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Fourier transformed infrared spectroscopy analysis of constituents of *Rosmarinus officinalis* L. essential oil from Algeria

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Abstract

Three main tools are used to determine the structures of organic molecules. These tools are infrared (IR) spectroscopy, mass spectrometry (MS) and nuclear magnetic resonance (NMR) spectroscopy. Infrared Spectroscopy (IR), Mass Spectrometry (MS) and Nuclear Magnetic Resonance Spectroscopy (NMR). Organic molecules absorb light (infrared, ultraviolet, etc.) at particular wavelengths based on different vibrational modes unique to the specific functional groups and structural features. In the present study, the volatile compounds of Rosemary (*Rosmarinus officinalis* L.) collected from Azzaba, Skikda city (Algeria), were detected and identified by Fourier Transformed Infrared Spectroscopy (FTIR) analysis. FTIR allowed us to identify 10 volatile compounds and indicated that the functional groups of the essential oils are Aromatic C=C Bending, C-H (Aromatic) and Carboxylic Acid O-H Stretch (broad, v). The obtained results have shown that the essential oil can be fully utilized for pharmacy, cosmetology and industry.

Keywords: Rosemary, *Rosmarinus officinalis* L., essential oil, Fourier Transformed Infrared Spectroscopy (FTIR), functional groups

1. Introduction

Rosemary (*Rosmarinus officinalis* L.) is an aromatic, medicinal and condiment plant that belongs to the family Labiatae. It is widely spread in Algeria and broadly used in traditional medicine [1]. Different parts of plants have been used to obtain essential oil. These include flowers, leaves, seeds, roots, stems, bark, and wood though secretory parts. Rosemary essential oil is of immense medicinal importance for its powerful anti-mutagenic, anti-phlogistic, anti-oxidant, chemo-preventive and anti-bacterial properties, anti-inflammatory, anti-septic, anti-spasmodic and anti-diabetic [2-3]. The essential oil of *Rosmarinus officinalis* L. has been the object of several studies as anti-oxidant activity [4-5], anti-bacterial [6, 7-8], toxicity insecticidal [9-10], anti-inflammatory and anti-nociceptive [11], anti-fungal and recently as a pest control product [12-13].

2. Materials and methods

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 [14].

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 [15].

2.1. Material

Leaf sample of *Rosmarinus officinalis* L. growing wild in Azzaba located at Skikda city (North-east of Algeria) were collected on March 2013. The taxonomic identity of the plant was confirmed by the well-known Algerian flora of Quezel and Santa (1962) [16], we gave also the following voucher specimen number: H. Boughendjioua & Z. Boughendjioua: 03/2013.

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2.2. Isolation of the Essential Oil

The extraction of essential oil from the leaves of rosemary was performed by hydro distillation in a Clevenger-type apparatus [17]. We conducted three distillations by boiling 200 g of dry plant material. The extraction time was about 3 hours in average. Yields are expressed in ml per 100 g of dry matter. Steam distillation is a special type of distillation (a separation process) for temperature sensitive materials like natural aromatic compounds. After distillation the vapors are condensed. The water vapor carries small amounts of the vaporized compounds to the condensation flask, where the condensed liquid phase separates, allowing for easy collection. Usually the immediate product is a two-phase system of water and the organic distillate, allowing for separation of the components by decantation, partitioning or other suitable methods. The essential oil obtained was dried by anhydrous sodium sulfate and then stored at low temperature (below 4°C) and dark before use.

2.3. Fourier Transformed Infrared Spectroscopy 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.

Qualitative information: The wavelengths to which the sample absorbs are characteristic of the chemical groups present in the analyzed material.

Quantitative Information: The intensity of absorption at the characteristic wavelength is related to the concentration of the chemical group responsible for absorption.

This method of analysis is simple to implement and not destructive. It allows the analysis of both organic and inorganic materials [14-15].

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 02 and Table 01 showed the infrared spectra and the characteristic bands observed in Rosemary essential oil in the range of 4000-600 cm⁻¹:

