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The effect of a simulated volumetric expansion: Calculated vibrational properties and elastic constants of pentaerythritol[1] J. CRISWELL, W. PERGER, W. SLOUGH, L. VALENZANO, Michigan Technological University — Current *ab-initio* calculations do not include the van der Waal's interactions. These long range forces are important in the binding of many molecular crystals. Using current theory one may include empirical van der Waal's forces to describe the binding of a molecular solid. The results of *ab-initio* calculations are at 0K. But, experiments measuring material properties are often at ambient conditions. The exclusion of thermal effects produces an inherent disparity between measurements and first-principles calculations of physical properties. In this work, the vibrational spectra and second-order elastic constants (SOECs) of pentaerythritol (PE) are found using density functional theory (DFT) with the B3LYP-D* functional. B3LYP-D* is the B3LYP functional with an empirical description of the van der Waal's dispersion force. PE is chosen because it has a small, highly symmetric, unit cell and exhibits anisotropic binding. Also, recent experimental and theoretical vibrational studies show an interesting behavior of the OH-stretch mode for PE. Using DFT, the SOECs and vibrational spectra of PE are calculated at 0K. The volumetric expansion to ambient temperature is simulated by fixing the unit cell to an experimental volume, optimizing the structure, and recalculating properties. Results of elastic and vibrational properties for 0K, simulated ambient temperature, and experiment are compared.

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