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Raman Spectroscopy of RDX Single Crystals under Static Compression ZBIGNIEW DREGER, YOGENDRA GUPTA, Washington State University — To gain insight into the high pressure response of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), an energetic crystal, Raman spectroscopy results were obtained for hydrostatic (up to 15 GPa) and non-hydrostatic (up to 22 GPa) compressions. These results are needed to properly interpret the shock data. Several distinct changes in the spectra were found at 4.0 \pm 0.3 GPa, confirming the $\alpha - \gamma$ phase transition previously observed in polycrystalline samples. Symmetry correlation analyses indicate that the γ -polymorph may assume a space group isomorphous with a point group D_{2h} with eight molecules occupying the C_1 symmetry sites, similar to the α -phase. It is also proposed that the factor group splitting can account for the observed increase in the number of modes in the γ -phase. Spatial mapping of Raman modes in a non-hydrostatically compressed crystal up to 22 GPa revealed a large difference in mode position indicating a pressure gradient across the crystal. No apparent irreversible changes in the Raman spectra were observed under non-hydrostatic compression. Work supported by DOE and ONR.

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