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Low-frequency vibrations of water molecules in the hydration spine of DNA minor groove

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Under the natural conditions, DNA macromolecule takes the form of a double helix which structure is stabilized by water molecules and metal ions. The organization of the ion-hydration environment of the macromolecule depends on a region of the double helix. In particular, in the minor groove of the macromolecule the water molecules are highly structured and the spine of water molecules, bridging the N_3 atoms of purine and O_2 atoms of pyrimidine bases, is formed. The dynamics of water molecules in the DNA water spine should be characterized by the vibrations in the same spectra range as the conformational vibrations of DNA. Therefore, the goal of our study was the determination of distinctive vibration modes of water molecules in the DNA minor groove that may be observed in the low-frequency spectra. On the basis of the approach for the description of DNA conformational dynamics [2], the vibrational model has been elaborated. In the model the nucleosides are considered as physical pendulums, rotating around phosphate groups in the plane perpendicular to the helical axis, and water molecules are presented as the masses attached to physical pendulums in different pairs. The parameters of the model [2] and the results of molecular dynamics simulations [3] were used for the estimation of the frequencies and amplitudes of vibrations. As a result the mode of water translational vibrations in the hydrated spine of DNA minor groove has been established. This mode characterizes the displacements of water molecule as a single whole from the equilibrium position in the frequency range within 170 – 270 cm^{-1}. The comparison of the obtained results with the experimental spectra of DNA in an aqueous environment showed that in this region of the vibrational spectra the translational vibrations of water molecules in the bulk phase as well as ion-phosphate vibrations of DNA are observed. Thus, the obtained results ground the presence of the mode of vibrations of water molecules in the hydration spine of the DNA minor groove among the modes of DNA conformational vibrations.

[1] Drew H.R., Dickerson R.E., J. Mol. Biol., **151**, 535–556 (1981)
[2] Volkov S.N., Kosevich A.M., J. Biomol. Struct. Dyn. **8**, 1069 (1990)
[3] Perepelytsya S.M., Journal of Molecular Modeling, **24**, 171 (2018).

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