Clustering processes in hydrogen-bonded liquids by matrix-isolation FTIR spectroscopy

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Clusters, by definition, are aggregates of atoms/molecules with more or less regular and arbitrarily scalable repetition of basic building blocks. Their size is intermediate between that of atoms/molecules and the bulk. The growing interest to the clustering phenomena that produce partially ordered atomic or molecular structures is due to the recent developments and challenges in nanotechnologies, smart materials, heterogeneous systems, basic biochemical research, etc.

The processes of molecular cluster formation in hydrogen-bonded liquids were investigated using FTIR spectroscopy and a matrix isolation technique [1-3]. The methods of cluster isolation in low-temperature matrices provide the possibility to study individual clusters of different sizes. FTIR spectra of water and monohydric alcohols (from methanol to decanol) in argon and nitrogen matrices were registered in the frequency range from 500 cm^{-1} to 4000 cm^{-1}. The gradual transformation of the spectral bands assigned to different vibrations was observed with matrix heating from 10 to 50 K, indicating a transformation of the structure of the isolated clusters. Main changes with the temperature increasing were observed in the spectral regions of stretch O-H and C-O vibrations.

Spectral data were processed with modern methods of data analysis – principal component analysis and 2D correlation spectroscopy. Experimental spectra were compared with results of quantum-chemical simulations.

The observed temperature dependence of the registered spectra may be considered as a model of structural transformations in the studied objects during the phase transition from gas to liquid state.

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References

[1] V. Pogorelov, I. Doroshenko, P. Uvdal, V. Balevicius, V. Sablinskas, Mol. Phys., 108, 2165-2170 (2010).

[2] P. Golub, V. Pogorelov, I. Doroshenko, J. Mol. Liq., 169, 80-86 (2012).

[3] P. Golub, I. Doroshenko, V. Pogorelov, Phys. Lett. A, 378, 1937-1944 (2014).

[4] V. Pogorelov, Ye. Chernolevska, Ye. Vaskivskyi, L.G.M. Pettersson, I. Doroshenko, V. Sablinskas, V. Balevicius, Ju. Ceponkus, K. Kovaleva, A. Malevich, G. Pitsevich, Journal of Molecular Liquids, 216, pp. 53-58 (2016).