

AROMA CHEMICALS

1. Introduction

Aroma chemicals are an important group of organic molecules used as ingredients in flavor and fragrance composition. Aroma chemicals consist of natural, nature-identical, and artificial molecules. Natural products are obtained directly from the plant or animal sources by physical procedures. Nature-identical compounds are produced synthetically, but are chemically identical to their natural counterparts. Artificial flavor substances are compounds that have not yet been identified in plant or animal products for human consumption.

There are ca 3000 different molecules that find use in the production of flavor and fragrance compositions. Synthetic ingredients play a major part as components due to their convenient availability and the relatively lower costs compared to natural molecules from isolation of relatively limited natural sources.

2. Odors Descriptors

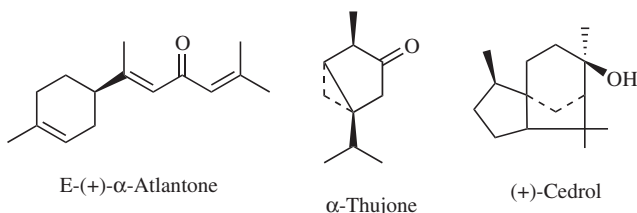
The odors of single chemical compounds (aroma chemicals) are very difficult to describe unequivocally. The odors of complex mixtures called compounds are often impossible to describe unless one of the components is so characteristic that it determines the odor or flavor of the composition. Although an objective classification is not possible, an odor can be described by adjectives such as flowery, fruity, woody, or hay-like, which will relate to natural occurring or other well-known products with such odors characteristics.

A few terms (1) used to describe odors are listed in Table 1, with a few examples.

3. General Production Routes

Aroma chemicals are specific molecules of particular aroma, which can be obtained (1) by isolation from natural sources, with or without chemical modifications, using natural molecules as precursors for many aroma chemicals (partial synthesis); (2) from petrochemical raw materials; or (3) by synthesis from cyclic and aromatic precursors.

For example, cedarwood oils obtained from plants like *Cedrus atlantica*, *Chamaecyparis funebris*, or *Juniperus mexicana*, contain aromatic molecules, eg, (*E*)-(+)- α -atlantone, α -thujone, or (+)-cedrol:



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Table 1. Terms to Describe Odors



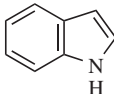
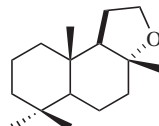
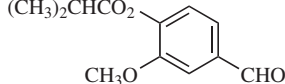
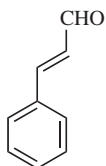
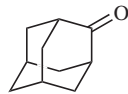
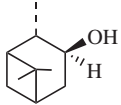
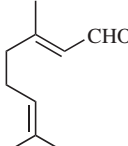
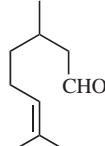

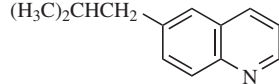
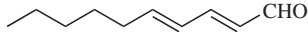
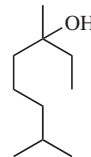
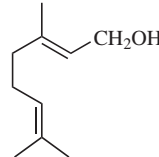
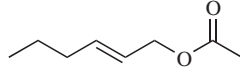
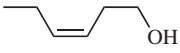
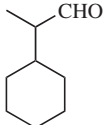
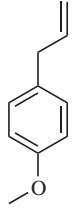
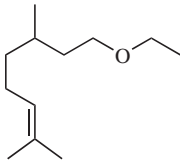
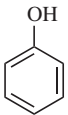
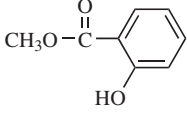
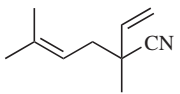
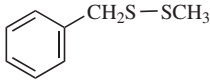
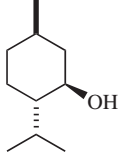
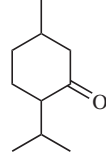
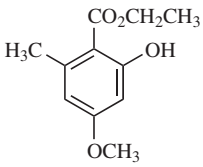
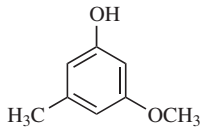
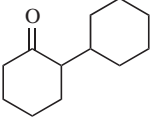
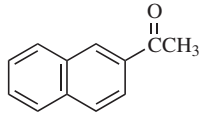
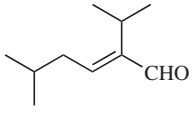
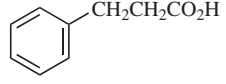
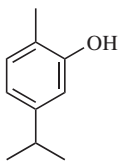
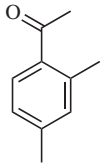
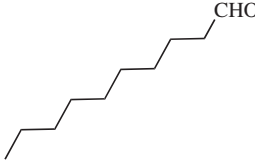
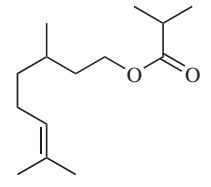
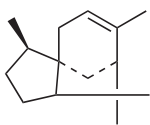

Odor	Description	Examples	
aldehydic	note of the long-chain fatty aldehydes, eg, fatty-sweaty, ironed laundry, seawater	 <i>n</i> -Decanal	 <i>n</i> -Octanal
animalic	typical notes from the animal kingdom, eg, musk, castoreum, skatol, civet, ambergis	 Indole	 Ambrox
balsamic	heavy, sweet odors, eg, cocoa, vanilla, cinnamon	 Vanillin isobutyrate	 Cinnamaldehyde
camphor-aceous	reminiscent of camphor	 2-Adamantanone	 (+)-Isoborneol
citrus	fresh, stimulating odor of citrus fruits such as lemon or orange	 Citral	 Citronellal
earthy	humus-like, reminiscent of humid earth	 2-Ethylfenchol	 6-Isobutylquinoline
fatty	reminiscent of animal fat and tallow	$\text{CH}_3(\text{CH}_2)_8\text{CO}_2(\text{CH}_2)_4\text{CH}_3$ Amyl decanoate	 (<i>E,E</i>)-2,4-Decadienal
floral, flowery	generic terms for odors of various flowers	 Tetrahydrolinalool	 Geraniol

Table 1. (Continued)

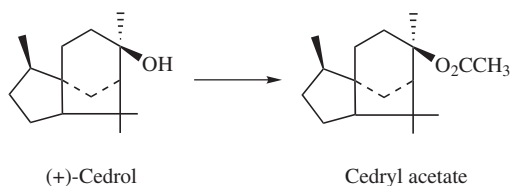
Odor	Description	Examples
fruity	generic terms for odors of various fruits	$\text{CH}_3\text{CO}_2(\text{CH}_2)_7\text{CH}_3$ <i>n</i> -Octyl acetate  <i>trans</i> -2-Hexenylacetate
green	typical odor for freshly cut grass and leaves	 <i>cis</i> -3-Hexenol  2-(Cyclohexyl)-propanal
herbaceous	noncharacteristic, complex odor of green herbs with, eg, sage, minty, eucalyptus-like, or earthy nuances	 Estragole  Citronellylethyl ether
medicinal	odor reminiscent of disinfectants, eg, phenol, lysol, methyl salicylate	 Phenol  Methyl salicylate
metallic	typical odor observed near metal surfaces, eg, brass or steel	 2,5-Dimethyl-2-vinyl-4-hexenenitrile  Benzyl methyl disulfide
minty	peppermint-like odor	 (-)-Menthol  Menthone
moissy	typical note reminiscent of forests and seaweed	 Ethyl 2-hydroxy-4-methoxy-6-methylbenzoate  3-Methoxy-5-methylphenol

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Table 1. (Continued)

Odor	Description	Examples	
powdery	odor identified with toilet powders, sweet-diffusive	 2-(1-Cyclohexenyl)-cyclohexanone	 Methyl- β -naphthyl ketone
resinous	aromatic odor of tree exudates	 2-Isopropyl-5-methyl-2-hexenal	 3-Phenylpropionic acid
spicy	generic term for odors of various spices	 Carvacrol	 2,4-Dimethyl-acetophenone
waxy	odor resembling that of candle wax	 <i>n</i> -Decanal	 Citronellyl-isobutyrate
woody	generic term for the odor of wood, eg, cedarwood, sandalwood	 α -Cedrene	 <i>cis-p-tert</i> -Butyl-cyclohexylacetate

Acetylation of (+)-cedrol gives cedryl acetate, a woody-earthy odorous molecule, applied in woody compounds for all purposes.



3.1. The Use of Natural Molecules as Precursors. One of the most useful sources for natural molecules as chemical precursors is turpentine oil, originated from *Pinus* sp. The oil contains 60–70% of α -pinene and β -pinene, along with other natural molecules, ie, α -phellandrene, γ -terpinene, anethole, caryophyllene, 3-carene, and camphene (see Figs. 1 and 2).

3.2. The Use of Petrochemicals as Precursors. Synthesis from petrochemical precursors of one-to-five carbon atoms, ie, carbon monoxide/formaldehyde, acetylene, isobutylene, and isoprene, represents one of the most important routes to produce aroma chemicals.

Aromatic molecules, eg, benzene, toluene, xylenes, phenol, cresols, and naphthalene, are also important precursors for aroma chemicals (see Figs. 3–5).

