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Stability of LLM 172 under high pressure. ISKANDER G. BATYREV, JENNIFER A. CIEZAK-JENKINS, GUSTAV M. BORSTAD, US Army Research Laboratory — LLM-172 or 3, 4-bis (4-nitro-1,2,5- oxadiazol-3-yl)-1,2,5-oxadiazole has been studied experimentally and computationally modeled at high-pressure. Minimum enthalpy structures were relaxed using norm-conserving pseudo potentials which provided a high level of convergence for the final computational structures. The calculated P-V curve fits reasonably well to the experimental X-ray diffraction data. The best fit for calculated values (using Vinet, Birch-Murnaghan, and Tait equations of state) was obtained with bulk modulus K_0 =17.70 GPa. No phase transitions or deviations from the $P2_12_12_1$ (D2-4) space group of the LLM-172 crystal were observed to near 35 GPa, although slight modifications to the molecular geometry were noted in the Raman spectra. Variational density functional perturbation theory was used to obtain calculated Raman spectra; these calculated spectra were then used for comparison with experimental Raman spectra and the identification of the molecular motions associated with the vibrational modes. Based upon the modification of the experimental Raman spectra with pressure, potential decomposition mechanisms are proposed. The band gap, which was calculated with the GGA-PBE approximation and hybrid functional HSE06, shows a gradual decrease with pressure, although it is far from closing at 30 GPa.

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