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标题: Improved Mode Assignment for Molecular Crystals Through Anisotropic Terahertz Spectroscopy
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摘要: We report the anisotropic terahertz response of oxalic acid and sucrose crystals in the 0.2-3.0 THz range using terahertz time domain spectroscopy on large, single crystals. We compare the observed anisotropic response with the response calculated using solid-state density functional theory and find good agreement in the orientation dependence and relative intensities of the crystal phonons. It was found that oxalic dihydrate can be reversibly converted to anhydrous by controlled relative humidity. In addition, oxalic acid was found to have a large birefringence with Delta n = 0.3, suggesting the material may be useful for terahertz polarization manipulation. Sucrose has a smaller birefringence of Delta n = 0.05, similar to that of x-cut quartz. The anisotropic measurements provide both mode separation and symmetry determination to more readily achieve mode assignment for the more complex sucrose spectrum.
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