Characterization of Some Volatile Constituents of Carrots

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A steam volatile oil obtained from carrot root (*Daucus carota* L. var. Sativa; type Imperator), amounting to 40 p.p.m. of the carrot root, has been analyzed, using capillary and conventional gas-liquid chromatography separation with characterization by mass and infrared absorption spectrometry. Major components identified were terpinolene, γ-bisabolene, γ-terpinene, caryophyllene, sabinene, eight other terpenoid hydrocarbons, falcarinol, terpinene-4-ol, bornyl acetate, α-terpineol, myristicin, 2-nonenal, octanal, and eight other oxygenated compounds. Odor thresholds of a number of these components were measured in water solution; 2-nonenal appeared to contribute most to the total odor of dilute water solutions of the oil.

Carrots are a relatively important food crop in the U.S.A., and are used extensively for processing into canned, frozen, and dehydrated products. Consequently a knowledge of what compounds cause their characteristic odor and taste is desirable for controlling flavor in the various processed forms of carrot. Pigulevskii and coworkers in Russia (Pigulevskii and Motskus, 1962) and other workers have made fairly extensive studies of the composition of carrot seed oil (Seifert *et al.*, 1968). Very little work has, however, been done on the volatile oil of the carrot root, which is quite different in odor and taste from carrot seed oil. This paper deals with the identification of the components of the volatile oil of carrot roots and estimates their contribution to the total odor intensity of carrot root oil in water.

EXPERIMENTAL

Isolation of Steam Volatile Oil. Carrots (*Daucus carota* L. var. Sativa; type Imperator), freshly obtained from a local market with their tops removed, were cut into pieces about 1 to 2 inches long and treated in a steam distillation: continuous extraction apparatus of the type described by Likens and Nickerson (1964). In a typical isolation, 7 kg. of carrots were refluxed with 2 liters of water in a 12-liter flask and the condensed water returning to the flask was continually extracted with pentane in the Likens extraction head. A total of 100 ml. of purified pentane was used. The Likens extraction head was modified slightly by adding an additional condenser in the steam side arm. The apparatus was used both at atmospheric pressure with the carrots at approximately 100° C. and at reduced pressure (60 to 80 mm. of Hg) with the carrots at 40° to 45° C. and heptane instead of pentane as the extracting solvent. Ice water was used to cool the condensers.

The pentane or heptane extracts were extracted with $NaHCO_3$ solution (1 × 50 ml.), dried over Na_2SO_4, and concentrated at atmospheric pressure using low holdup fractionating columns and progressively smaller containers. A 5-minute period on a Rotovac at room temperature removed the last traces of pentane.

A typical steam distillation–extraction at atmospheric pressure with this apparatus for 2 hours gave 0.28 gram of oil from 7 kg. of carrots, a concentration in the original carrot of 40 p.p.m. A similar value was obtained when using reduced pressure.

Preliminary GLC Analysis of Whole Oil. The carrot root from above was examined by GLC on a 150-foot × 0.01-inch I.D. stainless steel capillary coated with silicone SF 96-100 (5% Igepal CO-880) programmed linearly from 50° to 160° C. at 0.5° per minute. This gave a general idea of the range and types of compounds present by comparison of peak retention times with those of authentic compounds. A preliminary separation of components was also carried out by GLC on a 500-foot long × 0.03-inch I.D. stainless steel capillary coated with silicone SF 96-100 (+5% Igepal CO-880) programmed nonlinearly from 50° to 160° C. Components were collected in boro-

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silicate glass capillary tubes and examined by mass spectrometry.

Separation into Hydrocarbon and Oxygenated Fractions. The carrot root oil was separated into its oxygenated and hydrocarbon components by selective absorption on silica gel. The oil (0.28 gram) was placed on a column of silica gel (11 cm. long × 1-cm. diameter) in pentane (10 ml.). The hydrocarbon fraction was eluted with 150 ml. of pentane. The oxygenated fraction was then eluted with 50 ml. of ether. The solvent was removed as before to give the hydrocarbon fraction (0.16 gram) and the oxygenated fraction (0.085 gram). These amounts were typical of a number of separations.

