Abstract Submitted
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Ammonium Azide under High Pressure – a combined Theoretical and Experimental Study[1] HARRY RADOUSKY, JONATHAN CROWHURST, JOSEPH ZAUG, Lawrence Livermore National Laboratory, BRADLEY STEELE, AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida — Efforts to synthesize, characterize and recover novel polynitrogen energetic materials have driven attempts to subject high nitrogen content precursor materials (in particular metal and non-metal azides) to elevated pressures. Here we present a combined theoretical and experimental study of the high pressure behavior of ammonium azide (NH_4N_3). Using density functional theory we have considered the relative thermodynamic stability of the material with respect to two other crystal phases, namely trans-tetrazene (TTZ), and also a novel hydronitrogen solid (HNS) of the form $(NH)_4$, that was recently predicted to become relatively stable under high pressure. Experimentally we have measured the Raman spectra of NH_4N_3 up to 71 GPa at room temperature. Our calculations demonstrate that the HNS becomes stable only at pressures much higher (89.4 GPa) than previously predicted (36 GPa). Our Raman spectra are consistent with earlier reports up to lower pressures, and at higher pressures, while some additional subtle behavior is observed (e.g. mode splitting) there is again no evidence of a phase transition to either TTZ or the HNS.

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Harry Radousky
Lawrence Livermore National Laboratory

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