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Structural study of Adipic esters by IR spectroscopy

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Abstract
In this article, we determined by IR spectroscopy the composition of the following adipic esters: isotridecyl adipate and 2-(p-nonyl-phenoxy) ethyl, isotridecyl adipate and 2-(o-sec-butyl-phenoxy) ethyl and isotridecyl adipate and 2-phenoxy ethyl. The absorption spectrum of isotridecyl adipate and 2-(p-nonyl-phenoxy) ethyl is between the wave numbers 2958 cm^{-1} and 629 cm^{-1}. The absorption spectrum of isotridecyl adipate and 2-(o-sec-butyl-phenoxy) ethyl is between the wave numbers 2959 cm^{-1} and 751 cm^{-1}. The absorption spectrum of isotridecyl adipate and 2-phenoxy ethyl is between the wave numbers 2958 cm^{-1} and 752 cm^{-1}. IR spectra for adipic esters were obtained on a Jasco 430 FT-IR spectrophotometer.

Keywords: Ester, spectroscopy, structure, adipic

Introduction
FTIR is an acronym determined from Fourier Change Infrared Spectroscopy, which stands for Fourier Change Infrared Spectroscopy. This examination strategy, known as FTIR investigation or FTIR spectroscopy, is an explanatory testing strategy utilized to distinguish natural, polymeric, and in a few cases, inorganic materials.
The FTIR item composition examination strategy employments infrared light to filter the tried tests and watch the chemical properties [1, 7].
The gadget utilized within the examination sends infrared radiation from a test by retaining a few radiation and passing a few radiation. The ingested radiation is changed over into rotational or vibrational vitality by the particles of the test.
The coming about flag within the finder speaks to the atomic unique finger impression of the test, and each particle or chemical structure creates a interesting ghastly unique finger impression, making it an amazing device for chemical recognizable proof.
FTIR examination, or FTIR spectroscopy, is an built up quality control method for assessing materials created in different businesses and regularly serves as the primary step within the materials examination handle. On the off chance that fabric issues are recognized by visual assessment, the source is more often than not decided by FTIR micro-analysis. This method is valuable for analyzing bigger surface zones as well as the chemical composition of littler particles, for the most part between 10 and 50 microns [7, 14].

Item composition investigation with FTIR is primarily utilized for the taking after purposes
- Distinguishing proof and characterization of obscure materials such as movies, solids, powders or fluids
- Recognizable proof of defilement on or in a fabric such as particles, filaments, powders or fluids
- Distinguishing proof of added substances after extraction from a polymer framework

To recognize oxidation, isolation or tainted monomers in disappointment examination examinations.
In industry, FTIR spectroscopy could be a exceptionally effective apparatus in many applications, but deciphering the information isn't easy. By its exceptionally nature, the whole range created could be a set of retained vitality reaction capacities.
For case, within the makeup industry, fast distinguishing proof of corrective items is especially vital in distribution centers that have huge amounts of item entries each day. FTIR spectroscopy offers the advantage of measuring a small amount of test (some milligrams or

milliliters) within the most limited conceivable time.

Makeup are broadly utilized by a expansive portion of the populace. Opposite to prevalent conviction, makeup are not totally secure to utilize and cause genuine side impacts. The long-term harm caused by sporadic utilize of these items is still obscure.

In this respect, it is fundamental to create expository methods utilized to look at a exact and fast number of clumps. One of these strategies is the FTIR (Fourier Change Infrared Spectroscopy) strategy.

This procedure may be a classic technique widely utilized within the pharmaceutical industry, because it is fast and non-destructive and requires negligible test arrangement.

As of late, this procedure has been utilized within the corrective industry for item characterization, soundness, recognizable proof of contaminants and scientific recognizable proof of wrongdoing scene tests.

In brief, FTIR (Fourier Change Infrared Spectroscopy) may be a strategy connected to analyze both natural and inorganic materials. With this strategy, the chemical structure of a fabric is analyzed by looking at the chemical bonds and composition.

The FTIR procedure is valuable for both natural and inorganic materials. In expansion, with this strategy, the covalent bond sets and utilitarian bunches in a fabric are too decided. The FTIR strategy employments the assimilation of light by a fabric by utilizing the way diverse atomic compounds respond to infrared light to decide the structure of the fabric being analyzed. This strategy is additionally known as retention spectroscopy and is connected in a assortment of ways, counting sparkling a bar of light with a constrained recurrence band or utilizing monochromatic light.

