

Unsaturated Trimethyl Undecanals— Chemistry and Odor



Floral notes

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The trimethylundecane unsaturated aldehydes are mostly floral aliphatic aldehydes, having rather related olfactory properties and similarity in the molecular structure, suggesting a possible SOR (structure-odor-relationship).

2,6,10-Trimethyl-9-undecenal (**F-1**) is a fresh, aldehydic, marine, powerful, floral ingredient. 2,6,10-Trimethyl-9-undecenal blends extremely well with floral notes such as lily of the valley and cyclamen, as well as with fruity and woody compositions. It can also be seen as having a typical fresh linen odor which makes it very useful for detergent perfumes. 2,6,10-Trimethyl-9-undecenal has a natural, ozonic aspect and due to its high ϕ value it must be used carefully^a.

2-Methyl-4-(2,6,6-trimethyl-2(1)-cyclohexen-1-yl) butanal (CAS# 65405-84-7, cetonal) is another aliphatic unsaturated aldehyde; having an orris, woody, powerful odor, it is an elegant ingredient used in woody, orris accords as well as with leather, tobacco and animal notes where it acts as an excellent blending agent and adds to the harmony of a fragrance (**F-2**).

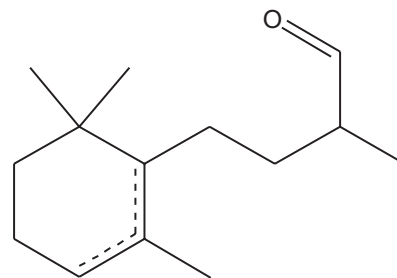
^a Organoleptic descriptions are mostly taken from commercial producers' specs, e.g., Givaudan, Symrise.

2,6,10-Trimethylundeca-5,9-dienal (CAS# 54082-68-7, profarnesal) has an aldehydic-floral odor, reminiscent of nuances in lily of the valley and orchid flowers, with fruity, green, waxy and fresh-air accents (**F-3**).

Using 2,6,10-trimethyl-5,9-undecadienal for improving tobacco smoke taste in cigarettes was claimed by Takasago Perfumery Co. Ltd. and Japan Tobacco Inc. According to

2-Methyl-4-(2,6,6-trimethyl-2(1)-
cyclohexen-1-yl) butanal

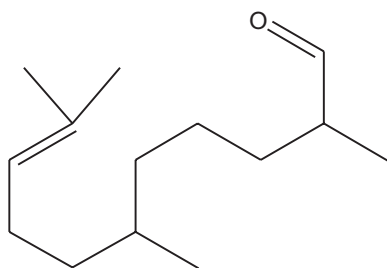
F-2



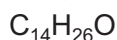
2-Methyl-4-(2,6,6-trimethyl-2(1)-
cyclohexen-1-yl) butanal

2,6,10-Trimethyl-9-undecenal

F-1



2,6,10-Trimethyl-9-undecenal

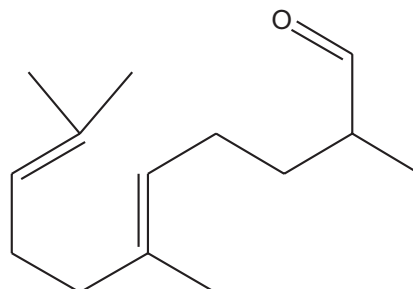


CAS# 141-13-9

Adoxal, farenal

2,6,10-Trimethyl-undeca-5,9-dienal

F-3



2,6,10-Trimethyl-undeca-5,9-dienal

Physical Data for 2,6,10-Trimethyl-9-undecenal

| | |
|-------------------|------------------------------------|
| Appearance: | Colorless pale yellow clear liquid |
| M.W.: | 208.18 |
| Specific Gravity: | 0.845 to 0.850 20°C |
| Refractive Index: | 1.451 to 1.455 20°C |
| Flash Point: | >93°C TCC (>200°F) |
| logP (o/w): | 5.35 (estd.) |

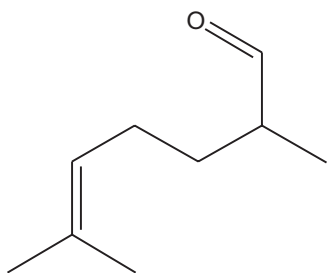
the patent, 2,6,10-trimethyl-5,9-undecadienal is capable of significantly favorably adding sweetness to cigarettes with an extremely small amount (<15 ppm), increasing softness in cigarette smoke, imparting the cigarette aroma with both broadness and powerfulness, thus ensuring the sweetness inherent in cigarettes.

