

## Analysis of water state adsorbed by cellulose fibers

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### Abstract

Modernized model of microfibril cellulose layered structure is proposed. This model considers presence of slit-shaped micropores in space between elementary fibrils and cellulose microfibrils. It is discussed the nature of donor-acceptor hydrogen bonds formation: intra-, intermolecular, and interlayer bonds inherent in each glucopyranous cellulose link. It's described the mechanism of water molecules specific adsorption interactions in a monolayer with active centers located on the hydrophilic surfaces of elementary fibrils. Dipole-dipole energy transition into energy of hydrogen bond is discussed during adsorption process between active centers of cellulose and water adsorptive molecules. Analysis of water molecules dipole-dipole interactions with surface hydroxyl groups of cellulose showed that at distance of 2.5-3 Å energy of this interaction transforms into energy of hydrogen bond. It is discussed the formation mechanism of water molecules donor-acceptor bonds with cellulose surface hydroxyl groups. Thermodynamic parameters characterizing adsorbate state the in these layers are determined by proton magnetic relaxation and sorption measurements. It's established the possibility of determining adsorption net heat in bilayer considering Arrhenius nature of adsorbate thermal molecular motions correlation times. Increase in entropy of adsorbed water during adsorption process is revealed basis on Vant Hoff equation and certain adsorption equilibrium constant. The calculation established that distance between nearest active centers of cellulose is 6.5 Å. This leads to disunity of adsorbed water molecules and allows application of Langmuir and BET adsorption theory. Analysis of spin-lattice relaxation times dependence on cellulose moisture content made it possible to establish the cause of its crystallite wedging from adsorbed water molecules at adsorption initial stages. Decline of the spin-lattice relaxation unambiguously indicates the process of cellulose dispersion into its structural elements. It was established that during adsorption a part of the internal regions of crystallites passes to their surface with participation of cellulose hydroxyl groups. During desorption reverse process is observed.

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