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Experimental and theoretical investigation of pressure-dependent Raman spectra of triaminotrinitrobenzene (TATB) at high pressures AARON LANDERVILLE, University of South Florida, CHRISTIAN GRANT, JOSEPH ZAUG, JONATHAN CROWHURST, Lawrence Livermore National Laboratory, IVAN OLEYNIK, University of South Florida — The experimental pressure dependent Raman spectra of triamino-trinitrobenzene (TATB) are determined up to 27 GPa, and compared with those obtained using density functional theory (DFT). The density functional perturbation theory calculations include the Grimme empirical van der Waals correction, as well as corrections for both thermal and zero-point energy contributions to pressure. DFT calculations of the crystal structure of TATB at ambient conditions, the equation of state, and Raman spectra up to 25 GPa are in good agreement with experiment. Pressure-dependence of specific vibrational modes is discussed in detail. Further, the comparison of experimental and calculated Raman spectra of TATB offers evidence that no first-order polymorphic phase transition occurs at least up to 25 GPa.

Ivan Oleynik
University of South Florida

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