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Calculation of PETN molecular crystal vibrational frequencies under hydrostatic pressure WARREN PERGER, Michigan Tech University, JI-JUN ZHAO, J.M. WINEY, Y.M. GUPTA, Washington State University — First-principles calculations of the effects of hydrostatic pressure on pentaerythritol tetranitrate (PETN) are performed using the all-electron CRYSTAL03 program. The procedure for applying hydrostatic pressure by performing a series of volumetric changes coincident with lattice constant and internal coordinate optimization using various scripts and support programs is described. Once the optimized internal coordinates and lattice constants have been obtained for a given hydrostatic pressure, a separate algorithm consisting of additional scripts and programs is employed for performing a complete normal-mode analysis, with analytic first derivatives and numeric second derivatives of the total energy. The eigenvalues obtained provide the vibrational frequencies and the eigenvectors are used for mode identification. The role of the Gaussian basis sets chosen and the exchange-correlation potential used is discussed. The vibrational frequencies obtained at ambient pressure are shown to compare well with experiment and gas-phase calculations. The shift of the vibrational frequencies under hydrostatic pressure is compared with experiment.

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