Ocimene

A versatile floral ingredient

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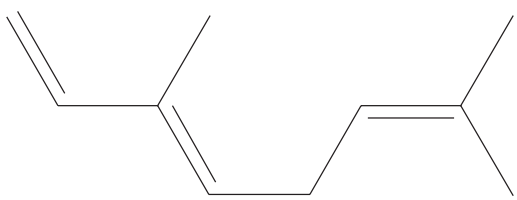
Ocimene (**F-1**) has a warm-herbaceous, citrus, tropical, green, terpene, woody odor that is very diffusive with relatively low tenacity. Its sweetness is almost floral, evoking an immediate similarity to neroli oil in the odor of pure ocimene.[1] It also has vegetable nuances, and when tasted it has a green, tropical, woody flavor with floral and vegetable nuances.[2] Ocimene occurs in ho leaf oil, hop oil, kumquat, mango, mint, neroli, bigarde oil, parsley, pepper, petitgrain, bergamot oil, lavender and more.

F-1. 3,7-Dimethyl-1,3,6-octatriene; (E)-β-ocimene; C10H16; CAS# 13877-91-3; FEMA# 3539



Pure ocimene can be used in numerous artificial essential oils, bergamot, lavandin, neroli, orange, basil, etc., but it is also in itself an interesting material for a new and powerful top-note effect in citrus colognes, lavender and fougere. It also has applications in mango and spicy-herbaceous fragrances, as well as limited use in household product fragrances.

There is a very considerable difference in price between ordinary grade ocimene and pure ocimene, but the terpene is often used so sparingly that it compensates for its relatively high cost. Commercial-grade ocimene is used as a starting material for the manufacture of a number of perfume chemicals, and it is also used occasionally as a perfume material since it creates very pleasant effects with bay oil in modem spicy-herbaceous fragrances.[1]

(E)-β-Ocimene is recommended for use in fragrances at levels up to 3%.[a, b]

The ocimenes (*trans-* or *cis-*) undergo oxidation most readily and with relatively shorter exposure to air to form a yellow resin. However, ocimene may be preserved unaltered in an atmosphere free from oxygen. **F-2** describes a list of additional isomers of ocimene. Ocimene derivatives used in the F&F industry are shown in **F-3**. The biosynthetic pathway for ocimene is shown in **F-4**.

Physical Data for Ocimene[a, b]

Appearance: Colorless to straw-colored liquid

M.W.: 136.2

Assay (min.): 80%

Boiling point: 176°–178°C

Specific gravity: 0.801–0.805 (25°C)

Refractive index: 1.4780–1.4910 (20°C)

Acid value (mgKOH/g): 1.00 max.

Flash point: 143°F TCC

LogP(o/w): 4.70 (estd.)

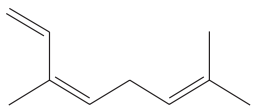
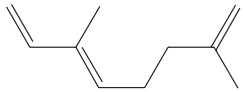
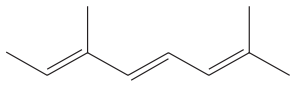
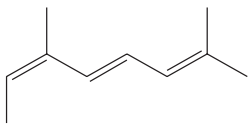
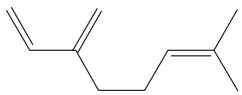
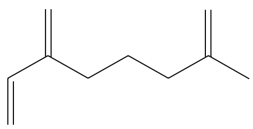
Monoterpene compounds, such as (E)-β-ocimene and myrcene, contribute significantly to the floral odors of numerous plant species.[5] (E)-β-Ocimene constitutes 87% of the scent of the orchid *Laelia anceps*, whereas the scent of *Brugmansia* x *candida*, a member of Solanaceae, contains as much as 52% (E)-β-ocimene.[6,7] In snapdragon (*Antirrhinum majus*), the monoterpene fraction of the floral scent bouquet is dominated by (E)-β-ocimene and myrcene, which account for 20% and 8% of total floral volatiles, respectively.[8] Snapdragon flowers emit these two monoterpene olefins—myrcene and (E)-β-ocimene—biosynthetically derived from geranyl diphosphate, in addition to a major phenylpropanoid floral scent component, methylbenzoate.

Emission of myrcene and (E)-β-ocimene is regulated developmentally and follows diurnal rhythms controlled by a circadian clock.[9]

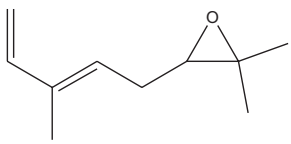
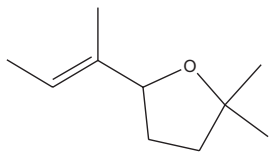
E-β-Ocimene is also a pheromone involved in social regulation in the honey bee colony (*Apis mellifera L.*). In honey bee colonies, the brood is able to manipulate and chemically control the workers in order to sustain their own development. A brood ester pheromone produced primarily by old larvae was first identified as acting as a contact pheromone with specific effects

[a] The Good Scents Company site database *www.thegoodscentscompany.com/*
[b] Ocimene PQ spec. sheet of Innospec for a product containing *cis*-β-ocimene >69%

