

## W0360

**The Molecular Structure of RDX at High Pressure.** Wayne H. Pearson<sup>1</sup>, Suhithi M. Peiris<sup>2</sup>, <sup>1</sup>Chemistry Dept., United States Naval Academy, Annapolis, MD; <sup>2</sup> Indian Head Div., Naval Surface Warfare Center, Indian Head, MD.

RDX, 1,3,5-trinitrohexahydro-1,3,5-triazine, is an explosive material used for military applications. We have undertaken a study of the crystal structure of RDX to determine how the geometry of the molecule changes in high-pressure environments. Data were collected at Cornell University's synchrotron source (CHESS) with crystals loaded in Merrill-Bassett type DACs at various pressures. Omega scans of 4° were performed at different chi settings on a two-circle goniometer. The images were recorded on a MARS 3450 image-plate detector and the resulting data were indexed and integrated using DPS/Mosflm. Full structural analyses of the data were performed using SHELX. Significant changes in bond lengths, angular distortions and ring puckering are evident at 1.5 GPa when compared to the ambient pressure structure. The 2 and 3.5 GPa data appear to reveal the existence of two separate phases, indicating that the phase transition previously seen at 3.8 GPa may start occurring at lower pressure.