

Harmonic and anharmonic vibrational computations for biomolecular building blocks: Benchmarking DFT and basis sets by theoretical and experimental IR spectrum of glycine conformers

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Advanced vibrational spectroscopic experiments have reached a level of sophistication that can only be matched by numerical simulations in order to provide an unequivocal analysis, a crucial step to understand the structure-function relationship of biomolecules. While density functional theory (DFT) has become the standard method when targeting medium-size or larger systems, the problem of its reliability and accuracy are well-known and have been abundantly documented. To establish a reliable computational protocol, especially when accuracy is critical, a tailored benchmark is usually required. This is generally done over a short list of known candidates, with the basis set often fixed a priori. In this work, we present a systematic study of the performance of DFT-based hybrid and double-hybrid functionals in the prediction of vibrational energies and infrared intensities at the harmonic level and beyond, considering anharmonic effects through vibrational perturbation theory at the second order. The study is performed for the six-lowest energy glycine conformers, utilizing available “state-of-the-art” accurate theoretical and experimental data as reference. Focusing on the most intense fundamental vibrations in the mid-infrared range of glycine conformers, the role of the basis sets is also investigated considering the balance between computational cost and accuracy. Targeting larger systems, a broad range of hybrid schemes with different computational costs is also tested.

Słowa kluczowe

benchmark, biomolecules, database, DFT, vibrational spectroscopy, VPT2

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