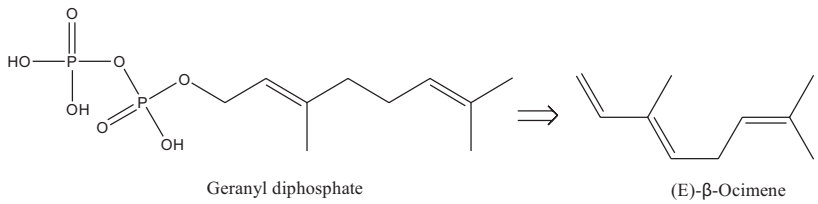
F-2. Ocimene isomers

Substance synonym [CAS no.]	Structure	Organoleptic properties
(Z)-β-Ocimene cis-3,7- dimethylocta-1,3,6-triene [3338-55-4]		Warm, floral, herbaceous, sweet
α-Ocimene 3,7-Dimethyl-1,3,7-octatriene [502-99-8]		Fruity, floral, wet cloth
(E,E)-2,6-Alloocimene (4E,6E)-2,6-dimethylocta-2,4,6-triene [3016-19-1]		Terpeny, sweet, fresh, floral
(E,Z)-Alloocimene (4E,6Z)-2,6-Dimethylocta-2,4,6-triene [7216-56-0]		n.a.
β-Myrcene 7-Methyl-3-methylene-1,6-octadiene [123-35-3]		Terpeny, herbaceous, woody with a rosy celery and carrot nuance[3]
α-Myrcene 2-Methyl-6-methylene-1,7-octadiene		n.a.

F-3. Ocimene derivatives

Substance synonym [CAS no.]	Structure	Organoleptic properties
Ocimene oxirane 2,2-Dimethyl-3-(3-methylpenta-2,4-dienyl)oxirane Myroxyde [69103-20-4]		Sweet, metallic, fresh, herbal, lavender, opoponax, clary, pear[a]
Ocimene quintoxide 5-[(E)-but-2-en-2-yl]-2,2-dimethyloxolane		Citrus, cooling, woody, camphoraceous, minty, with a green and fresh spicy nuance[5]

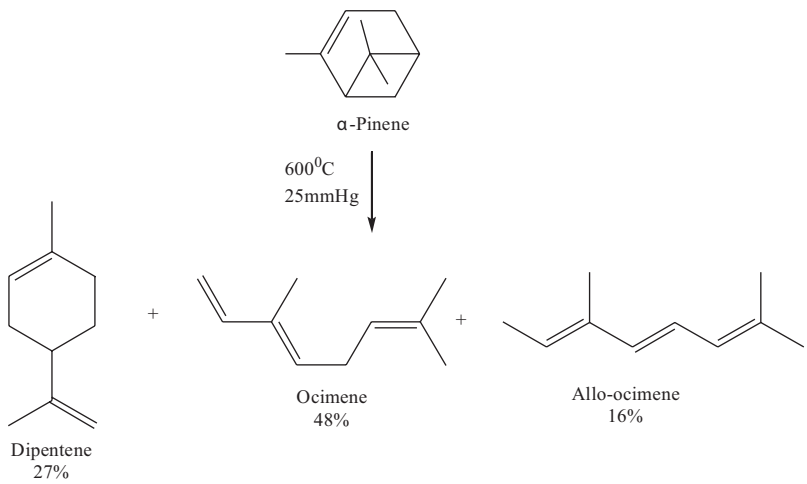
F-4. General biosynthetic pathway for ocimene



Geranyl diphosphate

(E)-β-Ocimene

F-5. Thermal rearrangement of α-pinene (pyrolysis)

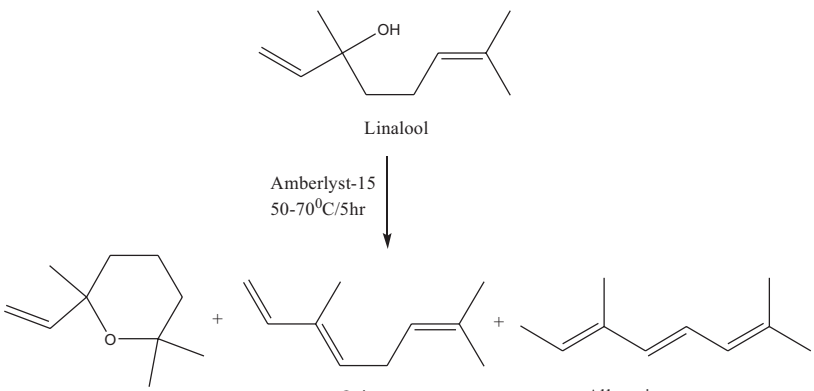


Dipentene
27%

Ocimene
48%

Allo-ocimene
16%

F-6. Dehydration of linalool



2-Vinyl-2,6,6-trimethyl-
3,4,5,6-tetrahydro-2H-pyran
9%

Ocimene
40%

Allo-ocimene
30%

on nurses in the colony. E-β-Ocimene has been identified recently as a new volatile brood pheromone, which partially inhibits ovary development in workers.[10] Ocimene is prepared by two main routes: 1) thermal rearrangement of α-pinene (pyrolysis) **(F-5)** and 2) by dehydration of linalool **(F-6)**.[11, 12]

References

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