

Ab initio molecular dynamics study of overtone excitations in formic acid and its water complex.

Autorzy

Teemu Järvinen

Jan Lundell

Przemysław Dopieralski

Rok wydania

2018

Czasopismo

Theoretical Chemistry
Accounts

Numer woluminu

137

Strony

100/1-100/8

DOI

10.1007/s00214-018-2280-6

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

In this article, we present results from ab initio molecular dynamics simulation of overtone excitation in formic acid monomer and its water complex in the gas phase. For the monomer, a conformation change is observed employing both OH and CH vibrational excitations, which supports experimental findings. In the formic acid–water complex, interconversion also takes place, but it proceeds via hydrogen exchange rather than via intramolecular reaction. Simulations raise a question on effect of quantum and matrix effects to the results. Also, a brief test of different computation methods was done on the system.

Słowa kluczowe

Formic acid, Overtone, Proton exchange, Vibration induced chemistry

Adres publiczny

<http://dx.doi.org/10.1007/s00214-018-2280-6>

Strona internetowa wydawcy

<http://link.springer.com>