



Infrared absorption spectra of Buriti (*Mauritia flexuosa* L.) oil

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Abstract

Room temperature infrared absorption spectra from 650 to 4000 cm^{-1} of Buriti (*Mauritia flexuosa* L.) oil, a fruit from the Amazon region, is given. It is composed basically of fatty acids, tocopherols and carotenoids. The assignment of the observed bands was done based on the correlations with the infrared spectra of its individual components and other compounds already published.

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1. Introduction

It is well known that the Amazon region presents a huge biodiversity. Many plants and animals are still to be identified. It is the largest water reserve in the world. Among the plants, there are several from which fats and oils can be extracted. Fats and oils play an important role in the food industry. They are very important to human nutrition because they are the main source of energy for the human body. Since abundant reserves of such plants can be easily found, they are potential sources of vegetable oils with high and healthy nutritional values. Unfortunately, the knowledge of the benefits of the large variety of natural products from the Amazon region is still the heritage of a native population. Exploiting and understanding the physical and chemical properties of these

natural products has been a challenge for researchers in the past few years. For instance, the development of processes to remove oily substances from different raw materials, such as canola seeds [1], Bacuri shell and seed [2,3] and Tucumã seed [4].

Supercritical CO_2 extraction of the pulp of the Buriti fruit (*Mauritia flexuosa* L.) released Buriti oil fractions with a high concentration of vitamins, mainly β -carotene [5]. Recently, important physical chemical properties of Buriti oil, such as thermal diffusivity [6] and phase transitions were observed from dielectric constant measurements [7]. Despite the fact that Raman spectroscopic data for several other vegetable oils have already been reported [8], no data for Buriti oil is available. Therefore, as part of an investigation program into the properties of Buriti oil, we present here a room temperature spectroscopic characterization of Buriti oil in the range 650–4000 cm^{-1} using the infrared absorption technique. For understanding its complex structure, we have also carried out infrared measurements for two of its basic components. Assignment of most of the

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bands was performed on the basis of pure long-chain saturated and monounsaturated fatty acids, methyl esters and triglycerides of fatty acids and correlations with previous data reported for similar compounds.

2. Experimental

Buriti oil was extracted from the Buriti fruit by grinding chips of fruit (shell and pulp) in a comminuting mill. Extracts were analyzed using a gas chromatograph (Hewlett-Packard—model 5890A), and following the procedure described elsewhere [5]. Fatty acids (palmitic and oleic) were purchased from Merck & Co. Inc. and used as received. Fourier-transform infrared spectra were obtained from a Spectrum One FTIR Spectrometer with a spectral resolution of 1 cm^{-1} . For palmitic acid, the spectrum was obtained from KBr pellets while for oleic acid and Buriti oil, the spectrum was obtained through the horizontal attenuated total reflectance (HATR) technique using a ZnSe crystal. Eight spectra in the region $650\text{--}4000\text{ cm}^{-1}$ were run and the averaged spectrum was plotted as a percent transmittance curve versus wavenumbers.

3. Results and discussions

The Buriti oil is basically composed of fatty acids, tocopherols and carotenes. Table 1 displays the composition of the oil used in this work. The carotenes are responsible for the yellowish/reddish color of most

Table 1
Composition of the Buriti oil used in this work

Substance	Amount
Carotenoids (ppm)	1700 (min)
Tocopherols (ppm)	800 (min)
Free fatty acid composition (%)	
Saturated fatty acid	
Miristic	0.1
Palmitic	17.34–19.2
Stearic	2.0
Unsaturated fatty acid	
Oleic	73.3–78.73
Linoleic	2.4–3.93
Linolenic	2.2

vegetable oils. Among the 70 identified carotenes, the most important to the human body is β -carotene, which is the precursor of Vitamin A. The tocopherols are natural anti-oxidants forming Vitamin E. Among the eight different natural tocopherols presenting Vitamin E activity, α -tocopherol is the most important and corresponds to 90% of the total amount of tocopherols in animal tissues and has the largest biological activity. The fatty acids present in the Buriti oil are said to be of long chain [5]. They are split into two groups: (i) saturated, where the carbon atoms are σ bonded, and (ii) unsaturated, where the carbon atoms are σ and π bonded. Palmitic acid is saturated, while oleic acid is an unsaturated acid.

