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**First-principles studies of PETN molecular crystal vibrational frequencies under high pressure** WARREN PERGER, Michigan Tech University, JIJUN ZHAO, J.M. WINEY, Y.M. GUPTA, Washington State University — The vibrational frequencies of the PETN molecular crystal were calculated using the first-principles CRYSTAL03 program which employs an all-electron LCAO approach and calculates analytic first derivatives of the total energy with respect to atomic displacements. Numerical second derivatives were used to enable calculation of the vibrational frequencies at ambient pressure and under various states of compression. Three different density functionals, B3LYP, PW91, and X3LYP were used to examine the effect of the exchange-correlation functional on the vibrational frequencies. The pressure-induced shift of the vibrational frequencies will be presented and compared with experiment. The average deviation with experimental results is shown to be on the order of 2-3%, depending on the functional used.

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