4. Functional Groups of Aroma Chemicals

As mentioned before, over 3000 specific chemical molecules are used in the F&F industry, but only a few hundreds are produced on a scale between 20 and 50 mt year. These molecules include most of the functional groups, from aliphatic molecules to heterocyclic ones, according to the following list:

- a. Hydrocarbons (aliphatic, acyclic terpenes, cyclic terpenes, benzenoids)
- b. Alcohols (aliphatic, alicyclic, cyclic)
- c. Ethers
- d. Aldehydes and ketones (including acetals and ketals)
- e. Carboxylic acids
- f. Esters and lactones
- g. Nitriles
- h. Amines
- i. Nitroaromatic compounds
- j. Thio compounds
- k. Heterocyclic molecules

The following sections contain selected examples of each functional group, the chemical structure, and organoleptic characteristics.

4.1. Hydrocarbons. Hydrocarbons include simple aliphatic molecules, terpenes—both acyclic and cyclic, and benzene rings.

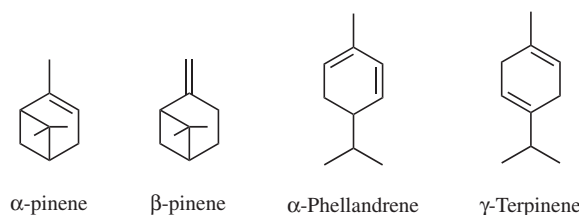


Fig. 1. α -Pinene as a natural precursor for aroma chemicals.

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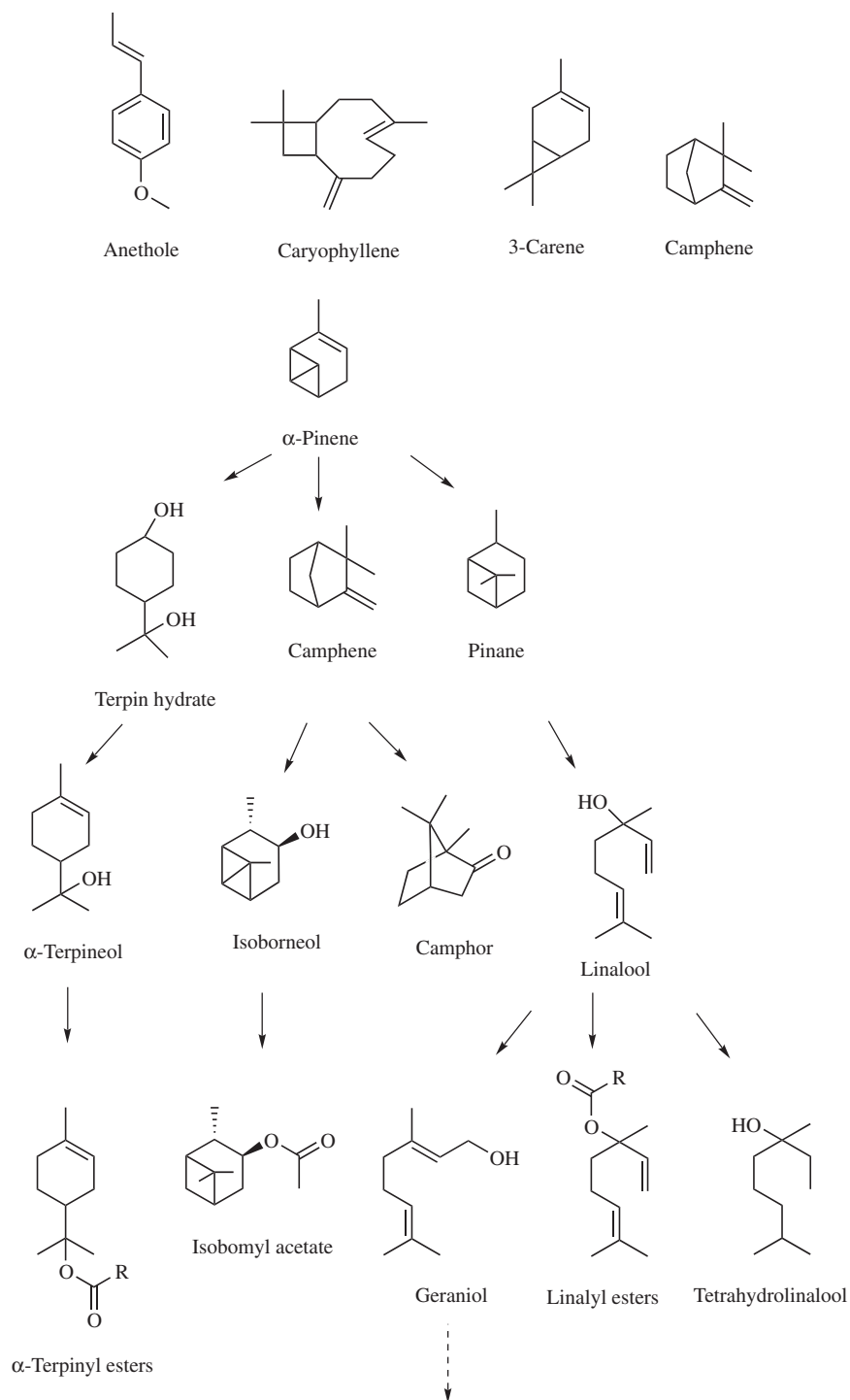


Fig. 1. (Continued)

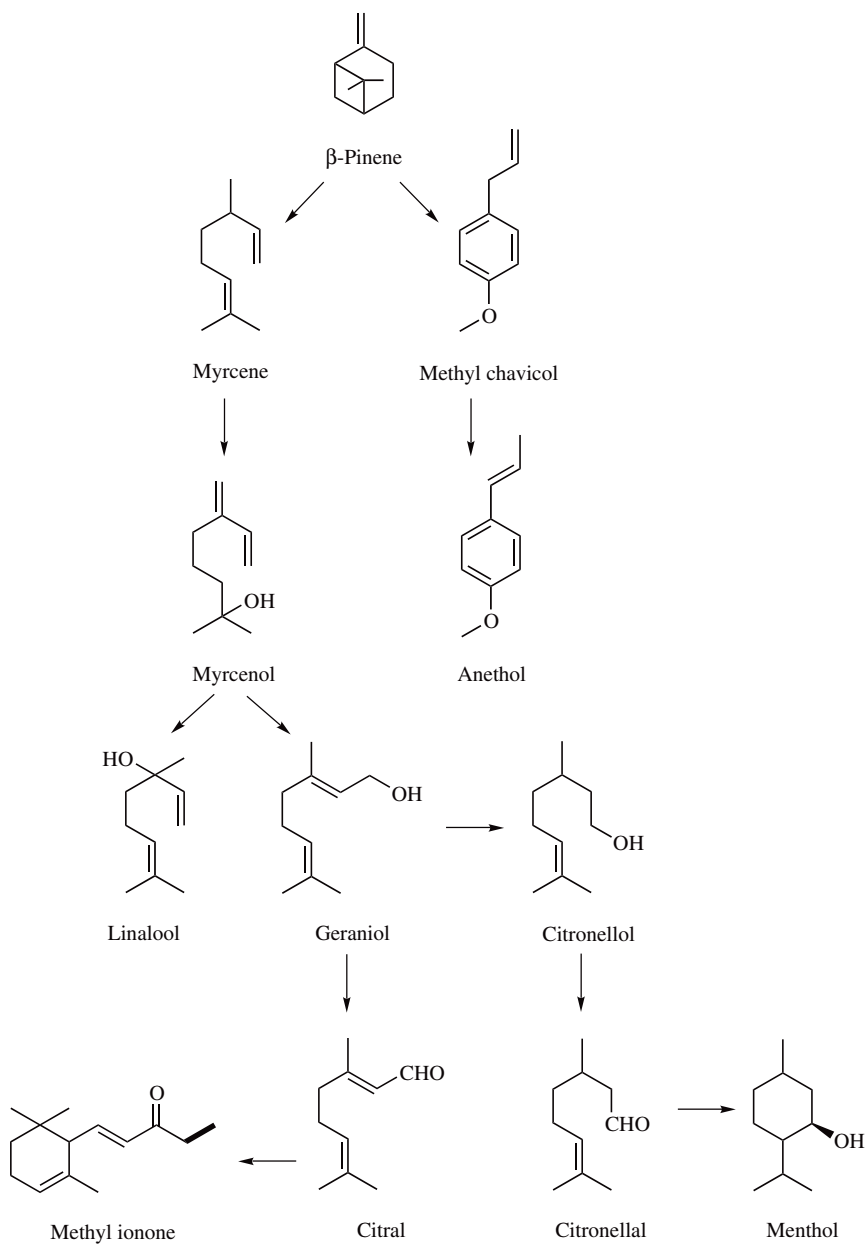


Fig. 2. β-Pinene as a natural precursor for aroma chemicals.

