Figure 1. Molecular geometry and symmetry-unique atom labels (for charge analyses in Figure 7) for the high explosives HMX (left, C_i symmetry) and PETN (right, S_4 symmetry). CPK renderings performed with VMD(1).
Figure 2. The eight solid-state GGA [functional]/DNP normal mode analyses (red) for the crystal forms $\beta$-HMX (left in oriented) and PETN I (right in oriented) from 20 to 120 cm$^{-1}$. Experimental THz spectra are shown in blue.
Figure 3. The isolated-molecule (top) and solid-state Hirshfeld (middle) and Mulliken (bottom) simulated THz spectra of HMX. Solid-state mode labels identify in- and out-of-phase ("+" and "−", respectively) combinations of the identified isolated-molecule modes. Remaining unlabeled modes are external modes between molecules in the β-HMX crystal cell.
Figure 4. The isolated-molecule (top) and solid-state Hirshfeld (middle) and Mulliken (bottom) simulated THz spectra of PETN. Solid-state mode labels identify in- and out-of-phase (“+” and “-”, respectively) combinations of the identified isolated-molecule modes. Remaining unlabeled modes are external modes between molecules in the PETN I crystal cell. Modes identified as “3,4” and “8,9” are combinations of these degenerate modes. See text.
Figure 5. The 0 to 120 cm\(^{-1}\) simulated Hirshfeld (red) and Mulliken (blue) solid-state THz spectra of \(\beta\)-HMX using the VWN-BP density functional and choice of basis set (DNP, DND, DN) and grid size (Medium Fine, XFine). The experimental THz \(\beta\)-HMX spectrum is shown in grey.
Figure 6. The 0 to 120 cm$^{-1}$ simulated Hirshfeld (red) and Mulliken (blue) solid-state THz spectra of PETN I using the BP density functional and choice of basis set (DNP, DND, DN) and grid size (Medium Fine, XFine). The experimental THz PETN I spectrum is shown in grey.
Figure 7. Variation in Mulliken (upper plots) and Hirshfeld (lower plots) population analyses with basis set and grid size for the individual molecules in the β-HMX (top, VWN-BP functional) and PETN I (bottom, BP functional) crystal cells. Atom labels correspond to those in Figure 1.
Figure 8. Single-processor compute times (in minutes) for the HMX and PETN crystal cells as a function of basis set and grid size. Calculations are for an AMD Opteron (280) workstation in single-processor mode running the SuseLinux 10.0 operating system.