

**XX Symposium
on High Resolution
Molecular Spectroscopy
HighRus-2023**

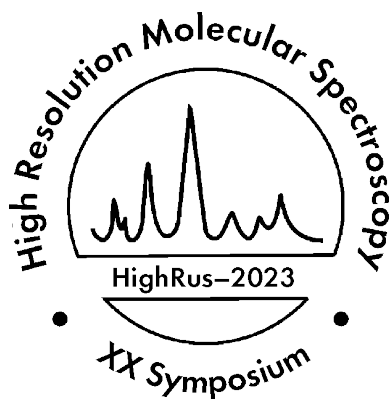
Lake Baikal, Russia
July 3–7, 2023

Abstracts of Reports



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**Institute of Quantum Physics,
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Parallel Oral Session I
Tuesday, July 4, 17³⁰ – 19⁰⁰
Chair: Petr M. Tolstoy

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**Calculation of structures, energetics and infrared absorption spectra
of hydrogen-bonded dimers and trimers formed by formaldehyde with hydrogen fluoride**

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Hydrogen-bonded complexes formed by H₂CO and HF may serve as model complexes of wide classes of carbonyl-containing and hydrogen halide molecules. Equilibrium nuclear configurations of (H₂CO)₂ and H₂CO⋯HF dimers and two stable H₂CO⋯(HF)₂ and four stable (H₂CO)₂⋯HF trimers were determined using the MP2/aug-cc-pVTZ *ab initio* method. The binding energies of complexes, the cooperativity of H-bonding effects in complexes of different composition and the structural changes upon formation of dimers and trimers were examined. Anharmonic values of frequencies and intensities for infrared absorption bands were computed using the second-order perturbation theory and variational approaches. The calculated spectral parameters relating to the H–F, C = O, and C–H stretches and the in-plane HF librations of H₂CO⋯HF were used to identify the spectrum of this heterodimer recorded in the matrix-isolation experiment in liquid N₂ at $T = 8$ K [1]. The changes in the spectral parameters of absorption bands upon formation of dimers and trimers were derived from comparison of the data obtained in the same approximation for the complexes and monomers [2]. For each complex, sufficiently strong and characteristic bands, including the H–F stretching band, were determined, which can be used for spectroscopic detection of these systems. It was found that three predicted trimers have sufficiently large binding energies and their H–F stretching bands are significantly shifted from strong bands of monomers and dimers, which can facilitate their experimental observation. The blue shifts of C–H stretching bands upon complexation were analyzed and explained. To study the isotope effects in the spectra of the considered complexes upon H/D substitution, the frequencies and intensities of absorption bands of (D₂CO)₂ and D₂CO⋯DF dimers and D₂CO⋯(DF)₂ and (D₂CO)₂⋯DF trimers were calculated in the same approximation [3].

References:

1. R.E. Asfin, V.P. Bulychev, M.V. Buturlimova, K.G. Tokhadze. *J. Mol. Struct.* **1225**, 129080 (2021). DOI: 10.1016/j.molstruc.2020.129080.
2. R.E. Asfin, V.P. Bulychev, M.V. Buturlimova, K.G. Tokhadze. *Comp. Theor. Chem.* **1217**, 113876 (2022). DOI: 10.1016/j.comptc.2022.113876.
3. V. P. Bulychev, M. V. Buturlimova, and K. G. Tokhadze. *Opt. Spectrosc.* **131** (4), (2023).