

## Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case

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### Streszczenie

An integrated computational approach built on quantum mechanical (QM) methods, purposely tailored inter- and intra-molecular force fields and continuum solvent models combined with time-independent and time-dependent schemes to account for nuclear motion effects is applied to the spectroscopic investigation of pyrimidine in the gas phase as well as in aqueous and  $\text{CCl}_4$  solutions. Accurate post-Hartree–Fock methodologies are employed to compute molecular structure, harmonic vibrational frequencies, energies and oscillator strengths for electronic transitions in order to validate the accuracy of approaches rooted into density functional theory with emphasis also on hybrid QM/QM0' models. Within the time-independent approaches, IR spectra are computed including anharmonicity through perturbative corrections while UV–vis line-shapes are simulated accounting for the vibrational structure; in both cases, the environmental effects are described by continuum models. The effects of conformational flexibility, including solvent dynamics, are described through time-dependent models based on purposely DFT-tailored force fields applied to molecular dynamics simulations and on QM computations of spectroscopic properties. Such procedures are exploited to simulate IR and UV–vis spectra of pyrimidine in the gas phase and in solutions, leading in all cases to good agreement with experimental observations and allowing to dissect different effects underlying spectral phenomena.

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