ROTATIONAL SPECTRA OF GLYCINE N-METHYL DERIVATIVES: N,N-DIMETHYLGLYCINE AND SARCOSINE

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The conformational behaviour of N,N-dimethylglycine (m.p. 180 °C) and sarcosine (m.p. 208 °C) has been studied for the first time in gas phase as an extension of our recent work on natural amino acids[a]. The solid amino acids were vaporized using laser ablation (LA) from a Q-switched Nd:YAG laser, and probed spectroscopically in a supersonic jet using molecular beam Fourier transform microwave spectroscopy (MB-FTMW)[b]. The rotational spectrum revealed the presence of three conformers of neutral N,N-dimethylglycine in the jet. A bifurcated methyl-to-carbonyl (C–H· · ·O=C) weak intramolecular hydrogen bond has been proposed to stabilize the most stable conformer of C_s symmetry. The second conformer of C_1 symmetry presents an intramolecular hydrogen bond N· · ·O–H analogue to glycine II. Substitution and effective structures have been derived for this conformer from the rotational data of seven isotopomers. A third conformer presents a cis-carboxylic functional group and C_1 symmetry.

Two conformers were observed for neutral sarcosine. The most stable conformer is stabilized by an intramolecular hydrogen bond N–H· · ·O=C, analogue to the interaction observed in the most stable conformer of glycine I. The second stable conformer exhibits an intramolecular hydrogen bond N· · ·O–H similar to glycine II. The observed conformers in both molecules are consistent with previous experiments using matrix-isolation FT-IR[c].

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[a] A. Lesarri, S. Mata, E. J. Cocinero, S. Blanco, J. C. López, J. L. Alonso, *Angew. Chem. Int. Ed.*, 41 (2002) 4673; A. Lesarri, E. J. Cocinero, J. C. López, J. L. Alonso, *Angew. Chem. Int. Ed.*, 43 (2004) 605; S. Blanco, A. Lesarri, J. C. López, J. L. Alonso, *J. Am. Chem. Soc.*, 126 (2004) 11675; A. Lesarri, E. J. Cocinero, J. C. López, J. L. Alonso, *J. Am. Chem. Soc.*, 127 (2005) 2572.

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

[c] A. Gómez-Zavaglia, I. D. Reva, R. Fausto, *Phys. Chem. Chem. Phys.* 5 (2003) 41; A. Gómez-Zavaglia, R. Fausto, *Vib. Spectr.*, 33 (2003) 105.