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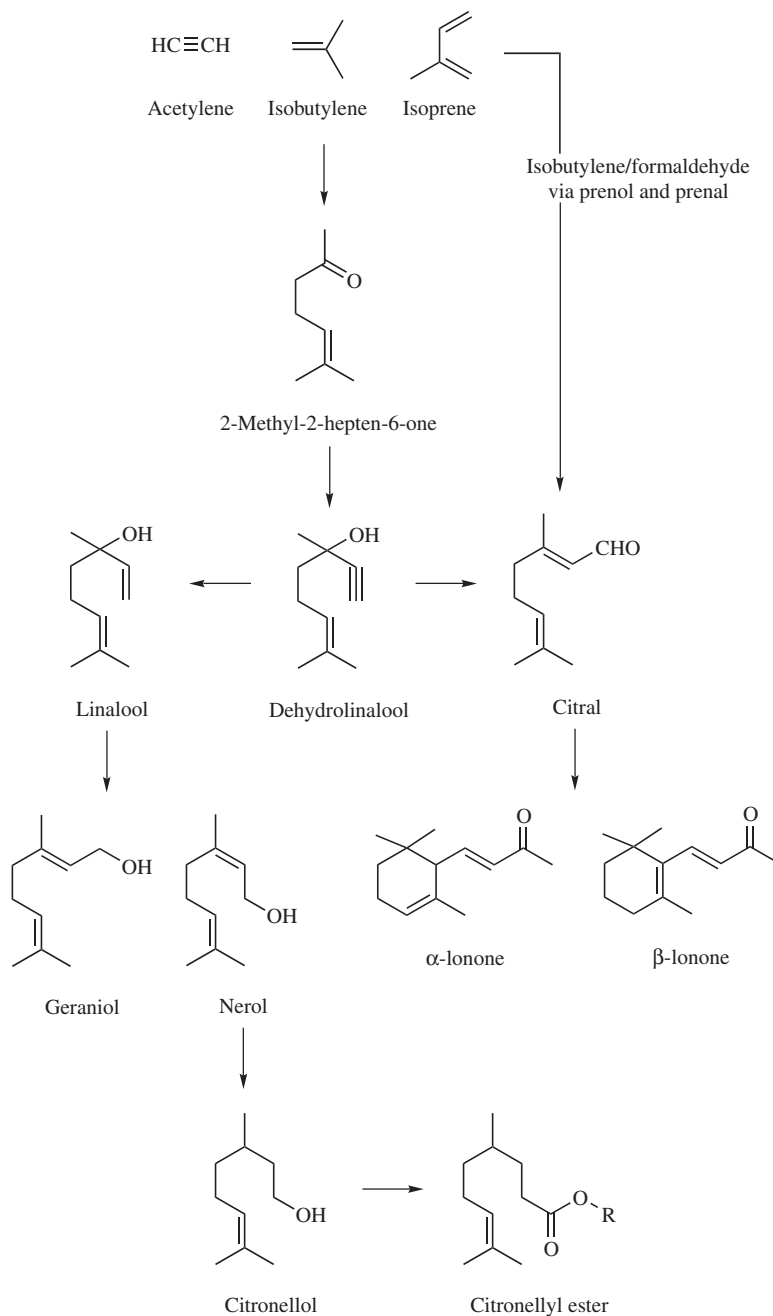


Fig. 3. General overview: Petrochemicals as a source for aroma chemicals.

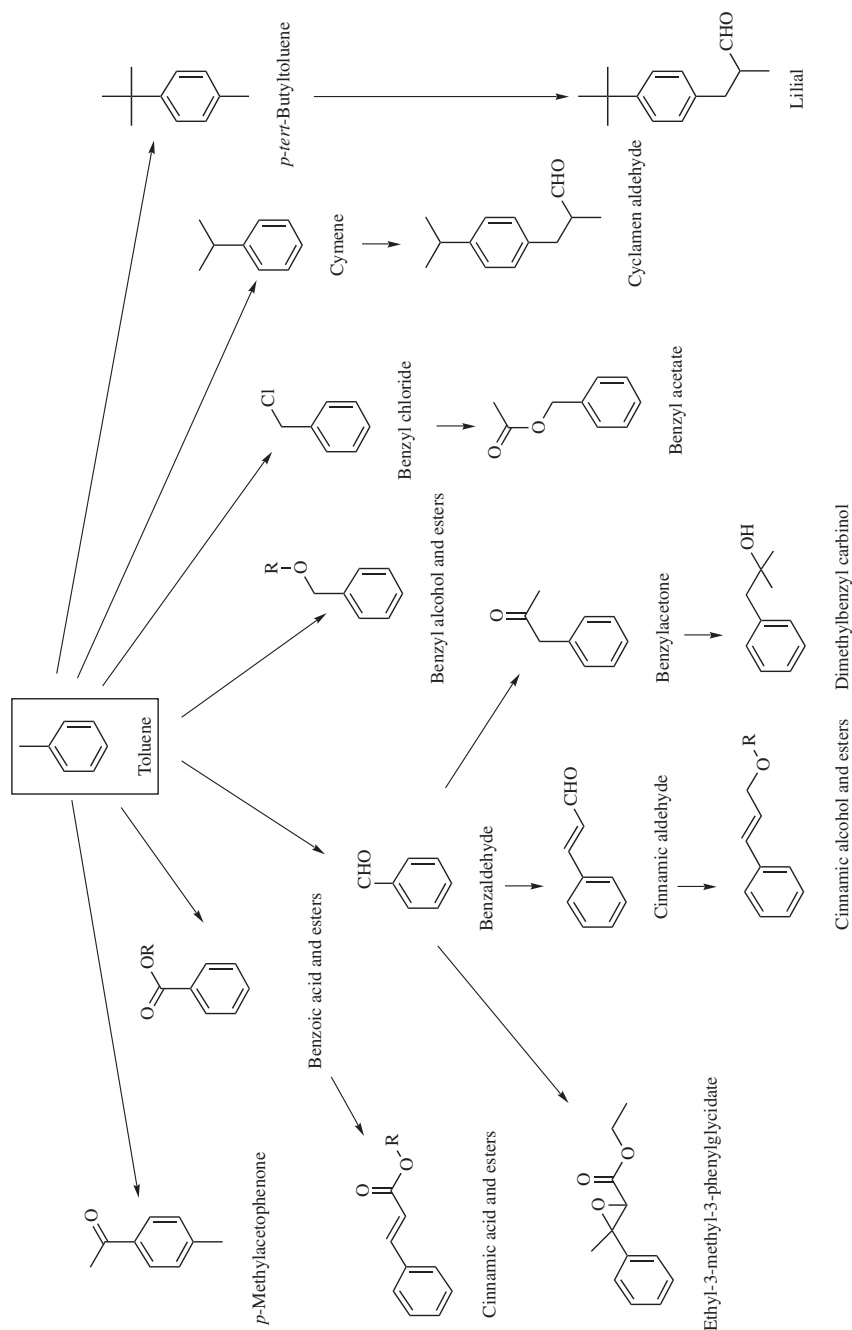


Fig. 4. Aroma chemicals derived from toluene.

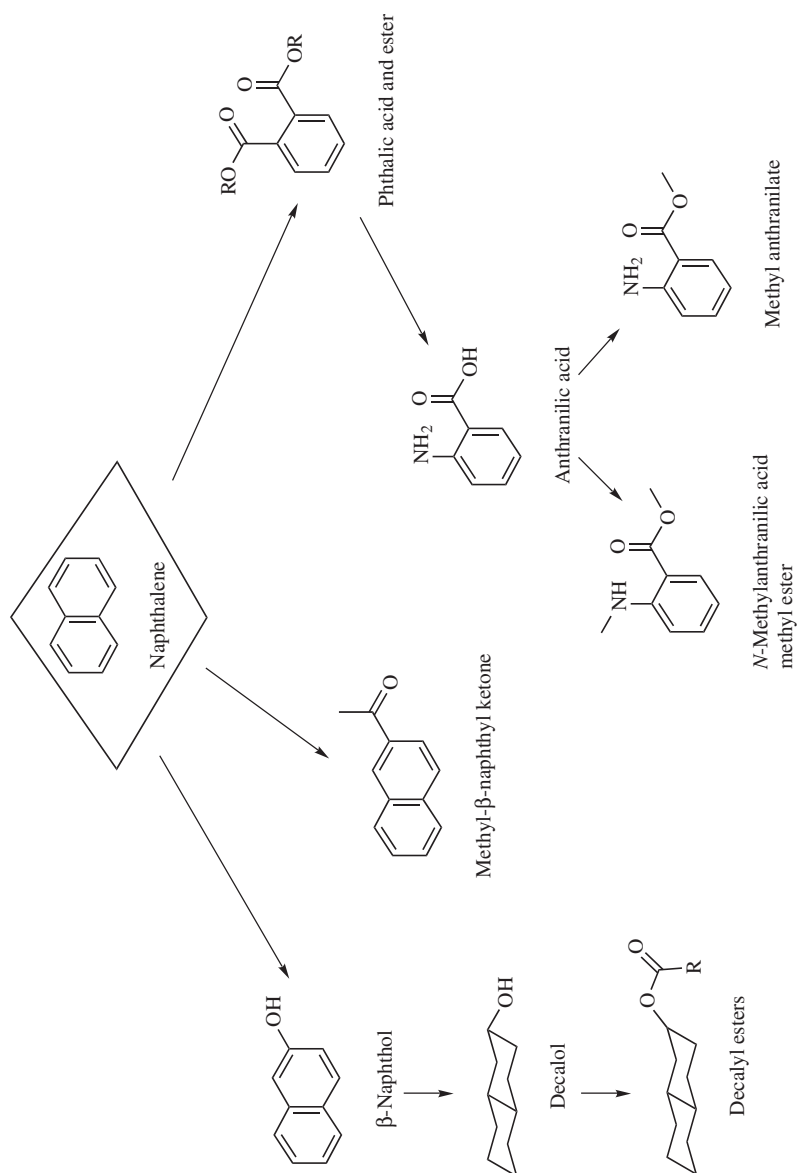

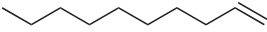
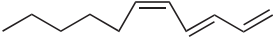


Fig. 5. Aroma chemicals derived from naphthalene.

