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**First-principles studies of RDX crystals under compression**[1] JIJUN ZHAO, J.M. WINEY, Y.M. GUPTA, Washington State University, WARREN PERGER, Michigan Tech University — Using the plane-wave pseudopotential technique (CASTEP program) within the generalized gradient approximation (GGA), we have performed first principles calculations to examine RDX crystals under hydrostatic and uniaxial strain compression. Crystal structures were calculated at ambient conditions for the orthorhombic structure and a vibrational analysis was performed. Second order elastic constants such as $C_{11}$, $C_{22}$, and $C_{33}$ were calculated by applying very small uniaxial strains along [100], [010], and [001] orientations. Unit cell dimensions and fractional coordinates of the RDX crystal were determined under hydrostatic and uniaxial compressions up to about 4 GPa. Compression-induced changes in the RDX molecular geometry for these two loading conditions are discussed.

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