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Structural diversity in the ammonium azide molecular crystal at high pressures AARON LANDERVILLE, BRAD STEELE, IVAN OLEYNIK, University of South Florida — Ammonium azide (NH_4N_3) seems to undergo phase transitions under compression as indicated by the experimentally measured Raman spectrum. However, X-ray diffraction studies of the NH_4N_3 crystal beyond the known first phase transition at $\sim$ 3 GPa have yet to be performed. Additionally, first-principles density functional perturbation theory calculations of the known phase of NH_4N_3 have been unsuccessful at reproducing Raman spectral evolution with pressure seen in experiment, while no evidence has been found that NH_4N_3 transitions to hydronitrogen solid at the predicted pressure of 36 GPa. This may indicate that the true lowest enthalpy configuration has yet to be discovered. Here, evolutionary structure prediction method coupled with density functional calculations are employed to calculate the lowest enthalpy phases of ammonium azide as a function of pressure. Novel structures are predicted, and ground state enthalpies and the Raman spectra are calculated as a function of pressure and compared with the experimental Raman spectra.

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