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Theoretical Vibrational Spectroscopy of Hydrogen-Bonded Complexes, Liquids and Solids

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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 an harmonicities. 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.