

Abstract Submitted
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Calculations and experimental studies of bis-triaminoguanidium azotetrazolate (TAGzT) under high pressure I.G. BATYREV, R.C. SAUSA, US Army Research Laboratory — Nitrogen-rich organic compounds may offer distinct advantages over conventional energetic materials for applications relating to gas generators, low-signature propellants, and additives to pyrotechnics and explosives. We have performed plane-wave, density functional theory calculations of TAGzT, an energetic, nitrogen-rich salt, up to 40 GPa, and report the pressure dependences of polarizability, x-ray diffraction patterns, and dipole moments. These results are compared to those we obtain experimentally from Raman Spectroscopy,¹ and x-ray diffraction analysis and infrared spectroscopy. Our results suggest TAGzT does not undergo any phase transitions within this pressure range. Mulliken and Hirshfeld population analysis of TAGzT at ambient and high pressure yields the change of charge distribution with an increase in pressure. We report and discuss this trend at the meeting. Also, we report trends in the pressure-induced modifications of both bond lengths and angles of TAGzT, and reveal how hydrogen bonding contributes to the stability of TAGzT under pressure. ¹K.D. Behler, J.A. Ciezak-Jenkins, R.C. Sausa, J. Phys. Chem A. 117(8), 1737 (2013)

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