Isolation of High Boiling Carotatoxin Fraction. A sample of whole carrot root oil as isolated above (0.6 gram) was distilled under vacuum at 120° C. and 0.1 mm. of Hg. This gave a residue (0.15 gram) which was examined by infrared spectra.

GLC Separation of Hydrocarbon Components. A 1000-foot long × 0.03-inch I.D. stainless steel capillary coated with silicone OV-17 (+5% Igepal CO-880) was used at 80° and 150° C. to resolve the hydrocarbon fraction into its terpene and sesquiterpene components, which were trapped separately and examined batchwise by mass spectrometry. The hydrocarbon fraction was also resolved into its components using a 10-foot × 1/4-inch aluminum column packed with 60- to 80-mesh Chromosorb P coated with 10% silicone SF 96-350 programmed nonlinearly to 180° C. and held. The components were collected in 1.5-mm. I.D. borosilicate glass tubes for infrared spectra.

Capillary GLC: Mass Spectral Analysis of Oxygenated Fraction. The oxygenated fraction was analyzed by the direct introduction of the effluent from a 600-foot × 0.02-inch I.D. capillary GLC column into the ionization chamber of a Bendix Time-of-Flight mass spectrometer. The technique used was similar to that described by McFadden *et al.* (1965). The capillary column used was 600 foot long × 0.02-inch I.D. stainless steel coated with silicone SF 96-100 containing 5% Igepal CO-880. A Watson and Biemann (1964) type molecular separator was used at the end of the column to reduce the percentage of helium entering the mass spectrometer. During the analysis a concurrent gas chromatogram was recorded by integrating a portion of the signal from the complete mass spectral output. This gave a GLC pattern very similar to that obtained with the flame ionization detector.

Compounds were identified by interpretation of the mass spectra followed by comparison with the mass spectra of authentic samples. This identification was further verified by comparison of the retention time of the authentic sample with that of the unknown on the 600-foot × 0.02-inch capillary. Exact location of an authentic peak was obtained by incorporating a sample of the authentic compound with the carrot root oxygenated fraction.

The oxygenated fraction was also separated into components in amounts large enough for infrared spectra by GLC separation on a 10 foot long × 1/4-inch O.D. aluminum column packed with 80- to 100-mesh Chromosorb P coated with 10% silicone SF 96-350 and 0.5% Igepal CO-880. The column was programmed from 80° to 160° C. at 1° per minute. A total of 29 components were collected and their infrared spectra measured.

Girard Separation of Carbonyls from Oxygenated Fraction. The oxygenated fraction (0.085 gram) was dissolved in 15 ml. of methanol and added to a solution of 8 grams of Girard T reagent in 40 ml. of methanol. The mixture was stirred for 3 hours at room temperature under an inert (argon) atmosphere, then added to 700 ml. of ice water, and extracted five times with 125-ml. portions of ether. The ether was dried over Na_2SO_4 and removed carefully in the usual way to give the noncarbonyl fraction. The aqueous layer from the extraction was mixed with 500 ml. of cold 4*N* HCl and 150 ml. of pentane containing a trace of the antioxidant Ionox 330. This mixture was then stirred for 3 hours at room temperature under an inert atmosphere (argon). It was then placed in a separatory funnel and the aqueous layer extracted three times with 100-ml. lots of pentane. The combined pentane extract was dried over Na_2SO_4 and the pentane removed carefully to give the carrot root carbonyl fraction.

The carbonyl fraction was separated into its components by GLC separation on a 500-foot × 0.03-inch I.D. stainless steel capillary coated with silicone SF 96-100 (containing 5% Igepal CO-880 by weight of the silicone). Using nonlinear programming from 110° to 160° C., individual fractions were collected in small tubes for batch introduction into the mass spectrometer.

Isolation of Sabinene and Myrcene from Carrot Top Stems. Carrot top stems (1280 grams) with the leafy material removed were treated with the Likens steam distillation: continuous extraction apparatus (2 liters of water) for 2 hours at atmospheric pressure and the pentane extract obtained (100 ml.) concentrated carefully as before to give an oil (0.28 gram), which was separated into its two major components with a 1000-foot × 0.03-inch I.D. stainless steel capillary coated with silicone OV-17. The mass and infrared spectra of the separated components were measured.

