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Molecular dynamics study of normal mode relaxation and infrared spectra in pentaerythritol tetranitrate ANDREY PEREVERZEV, THOMAS D. SEWELL, University of Missouri-Columbia — Vibrational properties of crystalline pentaerythritol tetranitrate (PETN) were studied using two different approaches based on classical molecular dynamics simulations. In the first approach relaxation of THz-active modes at 300 K and atmospheric pressure was studied by adding fixed amounts of kinetic energy to individual THz-active normal modes of the crystal and monitoring the time dependence of energy transfer from those selectively-excited modes. The THz absorption spectrum was constructed using linewidths obtained directly from the relaxation times of the excited modes for the case of low excitation energy. Dynamics of redistribution of the initial excitation energy among the other normal modes was also studied. In the second approach THz-region infrared spectra were obtained from the Fourier transform of the dipole-dipole autocorrelation function. Predictions of the two approaches are in reasonable agreement with each other and with experiment. Pressure effects and sensitivity to details of the force field were studied using both approaches.

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