

Inelastic neutron scattering, Raman, infrared and DFT theoretical studies on chloranilic acid.

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The vibrational spectra of chloranilic acid (2,5-dihydroxy-3,6-dichloro-[1,4]-benzoquinone) in the solid state were studied by using inelastic neutron scattering (INS), infrared (IR) and Raman (R) spectroscopy. The spectra were compared with simulated spectra using the Gaussian and Climax programs. Sufficiently good agreement between the experimental and theoretical (DFT) spectra is observed although the calculations show that in the crystalline state a bifurcation of hydrogen bonds takes place. Relatively strong intermolecular interactions are noticeable when the experimental (x-ray) and calculated bond lengths and angles with participation of OH groups are compared. The studies of the deuterium isotope effect in the IR and R spectra enabled us to analyse the low-frequency out-of-plane vibrations and particularly the $\nu(\text{OH})$ and $\nu(\text{OD})$ modes. In the case of the $\nu(\text{OH})$ and $\nu(\text{OD})$ vibrations, one observes a strong asymmetry of the bands (low-frequency wings), which can be interpreted in terms of a coupling of the $\nu(\text{OH})$ mode with low-frequency ones damped by the lattice phonons and no fine structure of the $\nu(\text{OH})$ and $\nu(\text{OD})$ bands is observed.

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