International Journal of Chemical Science
Online ISSN: 2523-2843, Print ISSN: 2523-6075
www.chemicaljournals.com
Volume 1; Issue 1; September 2017; Page No. 29-32

A complementary analysis of thyme essential oil by Fourier transformed infrared spectroscopy

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Abstract
The use of Fourier Transformed Infrared Spectroscopy (FTIR) techniques for the nondestructive analysis of biological specimens is a rapidly expanding research area. In the present study, the volatile compounds of Thyme (*Thymus numidicus* Poiret.) collected from Azzaba, Skikda city (Algeria), were detected and identified by Fourier Transformed Infrared Spectroscopy analysis. FTIR allowed us to identify 10 volatile compounds and indicated than the functional groups and the presence vibrational modes of the essential oils are CHx deformation (1500-1400 cm^{-1}), C-H (Aromatic) (3150-3050 cm^{-1}) and Alcohol/Phenol O-H Stretch (3550-3200 cm^{-1}). The obtained results have shown that the essential oils can be fully utilized for pharmacy, cosmetology and industry.

Keywords: thyme, *Thymus numidicus* Poiret., essential oil, fourier transformed infrared spectroscopy (FTIR), functional groups, vibrational modes

1. Introduction
The Algerian flora is characterized by its floral diversity: Mediterranean, Saharan and a tropical Palaeo flora, estimated at more than 3000 species belonging to several botanical families. These species are mostly spontaneous with a significant number (15%) of endemic species. This has given the traditional pharmacopoeia an inestimable richness [1].
Thymus numidicus Poiret.is an endemic species of Algeria and the Iberian Peninsula. It's a perennial plant with a short inflorescence or extended to verticillastres strongly interrupted and distant. The bracts and the bracteols minimized and the corolla may overstep or not the calyx, the flowering period extends from spring to summer. Due to the application of *Thymus* species growing wild in Algeria as a culinary herb and in folk medicine [2].
Most people either use essential oils for their therapeutic effect or for the fragrance alone but it is also interesting to take note of the chemistry, of which the oils are made up from.
Essential oils, like all organic compounds, are made up of hydrocarbon molecules and can further be classified as terpenes, alcohols, esters, aldehydes, ketones and phenols etc.
Every single oil normally has more than a hundred components, but this figure can also run into thousands, depending on the oil in question.
When you analyze essential oils with a chromatograph various organic components are found and the primary ones are as follows:

- Terpene hydrocarbons: Monoterpene hydrocarbons, Sesquiterpenes.
- Oxygenated compounds:Phenols, Alcohols.
- Monoterpene alcohols
- Sesquiterpene alcohols: Aldehydes, Ketones, Esters, Lactones, Coumarins, Ethers, Oxides [3].

Fourier Transformed Infrared Spectroscopy (FTIR) is based on the absorption of infrared radiation by the analyzed material. Through the detection of the characteristic vibrations of the chemical bonds, it makes it possible to carry out the analysis of the chemical functions present in the material [4].
The aim of this work was to clearly describe the functional groups of Thyme essential oil in order to better define the field of investigation of this natural product.

2. Material and Methods
2.1. Plant Material
Aerial parts of *Thymus numidicus* Poiret. (stems, leaves and flowers) growing wild in Azzaba located at Skikda city (North-east of Algeria) were collected on June 2013. The taxonomic identity of the plant was confirmed by the well-known Algerian flora of Quezel and Santa [1]. We gave also the following voucher specimen number: Boughendjioua & Djeddi: 01/2013.

2.2. Isolation of the Essential Oil
Aerial fresh parts of plant material (200 g) were submitted for 1 h 30 min to hydodistillation, using a Clevenger-type apparatus [5]. The obtained essential oil was dried with anhydrous sodium sulphate and stocked at 4 °C for later use.

2.3. FTIR Analysis
Spectroscopy is based on the study of the interactions between matter and electromagnetic radiation. This radiation consists of a particle beam having an undulating motion. All electromagnetic radiation forms the electromagnetic spectrum. In the spectrum, four regions are discernible: X-rays, ultraviolet (UV), visible and infra-red (IR). The emphasis will

be on infrared (IR) spectroscopy because spectrum analysis allows us to follow a reaction process, determine the dosage of a compound, check the purity of a product and identify an unknown. Moreover, it is an inexpensive and easy to use process which makes IR spectroscopy the most widely used spectral method used by chemists. The principle is based on molecular vibrations. The energy emitted as photons can be absorbed by the material causing vibration in the molecules. This vibration changes the angle and the distance between the atoms. When the molecule returns to its original form, energy will be released as heat. The absorption and release of energy by the molecule will be recorded by the apparatus and translated into a band spectrum. The analysis of this spectrum makes it possible to obtain the necessary information on the material analyzed.

