Abstract Submitted
for the SHOCK05 Meeting of
The American Physical Society

Equation of State of 1,1-diamino-2,2-dinitroethylene from First Principles FRANK ZERILLI, Naval Surface Warfare Center, Indian Head, Maryland, MAIJA KUKLJA, National Science Foundation, Arlington, Virginia — In recent work, the 0 K isotherms of 1,1-diamino-2,2-dinitroethylene (FOX-7), and β HMX were calculated with the ab-initio periodic structure code CRYSTAL. It was found that Hartree-Fock calculations gave the best agreement with experiment and a calculation with complete optimization of the internal molecular coordinates gives excellent agreement with experimental data. For the best results, especially for anisotropic materials, it was necessary to optimize both atomic coordinates and lattice parameters under a fixed volume constraint. The good results may be the result of cancellation of basis set superposition error with dispersion force errors. Here we report calculations of the full equation of state for the explosive FOX-7 that give results which compare well with experimental data reported by Peiris, et al. The above zero temperature contribution to the free energy was calculated from the phonon frequency spectrum obtained with density functional theory (DFT) in the local density approximation (LDA) with the code ABINIT.

Frank Zerilli
Naval Surface Warfare Center, Indian Head, Maryland

Date submitted: 01 Apr 2005 Electronic form version 1.4