Data related to the infrared absorption spectra of α -tocopherol quinone and β -carotene can be found in Refs. [9,10], respectively. Since, no significant contributions from α -tocopherol and β -carotene to the spectrum of Buriti oil were observed, in Fig. 1 we show the room temperature infrared spectrum of Buriti oil and two of its major components, namely, oleic and palmitic acids. The assignment of the vibration at 3475 cm^{-1} appearing in the spectrum of Buriti oil (band #1) will be given below. The vibration at 3006 cm^{-1} in the spectrum of oleic acid, observed from Raman measurements [11], is assigned as the CH stretching related to $=\text{C}-\text{H}$ bonding. Following this reference we also assign the band appearing at

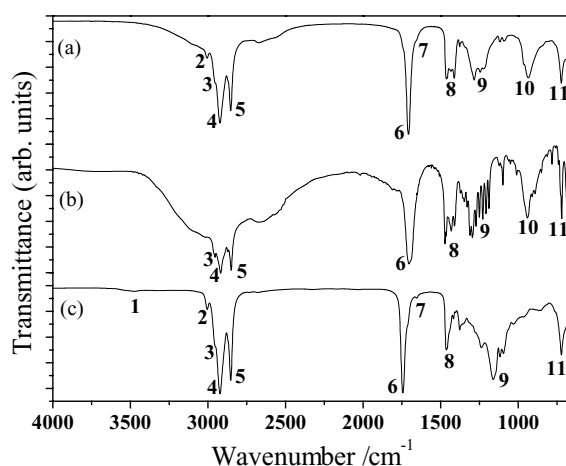


Fig. 1. Room temperature infrared absorption spectra in the range $650\text{--}4000\text{ cm}^{-1}$ of: (a) oleic acid, (b) palmitic acid, and (c) Buriti oil.

3006 cm^{-1} (band #2) in the spectrum of Buriti oil to the CH stretching of =C–H bonding. Similar vibrations were also observed for other vegetable oils [8]. Three vibrations are observed in the 2840–2960 cm^{-1} range. They appear not only in the spectrum of fatty acids [12] but also in those of triglycerides [13], and are assigned to the C–H stretching of methyl (CH_3) and methylene (CH_2) groups. The vibration at 2954 cm^{-1} (band #3) is assigned to the asymmetric stretching band of a CH_3 group. In the infrared spectrum of stearic acid this vibration also appears at around 2954 cm^{-1} [14]. The two intense bands at 2922 cm^{-1} (band #4) and 2854 cm^{-1} (band #5) are due to CH_2 asymmetric and symmetric stretching vibrations, respectively. From the Raman spectra of soybean, palm and palm kernel oils [8] these vibrations were observed at 2926 and 2855 cm^{-1} , respectively.

The band at 1744 cm^{-1} is assigned to the C=O stretching vibration of the carboxylic groups [13]. It appears around the same frequency for methyl esters and triglycerides; for long-chain fatty acids it appears at around 1700 cm^{-1} . Lie Ken Jie et al. [15] observed this band from infrared and Raman measurements of all 2,5-disubstituted C_{18} finanoid fatty esters. Hence, the observation of this band in the spectrum of the Buriti oil indicates the presence of the ester function. This vibration was observed at around 1743 cm^{-1} (see Ref. [8]). At 1655 cm^{-1} (band #7) we observe a very weak band which is assigned to a C=C stretching vibration [16]. This assignment seems to be correct once this vibration does not appear in the spectrum of the palmitic acid, which does not have such a bond in its structure (see Fig. 2). At 1464 cm^{-1} we observe a band (#8) which is assigned to CH_2 scissors deformation vibration [11,17]. In the room temperature spectrum of some fatty acids [12] it appears as a doublet. However in the spectrum of the oleic acid it appears as a single band which splits into a doublet with decreasing temperature [11,18]. In Ref. [8] this band was observed also as a single band at 1439 cm^{-1} . This vibration was observed also as a single band at 1439 cm^{-1} (see Ref. [8]).

