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Cesium Pentazolate: a New Nitrogen Rich Energetic Material BRAD STEELE, University of South Florida, ELISSAIOS STAVROU, HARRY RADOUSKY, JOSEPH ZAUG, JONATHAN CROWHURST, Lawrence Livermore National Laboratory, IVAN OLEYNIK, University of South Florida — Nitrogen, which forms strong triple bonds in molecular diatomic nitrogen N_2 at low pressures, was predicted to transform to single-bonded cubic-gauche crystal upon compression above 50 GPa. However, experimental realization of polymeric forms of nitrogen proved to be difficult. Here we report theoretical and experimental evidence for a new class of high-nitrogen content compounds consisting of molecular pentazoles, which are stabilized in the crystal phase upon introduction of elemental cesium. First-principles structural predictions show that the material with composition CsN_5 is thermodynamically stable above 30 GPa. Indexing of the measured X-ray diffraction spectra indicate the synthesis of this material at 60 GPa as well its stability upon decompression down to 24 GPa. Their energetic capacity and stability make these alkali-metal pentazolates excellent candidates for high-energy density materials.

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