Aldehydes and Acetals - Part 1*

Application as flavor and fragrance ingredients

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Aldehydes, one of the key aroma ingredient groups, have a considerable effect in both fragrances and flavors. Some of the first aldehydes to be used as synthetic molecules in a perfume were octanal, nonanal and decanal (**see F-1**); they were used in the formulation of *Chanel No. 5* by Chanel in 1921.** The odor note of these aliphatic linear aldehydes is green-floral and "aldehydic," usually described as the odor note of long-chain fatty aldehydes, e.g., fatty-sweaty, ironed laundry and sea water.

Aliphatic Aldehydes

Most aliphatic aldehydes occur in nature. Octanal (aldehyde C-8, caprylic aldehyde), nonanal (aldehyde C-9, pelargonic aldehyde) and decanal (aldehyde C-10, capric aldehyde) are found in many citrus oils and represent the saturated aliphatic group.

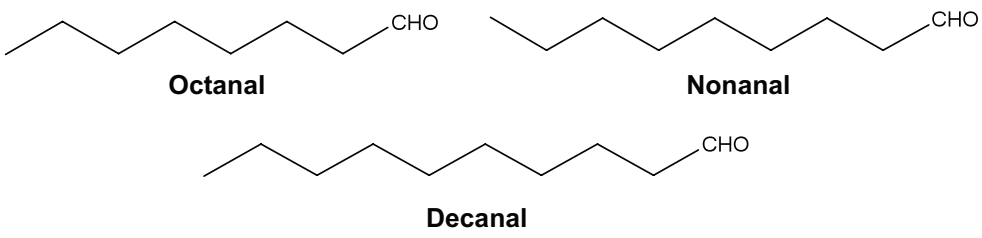
In addition, there are some branched aldehydes, such as aldehyde MOA (2-methyldecanal) and aldehyde MNA (2-methylundecanal) (**see F-2**). Aldehyde MOA, which is not yet reported to be found in nature, has a fresh, aldehydic, fatty odor, and an herbal-incense note on dilution. Aldehyde MNA, on the other hand, occurs in citrus and kumquat, and has a waxy, fatty, metallic odor, with citrus nuances.*** The preparation of these materials from the unsaturated aldehyde is shown in **F-3.**[1]

The unsaturated group of aldehydes contains several ingredients that are used in the formulation of flavors and fragrances. 7-Hydroxy-3,7-dimethyloctanal (Cyclosia Base, Firmenich) is a bifunctional molecule, and an hydroxyaldehyde possessing a smooth and flowery note

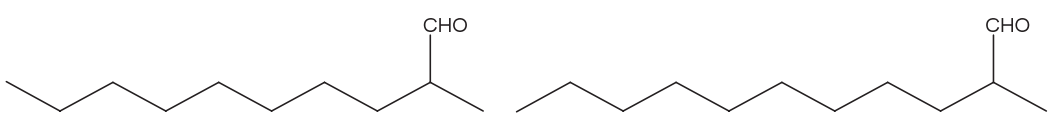
*Part 2 of this article will appear in the September 2009 issue.
**n-Octanal and n-decanal were first synthesized in 1912; n-nonanal earlier, in 1900.

***Most of the information on occurrence, organoleptic properties and uses is taken from: FRM 2001—Database of Flavour Raw Materials and PMP 96, *Database of Perfumery Materials & Performance*, Boelens Aroma Chemicals Information Services, Netherlands. Some of the organoleptic information is cited from suppliers specification sheets, *e.g.* IFF, Givaudan, Firmenich, Takasago, KAO, etc.

