RIAD MANAA, Lawrence Livermore Natl Lab — Equations of states (EOS) of unreacted energetic materials extending to high-pressure and temperatures regimes are provide fundamental information about the associated thermodynamic properties of these materials at extreme conditions. Using dispersion-corrected density functional theoretical calculations, we performed large-scale constant-volume, constant-pressure and temperature molecular dynamics simulations on crystal 2,6-diamino-3, 5-dinitropyrazine-1-oxide (LLM-105) for pressures ranging from ambient to 35 GPa, and temperatures ranging from 300 K to 1400 K. These calculations allowed us to construct an unreacted P-V-T EOS and obtain bulk modulus for each P-V isotherm. We also obtained the thermal expansion coefficient of LLM-105 in the temperature range of this study. Finally, we conducted a quantum-based molecular dynamics study at the C-J point to characterize the decomposition products of reacting LLM-105 at complete reactivity condition.

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