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Density Functional Theory Investigation of Sodium Azide at High Pressure BRAD STEELE, AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida — Sodium azide is being investigated as a potential precursor to a high-nitrogen content energetic material. Changes in the experimentally measured raman spectra under compression and high temperature indicate that a structural change may have taken place. Accurate mode assignments of new peaks arising in the raman spectra have been inconclusive. In this work, the first order raman spectra of sodium azide's alpha and beta phases are calculated using Density Function Pertubation Theory (DFPT) under compression and expansion. Normal mode assignments are made and compared to experiment. In addition, the equation of state of both phases is obtained up to 90 GPa.

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