Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Vibrational and Thermal Properties of β-HMX and TATB from Dispersion Corrected Density Functional Theory AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida, Tampa, FL — Dispersion Corrected Density Functional Theory (DFT+vdW) calculations are performed to predict vibrational and thermal properties of the bulk energetic materials (EMs) β-octahydrocyclotetramethylene-tetranitramine (β-HMX) and triaminotrinitrobenzene (TATB). DFT+vdW calculations of optimized unit cells along the hydrostatic equation of state are followed by frozen-phonon calculations of their respective vibration spectra. These are then used under the quasi-harmonic approximation to obtain zero-point and thermal free energy contributions to the pressure, resulting in PVT equations of state for each material that is in excellent agreement with experiment. Further, heat capacities, thermal expansion coefficients, and Gruneissen parameters as functions of temperature are calculated and compared with experiment. The vibrational properties, including phonon densities of states and pressure dependencies of individual modes, are also analyzed and compared with experiment.

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Date submitted: 23 Apr 2015 Electronic form version 1.4