MATHEMATICAL MODELLING OF SPATIAL ARRANGEMENT AND CALCULATION OF OPTICAL ACTIVITY OF DNA LIQUID-CRISTALLINE DISPERSION PARTICLES

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Nowadays nucleic acids biotechnology is being intensively developed, aimed at creation of spatial nanoconstructions with adjustable characteristics on the base of nucleic acids molecules or their complexes [1]. One of the effective methods of such nanostructures formation is the liquid crystalline approach, where as a result of double-stranded DNA molecules phase exclusion from the water-salt polymers solution, the composition of nucleic acids dispersions takes place. Herewith it is necessary to solve an essential problem – to determine the pattern of molecules arrangement in theses molecular aggregates.

For the problem solving it is reasonable to perform the investigation of dispersions optical activity, which gives the possibility to obtain meaningful information on their spatial package [2]. The most pictural manifestation of optical activity is the appearance of circular dichroism at frequencies, coinciding with the absorption band of DNA nitrogen bases.

Theoretical examination of DNA liquid crystalline dispersions circular dichroism is produced on the base of the theory of electromagnetic waves absorption by large molecular aggregates [3,4]. .The dispersion particles are modeled by the discrete set of absorbing dipoles, whose spatial order, for example helicoidal one in the case of cholesteric, corresponds to the type of spatial package of molecules, comprising complex. The developed approach gives the possibility together with the calculation of optical activity, according to the different kinds of arrangement of DNA molecules in dispersion particles, also to determine the changes of optical properties, connected with the perturbations due to the interaction with nanoparticles [4].

References.

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