To the above molecules, another one can be added, namely 2,6-dimethyl-heptenal (melonal), with its powerful, green, melon, cucumber odor character, and 6-methoxy-2,6-dimethylheptanal (Methoxymelonal, an old Bush Boake Allen name), having a light floral, slightly fruity note with watery citrus character.² In perfumery, methoxymelonal may be used to add a fresh

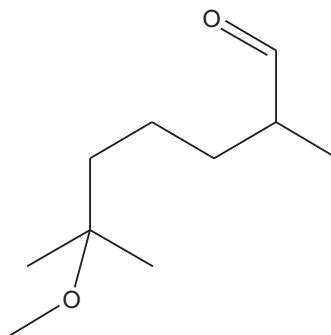
2,6-Dimethylhept-5-enal and 6-methoxy-2,6-dimethylheptanal

F-4

53



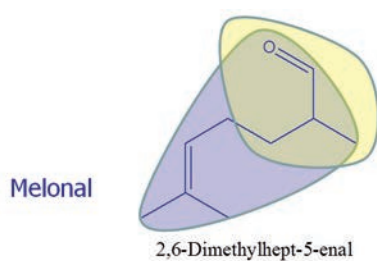
2,6-Dimethylhept-5-enal



6-Methoxy-2,6-dimethylheptanal

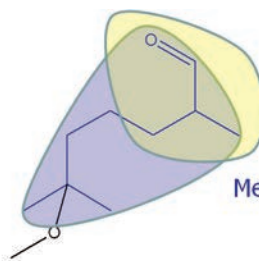
Aldehydes based on 2,6-dimethylheptane structure (containing α -methylpropanal moiety)

F-5



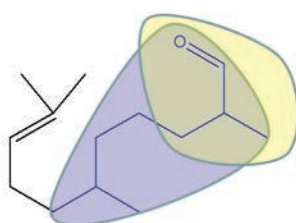
Melonal

2,6-Dimethylhept-5-enal

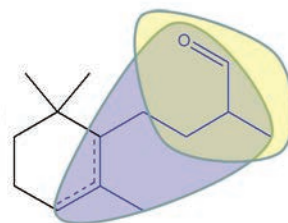


Methoxymelonal

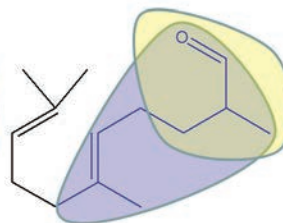
6-Methoxy-2,6-dimethylheptanal



2,6,10-Trimethylundec-9-enal
Adoxal; Farenal



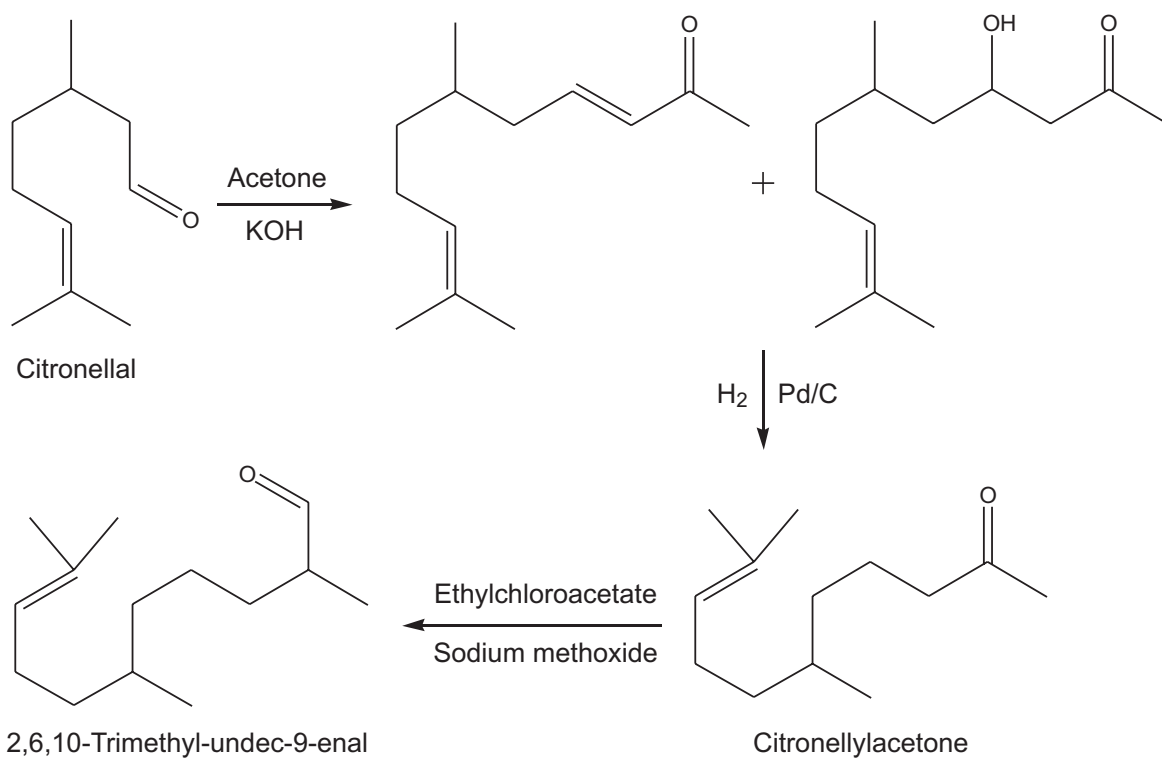
2-Methyl-4-(2,6,6-trimethyl-2(1)-
cyclohexen-1-yl)butanal
Cetonal



