HYDROGEN BONDING AND MOLECULAR STRUCTURE OF SINGLE ALCOHOLS, VIBRATION RELAXATION IN SINGLE ALCOHOLS

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We present the latest results of our investigations of determining of the structure peculiarities of such partially ordered substances as liquid monohydric alcohols. We have studied physical parameters of the clusters, which form the structure of liquid methanol and ethanol, the character of vibrational relaxation in these alcohols.

Quantum-chemical calculations of the associates forming the structure of liquid methanol and ethanol were performed. Their optimal space geometry, forming energy and electrical parameters were calculated. It was determined, that the structure of liquid methanol is formed mainly by cyclic trimers and tetramers. For the liquid methanol our results correspond to the infrared spectra, obtained using the technique of matrix isolation of three molecular methanol clusters in supercooled helium droplets. The changes in the molecular geometry of methanol and ethanol, which occur at the molecular association, were also studied.

The Raman profiles in methanol and ethanol were investigated in the temperature region of the condensed phase existance (160 - 340 K). The dynamical stability of liquid monohydric alcohols structure in the investigated temperature region was registered.

The correlation analysis of the Raman spectra of methyl alcohol was performed. The time of vibrational relaxation was calculated. The broadening of the vibrational bands in the spectra of alcohols can be explained by the process of hydrogen bond dissociation.