

IR spectra of crystalline nucleobases : combination of periodic harmonic calculations with anharmonic corrections based on finite models.

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Streszczenie

This work reports a theoretical study of infrared (IR) spectra of four nucleobases (adenine, cytosine, guanine, and thymine) in the crystalline state. The effects responsible for the fine spectral features were revealed, and the nonfundamental bands significantly contributing to the IR fingerprint region were successfully reproduced. Additionally, we compared the fundamental bands simulated for periodic models in harmonic approximation with the results obtained for finite models in anharmonic approximation. On this basis, we concluded that accurate description of the chemical neighborhood is more essential for the IR fingerprint region than the anharmonicity. Comparison with previous results indicates that the vibrational properties and the nature of intermolecular interactions of nucleobases in the crystalline state remain similar to those in solution. Therefore, the conclusions obtained for well-defined crystalline structures of nucleobases are general and helpful in understanding the vibrational spectra and properties of nucleobases and their derivatives. Finally, this work evidences that anharmonic force field based on finite models may be applied as an inexpensive correction to the harmonic spectrum of an infinite periodic system.

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