2,6,10-Trimethylundeca-5,9-dienal
Profarnesal

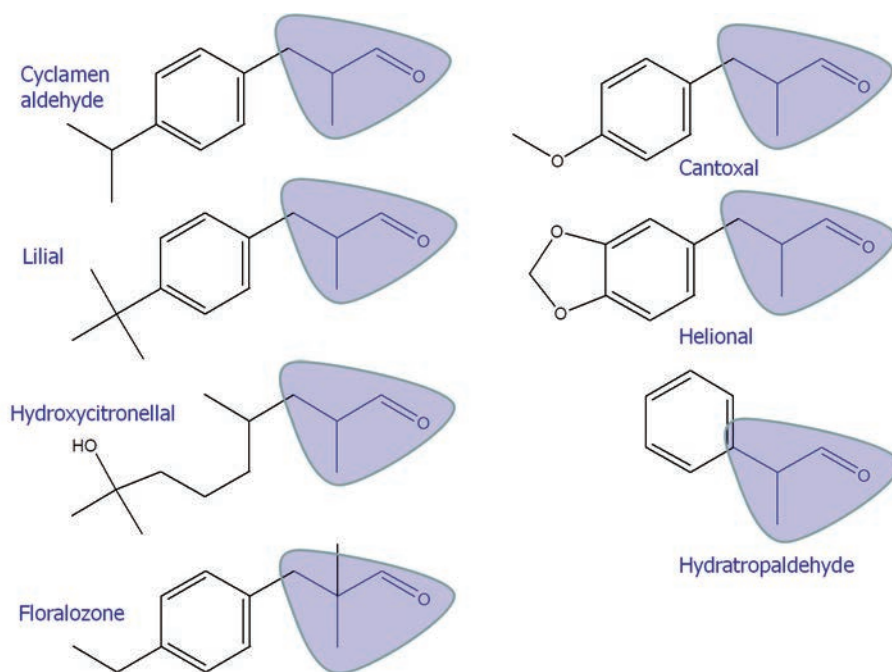
Process for 2,6,10-trimethyl-9-undecenal

F-6



Aldehydes for use in fragrance applications such as fine fragrance to household

F-7



florality to a variety of odor types.^{3,4} It combines especially well with green, citrus and floral bouquets (**F-4**).

This fundamental moiety—2,6-dimethylheptanal, with a double bond at position 5, as in Cetonal^b and partly in profarnesal, or without the double bond at position 5—as in adoxal/farnesal and methoxymelonol might direct toward the SOR of all these aldehydes, as having this general olfactophore, which will be studied in the future.

Aldehydes Based on 2,6-Dimethylheptane Structure (Containing α -Methylpropanal Moiety)

This moiety might be a generalization of a more basic olfactophore, i.e., α -methyl-propanal, as being very widespread in the following series of floral fragrance ingredients (the α -methylpropanal moiety is marked in both schemes above and below) (**F-5**).

Aldehydes Based on α -Methylpropanal Structure

There are several synthetic pathways toward 2,6,10-trimethyl-9-undecenal and its family, mostly based on Darzens reactions.³


In the following scheme, a route starting with a condensation between citronellal and acetone is used to obtain citronellylidene-acetone and the hydrated derivative. The double bond is then hydrogenated in the presence of a catalyst to get citronellyl-acetone. The last is condensed with ethyl chloroacetate in presence of sodium methoxide to give the glycidic ester, which undergoes basic hydrolysis to get the intermediate glycidic acid salt. After acidification and decarboxylation, 2,6,10-trimethyl-9-undecenal is obtained (**F-6**).

Many of the aldehydes are used in fine fragrance (alcoholic perfumes), beauty care (creams and lotions, antiperspirants/deodorants, hair conditioners) tablet and liquid soap, laundry care (liquid detergents), and different household items, e.g., talcum powder, candles, potpourri and incense (**F-7**).

For example, in *M/MINK* (Byredo Parfums and M/M) eau de parfum launched in 2010, Adoxal is used in the opening, accompanied by the perfume heart consisting of incense with a dry-down patchouli leaf, clover honey and amber, designed by Jerome Epinette of Robertet.

References

1. A Akira; N Tatsufumi, T Kazuhiko, K Tsuneyoshi, F Mine, M Mitsusachi and T Hidetoshi, JP 02131564 A, Jpn Kokai Tokkyo Koho (1990)
2. M Zviely, 6-Methoxy-2,6-dimethylheptanal, *Perfum Flavor*, 35, 22 (2010)
3. G Darzens, *Compt Rend*, 139, 1214 (1904)
4. U Huchel, Odor-Imparting Detergent, Cleaning or Care Product, Henkel AG & Co KGAA, DE102009026855 (2010)

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^b Cetonal is a trademark of Givaudan