The concentrations of myrcene and sabinene in the oil were calculated by injecting standard solutions and comparing peak areas.

Infrared Absorption Spectra. Infrared spectra were recorded on a Perkin-Elmer 237 double beam grating instrument. The samples were generally run neat as films between 3 × 9 mm. salt plates or in CCl_4 in a 0.05-mm. microcell.

Mass Spectra. A Bendix Time-of-Flight mass spectrometer was used in direct combination with the capillary separation of the oxygenated components as described above. Batch samples were generally collected for mass spectra in 15-cm. × 0.1-mm. borosilicate glass melting point tubes containing a spiral of Nichrome wire at the center of the tube of the type described by Teranishi *et al.* (1966). After collection the tube was sealed under vacuum. Samples were analyzed by breaking the tube inside the inlet system of a modified CEC Model 21-620 mass spectrometer.

Odor Evaluation of Fractions and Components. The principal effort in evaluating the various fractions and components for their contributions to the total odor intensity of the carrot root oil involved measurements of sensory thresholds (Guadagni *et al.*, 1966). The solutions for threshold measurements were made up in odor-free distilled water and submitted to a panel of 15 to 20 judges

in 8-ounce (*ca.* 250 ml.) flexible Teflon bottles equipped with short (10 cm.) Teflon tubes. The judges gently squeezed the bottles, forcing the vapor above the solution through the tubes and into the nose.

RESULTS AND DISCUSSION

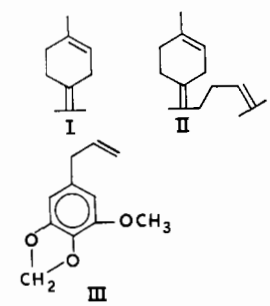
As carrots are usually eaten cooked, it was thought that isolation using steam distillation at atmospheric pressure would be a satisfactory method of isolating carrot root volatiles. A Likens extraction head was used.

The oil obtained (40 p.p.m. of the carrot root) possessed an odor similar to that of cooked carrots. The main study was carried out with this atmospheric pressure steam distilled oil. However, for comparison, carrots were also steam distilled under reduced pressure at 40° to 45° C. in the same apparatus described above. Capillary GLC analysis showed only minor differences in the composition of the two oils except for a few specific peaks. It was notable that the oil obtained under reduced pressure had an odor similar to that of raw carrots.

A preliminary study showed that the major constituents were terpene and sesquiterpene hydrocarbons. Compounds containing oxygen or other polar groups are generally more important to flavor than hydrocarbons. Analysis of the oxygenated material was difficult in the whole oil because the predominant hydrocarbons overlapped a high percentage of the oxygenated components even on the most efficient capillary columns. A useful, widely used technique in the analysis of an essential oil is to separate the oil into nonpolar (mostly hydrocarbons) and polar (mostly oxygenated components) fractions by selective adsorption on a silica gel column. Application of this technique to carrot oil divided it into 58% nonpolar fractions (hydrocarbons) and 30% polar (oxygenated). The polar or oxygenated fraction possessed the most characteristic cooked carrot odor. Calculations showed that the hydrocarbon fraction amounted to a concentration of 24 p.p.m. and the oxygenated fraction to 12 p.p.m. in the carrot root.

In the first GLC studies no peaks which might correspond to the known component of carrots, falcarinol or carotatoxin (Bentley and Thaller, 1967; Crosby and Aharonson, 1967), were detected and it was thought that such a large molecule would not be sufficiently steam volatile to occur in any appreciable amount in the carrot root oil. However, calculations of the percentages of oxygenated components from GLC of the oxygenated fraction compared to those calculated for the GLC of the whole oil indicated that a large part of the oxygenated fraction was not being detected by the GLC conditions used. Infrared analysis of the whole oxygenated fraction showed that it contained a large percentage of an acetylene compound which proved to be falcarinol (carotatoxin). This compound was obtained in relatively pure form by distilling off all of the other components. The infrared spectrum of the residue was essentially identical to that reported for falcarinol (Crosby and Aharonson, 1967) with maxima at (4 to 15 microns, S strong, M medium, W weak): S(5.86, 6.9, 7.3, 8.1, 9.8, 10.1), M(4.4, 8.6, 8.9, 10.7), W(6.1, 6.6, 7.9, 9.2, 11.4, 14.2 microns).