Unsaturated Aliphatic Non-Terpenes

	green, diary-like, creamy, apple, vegetable and strawberry flavor. Application in diary flavorings; cream, tomato, apple, vegetable, strawberry; general fresh green fruity notes (2)
1-Heptene	
	green, occurs in fresh apples
1-Decyne	
	oily, waxy, slightly fruity, peppery aroma, galbanum-like, green, musty, with an earthy rooty, fatty meat-like nuance flavor
(E,E,Z)-1,3,5-Undecatriene	

Terpenes. Terpenes are a group of plant originated natural products, which are usually composed of usually two, three, four, five, six or eight units of C_5 atoms. These units are formally derived from 2-methyl-1,3-butadiene (isoprene).

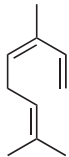


2-Methyl-1,3-butadiene (Isoprene)

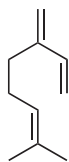
These molecules are named as follows:

Name	Number of isoprene units	Number of carbon atoms
monoterpenes	2	10
sesquiterpenes	3	15
diterpenes	4	20
sesterterpenes	5	25
triterpenes	6	30
tetraterpenes	8	40

Acyclic Monoterpenes

	harsh, terpene-like, somewhat citrus; green, woody and tropical fruity
Ocimene	
3,7-Dimethyl-1,3,6-octatriene	

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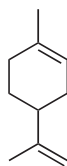


Myrcene

7-Methyl-3-methylene-1,6-octadiene

harsh, terpene-like, fresh somewhat citrus in dilution

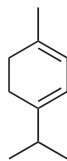
Cyclic Monoterpenes



Limonene

1-methyl-4-isopropenyl-1-cyclohexene

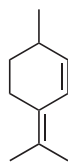
citrus, fruity, orange, berry-like, tarty



α -Terpinene

1-methyl-4-isopropyl-1,3-cyclohexadiene

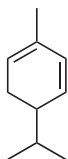
harsh, terpene-like; slightly citrus



Terpinolene

1-methyl-4-isopropylidene-1-cyclohexene

harsh, terpene-like, slightly citrus

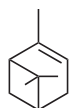


α -Phellandrene

1-methyl-4-isopropyl-1,5-cyclohexadiene

terpenic, citrus lime with a fresh green note

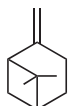
4.2. Bicyclic Monoterpenes



α -Pinene

2,6,6-trimethylbicyclo[3.1.1]hept-2-ene

harsh, terpene-like, coniferous



β -Pinene

6,6-dimethyl-2-methylenebicyclo[3.1.1]-heptane

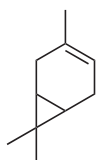
harsh, terpene-like, coniferous



Camphene

2,2-dimethyl-3-methylenebicyclo[2.2.1]-heptane

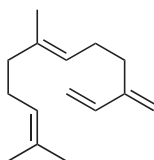
harsh, fresh camphoraceous,
terpene-like



Δ -3-Carene

harsh, terpene-like, coniferous

Acyclic Sesquiterpenes



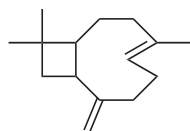
Farnesene

(3,7,11-trimethyl-1,3,6,10-dodeca-tetraene)

citrus, herbaceous

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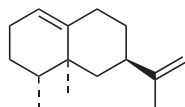
Bicyclic Sesquiterpenes



Caryophyllene

4,11,11-trimethyl-8-methylene-bicyclo-
[7.2.0]undec-4-ene

spicy, woody, dusty, oily; pepper-like,
camphoraceous, with a citrus
background

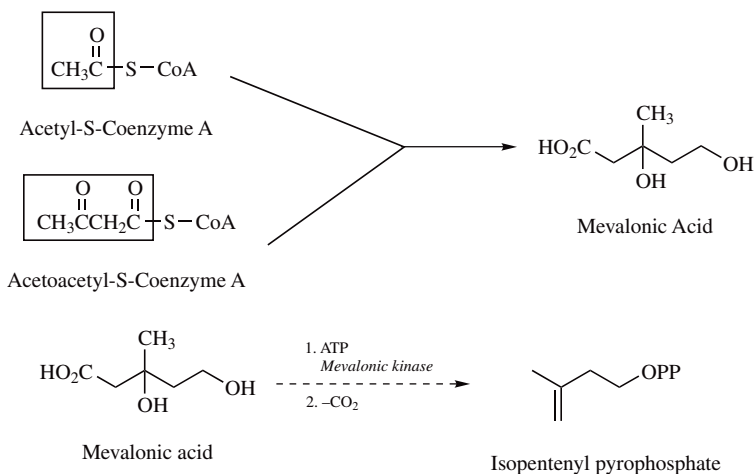


Valencene

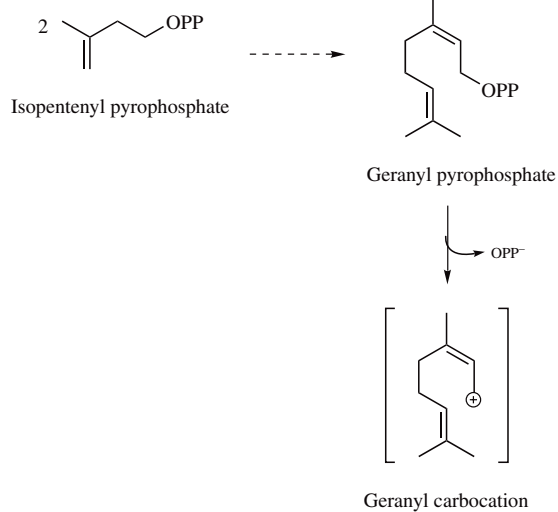
5,6-dimethyl-8-iso-propenylbicyclo- [4.4.0]-
dec-1-ene

paraffin, oily, somewhat citrus,
grapefruit-like

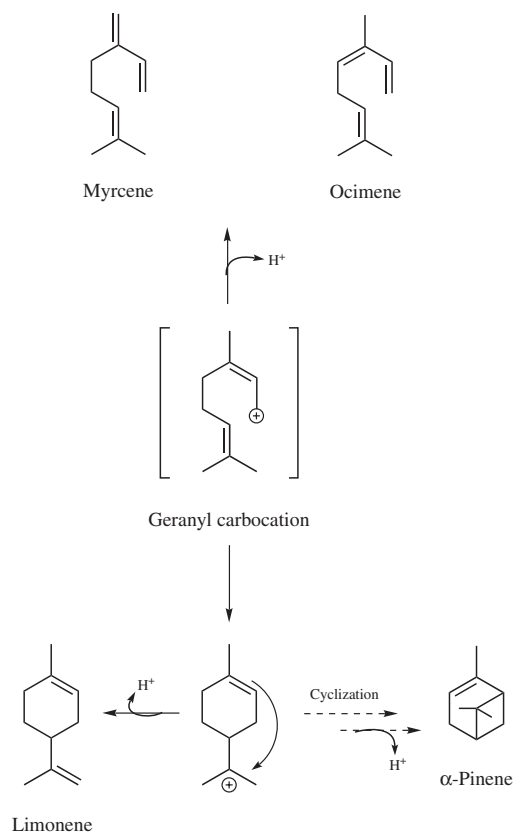
Terpenes are formed in nature via the “two carbons metabolism”, a process enabled by acetyl coenzyme A (CoA), which is produced from pyruvic acid. Acetyl-CoA forms mevalonic acid, which loses one carbon atom by decarboxylation to yield a C₅ unit—*isopentenyl pyrophosphate*:



Two units of isopentenyl pyrophosphate are combined with one C₁₀ atom unit—geranyl pyrophosphate, which loses its pyrophosphate group to form a unstable intermediate—geranyl carbocation:

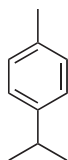


The geranyl carbocation can be stabilized by the following possibilities:



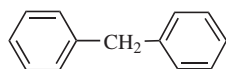
16 AROMA CHEMICALS

Benzenoids



p-Cymene

harsh, gasoline, terpene-like

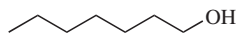


Diphenylmethane

aromatic oily, spicy on dilution

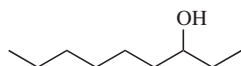
4.3. Alcohols. The alcohol function is found in simple aliphatic molecules, in acyclic and cyclic terpenes, and in molecules containing benzene rings. Phenols are also contained in this group of aroma chemicals.

Aliphatic Alcohols



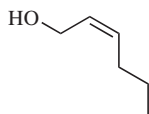
1-Heptanol

mild, oily, slightly caprylic fatty



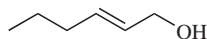
3-Octanol

oily, herbaceous, somewhat nut-like



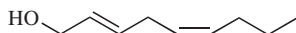
cis-3-Hexenol
Leaf Alcohol

strong, fresh, green grass



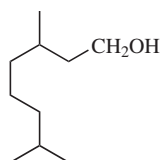
trans-2-Hexenol

sharp, green, leafy, slightly fruity odor,
and fruity, apple, green sweet, skin notes,
vegetable nuances, tropical grassy



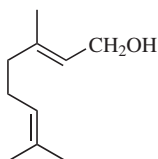
2-*trans*-6-*cis*-Nonadienol
Violet Leaf Alcohol

intense, heavy-fatty, green

Alcohols—Acyclic Terpenes

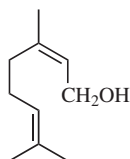
Tetrahydrogeraniol
3,7-dimethyloctanol

fresh floral, rosy, fatty



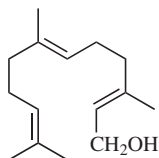
Geraniol [(*E*)-isomer]
3,7-dimethyl-(*E*)-2,6-octadienol

floral rose, citrus-like, fruity,
slightly fatty



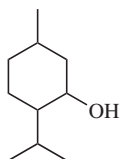
Nerol [(*Z*)-isomer]
3,7-dimethyl-(*Z*)-2,6-octadienol

floral rose, geranium; fruity, pear;
citrus-lemon



(*E,E*)-Farnesol
3,7,11-trimethyl-2,6,10-dodecatrieno

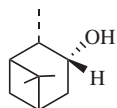
delicate, fresh green; floral (muguet)

