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Title:Noncovalent interactions in paired DNA nucleobases investigated by terahertz spectroscopy and solid-state density functional theory
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Abstract: Cocrystallized adenine and thymine derivatives, along with the pure monomeric crystals, were investigated by terahertz spectroscopy and solid-state density functional theory (DFT). The methylated nucleobase derivatives crystallize in planar hydrogen-bonded adenine-thymine pairs similar to the manner found in DNA. The spectra obtained for 1-methylthymine, 9-methyladenine, and the 1:1 cocrystal in the range of 10−100 cm−1 clearly demonstrate that absorptions in this spectral range originate from the uniquely ordered assembly and the intermolecular interactions found in each individual crystal system. The quality of spectral reproduction for the DFT simulations of each system was clearly improved by the inclusion of an empirical correction term for London-type dispersion forces to the calculations. Notably, it was found that these weak dispersion forces in the adenine-thymine cocrystal were necessary to produce a properly converged crystal structure and meaningful simulation of the terahertz vibrational spectrum.
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