

Abstract Submitted  
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**Sodium Pentazolate: a Nitrogen Rich Energetic Material** IVAN OLEYNIK, BRAD STEELE, University of South Florida — Sodium pentazolates  $\text{NaN}_5$  and  $\text{Na}_2\text{N}_5$ , new energetic materials, are discovered using first principles crystal structure search for the compounds of varying amounts of elemental sodium and nitrogen. The pentazole anion ( $\text{N}_5^-$ ) is stabilized in the condensed phase by sodium  $\text{Na}^+$  cations at pressures exceeding 20 GPa, and becomes metastable upon release of pressure, i.e. at ambient conditions. The sodium azide ( $\text{NaN}_3$ ) precursor for the new compounds is predicted to undergo a chemical transformation above 50 GPa into sodium pentazolates  $\text{NaN}_5$  and  $\text{Na}_2\text{N}_5$ . The calculated Raman spectrum of  $\text{NaN}_5$  is in agreement with the experimental Raman spectrum of a previously unidentified substance appearing upon compression and heating of  $\text{NaN}_3$  precursor, thus confirming the appearance of the new compound.

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