# Anharmonic interactions and infrared bandshape of the hydrogen bond vibration of potassium hydrogen (deuterium) maleate crystals.

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The spectral profiles of the hydrogen bond vibrations in the potassium hydrogen maleate (KHM) crystal and its deuterated analogue (KDM) were studied theoretically taking into account the Fermi resonance (FR) effect and strong coupling between the hydrogen bond vibration and lattice phonons. In addition, *ab initio* calculations of the frequencies and intensities of the H(D)-maleate ion for both $C_{2v}$ and $C_s$ symmetry were made. It was found that $C_s$ symmetry has to be used and that practically all intense bands have a contribution from the OH vibration. It was shown that, taking into account all the factors: *ab initio* results, FR and anharmonicity of vibrations, the experimental spectra for both KHM and KDM crystals can be explained adequately. Anharmonic constants were obtained as a result of fitting theoretical spectra to the experimental ones.

Słowa kluczowe

Infrared spectra, Hydrogen bond, Fermi resonance, Anharmonic interaction

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