

Spectra–structure correlations in isotopomers of ethanol (CX_3CX_2OX ; $X = H, D$): combined near-infrared and anharmonic computational study.

Autorzy

Krzysztof B. Beć
Justyna Grabska
Christian W. Huck
Mirosław A. Czarnecki

Rok wydania

2019

Czasopismo

Molecules

Numer woluminu

24

Strony

2189/1-2189/23

DOI

10.3390/molecules24112189

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The effect of isotopic substitution on near-infrared (NIR) spectra has not been studied in detail. With an exception of few major bands, it is difficult to follow the spectral changes due to complexity of NIR spectra. Recent progress in anharmonic quantum mechanical calculations allows for accurate reconstruction of NIR spectra. Taking this opportunity, we carried out a systematic study of NIR spectra of six isotopomers of ethanol (CX_3CX_2OX ; $X = H, D$). Besides, we calculated the theoretical spectra of two other isotopomers (CH_3CD_2OD and CD_3CH_2OD) for which the experimental spectra are not available. The anharmonic calculations were based on generalized vibrational second-order perturbation theory (GVPT2) at DFT and MP2 levels with several basis sets. We compared the accuracy and efficiency of various computational methods. It appears that the best results were obtained with B2PLYP-GD3BJ/def2-TZVP//CPCM approach. Our simulations included the first and second overtones, as well as binary and ternary combinations bands. This way, we reliably reproduced even minor bands in the spectra of diluted samples (0.1 M in CCl_4). On this basis, the effect of isotopic substitution on NIR spectra of ethanol was accurately reproduced and comprehensively explained.

Słowa kluczowe

near-infrared spectroscopy, ethanol, anharmonic quantum mechanical calculations, isotopic substitution, Overtones, combinations bands

Licencja otwartego dostępu

CC-BY

Licencja na prawach której można swobodnie kopiować, rozprowadzać, zmieniać i remiksować objęty prawem autorskim utwór (Utwór-przedmiot prawa autorskiego) pod warunkiem podania imienia i nazwiska autora utworu pierwotnego oraz źródła pochodzenia utworu.

Pełny tekst licencji:

<https://creativecommons.org/licenses/by/3.0/pl/legalcode>

Adres publiczny

<http://dx.doi.org/10.3390/molecules24112189>

Strona internetowa wydawcy

<http://www.mdpi.com/journal/metals>