FTIR is performed with a PERKIN ELMER (universal ATR Sampling Accessory) apparatus, the operating conditions are as follows: technique: ATR, analysis range: 4000- 600 cm $^{-1}$. The results are directly compared with those of the internal bibliography of the apparatus; Euclidean, 02. PSU / peak, 03. MIX PSU, 04. Peak Match, 05. PEAK / psu06.MIX PEAK. In our study we used the Euclidean library. The FTIR analysis was performed at the Regional Police Scientific Laboratory (Constantine, Algeria).

3. Results and Discussion

3.1. Determination of the functional groups present using FTIR

Fourier transform infrared spectroscopy is one of the most widely employed techniques for functional groups identification. Figures 01 to 03 and Table 01 showed the infrared spectra and the characteristic bands observed in Thyme essential oil in the range of 4000-600 cm[1]:

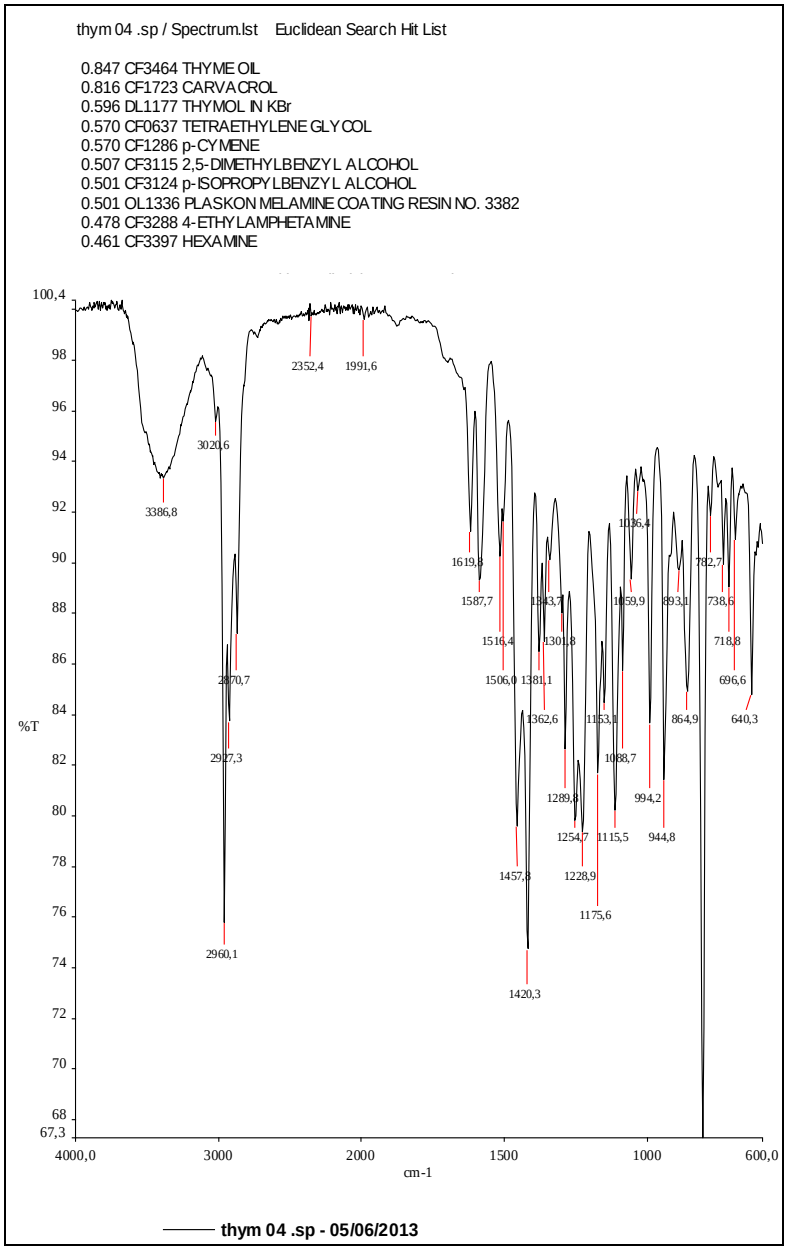

Fig 1: FTIR of Thyme essential oil

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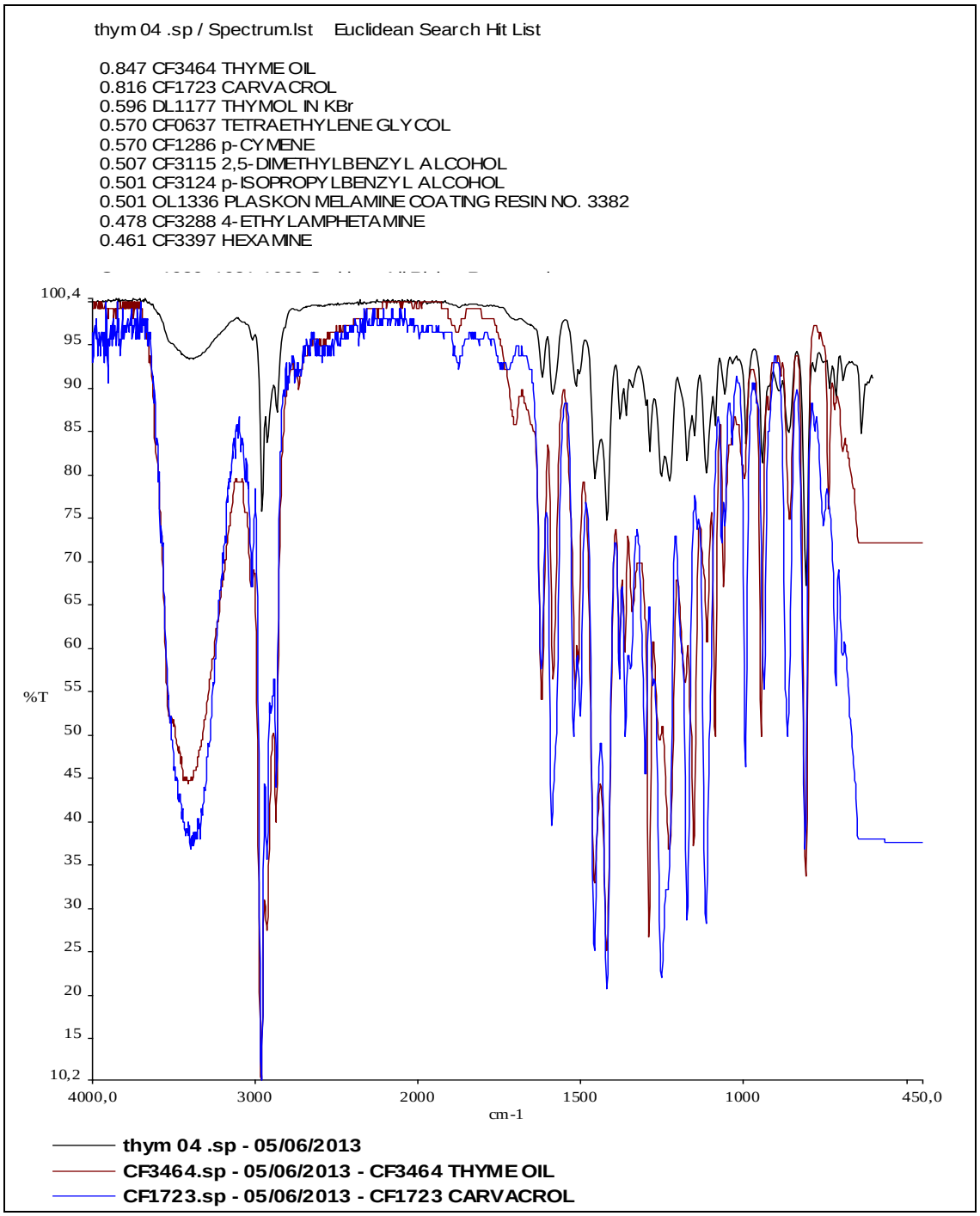

Fig 2: FTIR of Thyme essential oil compared to the bibliography.

Table 1: Links present in the Thyme essential oil.

Present links in essential oil	Theoretical frequency of the band (cm^{-1})	Presence of the band in the spectrum
CHx deformation	1500-1400	Yes
C-H (aromatic)	3150-3050	Yes
Alcohol/Phenol O-H Stretch	3550-3200	Yes

In an earlier work developed by Boughendjioua (2014) [6], the chemical composition of the essential oil of *Thymus numidicus* detected by GC–MS allowed us to identify 31 compounds and indicated that the main compounds constituting the volatile oil were mainly carvacrol (27.38%), thymol (22.47%) and *p*-cymene (9.41%).

Among the ten compounds revealed by FTIR: (1).thyme oil, (2).carvacrol, (3).thymol in kbr, (4).tetraethylene glycol, (5).p-

cymene, (6).2,5-dimethylbenzyl alcohol, (7).p-isopropylbenzyl alcohol, (8).plaskon melamine coating resin no. 3382, (9).4-ethylamphetamine, (10).hexamine.

On the other hand, the complete and detailed study of a spectrum is an operation rarely practiced in current interpretation because of the complexity of the analysis. It is therefore often limited to the identification of functional groups through the location of the different bands on the spectrum.

