# Aiming at an accurate prediction of vibrational and electronic spectra for medium-to-large molecules: An overview

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Rok wydania

2016

Czasopismo

International Journal of Quantum Chemistry

Numer woluminu

116

Strony

1543-1574

DOI

10.1002/qua.25188

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

In this tutorial review, we present some effective methodologies available for the simulation of vibrational and vibrationally resolved electronic spectra of medium-to-large molecules. They have been integrated into a unified platform and extended to support a wide range of spectroscopies. The resulting tool is particularly useful in assisting the extensive characterization of molecules, often achieved by combining multiple types of measurements. A correct assessment of the reliability of theoretical calculations is a necessary prelude to the interpretation of their results. For this reason, the key concepts of the underlying theories will be first presented and then illustrated through the study of thiophene and its smallest oligomer, bithiophene. While doing so, a complete computational protocol will be detailed, with emphasis on the strengths and potential shortcomings of the models employed here. Guidelines are also provided for performing similar studies on different molecular systems, with comments on the more common pitfalls and ways to overcome them. Finally, extensions to other cases, like chiral spectroscopies or mixtures, are also discussed.

Słowa kluczowe

anharmonic vibrational spectroscopy, computational spectroscopy, large amplitude motion, medium to-large molecules, vibronic spectroscopy

Adres publiczny

http://dx.doi.org/10.1002/qua.25188

Strona internetowa wydawcy

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