Kurt Bauer/Dorothea Garbe

Common Fragrance and Flavor Materials

Preparation, Properties and Uses

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Preface

Fragrance and flavor materials are used in a wide variety of products, such as soaps, cosmetics, toiletries, detergents, alcoholic and non-alcoholic beverages, ice cream, confectioneries, baked goods, convenience foods, tobacco products, and pharmaceutical preparations. This book presents a survey of those natural and synthetic fragrance and flavor materials which are produced commercially on a relatively large scale, or which are important because of their specific organoleptic properties. It provides information concerning their properties, methods employed in their manufacture, and areas of application. Therefore, the book should be of interest to anyone involved or interested in fragrance and flavor, *e. g.*, perfumers, flavorists, individuals active in perfume and flavor application, food technologists, chemists, and even laymen.

The book is, essentially, a translation of the chapter on fragrance and flavor materials in *Ullmanns Encyklopädie der technischen Chemie,* Volume 20, 4th Edition, Verlag Chemie GmbH, Weinheim (Federal Republic of Germany), 1981. The original (German) text has been supplemented by inclusion of recent developments and of relevant information from other sections of the Encyclopedia. The present English version will make the information available to a wider circle of interested readers.

The condensed style of presentation of "Ullmann's" has been maintained. A more detailed treatment of various items and aspects was considered but was believed to be outside the scope of this book. Additional information, however, can be obtained from the literature cited.

To improve its usefulness, the book contains

- a formula index, including CAS registry numbers;
- an alphabetical index of single fragrance and flavor compounds, essential oils, and animal secretions.

Starting materials and intermediates are not covered by these indexes.

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K. Bauer
D. Garbe

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1 Introduction

History. Since early antiquity, spices and resins from animal and plant sources have been used extensively for perfumery and flavor purposes, and to a lesser extent for their observed or presumed preservative properties. Fragrance and flavor materials vary from highly complex mixtures to single chemicals. Their history began when mankind discovered that components characteristic of the aroma of natural products could be enriched by simple methods. Recipes for extraction with olive oil and for distillation have come down to us from pre-Christian times.

Although distillation techniques were improved, in particular in the 9th century A. D. by the Arabs, the production and application of these concoctions remained essentially unchanged for centuries. Systematic development began in the 13th century when pharmacies started to prepare so-called remedy oils and later recorded the properties and physiological effects of these oils in pharmacopoeias. Many essential oils used by perfumers and flavorists today were originally prepared by distillation in pharmacies in the iatrochemical era of the 16th and 17th centuries.

Another important step forward in the history of natural fragrance materials occurred in the first half of the 19th century when the production of essential oils was industrialized due to the increased demand for these oils as perfume and flavor ingredients. Companies such as Schimmel & Co., in Miltitz (Germany), were founded at this time.

Around 1850, single organic compounds started to be used for the same purposes. This development resulted from the isolation of cinnamaldehyde from cinnamon oil by J. B. Dumas and E. M. Péligot in 1834, and of benzaldehyde from bitter almond oil by J. Liebig and F. Wöhler in 1837. The first synthetic "aroma oils" were introduced between 1845 and 1850. These consisted of lower fatty acid esters of several alcohols and were produced synthetically by the chemical industry for their fruity odor. Methyl salicylate was to follow in 1859 as "artificial wintergreen oil" and benzaldehyde in 1870 as "artificial bitter almond oil". With the industrial synthesis of vanillin (1874) and coumarin (1878) by Haarmann & Reimer, Holzminden (Germany), a new branch of the chemical industry was founded. The number of fragrance and flavor chemicals produced synthetically has expanded ever since through systematic investigation of essential oils and fragrance complexes for odoriferous compounds. Initially, only major components were isolated from natural products, their structure elucidated and feasible processes developed for their isolation or synthesis. The present trend is to isolate and identify characteristic fragrance and flavor substances which occur in the natural products in only trace amounts. The isolation and structure elucidation of these components requires the use of highly perfected chromatographic and spectroscopic techniques. Interesting products can then be made synthetically.

