THE PECULIARITIES OF SOME LIQUID ALCOHOLS STRUCTURE

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The results of spectroscopic investigations and structure simulation of liquid methanol, ethanol, propanol, isopropanol and buthanol (the first members of the monohydric alcohols homologous series) are presented. The Raman spectra of the listed alcohols were registered and interpreted at room temperature. In the cases of methanol and ethanol in order to more precise specification of the vibrational bands the polarized measurements of their intensities were made. The results of liquid phase cluster nanostructure simulation for studied objects are discussed. The model quantum-chemical calculations were carried out using DFT method with B3LYP potential. The calculations were performed by using the program package GAUSSIAN 03. The hydrogen bond dissociation energies were determined, the geometry of molecular clusters was optimized, the geometrical parameters of these clusters are discussed. The results of the simulation (in the case of methanol)[a] are in good agreement with the results of the investigations presented in the work[b]. For the interpretation of the spectroscopic and model investigations results the vibrational spectra of methanol aggregations in helium droplets were used [c].

[a] Pogorelov V., Bulavin L., Doroshenko I., Fesjun O., Veretennikov O., J. Molec.Struct., 708, 61 (2004).
[b] S. L. Boyd, Russell J. Boyd, J. Chem. Theory Comput., 3, 5461 (2007)
[c] Huisken F., Slemmer M., J.Chem.Phys., 98, 7680 (1993)