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Novel LLM series high density energy materials: Synthesis, characterization, and thermal stability¹ PHILIP PAGORIA, MAOXI ZHANG, Lawrence Livermore National Laboratory, ROMAN TSYSHEVSKIY, MAIJA KUKLJA, University of Maryland College Park — Novel high density energy materials must satisfy specific requirements, such as an increased performance, reliably high stability to external stimuli, cost-efficiency and ease of synthesis, be environmentally benign, and be safe for handling and transportation. During the last decade, the attention of researchers has drifted from widely used nitroester-, nitramine-, and nitroaromatic-based explosives to nitrogen-rich heterocyclic compounds. Good thermal stability, the low melting point, high density, and moderate sensitivity make heterocycle materials attractive candidates for use as oxidizers in rocket propellants and fuels, secondary explosives, and possibly as melt-castable ingredients of high explosive formulations. In this report, the synthesis, characterization, and results of quantum-chemical DFT study of thermal stability of LLM-191, LLM-192 and LLM-200 high density energy materials are presented.

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