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Hydrostatic equation of state and anisotropic Constitutive Relationships in 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) MIKALAI BUDZEVICH, MICHAEL CONROY, AARON LANDERVILLE, YOU LIN, IVAN OLEYNIK, University of South Florida, CARTER WHITE, Naval Research Laboratory — TATB is an energetic molecular crystal which exhibits remarkable insensitivity to shock, heating and electrical sparks. Despite its high stability and relative safety, TATB is a highly powerful explosive which makes it an interesting target for both theoretical and experimental studies. We performed first-principles van-der-Waals Density Functional Theory (vdW-DFT) studies of the equilibrium properties and hydrostatic equation of state (EOS) for TATB and compared with experiment. The vdW-DFT showed better agreement with the experimentally determined hydrostatic EOS and unit cell parameters compared standard DFT, which suffers from the lack of proper description of long-range dispersive interactions. The anisotropic EOS as a function of uniaxial compression in the {001}, {010}, {011} , {100} , {101} , {110}, and {111} crystallographic directions was also studied. Calculated mechanical properties such as the principal and shear stresses, energy gap, and the energy per atom show a clear anisotropy in the TATB molecular crystal upon uniaxial compression.

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