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Title:Importance of accurate spectral simulations for the analysis of terahertz spectra: Citric acid anhydrate and monohydrate
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Abstract:The terahertz (THz) spectra of crystalline solids are typically uniquely sensitive to the molecular packing configurations, allowing for the detection of polymorphs and hydrates by THz spectroscopic techniques. It is possible, however, that coincident absorptions may be observed between related crystal forms, in which case careful assessment of the lattice vibrations of each system must be performed. Presented here is a THz spectroscopic investigation of citric acid in its anhydrous and monohydrate phases. Remarkably similar features were observed in the THz spectra of both systems, requiring the accurate calculation of the low-frequency vibrational modes by solid-state density functional theory to determine the origins of these spectral features. The results of the simulations demonstrate the necessity of reliable and rigorous methods for THz vibrational modes to ensure the proper evaluation of the THz spectra of molecular solids.
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