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**Ab Initio Studies of High Pressure States of Crystalline Nitromethane.** FRANK ZERILLI, Naval Surface Warfare Center, JOSEPH HOOPER, Tulane University, MAIJA KUKLA, National Science Foundation — We have calculated the mechanical compression curve for solid nitromethane with the ab-initio periodic structure code CRYSTAL using both Hartree-Fock and Density Functional Methods. In addition, calculations with both 6-21G and 6-31G** basis sets were performed and the effect of basis set superposition error was estimated using the counterpoise method. In each calculation the internal atomic coordinates and the crystal lattice parameters were relaxed at constant unit cell volume to the minimum energy configuration. The 6-31G** basis set was optimized by scaling the outer valence and polarization orbitals. It was found that Hartree-Fock calculations with a 6-21G basis set, uncorrected for basis set superposition error, gave the best agreement with experiment. These results may be due to the cancellation of basis set superposition error with dispersion force errors. While this result may be accidental, it appears that it extends to a number of other energetic organic molecular crystals, including beta HMX, PETN, and 1,1-diamino-2,2-dinitroethylene.

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