Analysis of Tautomeric Composition of Cytosine

Using Two-Photon Absorption Spectra

T.G. Burova, M.N. Nurlygaianova, G.N. Ten

Saratov State University n.b. N.G. Chernyshavsky, 83, Astrakhanskaya str., Saratov, 410012, Russian Federation

Investigation of the optical spectra of biomolecules became one of the most important methods of studying their structure and properties.

This work continues the analysis of two-photon absorption (TPA) spectra of nucleic acid bases by direct calculations of the intensity distribution using the quantum-mechanical method [1] for the adiabatic model in the Herzberg-Teller approximation. In [1] it is suggested that one- and two-photon absorption spectra as well as luminescence and resonance Raman spectra of polyatomic molecules can be described using a single approach, in line with the similarity of their physical nature. It allows one to calculate vibronic coupling and evaluate the relative intensities of lines in these spectra using the same set of initial data. So we used IR vibration absorption spectra results from [2]. Inclusion of the vibronic term makes it possible to explain the presence of lines corresponding to one-quantum nontotally symmetric vibrations, their odd overtones and combinations.

The most probable tautomeric forms of cytosine (canonical amino-oxo tautomeric form, cation, anion, cis-imino-oxo, cis-amino-hydroxy and trans-amino-hydroxy tautomers) were the objects of our investigation. It has been confirmed that in the aqueous solution of cytosine (pH= 3.0) there exist several tauromeric forms: canonical amino-oxo tautomeric form, cation, as well as cys-imino-oxo and cys-amino-hydroxy tautomers.

1. *T. G. Burova //* Khim. Fizika 13 (3), 29 (1994).
2. *Ermolenkov V., Lednev I.,Ten G., Burova T., Kadrov D., Nurlygayanova M., Baranov V.* Ionic and tautomeric composition of cytosine in aqueous solution: resonance and non-resonance Raman spectroscopic study // J.Phys.Chem. A. 2013. 117(48), P.12734-12748.