

Abstract Submitted  
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**Prediction of the anisotropic properties of energetic materials at elevated pressures and temperatures**<sup>1</sup> OSCAR OJEDA, TAHIR CAGIN, Texas A&M University — Localization of strain and changes under extreme conditions in energetic materials (EM) can cause runaway reactions and unexpected initiation. A clear understanding of the mechanical properties is a prerequisite in understanding the interplay between mechanical, chemical and thermodynamic properties that relate sensitivity and EM's before they undergo initiation. We have conducted first principles ground state studies, complemented by atomistic calculations at elevated temperatures and pressures, for energetic commonly used secondary EM's with varying sensitivities. Chemical information found from ab initio methods, and from compression at elevated temperatures show that external conditions relevant to impact and shock behavior can have different effects on the studied systems. These range from changes in local conformation, changes in the hydrogen-bonding network, and more drastically to a full crystallographic transition in which the symmetry of the system undergoes a transformation. Due to the chemical, mechanical and thermodynamic level information that provides, multiscale modeling methods, can then be applied to the understanding of other type of systems and give a clearer understanding of the molecular processes that undergo energetic materials, prior to initiation.

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