Alcohols—Cyclic Terpenes

Menthol (8-*p*-menthen-3-ol)

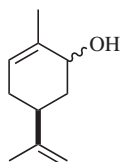
fresh, minty, with a dusty and earthy note

18 AROMA CHEMICALS



I-(-)-Borneol

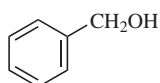
natural camphoraceous, pine-needlelike



L-Carveol

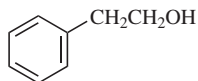
spearmint, caraway

Alcohols Containing Benzene Rings



Benzyl alcohol

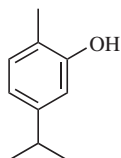
chemical, fruity with balsamic nuances



Phenethyl alcohol

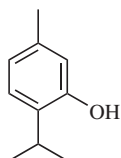
mild, warm honey, fruity, sweet floral-rose

Phenols



Carvacrol

spicy, somewhat herbal phenolic



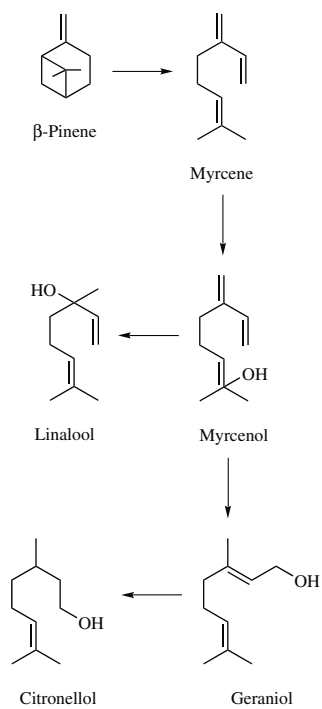
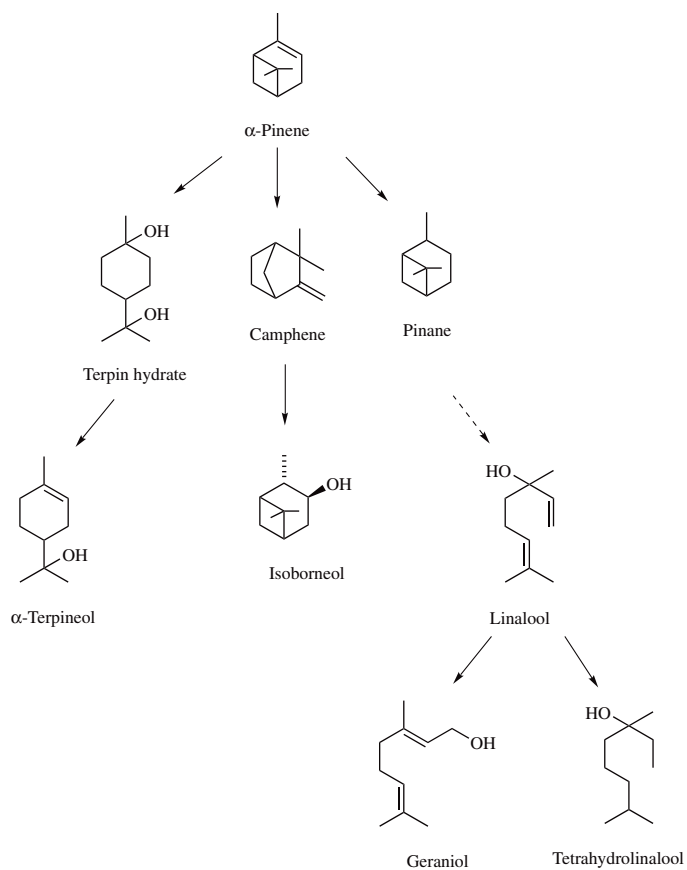
Thymol

herbal, spicy, aromatic, medicinal,
characteristic thyme

Preparation Methods of Alcohols

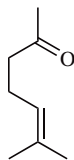
1. From Natural Sources

Conversion of α - and β -pinene to alcohols



20 AROMA CHEMICALS

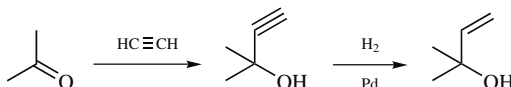
- From Chemical Precursors. The starting materials are isoprene, acetylene, formaldehyde, and acetone, which are used for the production of one of the possible key intermediates for linalool and geraniol - 6-methyl-5-hepten-2-one.



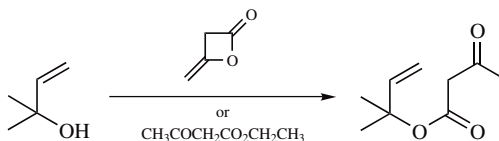
6-Methyl-5-hepten-2-one

6-Methyl-5-hepten-2-one is synthesized in several routes (3):

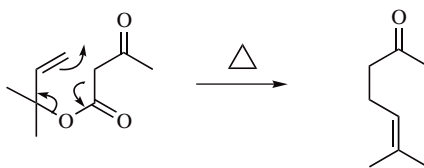
- From Acetylene and Acetone. Addition of acetylene to acetone, yielding 3-methyl-1-butyne-3-ol, which undergoes hydrogen addition to obtain 3-methyl-1-buten-3-ol, in presence of palladium catalyst:



3-Methyl-1-buten-3-ol reacts with diketene or with ethylacetoacetate as following:

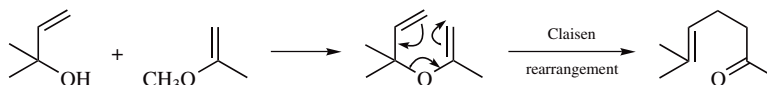


- This acetoacetate derivative, undergoes Carroll rearrangement, accompanied by decarboxylation to give the desired product:



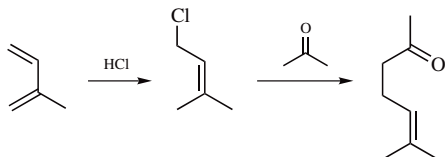
6-Methyl-5-hepten-2-one

- By Claisen Rearrangement. In this route, 6-methyl-5-hepten-2-one is prepared by reaction of 3-methyl-1-buten-3-ol with isopropenylmethyl ether, followed by Claisen rearrangement:

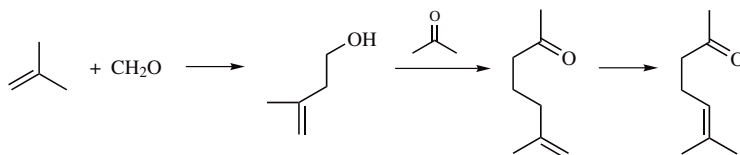


- From Acetone and Isoprene. In this route, hydrochloric acid is added to isoprene to obtain 3-methyl-2-butenylchloride. Reaction of the hydrogen chloride with acetone, in the presence of catalytic amount of organic

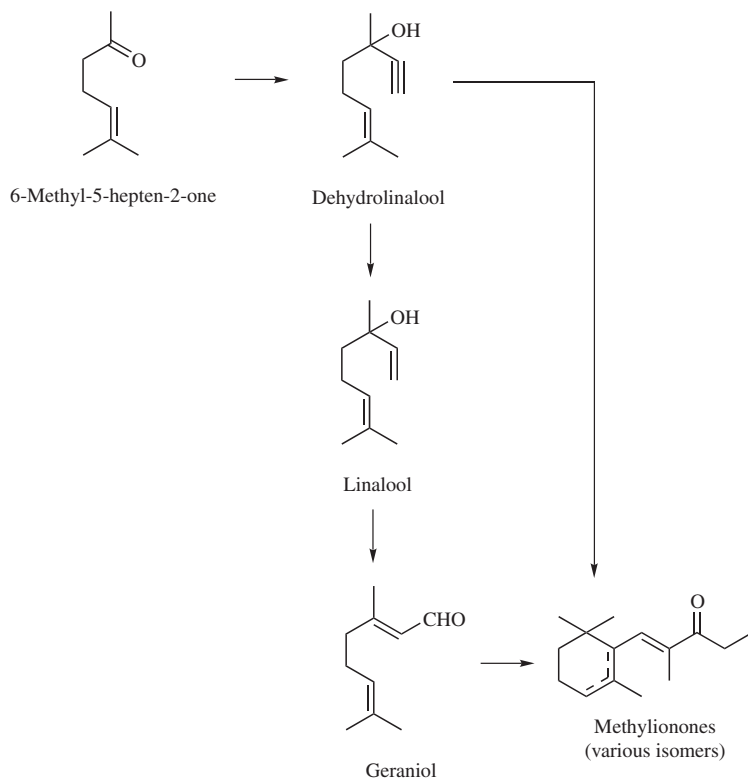
base, yields the desired product:



5. From Isobutylene and Formaldehyde. In this process 6-methyl-5-hepten-2-one is prepared via isoprenol by isomerization of 2-methyl-1-hepten-6-one. The starting material can be prepared in two steps from isobutylene and formaldehyde. The formed 3-methyl-3-buten-1-ol reacts with acetone to yield the desired product:

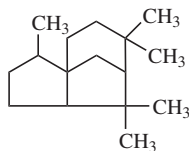


6-methyl-5-hepten-2-one, the main intermediate to linalool, can be further converted to important aroma chemicals such as geraniol, tetrahydrolinalool, methyl ionones, and others.



