ANALYSIS OF THE STRUCTURE OF CARBOHYDRATES WITH USE OF THE REGULARIZED DECONVOLUTION METHOD OF VIBRATIONAL SPECTRA

N.A. Nikonenko, D.K. Buslov, N.I. Sushko, R.G. Zhbarkov

B.I. Stepanov Institute of Physics, Academy of Sciences of Belarus, Skaryna Ave. 68, 220072, Minsk, Belarus; e-mail: nataly@dragon.bas-net.by

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In analyzing the composition and structure of complex chemical compounds vibrational (IR and Raman) spectroscopy have been successfully used. However, analytical potentialities of the method of vibrational spectroscopy are restrained, to a great extent, by the low resolution of bands in the spectra of complex substances. The effective way for solving this problem is the use of corresponding methods for mathematical treatment of vibrational spectra.

The infrared spectra of polysaccharides (amylose and cellulose) as well as of their constituent monosaccharides (α- and β- D-glucose) and the results of their deconvolution are presented. The number of bands separated upon deconvolution in the 1200-920 cm⁻¹ spectral ranges exceeds the number of visualized absorption maxima in the room temperature spectra by a factor of more than two. It is shown that the results of deconvolution of the IR spectra of monosaccharides are in good agreement with the data of normal coordinate analysis of these compounds in the crystalline state. The manifestation in IR spectra of the investigated monosaccharides of factor group splitting of a number of nondegenerate fundamental vibrational modes of molecules in the crystalline state has been found. It has been shown that the glycosidic linkage formation in polysaccharides with 1→4 glycosidic linkage is characterized by the appearance of new absorption bands in the 1175-1140 cm⁻¹ spectral range, as compared to the infrared spectra of their constituent monomers. In the 1000-970 cm⁻¹ range, in the deconvolved IR spectrum of cellulose, absorption bands, which are not observed in the monomer spectrum, are separated. The number of bands in the above region remains unchanged for amylose, as compared to the spectrum of monomer α-D-glucose.

The results obtained can be used in investigating of the vibrational spectra of carbohydrates with the aim of solving various practically important problems of molecular spectral analysis.

CHEMOMETRIC METHODS IN ANALYSIS WITH MULTICHANNEL DETECTOR SPECTROMETRY

Yu.P. Turov

Institute of Petroleum Chemistry, Russian Academy of Sciences, 3, Akademichesky Ave., 634021, Tomsk, Russia, e-mail: tur@ipc.tsc.ru

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Chemometrics is the discipline concerned with the application of statistical and mathematical methods, as well as those methods based on mathematical logic, to chemistry.