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Anharmonic vibrational properties of PETN, HMX, and TATB from temperature dependent Raman SHAWN MCGRANE, JEFFREY BARBER, JASON QUENNEVILLE, Los Alamos National Laboratory — Raman spectra from 50-3500 cm^{-1} and 4-296 K are analyzed for PETN, HMX, and TATB. Shock initiation of detonation is postulated to occur by vibrational up-pumping, which implies the presence of diagnostic features in the vibrational spectra of molecules with vastly different shock initiation properties. Temperature dependent Raman is utilized for its sensitivity to anharmonic couplings between thermally populated phonons and higher frequency vibrations. The data are analyzed with anharmonic perturbation theory (APT), which is shown to have significant fundamental limitations. Fitting to APT revealed no significant difference in averaged anharmonicities among the three explosives. Calculations of the multiphonon densities of states also failed to correlate clearly with shock sensitivity. However, striking differences in temperature dependent lifetimes were obvious: PETN has long lived phonons and vibrons, HMX has long lived phonons but short lived vibrons, while TATB has short lived phonons and vibrons. These data suggest the further hypothesis that hindered vibrational energy transfer in the molecular crystals is a factor in shock sensitivity.

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