TAUTOMERS OF CYTOSINE AND THEIR EXCITED ELECTRONIC STATES: A MATRIX ISOLATION SPECTROSCOPIC AND QUANTUM CHEMICAL STUDY

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We have measured the IR and UV spectra of cytosine in a low-temperature argon matrix. An attempt was made to determine the tautomeric ratios existing in the matrix, making use of the matrix-isolation IR spectrum and computed IR intensities of the tautomers in a least squares fitting procedure. The mole fractions are about 0.22 for oxo(-amino) form, 0.26 and 0.44 for the two rotamers, respectively, of the hydroxy(-amino) form and 0.08 for the (oxo-)imino tautomer. These ratios were then used to simulate the matrix-isolation UV spectrum as a composite of the individual spectra, the latter calculated *ab initio* at high levels of electron correlation theory. The agreement between simulated and experimental UV spectra seems satisfactory. This indicates that, in contrast to the solid state and solution spectra described up to now by the oxo(-amino) form alone, the reproduction of the matrix-isolation UV spectrum needs at least the hydroxy(-amino) and oxo(-amino) forms, and probably also the (oxo-)imino form.