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Title:Noncovalent interactions between modified cytosine and guanine DNA base pair mimics investigated by terahertz spectroscopy and solid-state density functional theory
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Abstract:Modified cytosine and guanine nucleobases cocrystallize in a hydrogen bonding configuration similar to that observed in native DNA. The noncovalent interactions binding these base pairs in the crystalline solid were investigated using terahertz (THz) spectroscopy and solid-state density functional theory (DFT). While stronger hydrogen bonding interactions are responsible for the general molecular orientations in the crystalline state, it is the weaker dipole - dipole and dispersion forces that determine the overall packing arrangement. The inclusion of dispersion interactions in the DFT calculations was found to be necessary to accurately simulate the unit cell structure and THz vibrational spectrum. Using properly modeled intermolecular potentials, the lattice vibrational motions of the cytosine and guanine derivatives were calculated. The vibrational characters of the modes exhibited by the DNA base pair mimic in the THz region were primarily rotational motions and are indicative of the energies and the nature of vibrations that would likely be observed between similar base pairs in DNA molecules. (Figure presented)
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