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First-principles studies of hydrostatic and uniaxial compression of a new energetic material – an energetic nitrate ester MICHAEL CONROY, AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida, CARTER WHITE, Naval Research Laboratory — Density functional theory calculations with an empirical vdW correction were performed on a new energetic material (EM), a nitrate ester, that was recently synthesized by Chavez *et al.* [Angew. Chem. Int. Ed. **47**, 8307 (2008)]. This EM was shown to have physical properties superior to another nitrate ester, PETN. The equilibrium structure was calculated by vdW-DFT in excellent agreement with experiment (to within about 0.1% of the equilibrium volume of the unit cell). From the hydrostatic-compression simulation, the isothermal EOS and bulk modulus were predicted prior to any known experimental results. In addition, uniaxial compressions were simulated in the <100>, <010>, <001>, <110>, <101>, <011>, and <111> directions to examine the anisotropic quality of the constitutive relationships. The calculated physical properties of the nitrate ester at extreme conditions are compared with other important energetic materials.

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