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Computational vibrational spectroscopy

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Streszczenie

Vibrational spectroscopies, in particular Infrared and Raman, represent commonly used, powerful analytical tools, which are nowadays routinely supported and complemented by quantum-mechanical (QM) computations. This chapter presents theoretical models and computational protocols of different sophistication levels and practical recipes to simulate reliable vibrational spectra. Among the methodologies accounting for the so-called anharmonic effects, vibrational second-order perturbation theory (VPT2) presents an appealing accuracy/cost ratio, allowing for the tailoring of medium-to-large-sized chemical systems. In this chapter, VPT2 is systematically employed in conjunction with potential energy and property surfaces obtained by QM methods ranging from density functional theory to coupled-cluster. It is stressed that the accuracy of QM computations is crucial to obtain “right results for the right reason.” It is also shown that accounting for both mechanical and electrical anharmonic effects leads to a correct description of the intensity of all kinds of transitions, as well as their band shape. A further discussion concerns the treatment of anharmonic resonances and the presence of highly anharmonic, floppy degrees of freedom. The latter can be (in a first approximation) treated by ad hoc reduced-dimensionality models, while more effective protocols involve the use of curvilinear internal coordinates for the description of molecular vibrations, replacing the rectilinear normal coordinates based on Cartesian displacements. The accuracy of such obtained results will be demonstrated by direct comparison with available experimental data for systems of increasing size and complexity.

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