Fully anharmonic IR and Raman spectra of medium-size molecular systems: accuracy and interpretation

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Computation of full infrared (IR) and Raman spectra (including absolute intensities and transition energies) for medium- and large-sized molecular systems beyond the harmonic approximation is one of the most interesting challenges of contemporary computational chemistry. Contrary to common beliefs, low-order perturbation theory is able to deliver results of high accuracy (actually often better than those issuing from current direct dynamics approaches) provided that anharmonic resonances are properly managed. This perspective sketches the recent developments in our research group toward the development of a robust and user-friendly virtual spectrometer rooted in second-order vibrational perturbation theory (VPT2) and usable also by non-specialists essentially as a black-box procedure. Several examples are explicitly worked out in order to illustrate the features of our computational tool together with the most important ongoing developments.

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