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FTIR Spectroscopy – A Technique for the Evaluation of Edible Oil Oxidation

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Abstract: ***Infrared (IR) spectroscopy is an old analytical technique that has been widely utilized as a routine tool by the fats and oils industry . The measurement of physicochemical properties by FT-IR spectroscopy, not only provide the benefit of rapid analysis but also avoid dangers associated with reagents used in the traditional chemical method. Mid IR spectra have been used to characterize edible oils and fats because they differ in the intensity and the exact frequency at which the max absorbance or transmittance of the band appears. According to the nature and composition of the oil sample exact positions of the band and a shift has been observed when the proportion of fatty acids changed. The present paper is an attempt to help researchers in order to identified fatty acid compositional changes occurred during heating of vegetable oils at elevated or frying temperature***.

Keywords: Fourier transforms infrared spectroscopy, Low density lipoproteins, High density lipoproteins, Hydro peroxide, Frequency

1. Introduction

Infrared (IR) spectroscopy is an old analytical technique that has been widely utilized as a routine tool by the fats and oils industry Since the first infrared spectra of fatty acids (FA) and vegetable oils were published by Coblentz in 1905, there has been a growing recognition by researchers and the food industry of the value of vibrational spectroscopy in lipid analysis Fourier transform infrared spectroscopy (FTIR) is a technique which is used to obtain an infrared spectrum of absorption or emission of a solid, liquid or gas. An FTIR spectrometer simultaneously collects high spectral resolution data over a wide spectral range. This confers a significant advantage over a dispersive spectrometer which measures intensity over a narrow range of wavelengths at a time. The term Fourier transform infrared spectroscopy originates from the fact that a Fourier transform (a mathematical process) is required to convert the raw data into the actual spectrum.

Vegetable oils are one of the major components of human diets, comprising as much as 25% of average caloric intake. The rate of saturated to unsaturated fatty acids is very important for human nutrition. While high levels of saturated fatty acids is desirable to increase oil stability, on the other nutritionally they became undesirable, because high levels of saturated fatty acids are frequently considered do have influence by increasing the concentration of low density lipoproteins (LDL),affecting the ratio of LDL to HDL (high density lipoproteins), promoting clotting and vascular smooth muscle proliferation on the other hand, nutritionally they became undesirable, because high levels of saturated fatty acids are frequently considered do have influence by increasing the concentration of low density lipoproteins (LDL), affecting the ratio of LDL to HDL (high density lipoproteins), promoting clotting and vascular smooth muscle proliferation

Deep frying is the most common and one of the oldest methods of food preparation worldwide. It involves heat and mass transfer. To reduce the expenses, the oils tend to be used repeatedly for frying. When heated repeatedly, changes in physical appearance of the oil will occur such as increased viscosity and darkening in colour which may alter the fatty acid composition of the oil. Heating causes the oil to undergo a series of chemical reactions like oxidation, hydrolysis and polymerization During this process, many oxidative products such as hydroperoxide and aldehydes are produced, which can be absorbed into the fried food. Vegetable oils are mixtures of glycerides, fatty acids and some other compounds in small quantities, like hydrocarbons, alcohols, phenols, tocopherols, phospholipides The quality of vegetable oils is evaluated by the means of their physico-chemical properties such as density, viscosity, refractive index, acid number, iodine number

Oil oxidation is an undesirable series of chemical reactions involving oxygen that degrades the quality of an oil. Oxidation eventually produces rancidity in oil, with accompanying off flavours and smells. Oxidation is not one single reaction, but a complex series of reactions. When oil oxidises it produces a series of break down products in stages, starting with primary oxidation products (peroxides, dienes, free fatty acids), then secondary products (carbonyls, aldehydes, trienes) and finally tertiary products. Oxidation progresses at different rates depending on factors such as temperature, light, availability of oxygen, and the presence of moisture and metals (such as iron). The type of oil also influences the rate of oxidation.

Gullien and Cabo (1999) developed a respective method which is based on Fourier transform infrared spectroscopy FTIR and assumes that frequency changes in specific band allow for the differentiation of stages of the oxidation process and detection of the oxidation level of the analyzed oil sample.

Table 1: Representing different frequency and related functional group

3633 cm^{-1}	secondary oxidized products
3473 cm^{-1}	O-H stretching vibration of hydro peroxide
3006-3009 cm^{-1}	C-H stretching vibration of the cis double bond
2854 cm^{-1}	C-H asymmetric stretching vibration aliphatic CH_2
2825 cm^{-1}	C-H symmetric stretching vibration aliphatic CH_2
1745. cm^{-1}	C=O ester carbonyl double bond stretching of triglycerides
1654- 1659 cm^{-1}	C=C stretching vibration of the cis olefins
1460–1462 cm^{-1}	deformations and bending of –C- H the CH_2 and CH_3 aliphatic groups
1373.2–1377 cm^{-1}	-C-H bending vibrations of CH_2 group
1163.0–1236.3 cm^{-1}	Stretching vibration of C-O
908.2–970.2 cm^{-1}	CH=CH trans unsaturation
723.3 cm^{-1}	(-CH2),-CH=CH- overlapping of the CH_2 rocking and the out of plane vibration of cis disubstituted olefins.

