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Low-frequency modes of water vibrations in the minor groove of DNA double helix

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Water and ions around DNA macromolecule are paramount for the stability of the double helix structure and found to mediate the vital biological process such as nucleic-protein recognition, and the interaction with the biologically active compounds. DNA interacts strongly with surrounding water molecules and counterions making the hydration shell with different structural and dynamical features in different regions of the double helix (minor and major grooves, phosphate groups). In the DNA minor groove water molecules are highly ordered and in the case of AATT nucleotide sequence, the spine of hydration is formed [1]. In the present research [2], the vibrations of hydration spine have been studied to establish the mode of translational vibrations of water molecules in the DNA low-frequency spectra (< 200 cm^{-1}). Within the framework of the developed phenomenological model, based on the approach of DNA conformational vibrations [3], the modes of water vibrations and DNA structural elements have been determined. The calculations for the case of DNA fragment CGCGAATTCGCG have shown that the frequencies of water vibrations are about 185 ± 20 cm^{-1} depending on nucleotide sequence. The obtained mode of water vibrations higher than the modes of internal conformational vibrations of DNA and observed in the same region of the vibrational spectra as translation vibrations of water molecules in the bulk phase. To distinguish the vibrations of water molecules from those in the bulk, the dynamics of DNA with heavy water (D_2O) has been considered. The estimations have shown that in the case of D_2O the frequency of vibrations decreases for about 10 cm^{-1} that may be used to identify the vibrations of water spine of the DNA minor groove experimentally.

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