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Phase Stability of Epsilon and Gamma HNIW (CL-20) at High-Pressure and Temperature

JARED GUMP, Indian Head Division - Naval Surface Warfare Center

Hexanitrohexaazaisowurtzitane (CL-20) is one of the few ingredients developed since World War II to be considered for transition to military use. Five polymorphs have been identified for CL-20 by FTIR measurements (α, β, γ, ε, and ζ). As CL-20 is transitioned into munitions it will become necessary to predict its response under conditions of detonation, for performance evaluation. Such predictive modeling requires a phase diagram and basic thermodynamic properties of the various phases at high pressure and temperature. Theoretical calculations have been performed for a variety of explosive ingredients including CL-20, but it was noted that no experimental measurements existed for comparison with the theoretical bulk modulus calculated for CL-20. Therefore, the phase stabilities of epsilon and gamma CL-20 at static high-pressure and temperature were investigated using synchrotron angle-dispersive x-ray diffraction experiments. The samples were compressed and heated using diamond anvil cells (DAC). Pressures and temperatures achieved were around 5GPa and 175^{o}C, respectively. No phase change (from the starting epsilon phase) was observed under hydrostatic compression up to 6.3 GPa at ambient temperature. Under ambient pressure the epsilon phase was determined to be stable to a temperature of 120^{o}C. When heating above 125^{o}C the gamma phase appeared and it remained stable until thermal decomposition occurred above 150^{o}C. The gamma phase exhibits a phase change upon compression at both ambient temperature and 140^{o}C. Pressure – volume data for the epsilon and gamma phase at ambient temperature and the epsilon phase at 75^{o}C were fit to the Birch-Murnaghan formalism to obtain isothermal equations of state.