SAND2015-0533C

Pressure dependence of Hexanitrostilbene Raman/ electronic absorption spectra to validate DFT EOS

Due to its thermal stability and low vapor pressure, Hexanitrostilbene (HNS) is often used in high-temperature or vacuum applications as a detonator explosive or in mild detonating fuse. Toward improving the accuracy of the equation of state used in hydrodynamic simulations of the performance of HNS, we have measured the Raman and electronic absorption spectra of this material under static pressure in a diamond anvil cell. Density functional theory calculations were used to simulate the pressure dependence of the Raman/Electronic spectra along the Hugoniot and 300K isotherm for comparison and to aid in interpreting the data. We will discuss changes in the electronic structure of HNS under pressure, validation of a DFT predicted equation of state, and using this data as a basis for understanding future pulsed Raman measurements on dynamically compressed HNS samples.