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Compositional changes upon compression of sodium azide predicted using density functional theory BRAD STEELE, AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida — The pressure induced phase transitions in sodium azide, which include a potential polymeric nitrogen phase transition, are investigated using evolutionary crystal structure prediction methods coupled with density functional theory calculations. Two new phases are predicted to be stable above 53 GPa that have an inequivalent ratio of sodium to nitrogen atoms as compared to sodium azide. The Raman spectrum is calculated from 0-100 GPa using these newly predicted structures, as well as the newly discovered I4/mcm phase of sodium azide. The predicted Raman spectrum is shown to give good agreement to experimental data above 30 GPa and below 15 GPa.

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