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Title:THz dielectric properties of molecular clusters of PETN and TNT calculated by density functional theory
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Abstract:The need for better detection of explosive devices has imposed a necessity for determining the dielectric response properties of energetic materials with respect to electromagnetic wave excitation. Among the range of different frequencies for electromagnetic excitation, the THz frequency range is of particular interest because of its nondestructive nature. The present study is based on significant progress in density functional theory (DFT), and associated software technology, which is sufficiently mature for the determination of dielectric response functions, and actually provides complementary information to that obtained from experiment. This point is further demonstrated in this study by calculations of ground state resonance structure associated with molecular clusters of the high explosives PETN and TNT using DFT, which is for the construction of parameterized dielectric response functions for excitation by electromagnetic waves at frequencies within the THz range. These dielectric functions provide for different types of analyses concerning the dielectric response of explosives. In particular, these dielectric response functions provide quantitative initial estimates of spectral response features for subsequent adjustment with respect to additional information such as laboratory measurements and other types of theory-based calculations. With respect to qualitative analysis, these spectra provide for the molecular level interpretation of response structure. The DFT software GAUSSIAN was used for the calculations of ground state resonance structure presented here. © 2012 ASM International.
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