ANHARMONIC IR SPECTRA OF BIOMOLECULES: NUCLEOBASES AND THEIR OLIGOMERS

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Computational spectroscopy techniques have become in the last years effective means to predict and characterize spectra, such as infrared, for molecular systems of increasing dimensions with account for different environments. We are actively developing a comprehensive and robust computational protocol, set within a perturbative vibrational framework [1], aimed at a quantitative reproduction of the spectra of biomolecules.

In order to model the vibrational spectra of weakly bound molecular complexes, dispersion interactions should be taken into proper account. In this work, we present critical assessment of dispersion-corrected DFT approaches for anharmonic vibrational frequency calculations. It is shown that fully anharmonic IR spectra, simulated through full and reduced-dimensionality generalized second-order vibrational perturbation theory (GVPT2)[1] with the potential energy surfaces computed with the B3LYP-D3 approach, may be used to interpret experimental data of nucleobases and their complexes[2] by the direct comparison of experimental IR spectra with their theoretical anharmonic counterpart, taking into account also overtones and combination bands.

[1] V. Barone, M. Biczysko, J. Bloino, Phys. Chem. Chem. Phys., 2014,16, 1759-1787

[2] T. Fornaro, M. Biczysko, S. Monti, V. Barone , Phys. Chem. Chem. Phys., 2014, DOI: 10.1039/C3CP54724H