

Molecule of the Month: Cyclooctenyl Methyl Carbonate

Characteristics and application in fragrance formulations

Michael Zviely, CIC; mzviely@cathay-israel-chemistry.com



Cyclooctenyl methyl carbonate (see **F-1**) is a colorless to pale yellow liquid with a floral, violet, banana odor. The material is neither found in nature, nor subject to EU fragrance allergen labeling. Its olfactory profile is floral, violet leaf, green and tagette, with fruity banana notes.*

The commercial material is a mixture containing (among others) carbonic acid methyl ester octahydro-pentalen-1-yl ester (see **F-2**), and cyclooct-4-en-1-yl methyl carbonate as the primary component.

Cyclooctenyl methyl carbonate is used in agrumen, aldehydic, alpine bouquet, amaryllis, apple and apple blossom fragrances. Its recommended use level in the final product is up to 2%. A part demonstration of a floral formulation using cyclooctenyl methyl carbonate is listed in **T-1**.

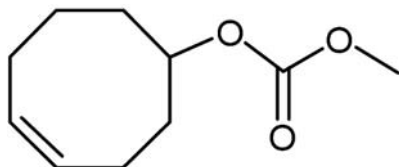
Cyclooctenyl methyl carbonate is stable in liquid detergents, concentrated fabric softeners, soaps, alcoholic fine fragrances, toiletries and antiperspirants. However, it is unstable in hypochlorite bleach and perborate powder detergents. Similarly, the material's substantivity is fair on skin, wet fabric and hair, and poor on dry fabric; its tenacity on blotter is more than 8 hours.**

* IFF and Takasago specifications data

** Takasago specification data

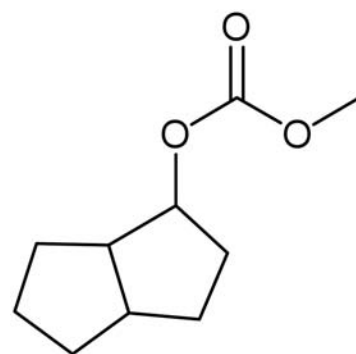
Cyclooctenyl methyl carbonate

F-1



Carbonic acid methyl ester octahydro-pentalen-1-yl ester

F-2

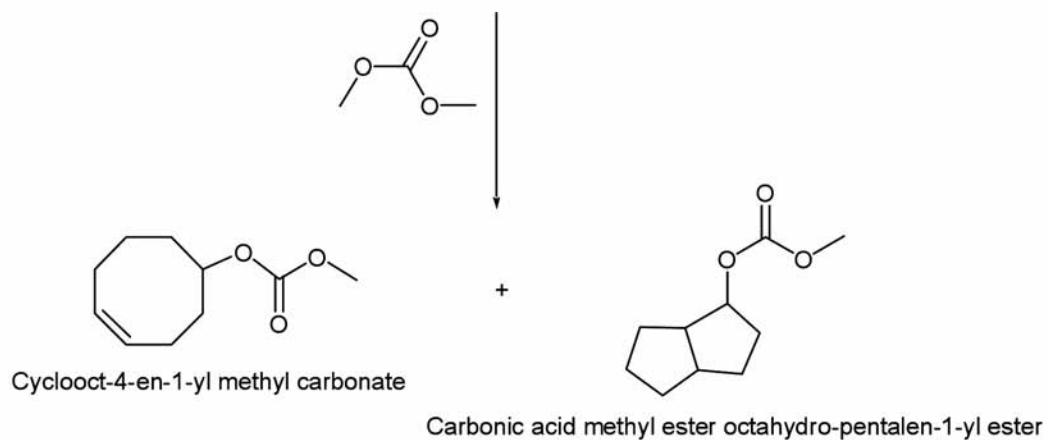
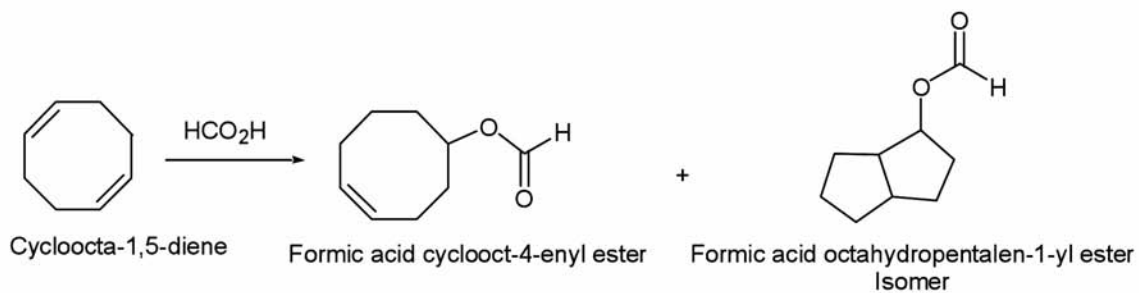


