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Simulations of the structure, vibrational spectra, and energy content of crystalline bis (4-amino-3,5-dinitropyrazolyl) methane under high pressures. ISKANDER G. BATYREV, JONNATHAN C. BENNION, JENNIFER A. CIEZAK-JENKINS, US Army Rsch Lab - Aberdeen — The crystalline structure of bis (4-amino-3,5-dinitropyrazolyl) methane (BDNAPM) was optimized from ambient pressure to 40 GPa using density functional calculations in order to understand pressure-induced instabilities. Raman spectra were calculated as a function of pressure using density functional perturbation theory and linear response for lattice dynamics. The zone center (k=0) optical modes provided information about the vibrational modes of the crystal. The calculated spectra were compared with high-pressure experimental spectroscopic measurements in the same pressure range. The enthalpy of formation was calculated along with the mass density for simulation of Chapman-Jouguet characteristics.

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