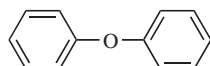
22 AROMA CHEMICALS

4.4. Ethers. The ether function is found both in aliphatic and aromatic molecules.



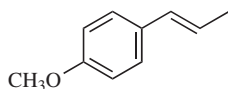
Cedrylmethyl ether

A colorless liquid with a fine cedarwood odor and a distinct amber nuance



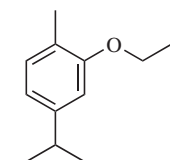
Diphenyl ether

aromatic, floral on dilution, rose-like



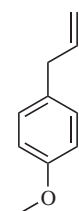
trans-Anethole

sweet, warm, herbaceous, strong anise-, licorice-, root beer-like



Carvacryl ethyl ether

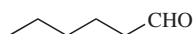
spicy, herbaceous, leafy



Estragole

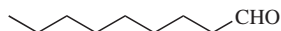
sweet, herbaceous, anise like

4.5. Aldehydes and Ketones. *Saturated Aldehydes*



Hexanal

aldehydic green, slightly fruity; somewhat green apple-like



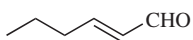
Nonanal

aldehydic, peely, floral (somewhat rosy), orange

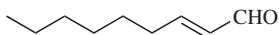


Decanal

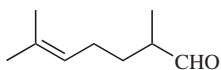
soft fatty; slightly green-fruity; cream, milk, cheese-like and green melon

Monounsaturated Aldehydes*trans*-2-Hexenal

strongly leafy green, slightly spicy, bitter
almond-like

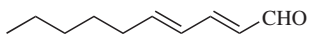
*trans*-2-Nonenal

green, soapy, cucumber/melon-like with an
aldehydic fatty nuance

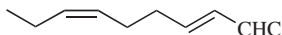


2,6-Dimethyl-5-heptenal

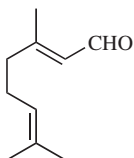
fresh, watery fruity (melon-like), with
herbal notes.

Diunsaturated Aldehydes*trans,trans*-2,4-Decadienal

powerful fatty, aldehydic, somewhat citrus

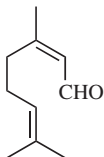
*2-trans-6-cis*-Nonadienal

powerful green cucumber, melon, violet leaf;
aldehydic with a fresh vegetable note

Terpene Aldehydes

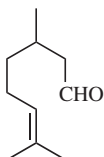
Geranial

fresh lemon-like, citrus and fruity



Neral

fresh, natural, citrus, slightly fruity-herbal.

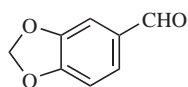


Citronellal

citrus, green, fruity, perfumistic,
aldehydic, soapy.

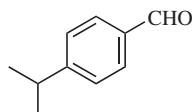
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Aldehydes Containing Benzene Ring



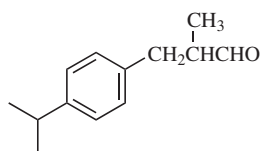
Heliotropin

sweet aromatic, somewhat vanilla,
characteristic heliotropic



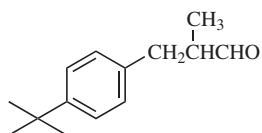
Cuminaldehyde

green, herbal, spicy; characteristic cumin



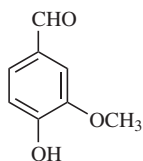
Cyclamen aldehyde

fresh, watery, floral, cyclamen-like



p-tert-Butyl- α -methyl
dihydrocinnamic aldehyde

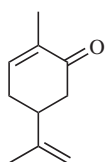
fresh, light, green, floral, reminiscent of
lily-of-the valley; notes of muguet



Vanillin

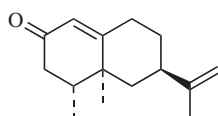
intensive sweet, tenacious creamy,
characteristic vanilla aroma

Ketones



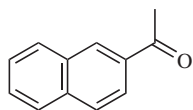
L-Carvone

fresh, herbal; characteristic spearmint note



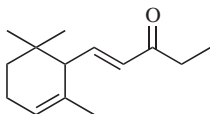
Nootkatone

full grapefruit character; slightly woody



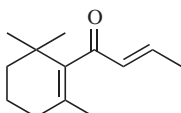
β -Methylnaphthylketone

powdery, sweet aromatic, floral; on dilution resembling neroli



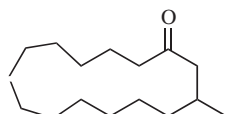
α -*n*-Methylionone

floral, woody; violet-like



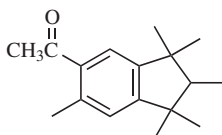
β -Damascone

fruity-floral, slightly woody, herbal; somewhat raspberry connotation



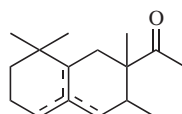
3-Methylcyclopentadecanone

natural, erogenic, animal-like musk



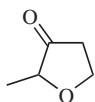
5-Acetyl-1,1,2,3,3,6-hexamethylindan

nitro-free musk compounds, herbal, and floral aspects



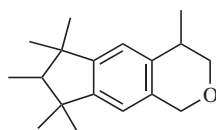
3-Acetyl-3,4,10,10-tetramethylbicyclo[4.4.0]decane

woody, amber



2-Methyltetrahydrofuran-3-one

breadlike, buttery top-note; nutty and astringent with a slight creamy almond nuance flavor; sweet, somewhat fruity, caramellic

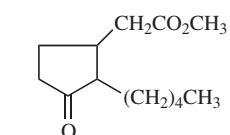
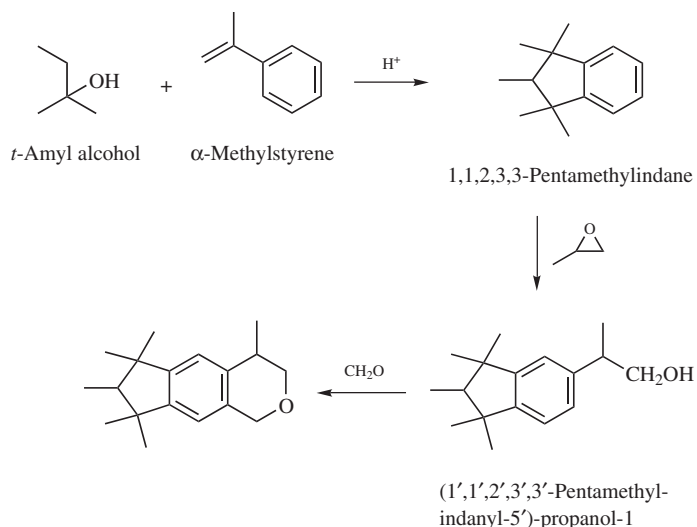


1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethylcyclopenta-(*g*)-2-benzopyran

powerful and clean musk, approaching the aspects of macrocyclic musks

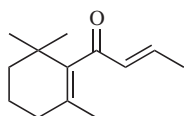
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Last isochormanic system drawn, 1,3,4,6,7,8-hexahydro-4,6,6,7,8-hexamethylcyclopenta-(g)-2-benzopyran, which was developed in the middle 1960 (3) by Beets and Heeringa from IFF is now also commercially as eg, Galaxolide, Abbalide. This molecule is synthesized as following; There is a condensation-cyclization stage of *tert*-amyl alcohol and α -methyl styrene in acidic conditions to obtain the indane system, followed by a Friedel-Crafts reaction with propylene oxide to get the side chain. The side chain is finally closed to the isochroman system using formaldehyde:



Methyl dihydrojasmonate

extremely persistent and powerful floral, fruity; characteristic of natural jasmin flower

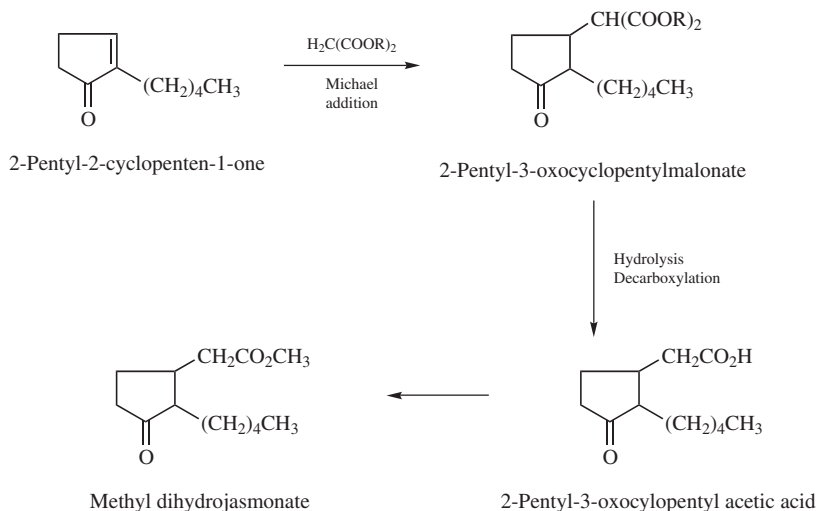


β -Damascone

fruity-floral, slightly woody, herbal; somewhat raspberry connotation

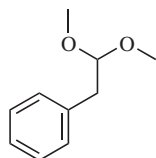
Methyl dihydrojasmonate is known also commercially by the names Hedione, Claigeon.

