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Accession number:20114114423954
Title:Molecular dynamics study of the effect of pressure on the terahertz-region infrared spectrum of crystalline pentaerythritol tetranitrate
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Source title:Chemical Physics Letters
Abbreviated source title:Chem. Phys. Lett.
Volume:515
Issue:1-3
Issue date:October 17, 2011
Publication year:2011
Pages:32-36
Language:English
ISSN:00092614
CODEN:CHPLBC
Document type:Journal article (JA)
Publisher:Elsevier, P.O. Box 211, Amsterdam, 1000 AE, Netherlands
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.
Number of references:26