WATCHING CONFORMATIONS OF BIOMOLECULES: A MICROWAVE SPECTROSCOPY APPROACH

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The combination of laser ablation with Fourier transform microwave spectroscopy in supersonic jets (LA-MB-FTMW) has made possible the gas-phase study of solid biomolecules with high melting points. In the experiment, solids are efficiently vaporized by a high-energy laser pulse, supersonically expanded into a evacuated Fabry-Perot cavity and characterised by their rotational spectra. Recent improvements such as the use of picosecond pulse lasers, new ablation nozzles and the extension of the range of the spectrometers to low frequecy have notably increased the sensitivity of our experimental setup. To date different α-, β- and γ-amino acids[a] have been studied using this technique, making possible the characterization of their preferred conformations and gaining insight in the role of intramolecular interactions. Even in conformationally challenging systems the different rotamers of such biomolecules can be identified by rotational spectroscopy as can be illustrated by the assignment of six low-energy conformers in cysteine and aspartic acid,[b] seven in serine and threonine,[a] and nine in γ-amino butyric acid (GABA).[c] In all cases the low-energy conformers have been conclusive identified from their experimental rotational and ^{14}N quadrupole coupling constants. The spectra of neurotransmitters[d] and of the nucleic acid bases uracil, thymine, cytosine and guanine[e] have also been studied and their preferred conformers or tautomeric forms determined. The complexes between amino acids and nucleic acid bases with water[f] have also been investigated to obtain information on the possible changes induced in the conformational or tautomeric preferences by the addition of solvent molecules.

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