Hydrocarbon Fraction. Figure 1 shows a capillary GLC analysis of the hydrocarbon fraction. Table I lists the identities of the peaks, with the evidence used for their identification. Terpinolene (I), peak 13, the major monoterpene, formed more than 60% of the hydrocarbon fraction. The major sesquiterpenes were γ-bisabolene (II), peak 28, and caryophyllene, peak 18. γ-Bisabolene was identified by comparison with infrared and NMR spectra reported by Minyard *et al.* (1966) who also noted its structural relationship to terpinolene.



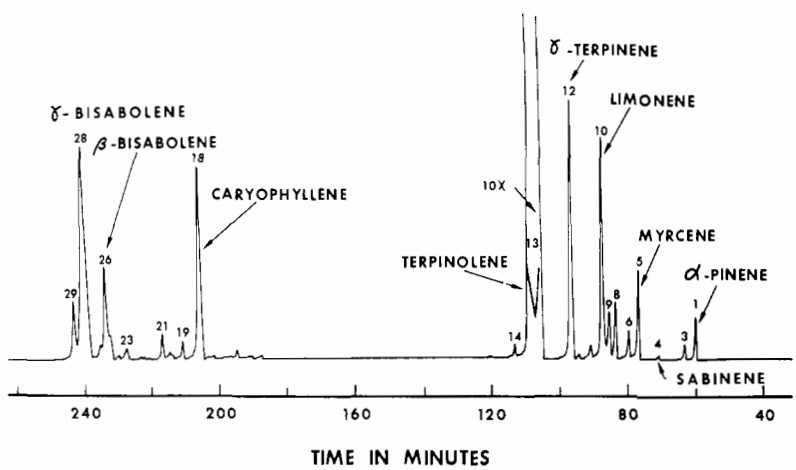


Figure 1. Capillary GLC chromatogram of hydrocarbon fraction from carrot root oil (atmospheric steam distilled) using a 150-foot × 0.01-inch I.D. silicone SF 96 coated capillary programmed from 50° to 160° C. at 0.5° C. per minute and held

Table I. Identity of Hydrocarbon Components in Carrot Root Oil (Atmospheric Steam Distilled)

Peak No. (Figure 1)	Confirmed Identity[a,b]	Relative % in[c] Whole Oil
1	α-Pinene, MS, RT	0.6
3	Camphene, MS, RT	0.2
4	Sabinene, MS, RT	4.0[d]
4a	β-Pinene, MS, RT	0.1
5	Myrcene, MS, RT	0.8
8	α-Terpinene, MS, RT	0.7
9	*p*-Cymene, MS, RT	0.3
10	Limonene, MS, RT	3.8
12	γ-Terpinene, MS, RT	5.4
13	Terpinolene, MS, IR, RT	38
18	Caryophyllene, MS, IR, RT	5.1
26	β-Bisabolene, MS	2.9
28	γ-Bisabolene, IR, NMR	6.6

[a] MS, IR, RT = mass spectral, infrared absorption spectral, and GLC retention time evidence, respectively. [b] Evidence cited consistent with that of authentic compound or published data. [c] Calculated from GLC of hydrocarbon fraction. [d] Calculated from GLC of whole oil.

Of the monoterpenes, sabinene was next highest in concentration to γ-terpinene in the whole oil but was almost completely rearranged on the silica gel to α- and γ-terpinene (Wrolstad and Jennings, 1965). Direct injection of the vapor above carrots into a sensitive GLC apparatus also showed larger amounts of sabinene and confirmed the presence of the other monoterpenes shown in Table I, particularly α- and γ-terpinene in the original carrot, although their concentration is increased in the hydrocarbon fraction by the sabinene rearrangement. No other rearrangements on the silica gel were observed.

Sabinene and myrcene in dilute water solution gave odors somewhat similar to that of the green tops of carrots rather than the root. Subsequent analysis of the steam volatile oil of carrot top stems showed that myrcene and sabinene were the principal components (infrared and mass spectra identical to that of authentic samples). They occurred in amounts much greater than that of any other components detected by GLC, in approximately equal concentration at 40 p.p.m. each in the carrot top stems (wet weight).

