Renewed spectroscopic and theoretical research of hydrogen bonding in ascorbic acid

Autorzy

Kinga Jóźwiak

Aneta Jezierska

Jarosław J. Panek

Barbara Łydżba-Kopczyńska

Aleksander Filarowski

Rok wydania

2024

Czasopismo

Spectrochimica Acta Part A-Molecular and Biomolecular Spectroscopy

Numer woluminu

320

Strony

124585/1-124585/9

DOI

10.1016/j.saa.2024.124585

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The studies of two isomers of ascorbic acid and their deuteroanalogues, presented in the paper, have been accomplished by vibrational spectroscopy methods and quantum-chemical simulations. The spectroscopic research of L-ascorbic and D-isoascorbic acids have been carried out by the infrared (IR) and Raman (R) techniques. On the basis of the obtained results the spectral interpretation of the hydrogen bonded groups of ascorbic acids has been performed. Car-Parrinello Molecular Dynamics (CPMD) and Density Functional Theory (DFT) have been employed to support spectroscopic experimental findings and shed light onto the bridged proton dynamics in the L- and D- isomers of ascorbic acids. The accurate assignments of the hydrogen bond modes have been accomplished with the application of deuterosubstitution, CPMD-solid state simulations and Potential Energy Distribution (PED) analysis. The spectral and structural results have shown that dependency ν(OH) = f(γ(OH)) is the most common for the OHO hydrogen bond, whereas dependency d(OO) = f(γ(OH)) differs as for the ionic and resonance assisted hydrogen bonds.

Słowa kluczowe

Ascorbic acid, Vitamin C, intramolecular hydrogen bond, CPMD simulations, Isotopic effect

Adres publiczny

http://dx.doi.org/10.1016/j.saa.2024.124585

Strona internetowa wydawcy

http://www.elsevier.com