第378回触媒科学研究所コロキウム

Vibrational Spectroscopy of Hydrogen-Bonded Complexes, Liquids and Solids

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創成科学研究棟4階セミナー室A

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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-mechanicaly 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.

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"Research profile" Physical and theoretical chemistry; Molecular spectroscopy; Hydrogen-bonded systems
[Degrees in chemistry]: MSc with honours 1968, PhD 1973, habilitation 1980, all at the Jagiellonian University, Professor of Chemistry 1996. [Appointments]: Jagiellonian University (since 1968), Head of Laboratory of Molecular Spectroscopy (since 1981), Professor extraordinary (1996-2003), Professor ordinary (since 2003). [Foreign experience]: Research Associate, NRC Canada (1977-78), JSPS Research Fellow, University of Tokyo (1982-83), [Visiting Professor]: University of Uppsala (1981,1982,1988-89), University of Chicago (1984-86), Cambridge University (1990,1997), University of Munich (1990-1991), Oklahoma State University (1991-92), University of Illinois, Chicago (1992), NRC Canada (1993,1994), Kyushu University (1995,2011), University of Natal, South Africa (1996), IMS Okazaki (1997-98), University of Bordeaux (1999), KEK Tsukuba (2000,2001,2002), Tohoku University (2003), Purdue University (2004), University of Perpignan (2004), Emory University (2006), Kwansei Gakuin University (2007, 2013), Technical University of Munich (2007, 2008,2009,2010,2013), University of Malaya, Kuala Lumpur (2012).[Research areas]: (i) theoretical studies of hydrogen-bonded systems, water, aqueous ionic solutions and ices, (ii) quantum-mechanical calculations, (iii) theoretical studies of multidimensional proton tunneling, (iv) Car-Parrinello simulations.[Research staff]: Marek Boczar, PhD, DSc, Łukasz Boda, PhD.[More information]: www.chemia.uj.edu.pl/~wojcik
"Selected publications"[1]. Witkowski, A., Wójcik M., Infrared spectra of hydrogen bond. A general theoretical model, Chem. Phys. 1, 9-16, 1973.[2]. Wójcik, M.J., Theory of the infrared spectra of the hydrogen bond in molecular crystals, Int. J. Quant. Chem. 10, 747-760, 1976.[3]. Wójcik M.J., Buch V., Devlin, J.P., Spectra of isotopic ice mixtures, J. Chem. Phys., 99, 2332-2344, 1993. [4]. Wójcik M.J., Boda Ł., Boczar M., Theoretical study of proton tunneling in the excited state of tropolone. J. Chem. Phys., 130, 164306, 2009.　[5]. Wójcik M.J., Gług M., Boczar M., Boda Ł., Spectroscopic signature for ferroelectric ice, Chem. Phys. Lett. 612, 162, 2014.[6]. Brela M.Z., Wójcik M.J., Boczar M., Witek Ł., Yasuda M., Ozaki Y., Car-Parrinello molecular dynamics simulations of infrared spectra of crystalline vitamin C with analysis of double minimum proton potentials for medium-strong hydrogen bonds, J. Phys. Chem. B, 119, 7922, 2015.

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