The spectrum presents characteristic bands at 1500-1400 cm^{-1} corresponding to CHx deformation, the signals which appeared between 3150-3050 cm^{-1} corresponding to C-H (aromatic) stretching, groups. For Alcohol/Phenol O-H with characteristic absorption 3550-3200 cm^{-1} (broad, s), is one of the most distinct and easily recognizable peaks in an IR spectrum is the broad O-H absorption of alcohols and phenols (Table 01 and Figure 03) [7].

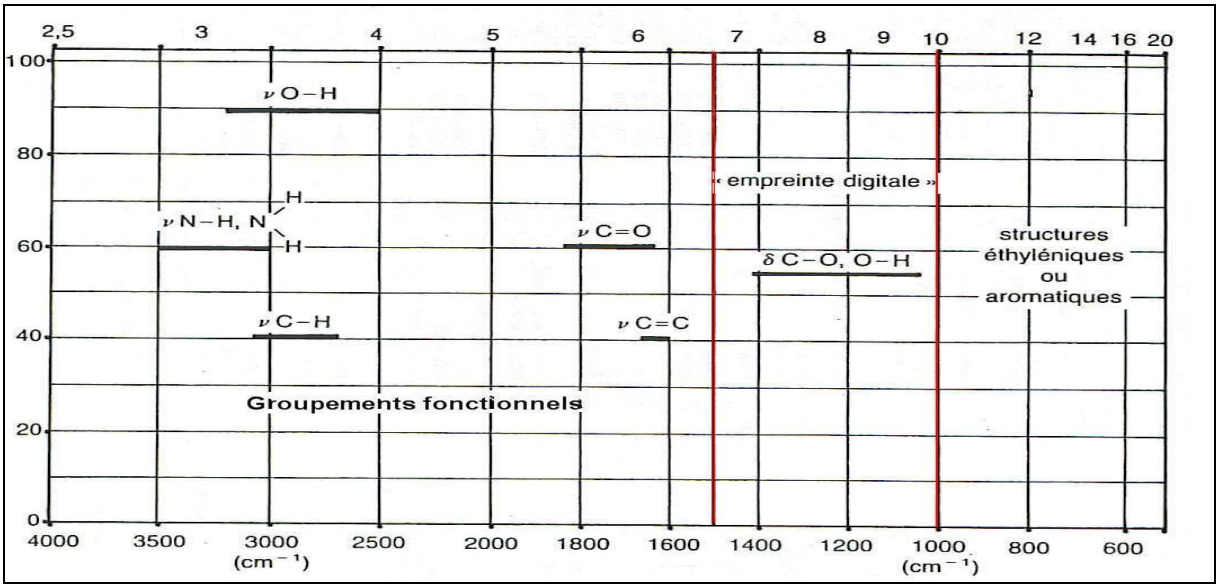

Fig 3: Graphs of IR spectroscopy.

4. Conclusion

IR Spectroscopy is an extremely effective method for determining the presence or absence of a wide variety of functional groups in a molecule; IR spectra can be used to identify molecules by recording the spectrum for an unknown and comparing this to a library or data base of spectra of known compounds. Computerized spectra data bases and digitized spectra are used routinely in this way in research, medicine, criminology, and a number of other fields. The ingredients obtained from this study indicate that the essential oil of Thyme (*Thymus numidicus* Poiret.) can be fully utilized for the manufacture of perfumery products, antimicrobial and antiseptic agents or even in petrochemical industry or alkenes serve as a feedstock for the petrochemical industry because they can participate in a wide variety of reactions, prominently polymerization and alkylation.

5. References

1. Quézel P, Santa S. Nouvelle flore de l'Algérie et des régions désertiques méridionales. Éditions du Centre National de la Recherche scientifique. Paris. 1962-1963; 2:1962-1170.
2. Boughendjioua H, Djeddi S, Seridi R. Chemical Composition, Antioxidant and Antimicrobial Activities of Thyme Essential Oil Wild-Growing in Algeria. European Journal of Scientific Research. 2014, 293-302.
3. The chemistry of essential oils, and their chemical components. http://essentialoils.co.za/components.htm. 27 may 2013.
4. Meskine M, Ouardi O. Analyse des fréquences rovibrationnelles des molécules octaédriques. Revue Algérienne de Physique. 2010; 04:62-68.
5. Clevenger JF. Apparatus for the determination of volatile oil. J Am Pharm Assoc. 1928; 17:346-1.
6. Boughendjioua H. Les plantes médicinales utilisées pour les soins de la peau. Composition chimique, activité antioxydante et antimicrobienne des huiles essentielles de *citrus limon*, *cinnamomum zeylanicum* et *thymus numidicus*. Doctorat en sciences spécialité: Biologie végétale. Université Badji Moktar, Annaba. 2014; 117:125-130.
7. Dias RF. Spectroscopy: How do we know what organic molecules look like? Organic Chemistry (CHEM311). 2005, 48-58.