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High-pressure and temperature investigations of energetic materials

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Static high-pressure measurements are extremely useful for obtaining thermodynamic and phase stability information from a wide variety of materials. However, studying energetic materials can be challenging when extracting information from static high-pressure measurements. Energetic materials are traditionally C, H, N, O compounds with low crystalline symmetry, producing weak signal in commonly performed x-ray diffraction measurements. The small sample volume available in a static high-pressure cell exacerbates this issue. Additionally, typical hydrostatic compression media, such as methanol/ethanol, may react with many energetic materials. However, characterization of their thermodynamic parameters and phase stability is critical to understanding explosive performance and sensitivity. Crystalline properties, such as bulk modulus and thermal expansion, are necessary to accurately predict the behavior of shocked solids using hydrodynamic codes. In order to obtain these values, equations of state of various energetic materials were investigated using synchrotron angle-dispersive x-ray diffraction experiments at static high-pressure and temperature. Intense synchrotron radiation overcomes the weak x-ray scattering of energetic materials in a pressure cell. The samples were hydrostatically compressed using a non-reactive hydrostatic medium and heated using a heated diamond anvil cell. Pressure – volume data for the materials were fit to the Birch-Murnaghan and Vinet formalisms to obtain bulk modulus and its first pressure derivative. Temperature – volume data at ambient pressure were fit to obtain the volume thermal expansion coefficient. Data from several energetic materials will be presented and compared.