PROBING GUANINE AND CYTOSINE TAUTOMERS IN THE GAS PHASE

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Using laser ablation molecular beam Fourier transform microwave spectroscopy (LA-MB-FTMW) we have recently studied the nucleic acid bases uracil[a] and thymine.[b] We have now successfully probed in isolation conditions in the gas phase cytosine and guanine which are solids with high melting points (m.p.>300C) and a low vapour pressure, and consequently, they are elusive to gas-phase rotational studies. Five rotational species have been detected in the supersonic expansion of cytosine. The unambiguous assignment of the observed species to the various tautomer/conformer structures is based on the markedly different values of the quadrupole coupling constants of the three ^{14}N nuclei, which act as fingerprints for the identification of the various species. Four species have been observed in the rotational spectra of Guanine. The comparison between the experimental rotational constants and those calculated ab initio provide a definitive test for the identification of the four lowest energy forms. The planarity of the tautomers is discussed on the basis of the inertial defect values (Δ=I_c-I_a-I_b).

[a] V. Vaquero, M.E. Sanz, J.C. López and J.L. Alonso, *J. Phys. Chem. A* 111, 3443 (2007)
[b] J.C. López, M.I. Peña, M.E. Sanz and J.L. Alonso, *J. Chem. Phys.* 126, 191103 (2007)