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Investigation of the Low-Frequency Vibrations of Crystalline Tartaric Acid Using Terahertz Spectroscopy and Solid-State Density Functional Theory

Source

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Abstract

The room temperature and cryogenic terahertz (THz) spectra (10-95 cm(-1)) of L-tartaric acid and DL-tartaric acid were investigated. At 293 K, the L-tartaric acid spectrum showed four absorption features at 36.4, 61.6, 781, and 87.3 cm(-1) in the experimental spectrum. Once cooled to 78 K, these features narrowed and shifted to 35.9, 63.4, 81.1, and 90.1 cm(-1). The THz spectrum of DL-tartaric acid is significantly different, containing only a single absorption at 79.9 cm(-1) at room temperature, which shifts to 82.9 cm(-1) at 78 K Solid-state density functional theory calculations [B3LYP/6-311G(2d,2p)] were performed to simulate the crystalline structure of both molecular solids and to assign the observed spectral features to specific atomic motions. The THz spectrum of L-tartaric acid is particularly interesting in that it contains a theoretically unaccounted for spectral feature that may arise from second-order phonon processes and also exhibits an anomalous red-shifting absorption feature with cooling that is shown to originate from negative thermal expansion of the crystal.