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Investigation Aminosaccharides and Their Derivatives Properties by Molecular Modeling Method. A.M. Levkovich, S.Sh. Rashidova, N.L. Voropaeva, I.N. Ruban, Inst. of Polymer Chemistry and Physics, Uzbekistan Ac.Sci., Tashkent, Rep. Uzbekistan.

In the field of macromolecular structures growing attention is devoted to computer modeling because it allows to save time and decrease expenditures on carrying of complex experiments. In system approach monomer-oligomer-polymer many specific properties of polysaccharides can be modeled, namely: stereochemical, investigations of polymer chains packing, estimation of molecular volumes in various conformational state, energetical and thermodynamical investigations, dynamics at various temperatures.

Understanding of possible spatial structures of crystalline polysaccharide systems, such as chitin, chitosan and cellulose has a great role. The investigation of surface relief for the surface of steric strain potential energy under a rotation around the bonds between two chains were fulfilled. Calculations were realized by two ways: method of regular lattice and that of Monte Carlo. The detailed investigation of such potential surfaces for dimeric systems (1-4)- β -D-glucose, (1-4)- β -D-aminoglucose, (1-4)- β -D-aminoacetylglucose was completed. Later this investigation was repeated with the oligomeric systems. The structure of chitin appears the most strong against structure of cellulose.

A comparative investigation of potential surface and influence of substituents in second position on these surface relief formations was carried out; oligomers systems up to 10 chains being modeled. The peculiarities of regular spiral structures, their energetic, charge and some specific stereochemical characteristics were investigated. In particular, the dependence of energy on spiral periodicity and its regularity were determined. Correlation between structure and crystallinity was found. The investigations were carried out by molecular mechanic methods. To control an interaction by hydrogen bonds AMBER was chosen to taking into account an electrostatic interaction on atoms. Charges at atoms were carried out in semi-empirical method PM3 without geometry optimization.