PREFERRED CONFORMERS OF NON-PROTEINOGENIC AMINO ACIDS HOMOSERINE AND HOMOCYSTEINE

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Vaporization of solid homoserine and homocysteine by laser ablation in combination with Fourier transform microwave spectroscopy techniques made possible the detection of their most stable structures in a supersonic expansion. All detected conformers have been identified through their rotational and ^{14}N quadrupole coupling constants. They show hydrogen bonds linking the amino and carboxylic group through N–H$\cdots$O=C (type I) or N$\cdots$H–O (type II) interactions. In some of them there are additional hydrogen bonds established between the amino group and the hydroxyl/thiol groups in the gamma position. Entropic effects related to the side chain have been found to be significant in determining the most populated conformations.