Frontier Chemistry Center
フロンティア化学教育研究センター

講演会

演 題：**Vibrational Spectroscopy of Hydrogen-Bonded Complexes, Liquids and Solids**

講 師：**Prof. Marek J. Wójcik**

Faculty of Chemistry,
Jagiellonian University, Poland

日 時：2017 年 5 月 24 日（水）15:00~16:00

場 所：理学部 7 号館 2 階　7-2-19・20 室

要旨：

Theoretical model is presented for the X-H(D) stretching vibrations in hydrogen-bonded systems. The model takes into account an adiabatic coupling between the high-frequency X-H(D) stretching and the low-frequency intermolecular X...Y stretching modes, linear and quadratic distortions of the potential energy for the low-frequency vibrations in the excited state of the X-H(D) stretching vibration, resonance interactions between hydrogen bonds, Fermi resonance between the X-H(D) stretching and the overtone of the X-H(D) bending vibrations, and mechanical and electrical anharmonicities. The effects of deuteration and temperature on spectra are successfully reproduced by the model. Comparison between experimental and theoretical spectra is presented for different hydrogen-bonded systems, including ices. We present also the method of Car-Parrinello molecular dynamics used to calculate infrared spectra of crystals.

Proton tunneling in tropolone is described by two-dimensional model potentials. The potentials have been fitted to quantum-mechanically calculated two-dimensional grid of energies, and used to analyze proton dynamics. The model PES well reproduces experimentally observed promotion of the tunneling by the excitation of the planar modes and suppression by the excitation of the out-of-plane modes.

本講演は、大学院総合化学院『化学研究先端講義（修士課程選択科目）／総合化学特別研究第二（博士後期課程選択科目）』の一部として認定されています。

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