Methyl dihydrojasmonate is synthesized by the following route (3) namely, Michael addition of diethyl malonate to the pentyl cyclopentenone to obtain the second side chain, followed by hydrolysis and decarboxylation, and finally esterification:



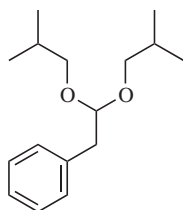
Diketones. The diketones used as aroma chemicals are mostly α -diketones.

	sweet, strongly buttery, creamy, milky
2,3-Butanedione (diacetyl)	
	creamy, sweet odor, buttery and cheesy
2,3-Hexanedione	
	buttery, cheesy, "oily", somewhat fruity
5-Methyl-2,3-hexanedione	
	"Oily", buttery, cheesy, pungent
2,3-Heptanedione	
	strong penetrating buttery, cheesy to slightly animal. In dilution: sweet "oily" berry note
2,3-Heptanedione	
	burnt caramellic flavor, and aromatic, burnt, caramellic
3,4-Hexanedione	

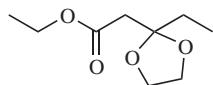
Acetals and Ketals

Phenylacetaldehyde dimethylacetal

dry, green-floral, fruity, citrus peel



Phenylacetaldehyde diisobutylacetal

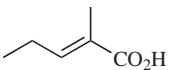
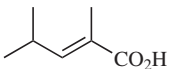
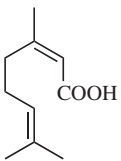
sweet aromatic, honey, brown,
somewhat floral (hyacinth-like)

Ethyl acetoacetate ethylene glycol ketal

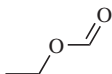
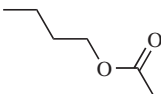
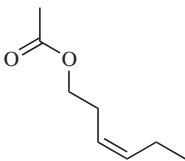
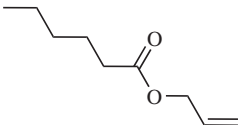
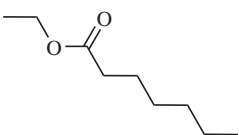
strongly fruity, slightly floral;
apple-, pear-, and berry-like**4.6. Carboxylic Acids. Saturated Carboxylic Acids**Table 2. **Saturated Carboxylic Acids**

Name	Organoleptic Characteristics	structure
formic acid	pungent, acidic, sour, astringent with a fruity depth	HCO_2H
acetic acid	sour, vinegar-like	$\text{CH}_3\text{CO}_2\text{H}$
propionic acid	sour, fruity on dilution	$\text{CH}_3\text{CH}_2\text{CO}_2\text{H}$
butyric acid	penetrating, reminiscent of rancid butter	$\text{CH}_3(\text{CH}_2)_2\text{CO}_2\text{H}$
valeric acid	strongly acidic, caprylic, cheese-like	$\text{CH}_3(\text{CH}_2)_3\text{CO}_2\text{H}$
caproic acid	acidic, caprylic, fatty	$\text{CH}_3(\text{CH}_2)_4\text{CO}_2\text{H}$
oenanthic acid	caprylic, fatty, green	$\text{CH}_3(\text{CH}_2)_5\text{CO}_2\text{H}$
caprylic acid	caprylic, fatty, oily	$\text{CH}_3(\text{CH}_2)_6\text{CO}_2\text{H}$
pelargonic acid	oily, fatty, caprylic; cheesy with a mild creamy background	$\text{CH}_3(\text{CH}_2)_7\text{CO}_2\text{H}$
capric acid	sour, fatty aroma	$\text{CH}_3(\text{CH}_2)_8\text{CO}_2\text{H}$
undecylic acid	fatty, fruity aspects	$\text{CH}_3(\text{CH}_2)_9\text{CO}_2\text{H}$
lauric acid	mild fatty	$\text{CH}_3(\text{CH}_2)_{10}\text{CO}_2\text{H}$
myristic acid	faint oily, fatty	$\text{CH}_3(\text{CH}_2)_{12}\text{CO}_2\text{H}$
palmitic acid	faint oily aroma	$\text{CH}_3(\text{CH}_2)_{14}\text{CO}_2\text{H}$
stearic acid	fatty, stearinic	$\text{CH}_3(\text{CH}_2)_{16}\text{CO}_2\text{H}$

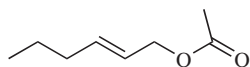
Unsaturated Carboxylic Acids

	acidic, fruity, somewhat cooked strawberry connotation
(E)-2-Methyl-2-pentenoic acid	
	acidic, caprylic, somewhat boiled strawberry connotations
2,4-Dimethyl-2-pentenoic acid	
	green, floral, weedy, woody aroma
cis-Geranic acid	

4.7. Carboxylic Acids Derivatives. Esters

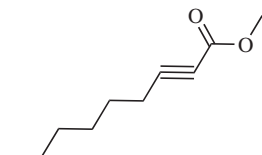
	sweet, ethereal-fruity; chemical with a clean fresh fruity lift
Ethyl formate	
	ethereal, fruity, apple- and banana-like
Butyl acetate	
	powerful, strongly green; slightly floral top-note
cis-3-Hexenyl acetate	
	strongly fruity, fatty; characteristic of fresh pineapple; rum and arak-note
Allyl caproate	
	strongly fruity, wine-brandy, apple, strawberry-like, with pungent note (reminiscent of pear)
Ethyl heptanoate	

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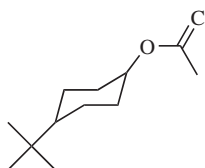
trans-2-Hexenylacetate

sweet, green, fresh, waxy and fruity;
banana- and apple-like



Methyl-2-nonynoate

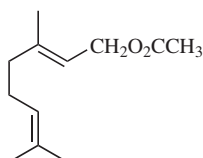
green, violet-leaf



p-*tert*-Butylcyclohexyl acetate

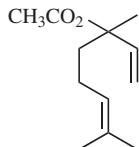
sweet and rich woody, pleasant floral,
with fruity note

Terpenic Esters



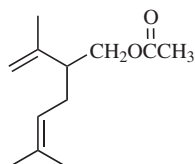
Geranyl acetate

sweet fruity-floral, rose-, and
lavender-like



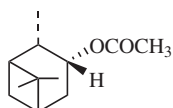
Linalyl acetate

freshly floral; bergamot-, petitgrain-,
lavender-, and cologne-like



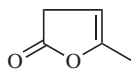
Lavandulyl acetate

fresh, floral-herbal, slightly fruity;
lavender-like

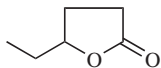
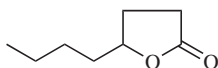


Bornyl acetate

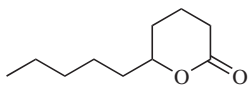
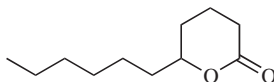
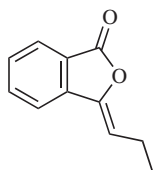
natural pinene-like, coniferous,
camphoraceous, slightly minty

Lactones α -Angelica lactone

nutty, maple, caramel, sweet, herbaceous

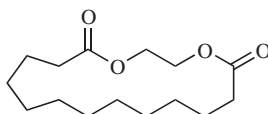
 γ -Hexalactonesweet, creamy, vanilla-like with green
lactonic powdery nuances γ -Octalactone

sweet creamy with coconut character

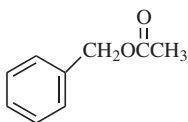
 δ -Decalactonesweet, dairy, creamy, fatty with a fruity
nuance; coconut- and peach-like δ -Undecalactonecreamy, fatty, somewhat fruit-like,
peach, coconut

3-Propylidene phthalide

powerful, warm, spicy, strongly celery-like



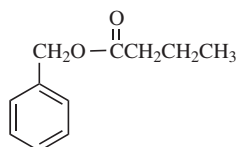
Ethylene brassylate

musk-like and oil-like scent, classical
macrocyclic musk with herbal
connotations*Benzylic and Homobenzylic Esters*

Benzyl acetate

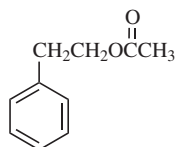
green, dry-powdery, fruity, somewhat
milky and estery

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Benzyl butyrate

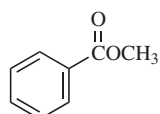
sweet aromatic, floral fruity, plum-like



Phenethyl acetate

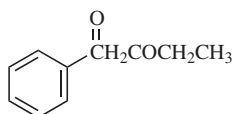
honey, sweet, floral

Benzoate and Homobenzoate Esters



Methyl benzoate

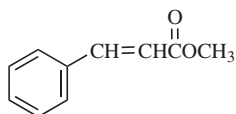
heavy sweet, slightly floral-fruity; berry-like



Ethyl phenylacetate

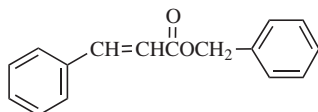
sweet aromatic, honey, waxy, fruity

Cinnamate Esters



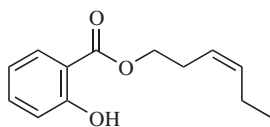
Methyl cinnamate

fruity, balsamic, somewhat strawberry-like

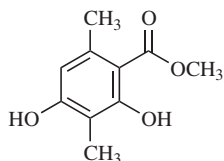


Benzyl cinnamate

sweet, floral, fruit, spicy; coumarin,
balsamic, honey

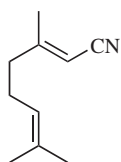
Salicylate Esters*cis*-3-Hexenyl-salicylate

long lasting, green floral, leathery note



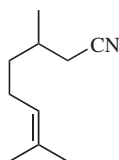
Methyl-3-methylorselinate

character-impact compound of oak- and treemoss; true moss-character

Nitriles

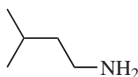
Geranyl nitrile

fresh, citrus, floral; lemon note of citral



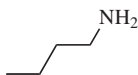
Citronellyl nitrile

fresh, lemon odor with greenish accent, citrus and herbal notes

Amines

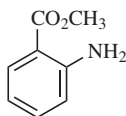
Isopentylamine

fishy, ammonia-like; in low concentration somewhat fermented

*n*-Butylamine

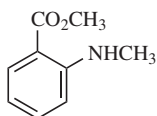
strong amine-like, fishy, on dilution slightly cheese like

