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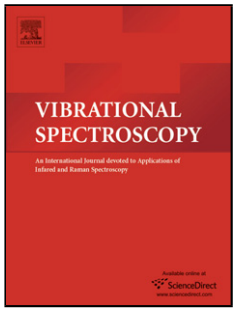

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On some controversy regarding ν_{OH} assignments in CsH_2PO_4

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Positive and negative/0 slopes

Abstract

Spectroscopic methods such as Raman scattering and IR absorption, as well as structural methods such as x-ray and n-diffraction, offer rather ambiguous interpretation of the high-frequency phonon spectrum of CsH_2PO_4 (CDP), especially regarding the proper assignment of proton vibrational modes. Empirical lattice dynamics (LD) simulations of the proton vibrational density of states (H-VDOS) in CDP also reveal a discrepancy in the frequency assignments of the O-H stretching modes of its two *non-equivalent* hydrogen bonds. This may be resolved by accounting for the LD simulated *directional* H-VDOS along the three Cartesian axes of CDP, from which the corresponding anisotropy of the proton kinetic energy tensor can be deduced. The results may then be tested by a simple deep inelastic neutron scattering (DINS) measurement on a single crystal of para-electric CDP at room temperature.