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A Theoretical Study of Vibrational Spectroscopy in Hydrostatically Compressed Nitromethane Crystal Using an Empirical Form Molecular Dynamics Force Field[1] ALI SIAVOSH-HAGHIGHI, RICHARD DAWES, THOMAS D. SEWELL, DONALD L. THOMPSON, Department of Chemistry, University of Missouri-Columbia, Columbia, MO 65211-7600 — Molecular dynamics simulations have been used with an unreactive but vibrationally accurate force field [Sorescu et al., J. Phys. Chem. B **104**, 8406 (2000)] to investigate the effects of isothermal hydrostatic stress on the vibrational spectrum of crystalline nitromethane. Power spectra corresponding to the classical vibrational density of states were obtained as Fourier transforms of the mass-weighted velocity-velocity autocorrelation functions at 298 K for seven hydrostatic pressures between 0.0 and 13.5 GPa. The goal is to provide an explanation for the pressure-induced shifts, splittings, and appearance/disappearance of bands in the infrared and Raman spectra observed in recent experimental [Ouillon et al., J. Raman Spectrosc. **39**, 354 (2008); Citroni et al., J. Phys. Chem. B **112**, 1095 (2008)] and electronic structure-based [Liu et al., J. Chem. Phys. **124**, 124501 (2006)] studies.

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