

Fully *ab initio* IR spectra for complex molecular systems from perturbative vibrational approaches: Glycine as a test case

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Streszczenie

Perturbative anharmonic computations have been used to simulate the IR spectrum of glycine, taking into account its three most stable conformers. The theoretical results have been directly compared with their experimental counterparts, showing good agreement between the latter and the spectra obtained after proper averaging of the contributions from the three most stable glycine conformers. The results show that direct simulation of the overall vibrational spectrum within a second-order perturbative treatment is feasible and leads to a better understanding of experimental data. Additionally, it has been shown that accurate results can be obtained even when several molecular species need to be considered simultaneously. The computations performed at the B3LYP/aug-N07D level have shown their reliability in the prediction of both vibrational energy levels and IR intensities beyond the harmonic approximation. This kind of computations represents an important tool for the analysis of vibrational spectra for complex medium-to-large molecular systems.

Słowa kluczowe

Vibrational spectroscopy, Computational spectroscopy, IR intensities, Anharmonicity, VPT2, DFT

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