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Methyl anthranilate

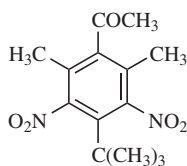
orange-flower-like, sweet fruity, tangerine and grape-note



Dimethyl anthranilate

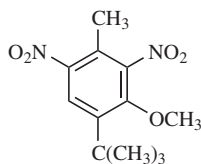
mandarin- and grape-like, tangerine note; somewhat orange-blossom

Nitroaromatic Compounds



Musk ketone

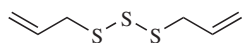
dry, powdery, nitro musk; somewhat floral-fruity connotations



Musk ambrette

strong nitromusk, with fruity (pear-like) note

4.8. Thio Compounds



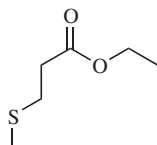
Diallyl trisulfide

sulfurous, characteristic garlic



Dimethyl disulfide

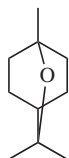
strong sulfurous, cabbage-, cauliflower- like



Ethyl 3-Methylthiopropionate

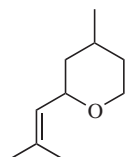
pineapple, tropical, onion at high levels

4.9. Heterocyclic Compounds. *Nonaromatic Compounds Containing Oxygen, Nitrogen, or Sulfur*

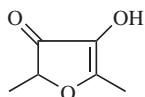


1,8-Cineole

fresh, strong eucalyptus-like, camphoraceous,
minty, cooling

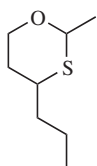
2-Isobutenyl-4-methyltetrahydropyran
(rose oxide)

floral, rose-like, fruity



4-Hydroxy-2,5-dimethyl-3(2H)-furanone

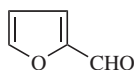
sweet, caramel-fruity (pineapple-like),
fried meat aspects



2-Methyl-4-propyl-1,3-oxathiane

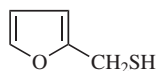
sulfurous, on dilution herbal, fruity

Furans



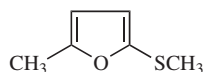
Furfural

sweet caramel-like, nutty, baked bread, almond



Furfuryl mercaptan

on dilution strong coffee-like

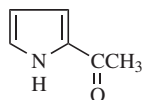


2-Methyl-5-(methylthio)furan

sulfurous, burnt, roasted (coffee-like) on dilution

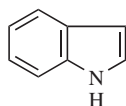
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Pyrrols and Indoles



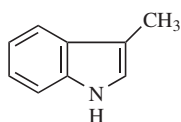
2-Acetyl pyrrole

sweet musty, nutty and tea-like



Indole

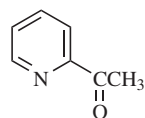
animalic, musk, cheese, slightly fecal on dilution



Skatole

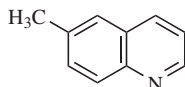
putrid, sickening, mothballs, decayed, fecal

Pyridines and Quinolines



2-Acetylpyridine

heavy oily, fatty, dusty, nutty, reminiscent of hazelnut and popcorn



6-Methylquinoline

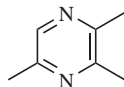
narcotic, earthy, green

Pyrazines and Quinoxalines



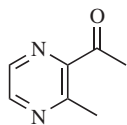
2-Methylpyrazine

musty, nutty, roasted, cocoa, peanut



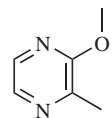
2,3,5-Trimethylpyrazine

burnt roasted, earthy, tobacco-like



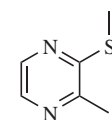
2-Acetyl-3-methylpyrazine

roasted potatoes, nutty, vegetable,
and cereal



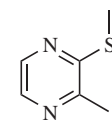
2-Methoxy-3-methylpyrazine

roasted peanuts



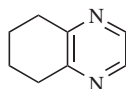
2-Methylthio-3-methylpyrazine

nutty, sweet, weakly green



2-Methylthio-3-methylpyrazine

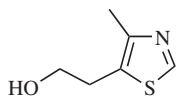
dusty, roasted



5,6,7,8-Tetrahydroquinixaline

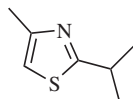
narcotic, fishy; on dilution fried and
roasted aspects

Thiazoles



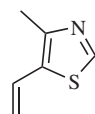
5-(2-Hydroxyethyl)-4-methylthiazole

meaty, nutty



2-Isopropyl-4-methylthiazole

green, vegetable character; nut-like, fruity



4-Methyl-5-vinylthiazole

nutty, musty, earthy, cocoa powder like

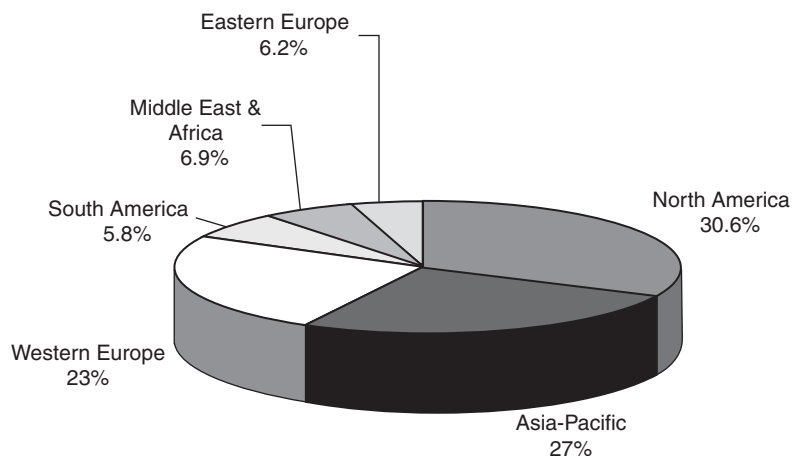


Fig. 6. Regional distribution of F&F market.

5. Economic Aspects

Aroma chemicals sales were expected to be $\$2,900 \times 10^6$ in 2011 up from $\$2,200 \times 10^6$ in 2006. Essential oils sales were expected to be $\$ \sim 5,000 \times 10^6$ up from $\$3,900 \times 10^6$ in 2006.

The regional distribution of the Flavor and Fragrance (F&F) market is shown in Fig. 6.

The top ten flavor and fragrance industry leaders and their estimated sales volume and market share are listed in Table 3.

6. Analytical Methods

Quality control of fragrance and flavor substances, as well as products derived from them, comprises the comparison of sensory, analytical, and it necessary, microbiological data with standards and specifications (5).

Table 3. Top Ten Fragrance and Flavor Industry Leaders^a

Company	Market share, %	Sales, \$ $\times 10^6$
Givaudan	20.6	4538.4
Firmenich	13.5	2978.0
IFF	11.9	2622.9
Symise	9.6	2106.6
Takasago	6.4	1416.2
Mane SA	2.9	643.4
Sensient Flavors	~ 2.6	582.6
T. Hasegawa	2.5	556.9
Robertet SA	2.2	484.5
Frutarom	2.1	451.1
<i>Total</i>	<i>74.5</i>	<i>~ 16381.6</i>
All others	25.5	~ 5618.4

^aFrom Ref. 4.

In the past few decades, a precise methodology has been developed for sensory evaluation. Increasingly in recent years, chemical sensor systems have been used for this purpose.

The analytical determination of identity and purity aids greatly in establishing the acceptability of fragrance and flavor materials. To meet customer requirements, all of these methods should be validated by quality assurance tools.

Single fragrance and flavor materials are identified by generally accepted analytical parameters such as density, refractive index, optical rotation, and melting point. The advantage of these methods is the short analysis time, which provides assessment criteria allowing comparison with other laboratories around the world. Spectroscopic methods such as IR and near IR are becoming more important for fast identity checks. NIR techniques may also be used for identification of single and complex fragrance and flavor materials.

Content as well as impurity determinations are done by gas chromatography (GC), high pressure liquid chromatography (HPLC), capillary electrophoresis (CE), and by spectroscopic techniques (UV, IR, MS, and NMR GC is used for quality and in-process control to give detailed results within a few minutes (6).

Classical sample preparation methods such as distillation and Soxhlet extraction are still used, but specific techniques such as supercritical fluid extraction (SFE) and, increasingly in recent years, adsorption techniques such as solid phase micro-extraction (SPME) and stir-bar extraction are also being used for isolation, separation, and identification of flavor and fragrance materials (7,8).

The determination of trace compounds such as halogens, heavy metals and pesticides, aflatoxins, residual solvents, and allergens in flavor and fragrance materials is becoming increasingly important (9–11).

For pesticides, a combination of GC-MS and LC-MS techniques is used to analyze quantities in the ppb range. Special detector systems such as electron capture detector (ECD) and atomic absorption spectroscopy (AAS) are used for detection and quantification of halogens and heavy metal content.

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