This method abuses the truth that each recurrence responds in an unexpected way to the fabric and works by utilizing a few distinctive frequencies within the bar. In this way, the composition of an obscure fabric is precisely decided (14-20). On the other hand, fabric disintegration is additionally recognized with the FTIR strategy. Materials are tried in genuine time or beneath quickened conditions. This procedure is utilized to test pollutions in a fabric or compound, as well as crude materials, drugs, and materials for therapeutic gadgets.

Our organization gives FTIR spectroscopy examination administrations to the asking undertakings inside the system of national and worldwide benchmarks, with a prepared and master staff and progressed mechanical hardware, among various test, estimation, investigation and assessment considers.

Material and Methods

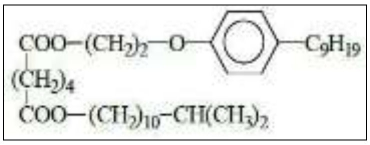
Structure Determination

IR spectra were obtained on a Jasco 430 FT-IR spectrophotometer. Samples were prepared in KBr pellets or in film between two KBr panes. FT-IR reactions were monitored in thermostated cuvettes with 0.137 mm thick silica panes on a Jasco 430 FT-IR spectrophotometer with a resolution of 1 cm^{-1}.

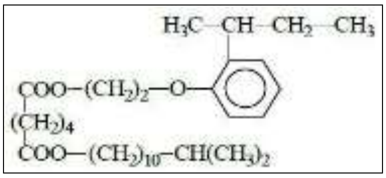
Fig 1: Jasco 430 FT-IR spectrophotometer

Synthesis of Adipic Esters

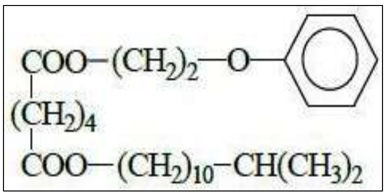
Isotridecyl adipate and 2-(p-nonyl-phenoxy) ethyl is obtained by synthesizing one mole of adipic acid with 1 mole of 2-(p-nonyl-phenoxy) ethanol and 0.035 moles of p-toluene sulfonic acid. In stage I: temperature 115-145 ^{0}C, time 5-7 hours, toluene 175 ml. In the second stage, one mole of isotridecanol is added at a temperature between 120 ^{0}C - 165 ^{0}C, time 5 - 7 hours.



Isotridecyl adipate and 2-(o-sec-butyl-phenoxy) ethyl is obtained by synthesizing 1.15 moles of adipic acid with 1.15 moles of 2-(p-sec-butyl-phenoxy) ethanol and 0.035 moles of p-toluene sulfonic acid. In stage I: temperature 115-145 ^{0}C, time 5-7 hours, toluene 175 ml. In the second stage, 1.15 of isotridecanol is added at a temperature between 120 ^{0}C-165 ^{0}C, time 5-7 hours.



Isotridecyl adipate and 2-phenoxy ethyl are obtained in the first stage from 1.3 moles of adipic acid, 2 phenoxy ethanol 1.3 moles and 0.04 moles of p-toluene sulfonic acid. In stage I: temperature 115 - 145 ^{0}C, time 5 - 7 hours, toluene 175 ml. In the second stage, 1.3 moles of isotridecanol are added at a temperature between 120 ^{0}C - 165 ^{0}C, time 5 - 7 hours.



Results and discussion

In figures 2-4 the absorption spectra for the following compounds are presented: isotridecyl adipate and 2-(p-nonyl-phenoxy)ethyl, isotridecyl adipate and 2-(o-sec-butyl-phenoxy)ethyl and isotridecyl adipate and 2-phenoxy ethyl.

In this spectrum, the fundamental absorption bands, located in the spectral range from 3000 cm^{-1} to 629 cm^{-1} , are clearly evident.

Figure 2 shows the IR spectrum of isotridecyl adipate and 2-(p-nonyl-phenoxy)ethyl.

