Investigation of Relaxation Processes and Phase Transitions in the Silica Gel-Undecylenic Acid System Using IR Spectra in a Wide Temperature Range

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1. Introduction

The study of relaxation processes in porous inhomogeneous systems by the method of dielectric and mechanical spectroscopy is associated with methodological difficulties. In addition, in these studies, it is necessary to take into account the properties of the matrix, which is not always possible. To understand how IR spectroscopy could be used in temperature dependence investigations, analyzed data are compared with previously measured data obtained with dielectric spectroscopy. The samples are bulk undecylenic acid and porous silica gel matrixes of three different sizes which are filled with undecylenic acid. The surface of porous samples are modified with SiO_2-OH (b) groups. The aim of this work is to study phase transitions and relaxation processes in the silica gel-undecylenic acid systems.

2. Method

To investigate physical properties of studied systems the method of IR spectroscopy is proposed to be used. It is shown that this method allows to obtain such characteristics as the values of the Davydov splitting $\Delta\nu_{1,2}$ of $\rho(CH_2)$ band in the temperature range of -160 °C to 40 °C and temperature dependence of the carboxyl O–H bending band ρ-OH at 950 cm^{-1} . Measures was performed with Nicolet Nexus 470 IR spectrometer in a temperature range of -160 °C to 40 °C .

3. Results

Output data were calculated with Origin and Peakfit Software and are shown on Fig. 3-4. The values of the $\Delta\nu_{1,2}$ were calculated by fitting of the 720 cm^{-1} peak profiles with two Voigt curves, as well as the values of O–H bending band peaks wavenumbers ν(ρOH) were obtained via fitting with one Voigt curve. Figures 3 and 4 show us that the lower pore's size the lower temperature of relaxation process. These conclusions are consistent with the data in Fig. 5.

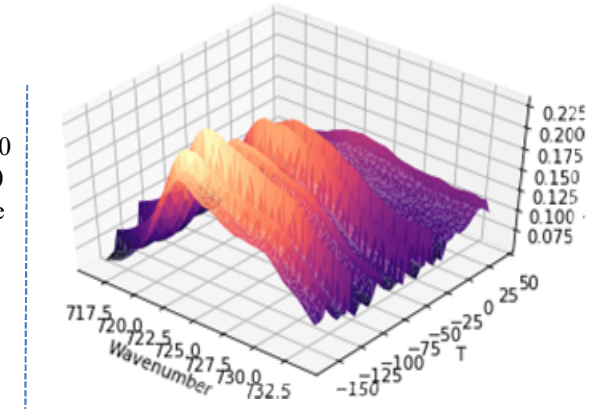

Fig. 2 Raw data which illustrate the Davydov splitting : wavenumber and temperature dependence of IR waves absorption.

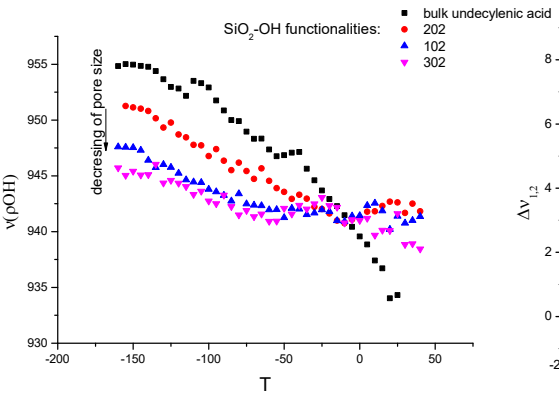

Fig. 3. Temperature dependencies of the of the ν(ρOH) of the samples .

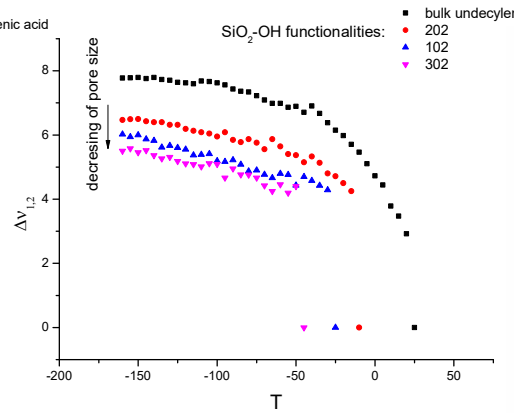

Fig. 4. Temperature dependencies of the of the $\Delta\nu_{1,2}$ of the samples .

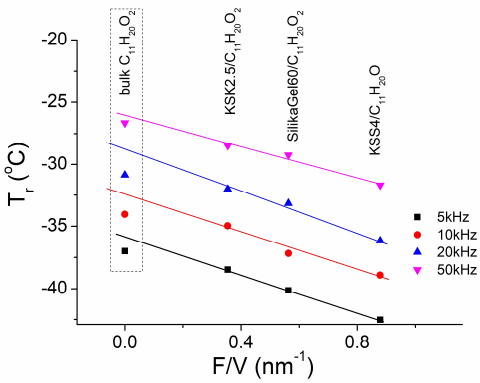

Fig. 5. The temperature of the relaxation process maximum dependence on the inverse effective size of pores recorded at different frequencies.

4. Conclusions

In this work, the systems of silica gel-undecylenic acid with different pore sizes is investigated with IR spectroscopy. The use of molecular spectroscopy methods, in particular in the IR region, in a wide temperature range, is shown to be able to provide additional information according to temperature dependence of the values of the Davydov splitting $\Delta\nu_{1,2}$ of $\rho(CH_2)$ band and the temperature dependence of the carboxyl O–H bending band ρ-OH at 950 cm^{-1}. These parameters can be new descriptors of samples relaxation processes and mechanisms therein.

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