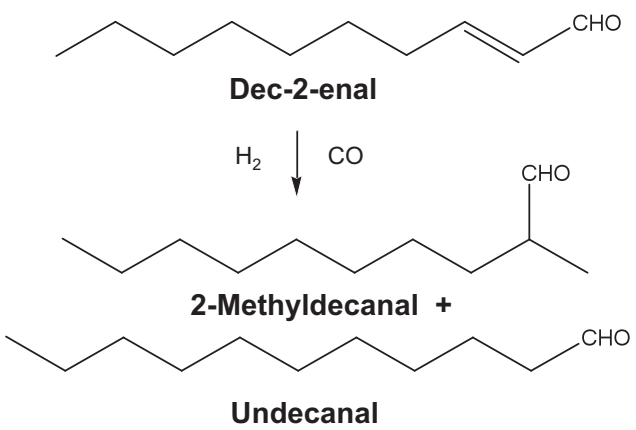
Octanal, nonanal, decanal **F-1**



Aldehyde MOA; aldehyde MNA **F-2**



Preparation of 2-methyldecanal and 2-methylundecanal **F-3**

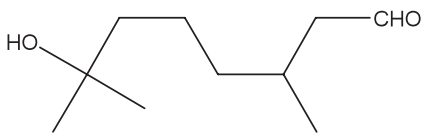


(**see F-4**). With a diffusion that sets it apart from that of hydroxycitronellal, this aldehyde is used in perfumes requiring muguet or white floral effects.

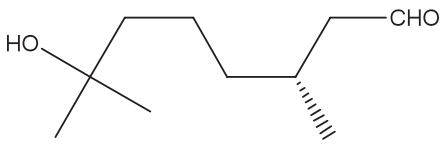
(3R)-7-Hydroxy-3,7-dimethyloctanal (l-Laurinal, Takasago) is one enantiomer of this optically active molecule, which is a volatile constituent of large cardamom (*Amomum subulatum* Roxb) (**see F-5**). It has a sweet-floral odor, and can be used in almost any floral accord, especially muguet and lilac.

Next, among bifunctional aldehydes is 3-methylthiopropionaldehyde (Methional; IFF), which occurs in vegetables, bread, dairy, meat, roasted products, tomato, cheddar cheese, whisky and potato chips (**see F-6**). It has a green sulfurous, aldehydic, caprylic, potatolike, musty, tomato and vegetative odor and flavor.

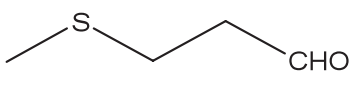
7-Hydroxy-3, 7-dimethyloctanal **F-4**



(3R)-7-Hydroxy-3,7-dimethyloctanal **F-5**



3-Methylthiopropionaldehyde **F-6**



Monounsaturated Aldehydes

trans-2-Hexenal (leaf aldehyde) occurs in citrus oils, apples, bananas, raspberries, strawberries, tomatoes and cucumbers (**see F-7**) and has a strong leafy green, slightly spicy, bitter almondlike odor and flavor. *trans*-2-Dodecenal (Cilantro Aldehyde, Frutarom; Aldehyde Mandarin, Firmenich), on the other hand, occurs in dairy products, heated chicken, coriander oil and roasted peanuts (**F-7**). It has a strong fatty odor and flavor that turns somewhat citrusy on dilution.

trans-2-Decenal, with its slightly fatty, citrusy on dilution, orangelike odor and flavor, and *trans*-4-decenal, with its aldehydic, orange, green, floral odor and flavor, are two isomers (**see F-8**).

2,6-Dimethyl-5-heptenal (Melonal, Givaudan) occurs in lemon peel, lime peel and ginger, and has a powerful, green, watery-fruity, melon and cucumber odor and flavor (**see F-9**). Due to its powerful, unique note this aldehyde is effective in all types of fragrances, and is especially important in the creation of natural-smelling marine and fruity-melon notes. The preparation of 2,6-dimethyl-5-heptenal starts from 6-methylhept-5-en-2-one, as is shown in **F-10**.

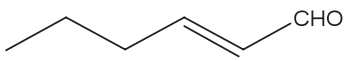
3,5,5-Trimethylhexanal (Vandor B, IFF) is an aldehydic, green, citrusy material, which has a powerful, almost pungent, aldehydic, green note and gives a fresh, clean impression on dilution (**see F-11**).