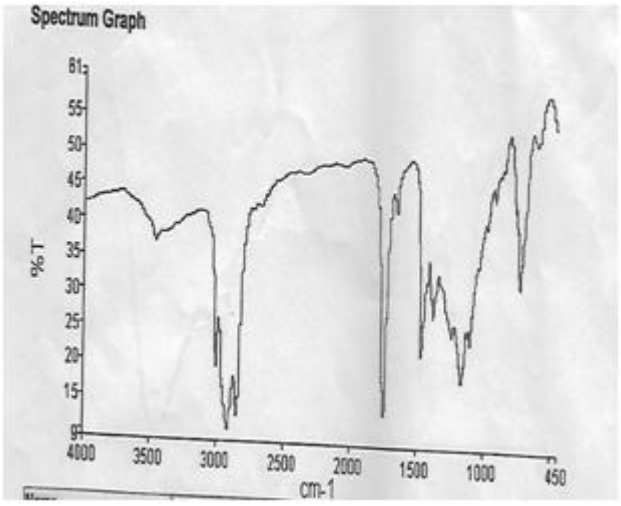

Figure 1: IR spectra of unheated soybean oil

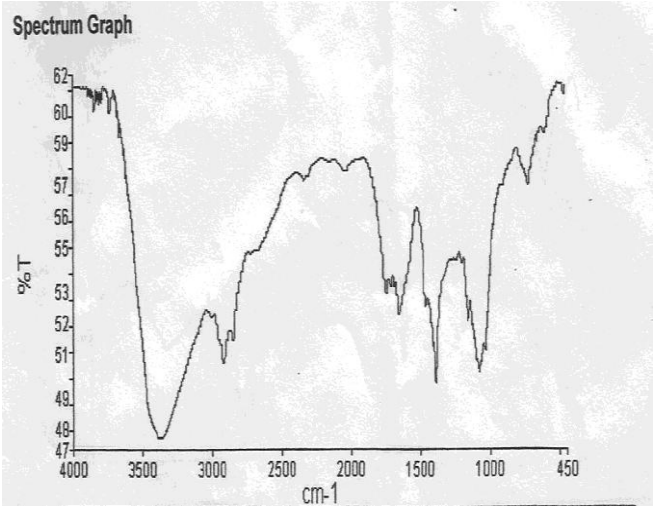

Figure 2: IR spectra of overheated soybean oil

FT-IR capability using finger print as tool to make a first differentiation and representative finger print (1163.0–723.3 cm^{-1}) in the infrared spectra All these changes in the spectral regions showed several changes during the oxidation process. The frequency of the 3007.0 cm^{-1} band depends on the oil composition as oil with a high proportion of linoleic or linoleic acyl groups show higher frequency data at this band than oils with a high proportion of oleic acyl group. The band at 2854 cm^{-1} and the shoulder at 2962 cm^{-1} increase their intensity but the band reduces its absorbance and increases percent transmittance.

2. Conclusion

The measurement of physicochemical properties by FT-IR spectroscopy, is rapid, simple and highly precise method, and avoids the reagents disposal problems associated with the traditional chemical method. FTIR spectroscopy may be able to substitute classic chemical method being a valuable tool to assess the oxidative stability of vegetable oil. FTIR method for determining trans isomer in fats and oils could also compete with gas chromatography FTIR method provides an automated efficient and low cost mean of evaluating oxidation in oils and has been considered as an important analytical tool for quality control in the industry

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Author Profile

Dr. Geeta Verma (*nee* Singh) received M.Sc (Organic Chemistry) from Lucknow University, U .P and completed her research work on the topic "Synthesis of Novel Peptides of Biological Significance" (having GH releasing and Immunosuppressant activity) from Central Drug Research Institute Lucknow, U.P and got Ph .D degree from Dr. Ram. Manohar .Lohia .Avadh University, Faizabad, U.P & M.A .(Eng) from Barkatullah University, Bhopal, M.P. Currently, she is working as an Assistant Professor in the Department of Chemistry in Chandra Shekhar Azad Govt Post Graduate Nodal College, Sehore, M. P. India. She has completed Minor research project sanctioned by UGC, CRO Bhopal and got Best paper award by International Academy of Science Engineering and Technology (IASET) in Sep 2015 edition for MRP work. Her major areas of interests are Chemistry including Astrology, Spirituality, Vastu Shastra, English Literatures Social & Family related issues *etc*. She has publications in following Journals.

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- *Journal of Aquaculture in Tropics,*
- *International Journal of English and Literature*
- *International journal of Educational Science and Research.*
- *Naveen shoadh sansar*
- *International Journal of Research in Applied Natural and Social Science (IMPACT),*
- *International Journal of Applied and Natural Science (IASET)*
- *One Indian Patent*.