Definition and physiological significance. Fragrance and flavor substances are comparatively strong smelling organic compounds with characteristic and usually pleasant odors. They are, therefore, used in perfumes and perfumed products, and also for the flavoring of regular and luxury food and beverages. Whether a particular product is called a fragrance or a flavor substance depends on whether it happens to be used in a perfume or in a flavor. In a way similar to the taste substances – among them the salty, sour, bitter, or pungent tasting compounds, which are not dealt with here – they are chemical messengers, the receptors being the olfactory cells in the nose and, to a lesser extent, the taste buds in the tongue [1].

Chemical signals are indispensable for the survival of many organisms, which use chemoreceptors to find their way, to hunt for food and inspect it, to detect enemies and harmful objects, and to find members of the opposite sex (pheromones). For humans, these functions are no longer vitally important, as is evident from the smaller number of receptors in humans as compared with other mammals. However, humans have retained the ability to detect odors. Undoubtedly, human beings can be affected in their behavior by fragrances and aromas, even without being aware of it.

Sensory information obtained from interaction between fragrance and flavor molecules and olfactory and taste receptors is processed in certain cerebral areas which are associated with these receptors, resulting in perception. Sometimes a single chemical compound suffices to transmit the information, but often a combination of compounds, which may originate from more than one source, *i.e.* a fragrance complex, is needed.

Since humans depend, for orientation, to a larger extent on acoustic and optical signals than do other mammals, the importance of flavor and fragrance substances has changed not only quantitatively but also qualitatively. Although food acceptance in humans is determined to a large extent by appearance and texture, flavor is nevertheless an essential part. For example, spices are added to food for their taste and flavor, not for their nutritional value. Also aromas formed during frying and baking enhance the enjoyment of food. Since enjoyment is defined as perception of beauty, flavor in food is an esthetic quality which, as in wines, can be described with words from the fine arts, such as harmonic or elegant.

Unlike flavoring substances, fragrances are not vitally important for humans. The use of fragrances in perfumery is primarily directed towards invoking pleasurable sensations, by shifting the organism's emotional level. Whereas in aromas, generally mixtures of many chemical compounds, "naturalness" is preferred, it is the talent and imagination of the perfumer which is essential in creating a perfume.

Natural, nature-identical, and artificial products. "Natural" products are those products which are obtained directly from plants and sometimes from animal sources by physical procedures. "Nature-identical" compounds are produced synthetically but are chemically identical with their "natural" counterparts. "Artificial" flavor substances are compounds which have not yet been identified in plant or animal products for human consumption.

"Nature-identical" aroma substances are with very few exceptions the only synthetic compounds used in flavors in addition to "natural" products. The initial function of our olfactory and taste receptors, as well as their evolutionary development, may explain why "artificial" flavor and fragrance substances are far less important. Also compounds used in fragrances only are, to a large extent, components of natural products, *e. g.* constituents of essential oils, resins, or animal secretions. The fragrance characteristics of artificial compounds nearly always mimic a natural example.