2,6,10-Trimethyl-9-undecenal (Adoxal, Givaudan; Farenal, Symrise) is a fresh, aldehydic, marine, powerful, floral ingredient that blends extremely well with floral notes such as muguet and cyclamen, as well as with fruity and woody compositions (**see F-12**). It can also possess a typical "fresh linen" odor, which makes it very useful for detergent perfumes. In addition, this ingredient has a natural, ozonic aspect.

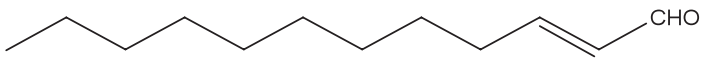
2,6,10-Trimethyl-9-undecenal is prepared from ψ-ionone, as shown in **F-13**.

2-Methyl-4-(2,6,6-trimethyl-2(1)-cyclohexen-1-yl) butanal (Cetonal, Givaudan) is yet another aliphatic unsaturated aldehyde that, due to its orris, woody,

trans-2-Hexenal (leaf aldehyde); *trans*-2-dodecenal — F-7

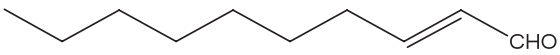


***trans*-2-Hexenal**
(Leaf Aldehyde)

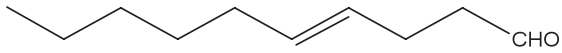


***trans*-2-Dodecenal**

trans-2-Decenal; *trans*-4-decenal — F-8

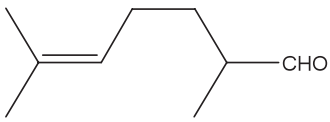


***trans*-2-Decenal**



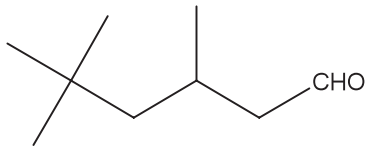
***trans*-4-Decenal**

2,6-Dimethyl-5-heptenal — F-9



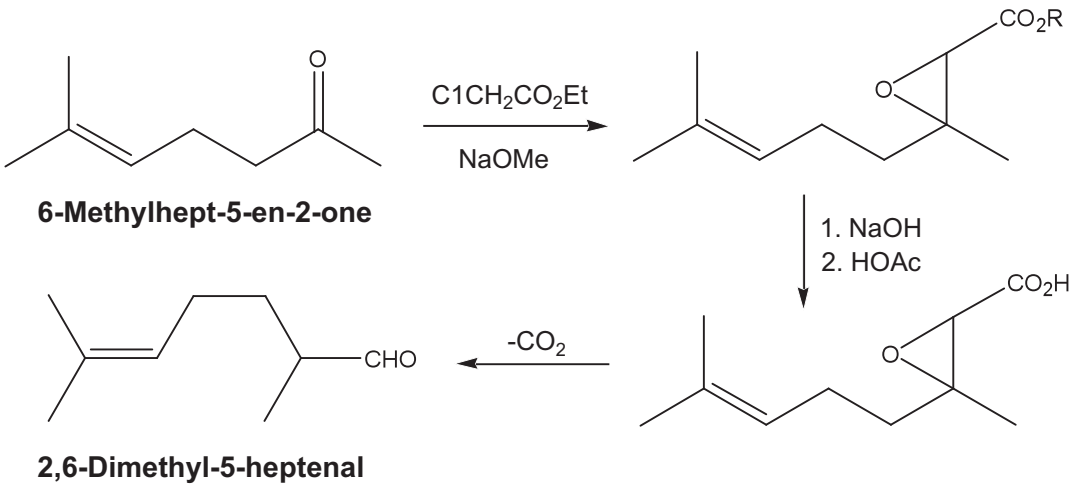
2,6-Dimethyl-5-heptenal

3,5,5-Trimethylhexanal — F-11



3,5,5-Trimethylhexanal

Preparation of 2,6-dimethyl-5-heptenal — F-10



6-Methylhept-5-en-2-one

2,6-Dimethyl-5-heptenal

powerful odor, is an elegant ingredient for application in woody, orris accords (**see F-14**). It also blends well with leather, tobacco and animal notes, where it acts as an excellent blending agent and adds to the harmony of a fragrance. Citronellyl oxyacetaldehyde, [synonym: (3,7-dimethyl-oct-6-enyloxy)-acetaldehyde, (Muguet Aldehyde, IFF)], an unsaturated ether-aldehyde, is a floral, aldehydic, fresh material, with a refreshing, aldehydic, rosy ozonelike note (**see F-15**). Traces of this material contribute a pleasant top note.

