Abstract Submitted
for the PSF13 Meeting of
The American Physical Society

Theoretical studies of terahertz spectra of crystalline energetic materials using molecular dynamics ANDREY PEREVERZEV, THOMAS SEWELL, DONALD THOMPSON, University of Missouri-Columbia — Terahertz infrared (THz IR) absorption spectra of crystalline pentaerythritol tetranitrate (PETN) and the α and γ polymorphs of 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX) were calculated at 300 K for pressures between 0 and 7 GPa using two different theoretical approaches based on molecular dynamics (MD). Beyond the choice of force field, neither method entails the specification of adjustable parameters. In the first approach spectral line frequencies and intensities were calculated using normal mode analysis of three-dimensionally periodic crystal supercells, while spectral line widths were calculated using relaxation times obtained from MD simulations of energy loss from selectively excited THz-region IR-active modes. The IR spectrum was then generated as a superposition of Lorentzian functions completely specified by the calculated frequencies, intensities, and line widths. In the second approach spectra were calculated from equilibrium MD simulations using the Fourier transform of the dipole autocorrelation function of the crystal. Spectra obtained using the two methods are similar and agree reasonably well with experimental results.

Thomas Sewell
University of Missouri-Columbia

Date submitted: 10 Oct 2013 Electronic form version 1.4