The next region to be analyzed runs from 1290 to 1040 cm^{-1} (band #9). In the spectrum of fatty acids with the formula $(\text{CH}_3(\text{CH}_2)_n\text{COOH}; n = 14–16)$, for example, palmitic acid, several narrow bands are observed. These bands are the so-called progressional bands [19,20] that arise from the CH_2 wagging and

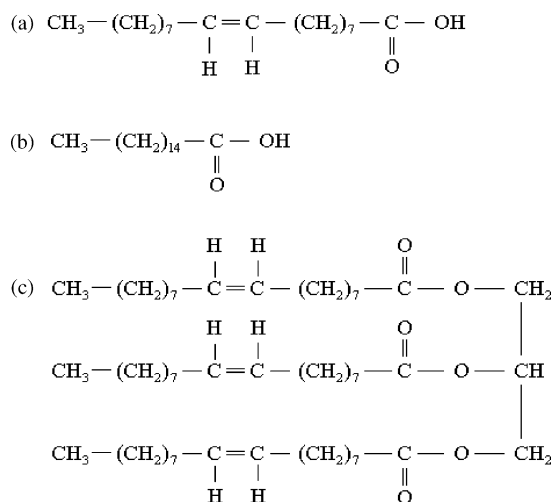


Fig. 2. Chemical structure of: (a) oleic acid, (b) palmitic acid, and (c) triolein.

twisting vibrations. However, for oleic acid, whose formula is $(\text{CH}_3(\text{CH}_2)_7\text{CH}=\text{CH}(\text{CH}_2)_7\text{COOH})$, a different pattern is observed; instead of several narrow bands, one sees a broad band with some structure. This vibration is assigned to the C–C (either COOH- or CH_3 -sided) stretching (see Ref. [11]). The difference observed is probably due to C=C bonding. In the spectrum of the Buriti oil, two changes are observed: (i) the pattern is different, and (ii) it shifts to lower frequency values. The broad band is replaced by a strong band at 1161 cm^{-1} flanked by weaker bands at 1238 and 1118 cm^{-1} . This profile is also observed in the spectrum of the triolein, a triglyceride of oleic acid [21,22]. The triolein molecule is formed by the reaction of three molecules of oleic acid with one of glycerol (see Fig. 2). So the mass of the right-hand side of C–C bond is increased, leading to a decrease in the frequency of this vibration. We therefore assign this mode as C=C–C–O stretching. Similar spectra were reported in Ref. [8]. These results indicate that the formation process of the Buriti oil molecule should be very similar to the triolein. Such characteristics can make the Buriti oil a candidate to prevent against LDL cholesterol.

The band (#10) observed in the spectrum of the fatty acids around 940 cm^{-1} has been assigned to either a C–C vibration [23] or a C=C–H out-of-plane vibration [11]. Due to the fact that this band is not observed in the spectrum of other vegetable oils [8,24], it suggests

