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First Principles Simulations of P-V-T Unreacted Equation of State of LLM-105[1] RIAD MANAA, I-FENG KUO, LAURENCE FRIED, Lawrence Livermore National Laboratory — Equations of states (EOS) of unreacted energetic materials extending to high-pressure and temperatures regimes are of particular interest since they provide fundamental information about the associated thermodynamic properties of these materials at extreme conditions. Very often, experimental and computational studies focus only on determining a pressure-volume relationship at ambient to moderate temperatures. Adding elevated temperature data to construct a P-V-T EOS is highly desirable to extend the range of materials properties. Atomic scale molecular dynamics simulations are particularly suited for such a construct since EOSs are the manifestation of the underlying atomic interactions. In this work, we report dispersion-corrected density functional theoretical calculations of unreacted equation of state (EOS) of the energetic material 2,6-diamino-3, 5-dinitropyrazine-1-oxide (LLM-105). We performed large-scale constant-volume and temperature molecular dynamics simulations for pressures ranging from ambient to 35 GPa, and temperatures ranging from 300 K to 1000 K. These calculations allowed us to construct an unreacted P-V-T EOS and obtain bulk modulus for each P-V isotherm. We also report the thermal expansion coefficient of LLM-105 in the temperature range of this study.

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