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Calculation of RDX molecular crystal geometry and vibrational frequencies under hydrostatic pressure[1] WARREN PERGER, WIL SLOUGH, Michigan Tech University — First-principles calculations of the effects of hydrostatic pressure on RDX are performed using the all-electron CRYSTAL06 program. The lattice constants and optimized internal co-ordinates are simulanteously obtained at ambient pressure and hydrostatic pressure up to 4 GPa. A variety of density functionals and basis sets are used and presented for comparison. The vibrational frequencies as a function of pressure are also calculated and compared with previous gas-phase calculations.

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