Thematic Section: Physicochemical Research. **Full Paper**
Subsection: Physical Chemistry. *Reference Object Identifier* – ROI: jbc-02/18-56-12-17
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings
Submitted on November 15, 2018.

The nature of the supramolecular rearrangements of native cellulose in the process of enzymatic hydrolysis

© **Yury B. Grunin**,[1]*+ **Maria S. Ivanova**,[1] and **Tatiana Y. Grunina**[2]
[1] *Department of Physics. Volga State University of Technology. Lenin Square, 3. Yoshkar-Ola, 424000. Mari El Republic. Russia. Phone: +7 (8362) 68-68-04. E-mail: GruninYB@volgatech.net*
[2] *Department of Biophysics. Lomonosov Moscow State University. Leninskie Gory, 3, bld.12. Moscow, 119991. Russia. Phone: +7 (495) 939-27-76. E-mail: info@mail.bio.msu.ru*

*Supervising author; +Corresponding author

Keywords: cellulose, NMR-relaxation, enzymatic hydrolysis, supramolecular structure.

Abstract

Based on the theories of NMR relaxation in multiphase systems and adsorption phenomena, methods is developed for determining the degree of crystallinity, specific surface area, and the average transverse size of native cellulose crystallites. In particular, using the Bloembergen-Purcell-Pound theory and the condition of fast exchange, a relation is obtained for determining the monomolecular adsorbed layer. A correlation is established between the capacity of the monolayer and the degree of crystallinity of the sample under study. This took into account the fact that the content of water molecules in the monolayer is equivalent to the number of glucopyranose rings in the surface chains of the cellulose, which made it possible to associate the capacity of the monolayer with the degree of crystallinity of the sample. Within the framework of modern ideas about the layered organization of elementary cellulose fibrils and about their entry into the structure of microfibrils, a technique is developed for estimating the average transverse dimensions of cellulose crystallites using an experimentally determined degree of crystallinity. It is established that sequential chemical treatment of the native starting cellulose with alcohol, ether and alcohol, ether and urea leads to a significant decrease in the degree of crystallinity, an increase in the specific surface. It is assumed that this effect should be associated with the weakening of intra-, intermolecular hydrogen bonds of cellulose under the action of these reagents. It is shown that preliminary chemical treatment of cellulose samples significantly affects the efficiency of its enzymatic degradation. Obviously, during the interaction with cellulose, the enzymatic complex switches its intra- and intermolecular hydrogen bonds of the -O-H..O type and neutralizes the interlayer hydrogen bonds of the -C-H..O type. It is confirmed that the main component of the cellulase complex, *endo*-1,4-β-glucanase, produces the greatest changes in the structure of cellulose.

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