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

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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*