Abstract Submitted
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The Equation of State of Triamino-Trinitrobenzene from Density Functional Theory Molecular Dynamics[1] RYAN R. WIXOM, Sandia National Laboratories — The U_S-u_P shock Hugoniot has long been the fundamental relationship used to experimentally define the unreacted equations of state of explosives. These experiments are typically performed on porous or composite samples, providing data that is specific to the density of the samples being tested. However, If the crystalline Hugoniot is known, analytical or numerical methods can be used to transform the U_S-u_P relationship to describe the shock response of the porous material. To obtain an accurate crystalline equation of state for TATB, density functional theory based molecular dynamics were used to map out points on the Hugoniot. Since this method provides the pressure, temperature, density, and internal energy at each point on the Hugoniot, a complete equation of state can be constructed. Isotropic, uniaxial, hydrostatic, and isothermal compression of the simulation cell were used to examine TATB under different thermodynamic conditions. A cusp is observed in the Hugoniot that correlates to loss of aromaticity of the molecule. Results of the calculations will be presented and compared to the available experimental data.

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