Abstract Submitted
for the SHOCK09 Meeting of
The American Physical Society

Analysis of α-phase RDX vibrational lattice modes under hydrostatic pressure[1] WILLIAM SLOUGH, WARREN PERGER, Michigan Technological University — Calculations employing density functional theory are performed on α-phase RDX using the all-electron CRYSTAL06 program. The lowest frequency infrared active lattice modes are investigated as a function of hydrostatic pressure from ambient conditions up to 3 GPa. The strength of coupling between lattice and molecular modes as a function of pressure is examined. The anharmonic deviation of each mode from simple harmonic behavior as a function of pressure is also illustrated.

[1]Supported by an ONR-MURI grant.

William Slough
Michigan Technological University

Date submitted: 17 Feb 2009 Electronic form version 1.4