INVESTIGATION OF MOLECULAR MOTION IN AMYLOSE, LICHENIN, AND CELLULOSE BY THE METHOD OF NUCLEAR MAGNETIC RESONANCE

Table 1

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Abstract

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INVESTIGATION OF MOLECULAR MOTION IN AMYLOSE, LICHENIN, AND CELLULOSE BY THE METHOD OF NUCLEAR MAGNETIC RESONANCE

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The physical and chemical properties of high-molecular compounds depend on the degree of regularity of the polymer and on molecular motion (^{1}). We have applied the method of nuclear magnetic resonance to the investigation of molecular motion. Amylose, lichenin, and cellulose, which have different degrees of regularity, were chosen as the objects of study. Investigation of these polysaccharides is of great practical and theoretical interest, since they are widely used in industry and, moreover, are important biopolymers playing various roles in nature. The investigations were carried out on samples dried in vacuum at temperatures from room temperature to −100°. The spectra of H nuclei were recorded at a frequency of 21 MHz on a previously described spectrometer with a permanent magnet. In the temperature range from 25 to −100°, we observed only a very slight increase in the line width and in the second moment as the temperature was lowered. Since theoretical calculation of the second moment is impossible because of the lack of experimental data on interatomic distances, we recorded the spectra of cellobiose and maltose, the polymers of which may be regarded as cellulose and amylose. The data obtained are given in Table 1 for 25°.

Table 1

	Maltose	Cellobiose	Amylose	Lichenin	Cellulose
ΔH, G	10.9	10.9	8.1	9.4	9.7
ΔH^2, G^2	10.8	10.7	7.3	9.0	8.8

The regularity observed in Table 1 in the change of ΔH and ΔH^2 can be explained by an increase in the angles of internal rotation of the pyranose rings about the C–O bonds in amylose, lichenin, and cellulose in comparison with maltose and cellobiose. An approximate calculation of the decrease in ΔH^2 on the basis of the assumption of an increase in the angles of internal rotation, according to data obtained by Burkhard and Husemann (^{2}), shows that ΔH^2 for cellulose is greater by 0.5 G^2 than for amylose when the angles are decreased by 1-5°. In addition, it was found (^{2}) that the radius of inertia of cellulose is 50% greater than that of amylose, which also should lead to a decrease in molecular motion and an increase in ΔH^2. Burkhard (^{3}) showed that the radius of inertia depends on the chain configuration of amylose and cellulose. Thus, our data can be explained by assuming that, in the samples studied, amylose is in the 3B configuration and cellulose in C1. To explain the observed regularities in the rates of the chemical reactions of amylose, cellulose, and lichenin (^{4}), and also to explain the more intense molecular motion in amylose, it should apparently be assumed that the poten-

the potential barrier of hindered motion in amylose is lower by 500 cal/mole than in lichenin and cellulose, which have close values of the barriers and similar chemical properties. From this point of view, the different biological role of cellulose, lichenin, and amylose, due to the different configuration of the chains, also becomes understandable. The observed correlation of the mean square radius of inertia and the angles of internal rotation with the second moment of the line width should also be observed in other polymers and probably has a simple dependence.

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