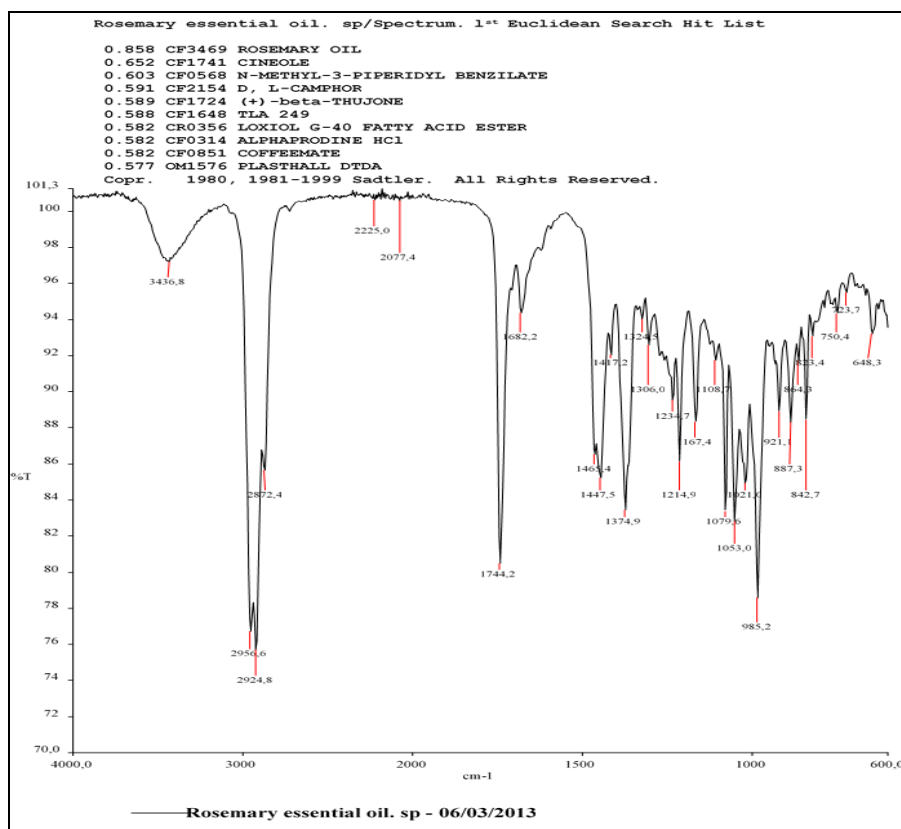


Fig 1: FTIR of *Rosmarinus officinalis* L. essential oil.

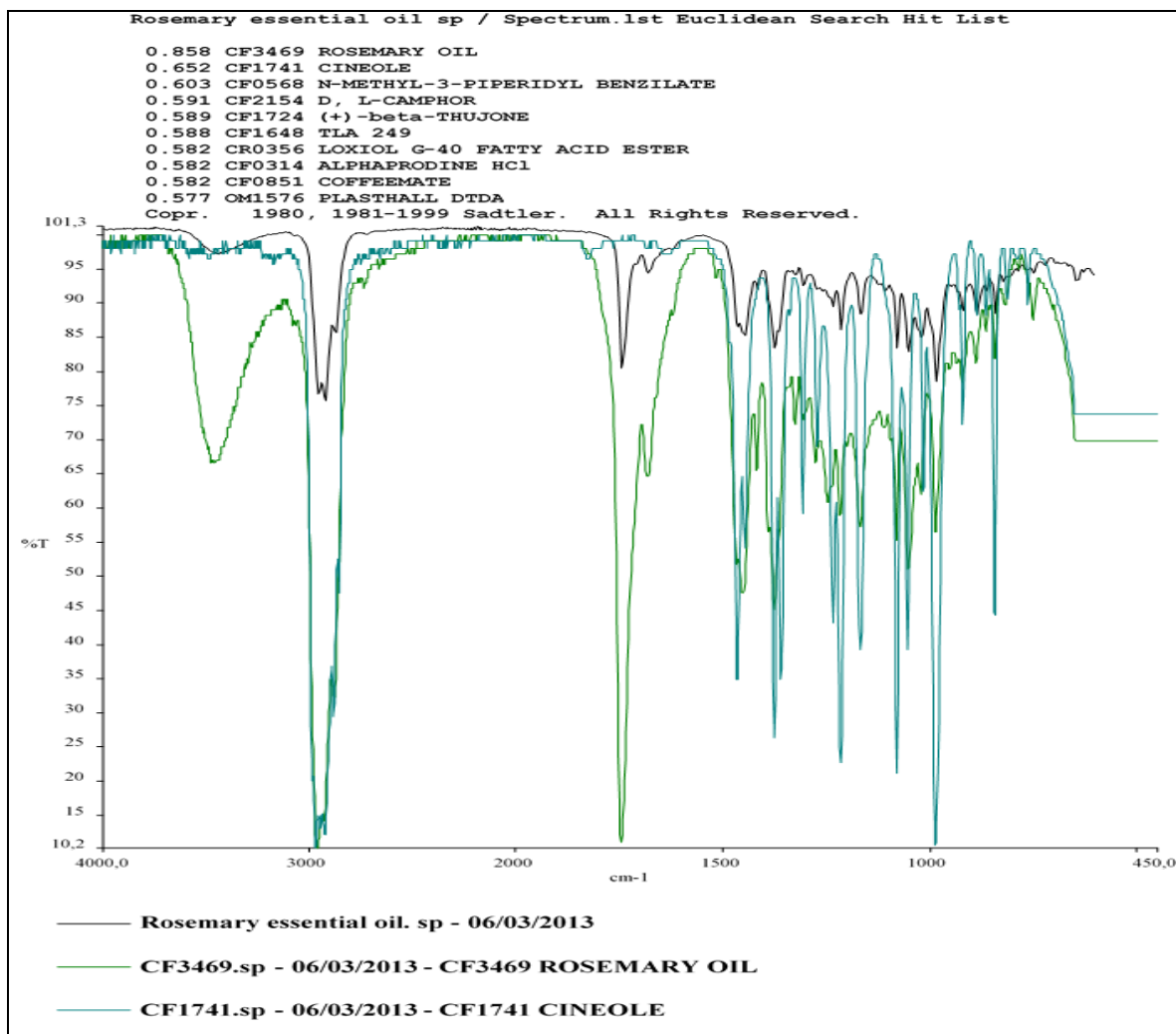


Fig 2: FTIR of *Rosmarinus officinalis* L. essential oil compared to the bibliography.

