Abstract Submitted
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Calculation of the vibrational spectra of RDX as a function of pressure using the Grimme DFT potential[1] WARREN PERGER, Michigan Tech University, K.M. FLURCHICK, North Carolina A&T University, WIL SLOUGH, LOREDANA VALENZANO, Michigan Tech University — The density-functional theory (DFT) potential by Grimme has been proposed for describing long-range dispersion corrections. This potential has been implemented into the CRYSTAL09 program and used to calculate the vibrational spectra in RDX at equilibrium and as a function of pressure. The intensities, Born charge tensor, and high-frequency dielectric constant are reported and compared with prior theory and experiment where possible.

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