Diploma thesis abstract Shpachenko I.G.

"Estimation of the rates of chemical reactions using vibrational spectroscopy data"

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The rate of chemical reaction, i.e. the rate of change of one of the reactants in the reaction mixture, is an essential characteristic of a chemical process, which depends on many variables, most important of which are the temperature and acidity. The purpose of this work is the experimental substantiation of the possibility of using vibrational spectroscopy, such as Raman spectroscopy and Fourier transform infrared spectroscopy by attenuated total reflection (ATR-FTIR), to measure the rates of chemical reactions and measuring the velocity characteristics of a well-studied chemical reaction.

Currently there are highly sensitive and specific methods for measuring the speed characteristics of chemical reactions, that in some cases making them indispensable. In addition, each method is effective, as a rule, when measuring the concentration of a particular product or reactant. Today does not exist universal method to determine the speed of a chemical reaction for any reactants or products.

The applicability of Raman spectroscopy is shown on example of the alkaline hydrolysis of ethyl acetate (EtOAc) in the presence of potassium hydroxide (KOH). The reaction rate is obtained by approximating the time dependence of the intensity of the selected line of the product or reagent in Raman spectrum by function, which is a solution of the corresponding kinetic equations. Control of the temperature allowed show the accuracy of the developed method by measuring the rate constants at temperatures in the range 15-45 °C. It was also demonstrated the possibility of using the developed technique for measuring the kinetic characteristics of the hydrolytic reaction with enzyme α-chymotrypsin for substrate 2,4-dinitrophenyl acetate (DNPA). Protein concentration and the initial concentration DNPA was 0.2 and 2 mM, respectively. Measurements were carried out at temperatures in the range 13-15 °C.

Using the method of ATR-FTIR measured velocity characteristics of alkaline hydrolysis of ethyl acetate in the presence of KOH at room temperature. Obtained values of the rate constants not coincide with the values obtained for reaction occurring in the volume, because the ATR-FTIR is a method of investigation of the surface layers of sample. Carried out the hydrolytic reaction for ethyl acetate involving α-chymotrypsin. It is shown that the analysis of the rate constants for this process in the selected configuration is not possible. It was found that the ATR-FTIR spectra of some pure substances and mixtures are changing over time. It shows that selected substances interact with the surface of the ATR-crystal (diamond). Physics of interaction with the surface of the diamond to be examined separately.