

Abstract Submitted
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Gamma phase RDX: vibrational features providing insight into the alpha-gamma phase transition¹ KEN FLURCHICK, North Carolina Agricultural and Technical State University, WARREN PERGER, WILLIAM SLOUGH, LOREDANA VALENZANO, Michigan Tech Univ — We present a full 3D periodic density functional theory study of the infrared spectra of gamma phase RDX. The B3LYP-D* functional as adjusted for molecular solids from Grimme's semi-empirical approach for molecules is used to better describe the van der Waals interactions in this system. Specifically, the low terahertz portion of the spectrum is explored in detail for modes that change substantially in behavior with respect to an alpha phase that is near the transition pressure for the system. These key modes provide possible clues into the nature of the alpha-gamma phase transformation. We also present infrared reflectance spectra and results for the refractive index, with the intent to guide experiments in achieving a more complete understanding of the vibrational features of this energetic molecular crystal.

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