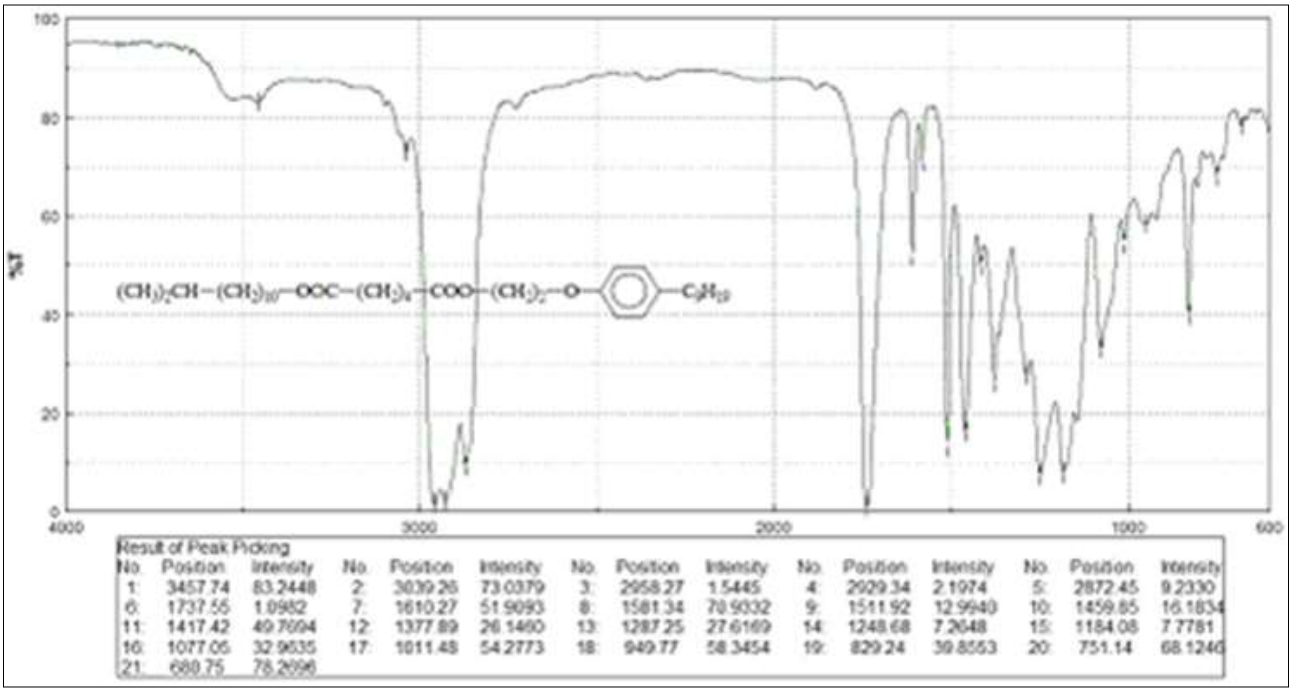


Fig 2: Spectrul IR al adipatul de izotridecil şi 2-(p-nonil-fenoxi) etil

As can be seen in the spectrum, 21 peaks appear for isodecyl adipate and 2-(p-nonyl-phenoxy) ethyl. The most important ones are listed in Table 1.

Table 1 shows the assignment of peaks in the FTIR spectrum for isotridecyl adipate and 2-(p-nonyl-phenoxy) ethyl.

Table 1: Assignment of peaks in the FTIR spectrum of isotridecyl adipate and 2-(p-nonyl-phenoxy) ethyl

Wave number, cm^{-1}	Functional grouping	Vibration mode
2958	CH_3	Asymmetric aliphatic
2929	CH_3	Asymmetric aromatic
1737	C=O	Saturated esters
1511	C-H	Stretch aromatic
1459	C-H	Stretch aromatic
1377	C-H	Stretch aromatic
1287	C-O	Symmetric
629	C-O	Intensive

At the wavelength of 2958 cm^{-1} the CH_3 functional group corresponding to asymmetric aliphatic appears. At the wavelength of 2929 cm^{-1} the CH_3 functional group corresponding to asymmetric aromatic appears. At the wavelength of 1737 cm^{-1} the C=O functional group corresponding to saturated esters appears. At the wavelength of 1511 cm^{-1} the C-H functional group corresponding to stretch aromatic appears. At the wavelength of 1287 cm^{-1} the C-O functional group corresponding to symmetric appears. At the wavelength of 629 cm^{-1} the C-O intensive functional group appears.

Figure 3 shows the IR spectrum of isotridecyl adipate and 2-(o-sec-butyl-phenoxy)ethyl.

Table 2 shows the assignment of peaks in the FTIR spectrum for isotridecyl adipate and 2-(o-sec-butyl-phenoxy) ethyl.

In the spectrum of isotridecyl adipate and 2-(o-sec-butyl-phenoxy) ethyl several absorption bands appear and the most important ones are presented in table 2.

At the wavelength of 2959 cm^{-1} the CH_3 functional group corresponding to asymmetric aliphatic appears. For the wavelength of 2929 cm^{-1} the CH_3 functional group corresponding to asymmetric aromatic appears. At the wavelength of 1737 cm^{-1} the C=O functional group corresponding to saturated esters appears. For the wavelength of 1491 cm^{-1}, 1377 cm^{-1}, 1356 cm^{-1} and 751 cm^{1} the C-H functional group corresponding to stretch aromatic appears.