Infrared spectral data for hydrocarbon components were (in the region 5 to 15 microns, S strong, M medium, and W weak):

Terpinolene S(6.9, 7.3), M(7.9, 8.2, 8.3, 8.6, 9.0, 10.9, 12.6), W(10.8, 7.7, 8.5, 9.3, 9.9, 10.8, 12.1, 12.6, 13.1) microns.

Caryophyllene S(6.9, 7.27, 7.33, 11.3, 11.4), M(6.15, 7.9, 8.5, 10.2), W(6.0, 6.3, 8.0, 8.2, 9.1, 9.4, 12.2, 12.3, 14.7) microns.

γ-Bisabolene S(6.9, 7.25), M(9.0, 12.1, 12.5), W(6.0, 6.6, 7.5, 7.7, 7.9, 8.2, 8.3, 8.5, 8.6, 9.3, 9.5, 9.8, 10.1, 10.4, 10.7, 10.9, 11.2, 13.0) microns.

Mass spectral data found for hydrocarbon components were (molecular ion and 5 to 10 major ions):

α-Pinene, mol. ion 136, major ions 93, 92, 91, 77, 79, 121, 68.

β-Pinene, mol. ion 136, major ions 93, 69, 79, 91, 77, 67, 80, 121.

Camphene, mol. ion 136, major ions 93, 121, 79, 67, 55, 77.

Sabinene, mol. ion 136, major ions 93, 77, 91, 69, 136, 80.

Myrcene, mol. ion 136, major ions 93, 69, 53, 79, 77, 67.

α-Terpinene, mol. ion 136, major ions 93, 121, 136, 91, 77, 79, 105, 65.

p-Cymene, mol. ion 134, major ions 119, 134, 91, 117, 77, 65.

Limonene, mol. ion 136, major ions 68, 93, 67, 53, 79, 121, 136.

γ-Terpinene, mol. ion 136, major ions 93, 91, 136, 77, 121, 92, 79.

Terpinolene, mol. ion 136, major ions 93, 121, 136, 79, 91, 77, 105.

Caryophyllene, mol. ion 204, major ions 69, 93, 79, 133, 91, 55, 67, 105.

β-Bisabolene, mol. ion 204, major ions 69, 93, 119, 79, 67, 55, 161, 94.

γ-Bisabolene, mol. ion 204, major ions 93, 107, 135, 119, 55, 79, 91, 69.

The above spectra were measured using a CEC Model 21-620 mass spectrometer and were consistent with the spectra of authentic samples run on the same instrument.

Oxygenated Fraction. Figure 2 shows an analysis of the oxygenated fraction on a 600-foot × 0.02-inch I.D. silicone SF 96-100 capillary. Table II lists the identity of the peaks, with the type of method used for their identification. Bornyl acetate, terpinene-4-ol, and α-terpineol were the major oxygenated terpenoids. Terpinene-4-ol and α-terpineol are related to our major terpenoid hydrocarbon terpinolene. At first sight, bornyl acetate appears to be unrelated, but the same positions in the basic menthane skeleton are involved. The only other major oxygenated terpenoid is the sesquiterpene alcohol carotol, a well-known component of carrot seed oil.

A second group of compounds found were related to eugenol. Peak 86 contains methyl eugenol (3,4-dimethoxyallylbenzene), peak 106 myristicin (111), and peak 91 a compound related to myristicin, probably 3-methoxy-4,5-methylenedioxypropylbenzene. Myristicin is a well-known constituent of parsley seed oil and other essential oils. Parsley is in the same family (umbelliferae) as carrots.

A third group of compounds were carbonyls, mostly aliphatic aldehydes. These were detected in the capillary GLC–mass spectral analysis of the oxygenated fraction but it was found advantageous to separate the carbonyls with Girard T reagent using a procedure similar to that described by Gaddis *et al.* (1964). The components were separated on a 500-foot long × 0.3-inch I.D. stainless steel capillary coated with silicone SF 96-100 and analyzed using batch introduction into the mass spectrometer. 2-Nonenal, octanal, 2-decenal, and heptanal were the major components. The steam distillation of carrots at atmospheric pressure gave an oil with a considerably higher concentration of these aldehydes than steam distillation under reduced pressure, indicating that the aldehydes are produced by the heating.

