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Calculation of the model of the spectrum of interaction with macromolecules by the method of finding symmetries

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Methods of X-ray diffraction analysis (XRD) have allowed us to determine the structure of many materials and substances around us. The configurations of crystal lattices of a variety of inorganic materials became known to science, which made it possible to create new compounds with specified properties and characteristics. Advances in the decoding of solid materials and crystals were attempted to be transferred to the field of biological substances. However, molecular compounds turned out to be more difficult to study XRD. Molecules practically do not lend themselves to high-quality crystallization, which does not allow the use of X-ray radiation for 40% of biological structures: proteins, macromolecules, and so on [1-2]. Nevertheless, alternative methods of research, for example, methods from the field of chemistry, do not allow us to decipher the structure of a molecule at the atomic level. That is why ultrashort laser pulses have now been used as a source of XRD in studies with molecular samples [3-5]. This made it possible to get rid of existing obstacles in research. For the use of ultrashort laser pulses, there is no need for crystallization of the sample, in addition, the pulse has time to fix the structure before its possible change (rearrangement of atoms, change of bonds), since it works on the same time scale as the molecule. To date, the world's leading laboratories are already using ultrashort laser pulses in working with biological substances[6-8]. But there are problems with decrypting the received data. In this paper, a new approach is proposed to describe the spectrum of interaction of a pulse with a complex polyatomic molecular structure.

Molecular structures are complex compounds that are difficult to analyze. The randomness of the arrangement of atoms in them makes it difficult to decipher the obtained spectra in XRD methods, since they are mainly aimed at working with inorganic substances whose crystal lattice is ordered. Complex biological structures such as proteins, amino acids, macromolecules, DNA and RNA do not have obvious symmetry and periodicity. However, most macromolecules are a set of repeating units formed from smaller molecules, which makes it possible to calculate the spectrum in an analytical form. In this paper, we propose a method for calculating the spectrum for a DNA molecule in an analytical form by finding symmetries in a macromolecule. Let's consider the calculation using the example of a DNA macromolecule. The nitrogenous bases repeated in it allow them to be put into separate groups for calculation –symmetry. When calculating a long chain of sequences, such groups are summed up, which simplifies the mathematical description of the interaction spectrum. For example, there is a piece of the DNA chain of the bacterium Escherichia coli str. K-12 substr. MG1655 of six nitrogenous bases: thymine, guanine, thymine, thymine, guanine, thymine (TGTTGT). Repeating nitrogenous bases according to the principle of complementarity create identical pairs: thymine-adenine, guanine -cytosine. These pairs can be combined in symmetry, thereby simplifying the calculation in an analytical form.

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Primary author: KHARLAMOVA, Anastasia (Northern (Arctic) Federal University named after M.V. Lomonosov)

Presenter: KHARLAMOVA, Anastasia (Northern (Arctic) Federal University named after M.V. Lomonosov)

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