

## Computational molecular spectroscopy

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### Streszczenie

Spectroscopic techniques can probe molecular systems non-invasively and investigate their structure, properties and dynamics in different environments and physico-chemical conditions. Different spectroscopic techniques (spanning different ranges of the electromagnetic field) and their combination can lead to a more comprehensive picture of investigated systems. However, the growing sophistication of these experimental techniques makes it increasingly complex to interpret spectroscopic results without the help of computational chemistry. Computational molecular spectroscopy, born as a branch of quantum chemistry to provide predictions of spectroscopic properties and features, emerged as an independent and highly specialized field but has progressively evolved to become a general tool also employed by experimentally oriented researchers. In this Primer, we focus on the computational characterization of medium-sized molecular systems by means of different spectroscopic techniques. We first provide essential information about the characteristics, accuracy and limitations of the available computational approaches, and select examples to illustrate common trends and outcomes of general validity that can be used for modelling spectroscopic phenomena. We emphasize the need for estimating error bars and limitations, coupling accuracy with interpretability, touch upon data deposition and reproducibility issues, and discuss the results in terms of widely recognized chemical concepts.

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