Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

High-pressure behavior of a novel, nitrogen-rich energetic material[1] R. STEWART MCWILLIAMS, Howard University, JENNIFER CIEZAK-JENKINS, Army Research Laboratory, YASMIN KADRY, University of Maryland College Park, VITALY PRAKAPENKA, Advanced Photon Source, MOHAMMAD MAHMOOD, Howard University, ALEXANDER GONCHAROV, Carnegie Institution of Washington — Energetic materials are of great interest in energy and defense applications. In the search for new energetic materials with improved properties, such as reduced environmental impact, a crystalline solid Triaminoguanidinium 1-methyl-5-nitriminotetrazolate (TAG), $C_3H_{12}N_{12}O_2$, has recently been synthesized (Klapötke et. al. 2008). We have studied the properties of TAG under static compression, and under reaction initiation at high pressure, using Raman and IR spectroscopy and x-ray diffraction. TAG appears to remain a stable, crystalline solid up to at least 35 GPa at room temperature. Laser initiation at 10-15 GPa reveals a rapid self-propagating reaction (deflagration) that consumes the sample, similar to other energetic materials such as nitromethane. Post-initiation products include crystalline molecular nitrogen (delta-phase), and nitrogen crystallites with regular defects. The formation of bulk molecular nitrogen during deflagration - in both phase segregated and impurity-hosting forms - distinguishes TAG from other known energetic materials, and suggests a pathway for the generation of novel phases from element-enriched energetic substances.

[1]This research was conducted under U.S. Army Research Office grant # 56122-CH-H.

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Date submitted: 27 Nov 2010 Electronic form version 1.4