which influence their stability. Relative populations of the conformers in the supersonic jet have been qualitatively determined by comparing the intensity ratio of several of their rotational transitions.

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