

Reliable Modeling of Anharmonic Spectra Line-Shapes from VPT2 and Hybrid QM Models: IR Spectrum of Uracil as a Test Case

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Streszczenie

Hybrid methods combining different levels of electronic structure quantum mechanical computations with vibrational perturbation theory have been increasingly used in anharmonic simulations of vibrational spectra to achieve accurate results with containable computational costs. However, energy has often been the main focus of these studies, so precision in predicting intensities was systematically overlooked. This situation is largely due to two aspects stemming from theory and experiment. Theoretically, implementations are fewer, and intensity-specific resonance analysis methods were not available until very recently and are still lacking extensive testing. Experimentally, high-resolution vibrational spectra of suitable molecular systems, which could really show the effects of different hybrid schemes on the vibrational intensities, remain scarce. A good candidate in this regard is uracil. Having been extensively studied experimentally, its IR spectrum is well-known over a wide range and at high definition. The patterns displayed by the band shapes represent an excellent challenge to validate and tune our recently developed automated tool to identify intensity-specific resonances. In this work, we compare the newly simulated spectra with state-of-the-art experimental data and propose an extensive analysis over a wide range covering 300 to 6200 cm^{-1} , including 3-quanta transitions. These will provide valuable guides and references for further measurements in the mid-infrared (MIR) and near-infrared (NIR) regions, which have not been reported until now. The methods and protocols applied in this article can also be used for other molecules with complex resonance patterns.

Słowa kluczowe

Chemical calculations, Energy, Infrared light, Potential energy, Uracil

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