

Car-Parrinello molecular dynamics and density functional theory simulations of infrared spectra for acetic acid monomers and cyclic dimers.

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Rok wydania

2009

Czasopismo

Chemical Physics Letters

Numer woluminu

477

Strony

249-254

DOI

10.1016/j.cplett.2009.07.010

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Acetic acid monomer, dimer and its deuterated analogue have been studied using *ab initio* Car–Parrinello molecular dynamics (CPMD). Full geometry optimization has been carried out in the gas phase in order to obtain minimum structures and hydrogen bonding properties. The results show a good agreement with the available experimental data. Infrared spectrum has been calculated and comparative vibrational analysis has been performed. CPMD vibrational results appear to be in a qualitative agreement with the experimental ones.

Adres publiczny

<https://doi.org/10.1016/j.cplett.2009.07.010>

Strona internetowa wydawcy

<http://www.elsevier.com>