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Research Direction:

Study of the mechanisms of molecular cluster formation and their properties using vibrational spectra. Determination and analysis of spectroscopic parameters of nanosized molecular clusters in biological objects and development of recommendations for practical use of these objects.

The main results of scientific research:

In substances consisting of highly polar molecules in liquid and crystalline states, the mechanisms of formation of clusters up to 10 molecules in number have been established, a complex system of molecular cluster formation processes has been established; the role of intramolecular and intermolecular hydrogen bonds in the formation of cluster structures of highly polar substances in liquid and isolated states, as well as geometric and electro-optical parameters of clusters have been established; a new spectroscopic interpretation of the bands associated with the O-H vibrations has been presented; a new spectroscopic interpretation of the bands associated with the O-H vibrations has been presented; the role of intramolecular and intermolecular hydrogen bonds in the formation of cluster structures of highly polar substances in liquid and isolated states, as well as geometric and electro-optical parameters of clusters.

Main scientific publications:

1. F.H. Tukhvatullin, V.Ye.Pogorelov, A. Jumabaev, H.A. Hushvaktov, A.A. Absanov, A.Usarov. Polarized components of Raman spectra of O-H vibrations in liquid water // Journal of Molecular liquids, 2011, 160, P.88-93.
2. Kh.A.Khushvaktov, A.Jumabaev, V.E.Pogorelov, U.N.Tashkenbaev, A.A.Absanov, G.Sharifov, B.Amrullaeva. Intermolecular hydrogen bond in acetic acid solutions. Raman spectra and ab initio calculations // American Journal of Physics and Applications. Received: December 7, 2018; Accepted: December 20, 2018; Published: January 15, 2019. V.6, No.6. PP.169-174. (IF=5,0).
3. H.Hushvaktov, F.H.Tukhvatullin, A.Jumabaev, U.N.Tashkenbaev, A.Absanov, B.Hudoyberdiev. Raman spectra and ab initio calculation of a structure of aqueous solutions of methanol // Journal of Molecular Structure, 1131 (2017) P. 25-29.
4. Jumabaev, A., Holikulov, U., Hushvaktov, H., Issaoui, N., Absanov, A. (2023). Intermolecular interactions in ethanol solution of OABA: Raman, FTIR, DFT, M062X, MEP, NBO, FMO, AIM, NCI, RDG analysis. Journal of Molecular Liquids, 377, 121552. https://doi.org/10.1016/j.molliq. 2023.121552
5. A.Jumabaev, H.Hushvaktov, I.Doroshenko, A.Absanov. Raman spectra and non-empirical

(ab initio) calculations of the structure of dimethylformamide molecular clusters // Journal of Vibrational Spectroscopy. 2021. Vol.117, P.103315 (8)
6. A.Jumabaev, H.Hushvaktov, I.Doroshenko, A.Absanov. Role of intermolecular interactions in formation of molecular clusters in liquid nitromethane and its solutions // Molecular Crystals and Liquid Crystals, 2022. pp. 1-9.
7. Hushvaktov H., Khudaykulov B., Jumabaev A., Doroshenko I., Absanov A., Murodov G. Study of formamide molecular clusters by Raman spectroscopy and quantum-chemical calculations // Molecular Crystals and Liquid Crystals. 2022. pp. 1-8. https://doi.org/10.1080/15421406.2022.2068478/
8. Pu, D., Zhou, S., Guan, H., Jia, P., Chen, G., Fang, H., Ke, W. (2024). Enhancing Efficiency and Intrinsic Stability of Large-Area Blade-Coated Wide-Bandgap Perovskite Solar Cells Through Strain Release. Advanced Functional Materials, 2314349.