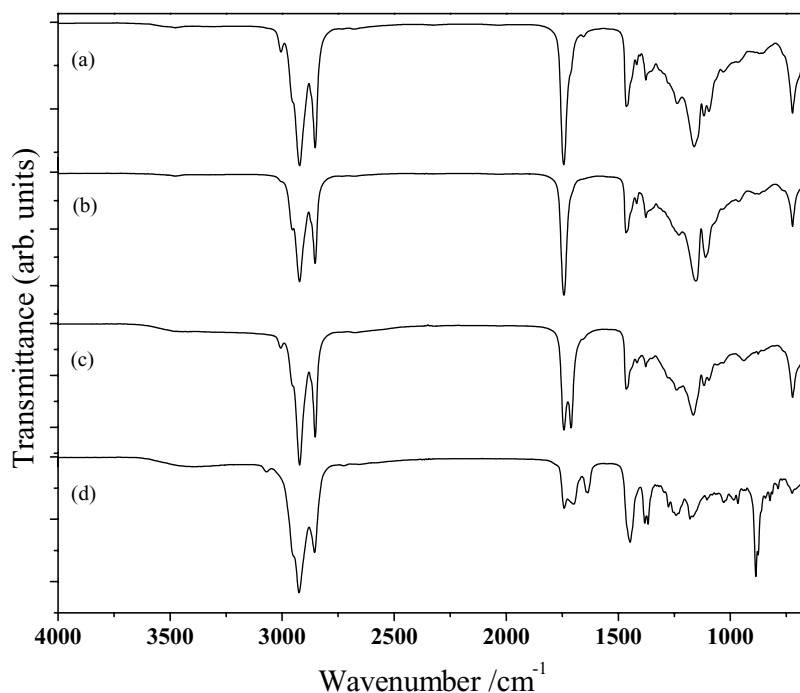


Fig. 3. Room temperature infrared absorption spectra in the range 650–4000 cm^{-1} of: (a) Buriti, (b) Babaçu, (c) Andiroba, and (d) copaiba oils.

that this band is indeed related to the $-\text{C}-\text{C}-\text{O}$ motion. The band at 722 cm^{-1} (#11) is observed in the spectrum of fatty acids and triglycerides; it is assigned to the CH_2 rocking mode [17]. Finally, let us discuss the assignment of band #1. In the spectra of fatty acids it is undoubtedly assigned to the stretching vibration of OH group. In the proposed model for the formation of Buriti oil molecule, no OH groups are present. However, due to humidity some H_2O molecules can be

present [25], therefore resulting in the observation of band #1.

For the sake of completeness, in Fig. 3 we display the infrared absorption spectra of other vegetable oils also obtained from the Amazon region. Despite the fact we do not have complete information about their chemical composition, Fig. 3 shows that their infrared spectrum are very similar indicating that oleic and palmitic acids are probably their major components.

Table 2
Relevant infrared bands and assignments of the oils investigated

Bands	Buriti (cm^{-1})	Babaçu (cm^{-1})	Andiroba (cm^{-1})	Copaiba (cm^{-1})	Assignments
1	3475	3478			OH stretching
2	3006	3007	3005	3070	(=C–H) stretching
3	2954	2955	2953	2950	CH_3 asymmetry stretching
4	2922	2923	2923	2924	CH_2 asymmetry stretching
5	2854	2854	2854	2855	CH_2 symmetry stretching
6	1744	1743	1741	1742	C=O stretching
7	1655	1664	1657		C=C stretching
8	1464	1464	1463	1447	CH_2 scissors
9	1040–1290	1040–1290	1040–1290		C=C–C–O
11	722	722	722	724	CH_2 rocking

Although they look very similar, there exists differences between the infrared spectra of the first three oils and that of copaiba. Two changes are clearly observed: (i) the pattern of the bands at around 1160 cm^{-1} and (ii) the appearance of a band at 886 cm^{-1} . The latter can be due to the vibration of the structure $\begin{array}{c} \diagup \\ \text{C}=\text{C} \\ \diagdown \end{array} \begin{array}{c} \text{H} \\ | \\ \text{H} \end{array}$, which is not present in the structures of fatty acids, esters and triglycerides of fatty acids. This explains why the pattern of the band at 1160 cm^{-1} is different. In fact, the copaiba oil is not obtained from either the kernel or the pulp of fruit, but rather is obtained from the trunk of the tree. It is therefore a resin oil which has several resinous and aromatic acids different from those found in the vegetable oils. The spectral differences mentioned above can therefore be used to distinguish pure vegetable oils from vegetable resin-oils. In Table 2 we display the observed infrared bands for the vegetable oils and their possible assignment.

4. Conclusions

Here we have used the infrared absorption technique to obtain the room temperature vibrational spectra of the Buriti oil and other vegetable oils from the Amazon region. The assignments for the infrared bands were based on the correlations with fatty acids, esters and triglycerides of fatty acids and similar results found for other vegetable oils. It is observed that the spectrum of Buriti oil is very similar to that of triolein, a triglyceride of oleic acid. This result not only indicates which is the formation process of the Buriti oil molecule but opens the possibility of using it to avoid LDL cholesterol. Other vegetable oils were also analyzed. We have found changes in the infrared spectra that make it possible to distinguish between pure vegetable oil from vegetable resin-oil.

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