

Abstract Submitted
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First principles calculation of the structure and vibrational modes for RDX crystals under static and shock compression¹ M.S. MIAO, Z.A. DREGER, J.M. WINEY, Y.M. GUPTA, Inst. for Shock Phys. Wash State Uni. — The structure and vibrational modes for RDX crystals, under hydrostatic pressures up to 4 GPa and uniaxial strains along [100] and [111] directions, were calculated at the first principles level by use of the VASP program. The PW91 generalized gradient approximated (GGA) exchange and correlation energy functional and ultrasoft pseudopotentials were employed and a cutoff of 550 eV was used for plane wave basis. The calculated volume and lattice constants at ambient pressure are larger than the experimental value. With increasing pressure, both volume and lattice constants agree better with experimental values. Despite the large deformation of the lattice, the geometry of each molecule changes only slightly as a function of pressure or uniaxial strain. For the vibrational modes, the calculated pressure dependencies of the frequencies agree well with experimental results. For example, the C-H stretching modes and lattice modes show large pressure dependences whereas many other modes such as the ONO stretching modes change only slightly with pressure. The comparison between the effects of hydrostatic pressure and uniaxial strain on vibrational modes will also be presented.

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