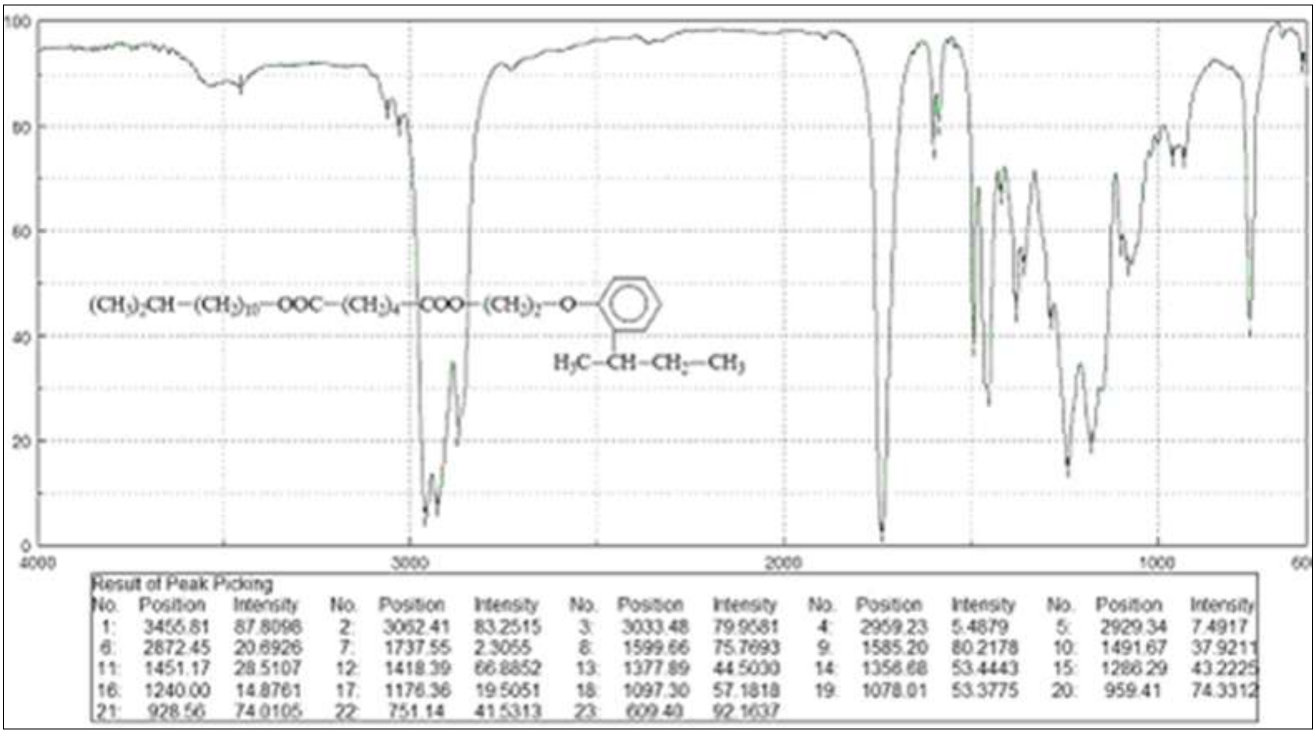


Fig 3: IR spectrum of isotridecyl adipate and 2-(o-sec-butyl-phenoxy) ethyl

Table 2: Assignment of peaks in the FTIR spectrum of isotridecyl adipate and 2-(o-sec-butyl-phenoxy) ethyl

Wave number, cm^{-1}	Functional grouping	Vibration mode
2959	CH_3	Asymmetric aliphatic
2929	CH_3	Asymmetric aromatic
1737	C=O	Saturated esters
1491	C-H	Stretch aromatic
1377	C-H	Stretch aromatic
1356	C-H	Stretch aromatic
751	C-H	Stretch aromatic

Figure 4 shows the IR spectrum of isotridecyl adipate and 2-phenoxy ethyl.

