

First-principles investigation of isomerization by proton transfer in β -fumaric acid crystal.

Autorzy

Przemysław Dopieralski

Jarosław Panek

Zdzisław Latajka

Rok wydania

2009

Czasopismo

Journal of Chemical Physics

Numer woluminu

130

Strony

164517/1-164517/9

DOI

10.1063/1.3124192

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Crystal structure of fumaric acid was investigated by Car–Parrinello molecular dynamics and Path Integral molecular dynamics. We propose a mechanism of isomerization by proton transfer in the solid state. It is shown that the three conformers of fumaric acid observed in cryogenic Ar matrix are also present in the solid. Standard *ab initio* Car–Parrinello dynamics of the studied solid at 100 K indicates that barrier height for proton transfer is too high to enable thermal jump over the barrier. Path Integral method in this particular case significantly changes proton behavior in the hydrogen bridge, and the proton tunneling process is observed. Vibrational spectra of investigated system HOOC-CH=CH-COOH and its deuterated analog DOOC-CH=CH-COOD were calculated and compared with experimental data.

Adres publiczny

<https://doi.org/10.1063/1.3124192>

Strona internetowa wydawcy

<https://www.aip.org/>