V.E. Zuev Institute of Atmospheric Optics

Institute of Quantum Physics

High Resolution Molecular Spectroscopy

HighRus–2023

XX Symposium

XX Symposium on High Resolution Molecular Spectroscopy HighRus-2023

Lake Baikal, Russia
July 3–7, 2023

Abstracts of Reports

V.E. Zuev Institute of Atmospheric Optics
Siberian Branch, Russian Academy of Science

Institute of Quantum Physics,
Irkutsk National Research Technical University

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Tomsk

2023

УДК 535+539

XX Symposium on High Resolution Molecular Spectroscopy HighRus-2023: Abstracts of Reports. — Томск : Издательство ИОА СО РАН, 2023. — 160 стр. — 1,4 МБ. — 1 электрон. опт. диск (CD-ROM). — Систем. требования: PC Pentium 1 или выше; Acrobat Reader 4.0 или выше. Загл. с экрана.

Сборник включает в себя программу и аннотации докладов, представленных на XX Симпозиуме по молекулярной спектоскопии высокого разрешения HighRus-2023 (Байкал, 3–7 июля 2023 г.).

Ответственный за выпуск – *Е.Н. Старикова*

Дизайн обложки *К.И. Власовой*

Электронное издание. PC Pentium 1 или выше; CD-ROM 16-х или выше; мышка; Acrobat Reader 4.0 или выше

Подписано к использованию 22.06.2023 г. 1,4 МБ. 1 CD-ROM. 110 экз.
Издательство ИОА СО РАН, 634055, г. Томск, пл. Академика Зуева, 1.
Тел. 8-3822-492384

ISBN 978–5-94458–195-2

Parallel Oral Session I
Tuesday, July 4, 17^{30} – 19^{00}
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 H_2CO and HF may serve as model complexes of wide classes of carbonyl-containing and hydrogen halide molecules. Equilibrium nuclear configurations of $(H_2CO)_2$ and $H_2CO\cdots HF$ dimers and two stable $H_2CO\cdots(HF)_2$ and four stable $(H_2CO)_2\cdots HF$ 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 $H_2CO\cdots HF$ were used to identify the spectrum of this heterodimer recorded in the matrix-isolation experiment in liquid N_2 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 $(D_2CO)_2$ and $D_2CO\cdots DF$ dimers and $D_2CO\cdots(DF)_2$ and $(D_2CO)_2\cdots DF$ trimers were calculated in the same approximation [3].

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