Table 1: Links present in *Rosmarinus officinalis* L. essential oil.

Present links in essential oil	Theoretical frequency of the band (cm ⁻¹)	Presence of the band in the spectrum
C=C Bending	1700 - 1500	Yes
C-H (aromatic)	3150 - 3050	Yes
Carboxylic Acid O-H Stretch	3000 - 2500	Yes

Among the ten compounds revealed by FTIR: (1). ROSEMARY OIL, (2). N-METHYL-3-PIPERIDYL BENZILATE, (3). CINEOLE, (4). D, L-CAMPHOR, (5). (+)-beta-THUJONE, (6). TLA 249, (7). LOXIOL G-40 FATTY ACID ESTER, (8). ALPHAPRODINE HCl, (9). COFFEEMATE, (10). PLASTHALL DTDA.

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 1700 – 1500 cm⁻¹ corresponding to C=C Bending, the signals which appeared between 3150-3050 cm⁻¹ corresponding to C-H (aromatic) stretching, groups. For Carboxylic Acid O-H Stretch with characteristic absorption 3000 – 2500 cm⁻¹ (broad, ν)^[18] (Table 01 and Figure 03).

Carboxylic acids exist predominantly as hydrogen bonded dimers in condensed phases. The O-H stretching absorption for such dimers is very strong and broad, extending from

2500 to 3300 cm⁻¹. This absorption overlaps the sharper C-H stretching peaks, which may be seen extending beyond the O-H envelope at 2990, 2950 and 2870 cm⁻¹. The smaller peaks protruding near 2655 and 2560 are characteristic of the dimer. In ether solvents a sharper hydrogen bonded monomer absorption near 3500 cm⁻¹ is observed, due to competition of the ether oxygen as a hydrogen bond acceptor. The carbonyl stretching frequency of the dimer is found near 1710 cm⁻¹, but is increased by 25 cm⁻¹ or more in the monomeric state. Other characteristic stretching and bending absorptions are marked in the spectrum.

According to Elzey *et al.*, (2016)^[19] the FTIR specter of the pure essential oil of Rosemary, showing the expected characteristic C-H stretch (~2900 cm⁻¹), C=O stretch (~1700 cm⁻¹), broad O-H stretch (~3400 cm⁻¹), and C-O stretch (~1100 cm⁻¹) of terpenoid components.

The compositions and constituents of essential oils may vary and highly depend on the geochemistry of the soil where it is cultivated. In general, essential oils are made up of terpenes such as terpineol, cineole, citronellal, and others.

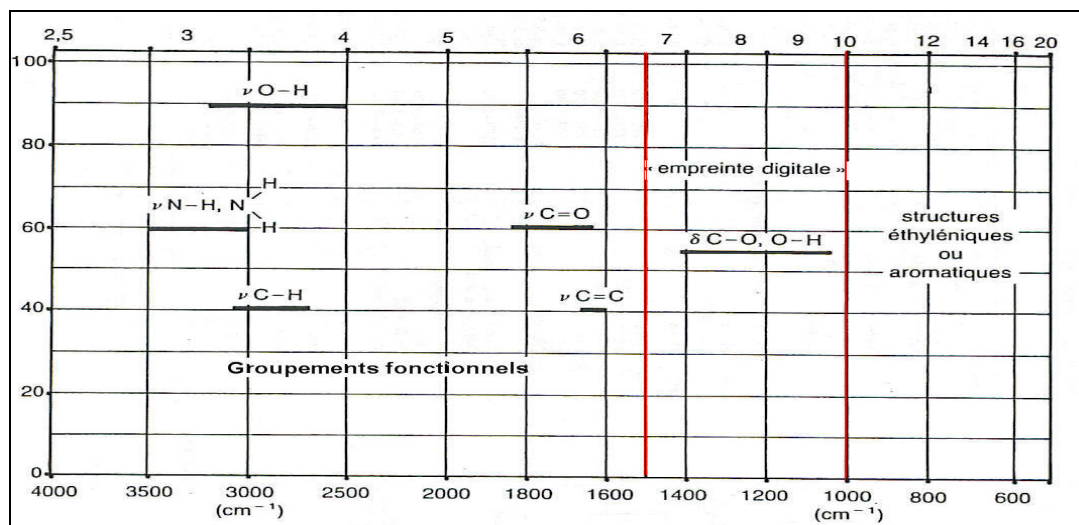


Fig 3: Graphs of IR spectroscopy.

4. Conclusions

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 Rosemary (*Rosmarinus officinalis* L.) can be fully utilized for the manufacture of perfumery products, antimicrobial and antiseptic products.

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