Investigation of Nucleosides Molecular Structure

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1 Introduction

The investigations of nucleoside molecular structures are of fundamental interest for molecular biology. Up to the present the main experimental information about their structure was obtained from the data for the crystals and solutions [1]. But the intermolecular interaction strongly influences on the conformational and tautomeric equilibrium. And their result can not be compared with quantum chemical calculations. Therefore it is very interesting to obtain an information about nucleoside structure in the isolated conditions. Owing to weak intermolecular interactions in the inert matrices and their optic transparent, matrix isolation spectroscopy is very useful tool for such investigations. The main problem is low thermostability of nucleosides and consequently it is difficult to obtain the molecular beam. Previously we solved this problem for uridine and thymidine [2]. In this work we compare the results of our calculation method PM3 with the data obtained from FTIR matrix isolation spectroscopy.

2 Method and Results

In our experiments all FTIR spectra were recorded with apodized resolution 0.24 cm^{-1} in the range 450-2500 cm^{-1} (KBr beamsplitter) and 0.4 cm^{-1}in the range 1400-4000 cm^{-1} (CaF_2 beamsplitter). The temperatures of evaporations were adenosine 183°C uridine -148°C, thymidine -147°C. Also for comparison with adenosine, the matrix spectra of adenine was recorded in Ar matrix. Matrix to sample ratio (M/S) was about 900:1. The noticeable traces of nucleosides thermodestruction (H_2O, CO_2, bases) were not detected. The quantum-chemical calculation method PM3, contrary to previous experimental data [1], show an ability of existence of sin-conformer due to stabilising of it structure by intramolecular hydrogen bond $O_{5'}HO_2$ for thymidine, uridine and $O_{5'}HN_3$ for adenine. On Fig. 1. The OH, NH region of stretching vibration of nucleosides in Ar matrix (T=12K) is given. In a similar to data for adenine [3], only amino tautomer of adenosine is present in matrices. As in the work [2] the band 3664 cm^{-1} can be assigned to the stretching vibration $\nu O_{5'}H$ of hydroxymethyl group and the wide band 3637 to the free $O_{3'}H$ and $O_{2'}H$ group. These bands coincide well with uridine (Fig.1 curve 3) and thymidine (Fig.1 curve 4) vibrations of free OH groups.

Appearing hydrogen shifted bands 3472 cm^{-1} in thymidine and 3458, 3493 cm^{-1} in uridine spectra confirm existence of syn-conformations for these substances. But contrary to thymidine and uridine we don't see appearance of this H-bonded vibration in the adenosine spectrum. This band may overlap with antisymmetric vibration of NH_2 group in adenosine spectrum (Fig. 1, curve 1). But relations between of the intensities of symmetric and antisymmetric vibration for adenine (1.35) and adenosine

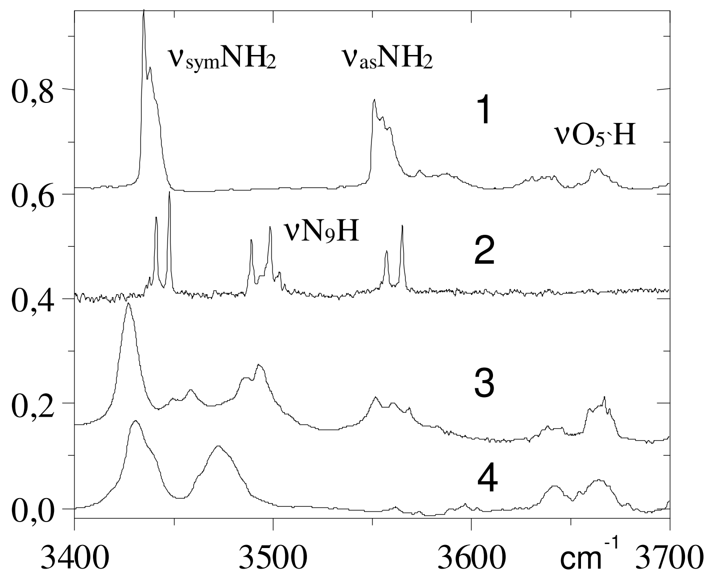

Figure 1: The OH, NH region of stretching vibration of nucleosides in Ar matrix (T=12K). Curve 1-adenosine (M/S=900), 2-adenine (M/S=1000), 3-uridine (M/S=1100), 4-thymidine (M/S=1000)

(1.4) are practically the same. That is way we can choose several the most probable structure from our calculations anti-conformation for adenosine and syn-conformations for thymidine and uridine. The situation for adenosine is the same as in a crystals [4].

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