Mass spectral data found for components separated from the oxygenated fraction were as follows (molecular ion and 5 to 10 major ions, Cons. spectra run on Consolidated 21-620 mass spectrometer, T. of F. spectra run on a

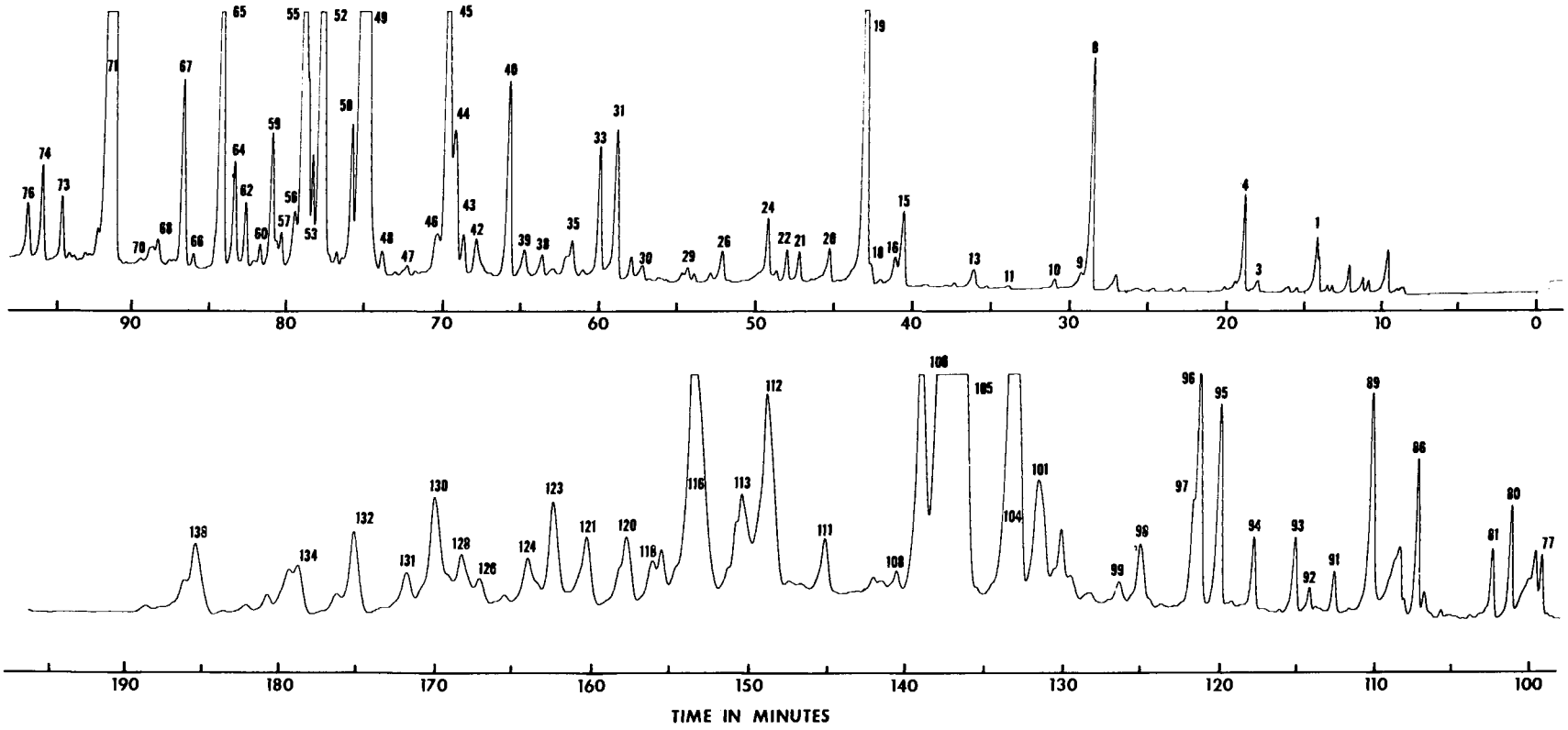


Figure 2. Capillary GLC chromatogram of the oxygenated fraction from carrot root oil (atmospheric steam distilled) using a 600-foot × 0.02-inch I.D. silicone SF 96 coated capillary programmed from 80° to 170° C. at 1° C. per minute and held

