Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Thermo-Physical Properties of Ammonium Azide under High Pressure from First-Principles AARON LANDERVILLE, BRAD STEELE, IVAN OLEYNIK, University of South Florida — Polynitrogen compounds offer tremendous promise for use as insensitive high-explosives or propellants. While the existence of such compounds have been observed in Diamond Anvil Cells (DAC) under high pressure, recovery to ambient pressure and temperature has proven problematic. A current thrust towards the recovery, and ultimate manufacture, of materials rich in polymeric nitrogen has brought renewed attention to various nitrogen-rich compounds, particularly crystalline azides, as possible precursors. We investigate the thermo-physical properties and Raman spectra of one azide candidate – ammonium azide – under hydrostatic compression using density functional theory with an empirical van der Waals correction. Additionally, we perform structural minima searches to discern possible polymorphs that may help to elucidate dynamical processes leading to the production of a material rich in polymeric nitrogen, as well as its recovery from DAC.

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Date submitted: 09 Nov 2012 Electronic form version 1.4