

Quantum chemical calculations of vibrational spectra, electronic and spatial structures of adenine and thymine molecules

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Adenine and thymine are part of many natural biologically active compounds, important intracellular intermediates and drugs. It is known that the hydrated environment mainly determines the formation of a stable structure of nucleic acids and their conformational variability. In this regard, studies of vibrational spectra of nucleotides and their derivatives are important, since the interaction of hydrogen bonds has an effect on stabilization the double-stranded DNA and its conformational mobility. Determination of the structural and electronic properties of biomolecules has a significant interest in describing the processes of formation of the hydrated environment as a whole. Moreover, the obtained geometric structures, distributions of electron density and the vibrational spectra of adenine and thymine biomolecules can be the basis for modeling the various processes in which these compounds are involved. On the other hand, the combination of biotechnology and materials science provides enormous opportunities for the creation of new materials and integrated components on basis of investigated biomolecules [1, 2].

All the calculations were performed with the GAMESS (US) quantum-chemistry package using the resources of the cluster at the V.M. Glushkov Institute of Cybernetics of the National Academy of Science of Ukraine. The calculations of the electronic properties, equilibrium geometric structures and vibrational spectra were performed by the spin-restricted Hartree–Fock (RHF) and density functional (DFT/ B3LYP) methods with the 6-31G basis set.

It follows from the results of calculations that under the geometry optimization conditions, the biomolecules studied remain stable. Calculated structural parameters of adenine molecule are shown in Fig. 1.

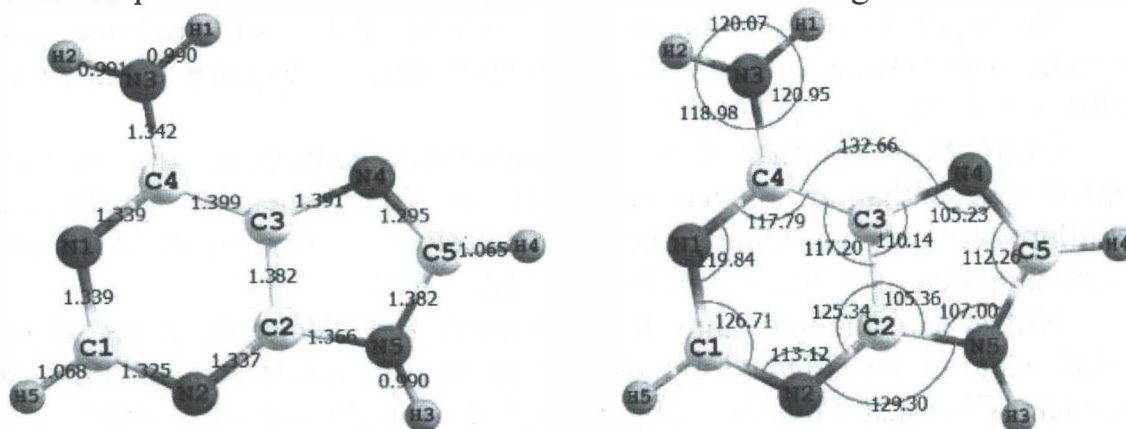


Fig.1. Calculated adenine bond lengths (left) and angles (right).

Comparison of calculated IR-spectrum by the DFT method for the investigated molecule with the available experimental spectrum of the adenine [3] is shown in Fig. 2.

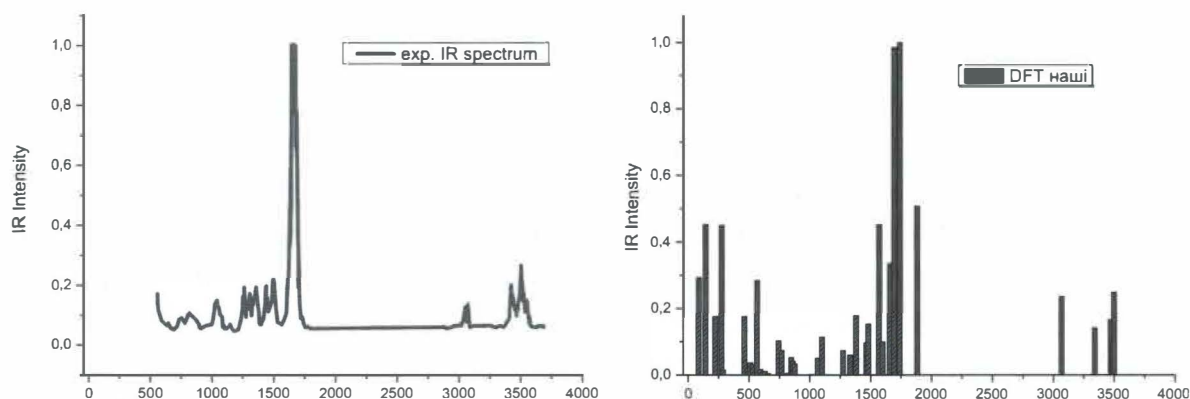


Fig. 2. Experimental (left) and calculated by DFT method (right) adenine IR-spectrum.

The analysis of the obtained results shows that the vibrational lines of the adenine IR-spectrum in the frequency ranges (87 cm^{-1} - 650 cm^{-1} and 3067 cm^{-1} - 3498 cm^{-1}) correspond to intra- and intermolecular vibrations of hydrogen bonds. The band of maximal intensity in range 1380 cm^{-1} - 1879 cm^{-1} appear due to the presence of C-N and C-B bonds in the structure of the six- and five-membered heterocycles of the adenine molecule. The analysis of vibrational spectra of the thymine molecule shows that planar valence vibrations of the double bonds C = O and C = C appear in the range between 1800 cm^{-1} and 1550 cm^{-1} and not-planar ring vibrations – in the vicinity of 800 cm^{-1} .

References:

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