STUDY OF SYNERGY MODELING OF COVID-19 PROCESSES BASED ON ORDERING IN BIOPOLYMERS

Bokhodir Askarov[1], Shukhrat Gulamov[2], Bekhzod Batirov[1]

[1]Andijan Mechanical Engineering Institute, Uzbekistan

[2]Andijan State Medical Institute, Uzbekistan

E-mail: shaqfiz@mail.ru

As is known, in the twenty-first century, mankind in all countries of the world is faced with wounds of unknown infectious diseases. Environmental factors, population growth and migration activity act and provoke an increase in the number of diseases.One of these viruses is the COVID-19 coronavirus.

As of January 2020, coronaviruses (lat. Coronoviridae) are a family of 40 types of RNA containing complexly organized viruses that have a supercapsid from which crown-shaped spine processes grow.

The size of the coronavirus is in the range of 80 - 220 nm, the appearance of its nucleocapsid is similar to a flexible helix, which consists of RNA and a huge number of N nucleoprotein molecules.

For a deeper understanding and analysis of the processes associated with the coronavirus COVID-19, the study of synergistic modeling of processes based on ordering in biopolymers can help.

Synergetics is becoming the most versatile method for studying complex systems and nonlinear phenomena. According to the principles of synergetics, ordering processes at the molecular level can qualitatively change the properties of a biological object at a higher level of its organization (biological activity, enzymatic catalysis, etc.). Previously, we introduced the concept of a local group of atoms (LHA) of a macromolecule and constructed the adiabatic potentials of LHA taking into account vibronic and low-symmetry perturbations in order to develop a method of synergetic modeling. This paper presents the main results of synergetic modeling of the processes of ordering of the ionic subsystem under the conditions of vibronic instability of the LHA macromolecule.

The main goal of the study is to determine the criterion for ordering the ionic subsystem of a double biopolymer.

To achieve this goal, we have solved the following tasks:

1. Criteria for the occurrence of vibronic instability of the local group of atoms (LHA) of the macromolecule have been determined;

2. Processes of LHA ordering of macromolecule have been investigated.

3. A synergistic modeling of the formation of a double copolymer from a homopolymer has been carried out.

The object of research is the electron-ion system of macromolecular structure. The main parameters of the object are the characteristic size and their electronic-vibrational characteristics.

The subject of research is the effects of ordering of local groups of atoms along the chain of a macromolecule.

Consider a linear chain of a homopolymer macromolecule. Each link is represented as a Jan-Teller system. We choose a trimer as the LHA macromolecule.

The process of modification of a certain link is described by the reaction equation of the following form: A $\geq$ B. Here, A is a monomeric link of a macromolecule before modification and B - after modification. In particular, this process is carried out during alkaline hydrolysis of chitin. The chitin macromolecule consists of N-acetylglucosamine. When deacetylation of monomeric chitin units is formed, a chitosan macromolecule is formed, which consists of two types of units: N-acetylglucosamine and glucosamine. Thus, to study the ordering of two types of units in the process of chemical modification, the linear chain of the homopolymer macromolecule is considered. If the initial composition of the macromolecule consists of the same units, then in the process of chemical modification, individual units undergo changes and, at the same time, both random and ordered structures are formed.

Vibronic effects are associated with mixing of the boundary orbitals of the HOMO (upper occupied molecular orbital) and LUMO (lower free molecular orbital) under the action of vibrations of atoms of the molecular system. If it is limited only to the Pz-Pz interaction of atomic orbitals between the trimer links, then the HOMO and LUMO have g - even and u - odd symmetry with respect to the LHA inversion center of the macromolecule. Consequently, the condition for the vibronic instability of the trimer is expressed by the following relation: $\frac{k\Delta}{2a^2} > 1$, where a is the vibronic constant, k is the force constant, is the energy gap between the one-electron energy levels corresponding to the boundary orbitals of HOMO and LUMO. Narrowing of the energy gap of the macromolecule leads to the vibronic instability of the LHA along a certain coordinate of its displacement, i.e. the reaction coordinates are the directions of the vibronic labilization of the adiabatic potential of the LGA. The energy gap between the energy levels of the HOMO and LUMO is determined by the formula $\Delta = \varepsilon_{k+1} - \varepsilon_k$; If the number n is even, then the energy levels of the LUMO and HOMO (the HOMO has a serial number k = n / 2) are calculated using the corresponding formulas.

As the obtained analytical expressions show, the energy gap narrows with an increase in n - the number of monomeric units of the macromolecule. Since L = na, where L is the chain length and a is the size of the monomer unit, the problem arises of revealing size effects in the formation of an ionic configuration under conditions of vibronic instability.

To study the process of ordering the arrangement of two types of units, the following features of the influence of low-symmetry perturbations on the rate of modification of each unit of the macromolecule were considered:

1. The modification process is inhibited under the action of a low-symmetry perturbation due to the static instability (Jahn-Teller effect) of the LGA.

2. The deacetylation reaction is accelerated due to vibronic instability leading to dynamic instability (pseudo Jahn-Teller effect) of the LHA macromolecule.

With an increase w_u, there is a decrease in the deacetylation reaction, which means that the process of modification of a link of a macromolecule can be realized only in the presence of a trimer inversion center. In the absence of an inversion center, the trim modification process does not occur.

It should be noted that, on the basis of synergetic modeling, the conditions for the formation of spatially periodic atherosclerotic structures in arterial vessels and the stability of isomers of tetrameric structures on the surface of nanoparticles were determined. All this shows the breadth of coverage of this method and its effectiveness in studying the features of modification of biological objects, especially those macromolecular structures that have a high molecular weight (DNA and viruses), including the coronavirus COVID-19.

Thus, in macromolecular structures with a linear chain, the vibronic instability of LHA inhibits and activates the processes of chemical modification of the composition, depending on the length and mutual arrangement of the units of the macromolecule. Low-symmetry perturbations in combination with vibronic instabilities determine the relative position of two types of units along the macromolecule.