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Spectroscopic and structural study of LLM-172 under pressure GUSTAV BORSTAD, JENNIFER CIEZAK-JENKINS, U.S. Army Research Laboratory — The properties of energetic materials have been investigated to permit the synthesis and scale-up of novel energetic materials possessing low sensitivity without sacrificing performance. To this end, there have been considerable efforts expended on the preparation of molecular crystals featuring unsaturated heterocycles with energetic functional groups such as LLM-105 and LLM-172 (BNFF-1)[1]. This permits the compounds to maintain high densities while controlling their stability and sensitivity. Due to the nature of energetic phenomena, varying pressure (and thus density) is a valuable tool to explore the properties of these materials. We will present data on LLM-172 compressed in diamond anvil cells to 50 GPa and characterized by Raman spectroscopy and synchrotron powder x-ray diffraction. These techniques allow for the exploration of the evolution of the structure and bonding with pressure. In particular, we will examine the changes as the sample approaches the detonation pressure (near 34 GPa)[2].

[1]A. DeHope, P. F. Pagoria, and D. Parrish, "New polynitro alkylamino furazans" (No. LLNL-CONF-624954), Lawrence Livermore National Laboratory (LLNL), Livermore, CA (2013).
[2]J. J. Sabatini and K. D. Oyler, *Crystals* **6**, 5 (2016)

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