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Study of supramolecular reorganizations of native cellulose at different stages of moistening

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Abstract

Based on the modernized scheme of the structural organization of microfibrils of native cellulose, the possibility of determining its degree of crystallinity, the transverse dimensions of crystallites, as well as the content of elementary fibrils in microfibrils using ^{1}H NMR and sorption measurements is shown. The mechanism of defibrillating cellulose at different stages of its wetting is established, which is associated with the appearance of a wedging pressure on the part of the condensed liquid in the micropores, which leads to changes in its supramolecular structure. In this case, the rate of spin-lattice relaxation of the "cellulose-water" system is sharply increased at low moisture contents, which is explained by the formation of new active centers at the interface of the forming section with water molecules adsorbed on them, which accelerate the energy exchange of the proton spin system with a "lattice". This process is accompanied by a decrease in the degree of crystallinity of the sample at all stages of cellulose moistening. The nature of the decrease in the transverse dimensions of crystallites in the framework of the proposed model of the layered structure of cellulose is established. The possibility of determining the content of elementary fibrils in a microfibril based on data on the degree of crystallinity of cellulose is shown. The process of penetration of adsorbed water molecules into the space between the elementary fibrils in the microfibril structure of cellulose is considered. A scheme is proposed for the formation of monolayer adsorption of water on the active surface of cellulose, which takes into account the dipole-dipole interaction in the "adsorbent – adsorbate" system, which turns into the formation of a hydrogen bond. A hypothesis is expressed about the formation of a V-structure of adsorbed water, when this molecule interacts with an active center to form an acceptor hydrogen bond with a hydroxyl group at the sixth carbon atom. In the adjacent glucopyranose ring of the surface cellulose chain, the adsorbate molecule forms two donor hydrogen bonds with the oxygen atoms of the hydroxyl groups at the second and third positions of the carbon atoms.

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