Odor and structure. The similarity between odors arises from the phenomenon that dissimilar substances or mixtures of compounds may interact with receptors in such a way as to create similar sensory impressions in the sensory centers of the brain.
On the other hand, small changes in structure, *e. g.* the introduction of one or more double bonds in aliphatic alcohols or aldehydes, may cause a different sensory impression or may intensify an odor by several orders of magnitude. Compounds having a similar odor despite totally different structures are, for example, the group of musk fragrances, comprising macrocyclic ketones and esters as well as aromatic nitro compounds and isochroman derivatives. In the near future, increasing knowledge of the structure and functioning of olfactory receptors may provide a better scientific basis for odor-structure correlation in fragrance and flavor substances and facilitate predicting the odor of still unknown compounds more accurately.
Alcohols, aldehydes, ketones, esters, and lactones are classes of compounds which occur most frequently in natural and artificial fragrances.
Fragrances must be volatile to be perceived. Therefore, in addition to the nature of the functional groups and the molecular structure of a compound, the molecular mass is an important factor. Molecular masses around 200 occur relatively frequently, masses over 300 are an exception.
Since fragrance compounds differ in volatility or tenacity, the odor of a perfume composition changes during evaporation. One distinguishes the topnote, the middle notes or body, and the dry out which consists mainly of less volatile compounds [2]. The odor perception also depends to a large extent on odor intensity. Therefore, the topnote is not made up of the most volatile compounds alone.
Due to the specificity of olfactory receptors, some compounds can be perceived in extremely low concentrations and significant differences in threshold concentrations are observed. The threshold concentration is defined as the lowest concentration in which a chemical compound, under standard conditions, can be distinguished with certainty from a blank.
For the compounds described in chapter 2, threshold concentrations vary by a factor 10^6 to 10^7. This is one of the reasons why some fragrance and flavor compounds are manufactured in quantities of a few kilograms per year, others in quantities of several thousands of tons.
The relative contribution of a particular compound (its odor or flavor value) to the odor impression of a composition can be expressed as the ratio between the concentration of the compound in the mixture and its threshold concentration, provided that threshold concentrations are not affected by the other fragrance and flavor compounds which are present [3]. Whereas it is extremely difficult to describe the odor of single chemical compounds unequivocally, it is often impossible to do so for complex mixtures; it is only possible when one of the components is so characteristic that it

determines to a large extent 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, hay-like, etc., thus relating fragrances to natural or otherwise known products with similar odors.

A few terms commonly used to describe odors are listed below:

aldehydic	odor note of the long-chain fatty aldehydes, *e. g.* fatty-sweaty, ironed laundry, sea-water;
animal(ic)	typical notes from the animal kingdom, *e. g.* musk, castoreum, skatol, civet, ambergris;
balsamic	heavy, sweet odors, *e. g.* cocoa, vanilla, cinnamon, Peru balsam;
camphoraceous	reminiscent of camphor;
citrus	fresh, stimulating odor of citrus fruits such as lemon, orange, etc.;
earthy	humus-like, reminiscent of humid earth;
fatty	reminiscent of animal fat and tallow;
floral, flowery	generic terms for odors of various flower types;
fruity	generic term for odors of various fruit types;
green	typical odor of freshly cut grass and leaves;
herbaceous	non-characteristic, complex odor of green herbs with, *e. g.*, sage, minty, eucalyptus-like, or earthy nuances;
medicinal	odor reminiscent of disinfectants, *e. g.* phenol, lysol, methyl salicylate;
metallic	typical odor observed near metal surfaces, *e. g.* brass or steel;
minty	peppermint-like odor;
mossy	typical note reminiscent of forest depths and seaweed;
powdery	note associated with toilet powders, diffusively sweet;
resinous	aromatic odor of exudates of trees;
spicy	generic term for odors of various types of spices;
waxy	odor resembling that of candle-wax;
woody	generic term for the odor of wood, *e. g.* cedarwood, sandalwood, etc.

2 Single Fragrance and Flavor Compounds

Compounds of commercial interest are arranged in this chapter following the Beilstein system of functional groups. They are not arranged according to organoleptic properties since the relationship between odor and structure is difficult to establish, as mentioned above. For practical reasons the Beilstein system has been abandoned in a few cases. Hydrocarbons and oxygen-containing compounds are described first. Nitrogen- and sulfur-containing compounds are incorporated in the chapter of parent compounds under the heading "Miscellaneous Compounds". Terpenes, a most important group of compounds, have been placed under separate headings (2.2 Acyclic terpenes, 2.3 Cyclic terpenes), after the aliphatic compounds (Sect. 2.1). The non-terpenoid cycloaliphatics are described in Sect. 2.4. In the aromatic series, phenols and phenol derivatives are arranged under a separate heading, accounting for their biogenetic and odor relationships. For the same reason methylenedioxyphenyl derivatives are also described under this heading although, systematically, they belong to the O-heterocycles. Compounds which are manufactured in minor quantities only, but which are important in applications due to their high odor intensity, are mentioned but not described in detail.

