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Title:Investigation of the low-frequency vibrations of crystalline tartaric acid using terahertz spectroscopy and solid-state density functional theory
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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, 78.7, 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.
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