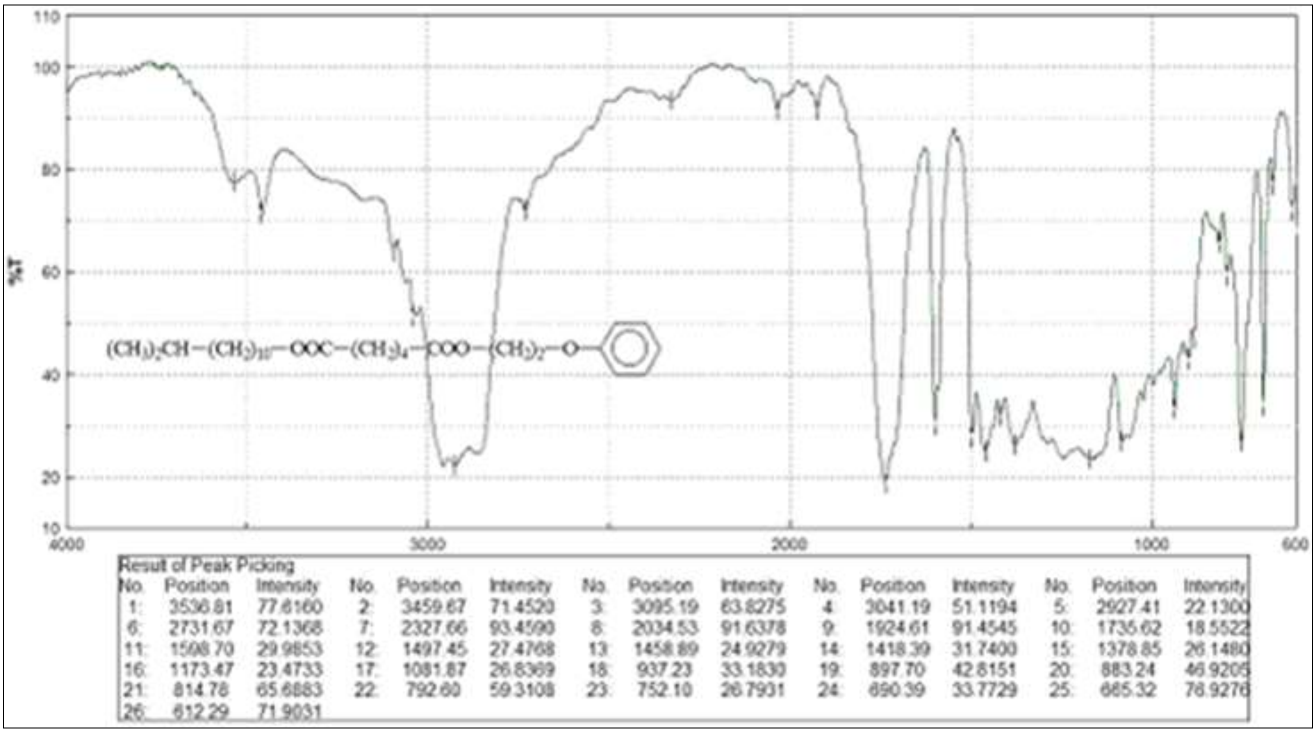


Fig 4: IR spectrum of isotridecyl adipate and 2-phenoxy ethyl

Table 3 shows the peak assignments in the FTIR spectra of isotridecyl adipate and 2-phenoxy ethyl.

The spectrum of isotridecyl adipate and 2-phenoxy ethyl shows fewer absorption bands and the most important ones are presented in Table 3.

At the wavelength of 2958 cm^{-1} the CH_3 functional group corresponding to asymmetric aliphatic appears. For the wavelength of 2872 cm^{-1} the CH_3 functional group corresponding to asymmetric aromatic appears. At the wavelength of 1735 cm^{-1} the C=O functional group corresponding to saturated esters appears. For the wavelength of 1241 cm^{-1} the C-O functional group corresponding to intense symmetrical appears. For the wavelength of 1173 cm^{-1} and 752 cm^{-1} the C-O functional group appears intensively.

Table 3: Peak assignments in the FTIR spectra of isotridecyl adipate and 2-phenoxy ethyl

Wave number, cm^{-1}	Functional grouping	Vibration mode
2958	CH_3	Asymmetric aliphatic
2872	CH_3	Asymmetric aromatic
1735	C=O	Saturated esters
1241	C-O	Stretch aromatic
1173	C-H	Stretch aromatic
752	C-H	Stretch aromatic

Conclusions

The absorption spectra of the following adipic esters isotridecyl adipate and 2-(p-nonyl-phenoxy) ethyl, isotridecyl adipate and 2-(o-sec-butyl-phenoxy) ethyl and isotridecyl adipate and 2-phenoxy ethyl contain the following functional groups: CH_3, C=O, C-O, C-H and were determined with FT-IR Jasco 430.

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