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Density Functional Theory Characterization of Potential Poly-Nitrogen Precursors IVAN OLEYNIK, AARON LANDERVILLE, BRAD STEELE, University of South Florida — The successful recovery of pure poly-nitrogen materials, such as cubic-gauche, from diamond anvil cells has proven both difficult and elusive. As it has been proposed that impurities within a polymeric nitrogen matrix may offer increased stability upon return of the material to ambient conditions, attention has turned to nitrogen-rich compounds, such as azides, as potential precursors to impure, but recoverable forms of poly-nitrogen compounds. To aid experimentalists in the search of novel poly-nitrogen compounds, thermophysical properties and Raman spectra of the candidate precursor ammonium-azide, along with a theoretically predicted polymorph, are calculated using Density Functional Theory with and empirical van der Waals correction. Additionally, we present preliminary results for another proposed nitrogen-rich precursor cyanuric-triazide.

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