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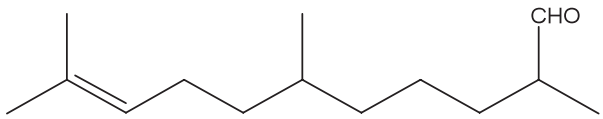
References

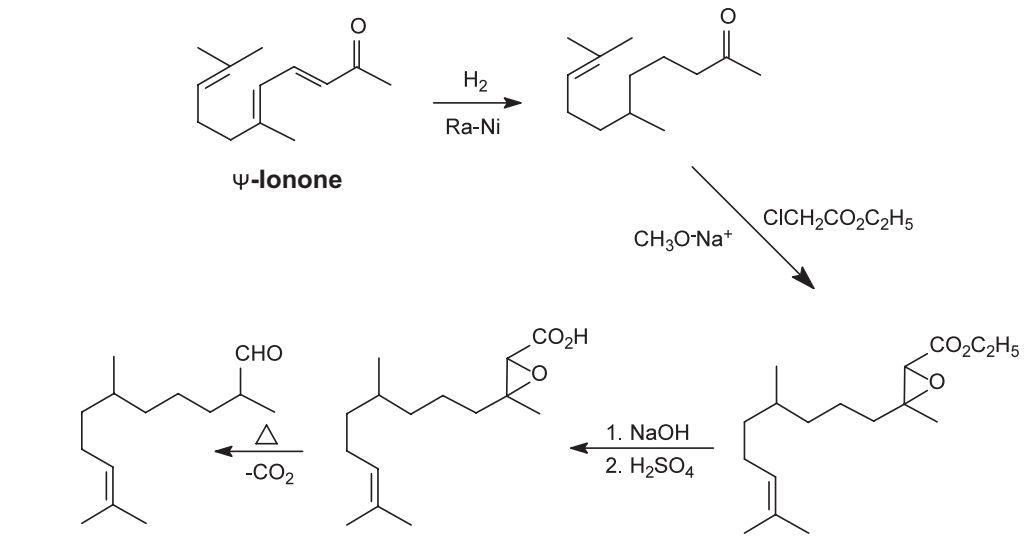
1. US 4258214, Process of the preparation of aldehydes, Bahrmann Helmut; Cornils Boy; Diekhaus Gerhard; Kascha Waldemar; Weber Juergen, assigned to Ruhrchemie AG (1981)

2,6,10-Trimethyl-9-undecenal F-12



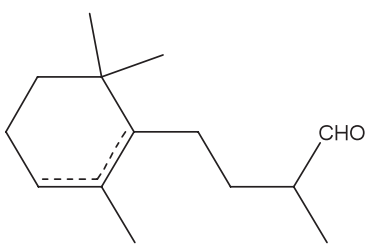
2,6,10-Trimethyl-9-undecenal

Preparation of 2,6,10-trimethyl-9-undecenal F-13



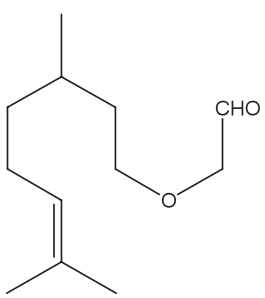
2,6,10-Trimethyl-9-undecenal

2-Methyl-4-(2,6,6-trimethyl-2(1)-cyclohexen-1-yl)butanal F-14



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

Citronellyl oxyacetaldehyde F-15



Citronellyl oxyacetaldehyde