

Advances in anharmonic methods and their applications to vibrational spectroscopies.

Autorzy

Krzysztof B. Beć

Justyna Grabska

Yukihiro Ozaki

Rok wydania

2018

Wydawca

Springer

Miejsce wydania

Singapore

Strony

483-512

DOI

10.1007/978-981-10-5651-
2_20

bookChapter.title

Frontiers of quantum
chemistry.

ISBN

978-981-10-5650-5

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Rozdział książki

Streszczenie

In this chapter, an overview of anharmonic time-independent approaches and their applications to vibrational spectroscopy will be presented. Attention to their significance for near-infrared (NIR) spectroscopy and studies on complex molecules in condensed phase will be paid. The benefits that are offered by NIR studies and particular difficulties that emerge in case of reproduction of NIR spectra due to the treatment of non-fundamental modes will be highlighted. A short introduction to available anharmonic methodologies, directly overviewed on the basis of the most recent reports in the field, will be presented. An exceptional possibility of elucidation of physicochemical properties, intermolecular interactions, hydrogen bonding, and solvent effects, through investigations of infrared and near-infrared modes, will be examined. Next, recent achievements allowing for accurate and efficient reproduction of experimental spectra in the entire NIR region will be presented. The perspectives for major advances approaching in the field of NIR spectroscopy due to the recent advances in anharmonic theoretical approaches will finally be deliberated.

Słowa kluczowe

Anharmonicity, Vibrational spectroscopy, IR and NIR spectroscopy

Adres publiczny

https://doi.org/10.1007/978-981-10-5651_20

Plik został wygenerowany dnia 2026-10-09 10:27:43

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/y-jgOzg>.