Physical data: Cyclooctenyl methyl carbonate

CAS#	87731-18-8
Synonyms	Carbonic acid, 4-cycloocten-1-yl methyl ester; Cyclooct-4-en-1-yl methyl carbonate; Violiff ^a ; Violet T ^b
Appearance	Colorless to pale yellow liquid
Molecular weight	184.2
Molecular formula	C ₁₀ H ₁₆ O ₃
Refractive index n ²⁰ /D	1.463–1.469
Specific gravity D ²⁵ /25	1.050–1.058
Purity (GC area)	68–78% (major peak)
Log Po/w	2.9
Flash point	94°C

^a Violiff is a trademark of IFF

^b Violet T is a trademark of Takasago



Floral formulation using cyclooctenyl methyl carbonate ‡

T-1

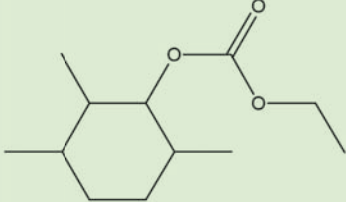
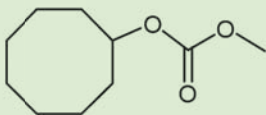
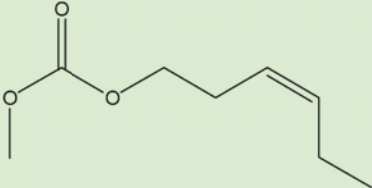
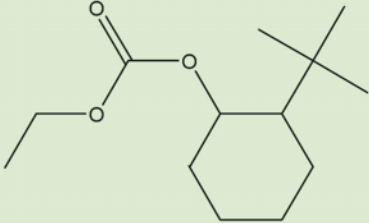
Ingredient	Parts
Benzyl acetate	9.1
Methyl dihydro jasmonate (Hedione [°])	35.5
Hexyl cinnamic aldehyde	11.4
Tetrahydro-3-pentyl-2h-pyran-4-yl acetate	5.9
Jasmone- <i>cis</i> 10% DPG	0.4
3-Butyltetrahydro-5-methyl-2h-pyran-4-yl acetate	9.9
3-and 4-(4-Hydroxy-4-methyl-pentyl) cyclohexene-1-carboxaldehyde (Lyrall ^d)	8.7
Phenyl ethyl alcohol	3.9
Styralyl acetate	2.4
Supalang ^e	4.9
3,7-Dimethyl-3-octanol and 2,6-dimethyl-2-octanol	3.9
Cyclooctenyl methyl carbonate 10% DPG	3.9

‡ IFF demonstration formula

[°] Hedione is the registered trademark of Firmenich

^d Lyrall is the trademark of IFF

^e Supalang is the trademark of IFF

Name	Structure	Olfactive description [△]
Carbonic acid, ethyl 2,3,6-trimethylcyclohexyl ester; Rholiate ^f		Herbal, fruity, floral, with aspects of saffron.
Methyl cyclohexyl carbonate; Jasmacyclat ^g		Floral-herbal, jasmine odor with fruity bottom note.
<i>cis</i> -3-Hexen-1-yl methyl carbonate; Leafarome ^h		Green, floral, violet.
Ethyl-2-tert-butyl-cyclohexyl carbonate; Floramat ⁱ		Herbaceous, fruity, musk.

[△]PMP 96, *Database of Perfumery Materials & Performance*, Boelens Aroma Chemicals Information Services, Netherlands.

^fRholiate is the trademark of Symrise

^gJasmacyclat is the trademark of Kao Chemicals

^hLeafarome is the trademark of IFF

ⁱFloramat is the trademark of Kao Chemicals

Cyclooctenyl methyl carbonate is prepared from cycloocta-1,5-dien; the process begins with the addition of formic acid to one double bond. Formic acid, octahydro-pentalen-1-yl ester is also obtained in this reaction. Both formate esters further react with dimethyl carbonate (by transesterification) to yield cyclooct-4-en-1-yl methyl carbonate and carbonic acid methyl ester octahydro-pentalen-1-yl ester, as shown in **F-3**. **T-2** lists other carbonates that are used as fragrance ingredients.

Address correspondence to Michael Zviely, CIC, 3, Haim-Hazaz St, Haifa, 34996, Israel.

References

1. US Pat 4397789, Alkyl-4-cyclooctenyl carbonates and uses thereof in augmenting or enhancing the aroma of perfume compositions, colognes and perfumed articles, RM Boden and M Licciardello, assigned to IFF (August 9, 1983)

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