Table II. Identities of Oxygenated Components in Carrot Root Oil (Atmospheric Steam Distilled)

Peak No. (Figure 2)	Confirmed Identity[a,b]	Tentative Identity	Relative % in Whole Oil[c]
8	Heptanal, MS, IR, RT		0.05
19	Octanal, MS, IR, RT		0.2
20–28		Oxygenated terpenoids, MS	
31		Oxygenated terpenoid, MS	
33	Nonanal, MS, RT		0.02
38–42		Oxygenated terpenoids, MS	
45	2-Nonenal, MS, IR, RT		0.3
46–48		Oxygenated terpenoids, MS	
49	Terpinene-4-ol, MS, IR, RT		0.7
52	α-Terpineol, MS, IR, RT		0.7
55–65		Oxygenated terpenoids, MS	
67	2-Decenal, MS, RT		0.04
71	Bornyl acetate, MS, IR, RT		0.6
73		Oxygenated terpenoid, MS	
74	2,4-Decadienal, (trans trans) MS, RT		0.01
76		MW 138 aromatic, MS	
80, 84		Oxygenated terpenoids	
86	Biphenyl, MS, IR, RT		0.1
89	Dodecanal, MS, RT 3,4-Dimethoxy-1-allylbenzene MS, RT		0.02
91		3-Methoxy-4,5-methylenedioxypropylbenzene MS	
93–104		Sesquiterpenoids, MS	
106	Myristicin, MS, IR, RT		0.4
111–113		Sesquiterpenoids, MS	
116	Carotol, MS, RT		0.2

[a] MS, IR, RT = mass spectral, infrared absorption spectral, and GLC retention time evidence, respectively. [b] Evidence cited consistent with that of authentic compound or published data. [c] Calculations based on GLC of whole oil.

Bendix Time-of-Flight instrument):

Heptanal (T. of F.) mol. ion 114, next prominent ion 96, major ions 70, 55, 57, 71, 81, 86, 96.

Octanal (T. of F.) mol. ion 128, next prominent ion 110, major ions 57, 56, 84, 55, 69, 82, 85, 68.

Nonanal (Cons.) no mol. ion, highest prominent ion 124, (mol. wt.–18), major ions 57, 56, 55, 70, 69, 98, 82.

2-Nonenal (Cons.) no mol. ion, highest prominent ion 122 (mol. wt.–18), major ions 55, 70, 57, 83, 69, 56, 84, 96.

Terpinene-4-ol (T. of F.) mol. ion 154, next highest prominent ion 136, major ions 71, 111, 136, 93, 86, 69, 55, 154.

α-Terpineol (T. of F.) mol. ion 154, next highest prominent ion 136, major ions 59, 93, 136, 121, 81, 92.

2-Decenal (Cons.) mol. ion 154, next prominent ion 136, major ions 55, 70, 57, 83, 56, 69, 71, 68, 67.

Bornyl acetate (T. of F.) mol. ion 196, major ions 95, 136, 121, 93, 55, 67, 80.

2,4-Decadienal (Cons.) mol. ion 152, next prominent ion 123, major ions 81, 67, 55, 83, 95, 54, 53.

Biphenyl (T. of F.) mol. ion 154, major ions 154, 153, 155, 152, 76, 51, 77.

Dodecanal (Cons.) no mol. ion, first prominent ion 166 (parent–18), major ions 57, 55, 82, 68, 67–71, 83, 81, 96.

3,4-Dimethoxyallylbenzene (Cons.) mol. ion 178, major ions 178, 163, 147, 91, 103, 51, 107, 77.

Myristicin (T. of F.) mol. ion 192, major ions 192, 91, 161, 165, 119, 65, 77.

Carotol (T. of F.) mol. ion 222, next prominent ion 189, major ions 161, 69, 55, 57, 81, 93, 79, 119, 123. All mass spectra were compared against those of authentic samples run on the same mass spectrometer.

Infrared spectral data found for the oxygenated components were (in the region 5 to 15 microns, S strong, M medium, and W weak):

Heptanal S(5.8, 6.8), M(7.1, 7.3, 9.0), W(7.8, 8.1, 9.4, 9.9, 10.5) microns.

