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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