

CONFORMATIONAL ANALYSIS OF LASER-ABLATED SERINE AND CYSTEINE

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The different conformers of the relevant natural amino acids serine (m.p. 240 °C) and cysteine (m.p. 225 °C) have been studied using Laser Ablation (LA) in combination with Molecular Beam Fourier Transform Microwave (MB-FTMW) spectroscopy^a, a technique that has been successfully applied to the investigation of proline^b, valine^c, alanine^d and hydroxyproline^e. The solids were vaporized by ablation of pressed rods using the 532 nm radiation of a Nd:YAG laser, seeded in Ne and probed with microwave radiation in a supersonic expansion inside the Fabry-Pérot cavity. Five different conformers of serine and four conformers of cysteine have been observed and their rotational and N-nuclear quadrupole coupling constants determined. Ab initio calculations at high level of theory predicted rotational and quadrupole coupling constants which helped us to identify the different conformations unequivocally. The observed conformers present different intramolecular hydrogen bonds involving the –COOH, –NH₂, –OH and –SH groups which influence their stability. An analysis of their relative intensities has been carried out and related, in a qualitative manner, to the stabilities of the conformers in our supersonic beam.

^aA. Lesarri, S. Mata, J. C. López and J. L. Alonso, *Rev. Sci. Instrum.*, 74 (2003) 4799.

^bA. Lesarri, S. Mata, E. J. Cocinero, S. Blanco, J. C. López, J. L. Alonso, *Angew. Chem. Int. Ed.*, 41 (2002) 4673.

^cA. Lesarri, E. J. Cocinero, J. C. López, J. L. Alonso, *Angew. Chem. Int. Ed.*, 43 (2004) 605.

^dS. Blanco, A. Lesarri, J. C. López, J. L. Alonso, *J. Am. Chem. Soc.*, 126 (2004) 11675.

^eA. Lesarri, E. J. Cocinero, J. C. López, J. L. Alonso, *J. Am. Chem. Soc.*, 127 (2005) 2572.