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Title

Molecular dynamics study of the effect of pressure on the terahertz-region infrared spectrum of crystalline pentaerythritol tetranitrate

Source

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Abstract

Terahertz infrared absorption spectra of crystalline pentaerythritol tetranitrate were obtained using classical molecular dynamics simulations for temperature  $T = 298$  K and hydrostatic pressures  $P = 0, 1, 2,$  and  $3$  GPa. Two approaches were used to calculate the spectra; one based on combined normal-mode analysis and mode-relaxation calculations and the other on Fourier analysis of the dipole-dipole time autocorrelation function. The two methods yield similar, though not identical, positions and relative spectral amplitudes for all pressures studied. The predicted spectra exhibit an overall blue shift with increasing pressure, accompanied by a decrease in the integral absorption.