Octanal S(5.8, 6.8), M(7.1, 7.2, 7.3, 9.0, 9.4), W(8.4, 10.2, 10.5, 11.2, 11.7, 13.8) microns.

2-Nonenal S(5.95, 6.1, 6.9, 8.8, 10.3), M(5.8, 9.1, 9.9, 13.8), W(7.3, 7.7, 9.5, 11.3) microns.

Terpinene-4-ol S(6.8, 6.9, 7.28, 7.3, 9.3, 9.8, 10.7, 11.3), M(8.5, 8.6, 8.9, 9.9, 10.0, 10.5, 11.6, 12.5), W(7.7, 8.0, 9.2, 9.5) microns.

α-Terpineol S(6.95, 7.3, 7.36, 8.6, 8.9, 10.8, 10.9), M (8.2, 9.8, 11.9, 12.4), W(7.8, 8.0, 9.2, 10.2, 10.5, 12.7, 13.2) microns.

Bornyl acetate S(5.75, 6.9, 7.24, 7.3, 7.34, 8.0, 9.5, 9.6), M(6.8, 7.7, 8.9, 10.0), W(6.35, 8.3, 8.6, 8.8, 9.2, 10.1, 10.4, 10.6, 11.0, 11.2, 12.1, 12.6, 13.3) microns.

Biphenyl S(6.75, 7.0, 9.9, 14.3), M(6.3, 9.6, 11.0), W(5.13, 5.17, 5.22, 5.25, 5.3, 5.35, 5.6, 5.75, 6.4, 6.5, 7.2) microns.

Myristicin S(6.14, 6.7, 6.9, 7.0, 8.8, 9.5), M(7.35, 7.6, 8.4, 9.2, 10.0, 10.5, 10.9), W(7.1, 7.8) microns.

Odor Significance of Carrot Root Components. The identity and amount of a volatile component of a food are not sufficient to tell how much the particular component contributes to the total odor of the food. One way of estimating fraction or component contribution to the total odor intensity of a mixture is by measuring the threshold concentration of the individual components. With hop oil the percentage of a fraction or component in the whole oil divided by its threshold concentration was proportional to the total odor intensity of the whole oil (Guadagni *et al.*, 1966). This relationship has been demonstrated for the hydrocarbon and oxygenated fraction of the carrot root oil (Table III). If we assume that this proportionality exists for the other components of the oil shown in Table III, the percentage contribution to the total odor intensity may be calculated on the basis of percentage composition

Table III. Odor Thresholds and Calculations of Relative Contribution of Some Components of Carrot Root Oil (Atmospheric Steam Distilled) to Total Odor Intensity of the Whole Oil in Water Solution

Compound	Threshold, P.P.B. in H_2O	Whole Oil, %	Odor Contribution, %
Heptanal	3	0.05	0.1
Octanal	0.7	0.2	2
2-Nonenal	0.08	0.3	22
2-Decenal	0.3	0.04	0.8
Terpinene-4-ol	340	0.7	0.01
α-Terpineol	350	0.2	<0.01
Bornyl acetate	75	0.6	0.05
Myristicin	25	0.4	0.1
Carotol	8	0.2	0.1
Terpinolene	200	37	1
Sabinene	75	6	0.5
Myrcene	13	0.8	0.4
Whole carrot root oil	6	100	100
Hydrocarbon fraction	75	58	5
Oxygenated fraction	2	30	90

and threshold concentrations where the intensities of various components behave in an additive fashion. When these conditions are met, the calculatons give an estimate of the order of relative importance of the various constituents to the total odor intensity. Of the compounds listed in Table III, only 2-nonenal appears to make a substantial contribution to the total odor intensity. An additional 2.8% was contributed by octanal and 2-decenal indicating the relative importance of aldehydes to the odor of this particular steam distilled oil. A number of other aldehydes were detected, 2,4-decadienal being the most potent odorant of these. Some tentative evidence was also obtained for the presence of the potent odorant 2,6-nonadienal (odor of cucumbers, Forss *et al.*, 1962), but it could not be separated in pure enough form to identify with any certainty.

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