

Accepted Manuscript

Conformational and vibrational studies of arachidonic acid, light and temperature effects on ATR-FTIR spectra

Tuğba Gocen, Sevgi Haman Bayarı, Mehmet Haluk Guven



PII: S1386-1425(18)30500-6
DOI: doi:[10.1016/j.saa.2018.05.100](https://doi.org/10.1016/j.saa.2018.05.100)
Reference: SAA 16134

To appear in: *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*

Received date: 2 February 2018
Revised date: 25 May 2018
Accepted date: 27 May 2018

Please cite this article as: Tuğba Gocen, Sevgi Haman Bayarı, Mehmet Haluk Guven , Conformational and vibrational studies of arachidonic acid, light and temperature effects on ATR-FTIR spectra. Saa (2017), doi:[10.1016/j.saa.2018.05.100](https://doi.org/10.1016/j.saa.2018.05.100)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Conformational and vibrational studies of arachidonic acid, light and temperature effects on ATR-FTIR spectra

Tuğba Gocen¹ Sevgi Haman Bayarı^{2*} Mehmet Haluk Guven¹

¹*Bülent Ecevit University, Department of Physics, 67100 Zonguldak, Turkey*

²*Hacettepe University, Department of Physics Eng., 06800 Beytepe-Ankara, Turkey*

Abstract

Arachidonic acid (AA) (*cis,cis,cis,cis*-5,8,11,14-Eicosatetraenoic acid) is an omega-6 polyunsaturated fatty acid (PUFA) constituent of the phospholipids of cell membranes. The conformational behavior of AA in the gas phase was investigated by means of density functional theory (DFT) using B3LYP method with 6-311++G(d,p) basis set. Theoretical calculations on the structures and infrared spectra of monomer conformers and dimer form of the most stable monomer conformer of AA were performed. Vibrational assignment of the fundamental modes was made based on calculated potential energy distribution (PED). Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) spectrum of AA in liquid phase was recorded in the region 4000-450 cm⁻¹. The theoretical spectrum of dimer AA in gas phase is in reasonably good agreement with the experimental liquid phase spectrum. The double bonds in unsaturated fatty acids are prone to oxidation. Oxidized PUFAs lead to adverse health effects. The effects of daylight and temperature on the oxidative stability of AA were investigated using ATR-FTIR Spectroscopy. The analysis reveals that the light and thermal treatment induce *cis-trans* isomerization in AA.

Keywords: *Arachidonic Acid, DFT, ATR-FTIR, Oxidation, Light, Temperature*

Download English Version:

<https://daneshyari.com/en/article/7668118>

Download Persian Version:

<https://daneshyari.com/article/7668118>

[Daneshyari.com](https://daneshyari.com)