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 ± 0.3 GPa, confirming the α – γ 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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