2.1 Aliphatic Compounds

The acyclic terpenes are discussed separately in Sect. 2.2. Some of the cycloaliphatic fragrance and flavor compounds are structurally related to the cyclic terpenes and are, therefore, discussed in Sect. 2.4 after the cyclic terpenes.

2.1.1 Hydrocarbons

Saturated and unsaturated aliphatic hydrocarbons, with straight as well as branched chain, occur abundantly in natural foodstuffs such as fruits. They contribute to the odor and taste only to a limited extent. The highly unsaturated hydrocarbons 1,3-*trans*-5-*cis*- and 1,3-*trans*-5-*trans*-undecatriene, however, do contribute to the odor of galbanum oil [4].

2.1.2 Alcohols

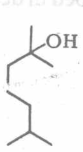
Saturated primary alcohols, free as well as esterified, occur widely in nature, *e.g.* in fruits. Since their odor is relatively weak, their use as components in fragrance compositions is limited. The alcohols are starting materials for aldehydes and esters. More important are some unsaturated alcohols, such as leaf alcohol with its intensely green odor. These alcohols may impart characteristic notes to compositions.
Naturally occurring fatty alcohols used in the fragrance industry are produced principally by reduction of the corresponding carboxylic acid methyl esters, which are obtained by transesterification of natural fats and oils with methanol. Technical processes for the reduction include catalytic hydrogenation in the presence of Adkins catalysts, and reduction with sodium (Bouveault-Blanc reduction). Unsaturated alcohols can be prepared by the latter method as well.
Specific methods of preparation are presented for alcohols which are mentioned individually for their characteristic organoleptic properties.

3-Octanol

$CH_3(CH_2)_4CH(OH)CH_2CH_3$, $C_8H_{18}O$, *M* 130.23, $bp_{976\,mbar}$ 176 – 176.5 °C, d_4^{20} 0.8264, n_D^{20} 1.4252.

May occur in its optically active form. It is a colorless liquid with a mushroomy-earthy odor. Occurs in champignons. Can be obtained by hydrogenation of 3-octanone and is used in lavender compositions and, in general, for imparting mushroom type odors.

2,6-Dimethyl-2-heptanol



$C_9H_{20}O$, *M* 144.26, $bp_{1013\,mbar}$ 170 – 172 °C, d_{20}^{20} 0.8186, n_D^{20} 1.4248.

Has not been found in nature to date. Colorless liquid with a delicate, flowery odor reminiscent of fresia. Synthesized by a Grignard reaction of 2-methyl-2-hepten-6-one and methylmagnesium chloride, followed by hydrogenation. Used in flowery perfume compositions.

***trans*-2-Hexen-1-ol**

$CH_3CH_2CH_2CH=CHCH_2OH$, $C_6H_{12}O$, *M* 100.16, $bp_{1013\,mbar}$ 155 °C, d_4^{20} 0.8459, n_D^{20} 1.4382.

Occurs in many fruits and has a fruity, green odor, which is sweeter than that of the isomeric *cis*-3-hexen-1-ol and is, therefore, preferred in aroma compositions.

***cis*-3-Hexen-1-ol, "leaf alcohol"**

$CH_3CH_2CH=CHCH_2CH_2OH$, $C_6H_{12}O$, *M* 100.16, $bp_{1013\,mbar}$ 156 – 157 °C, d_4^{20} 0.8495, n_D^{20} 1.4384.

Robinia pseudacacia and mulberry leaf oil contain up to 50% leaf alcohol, green tea up to 30%. Small quantities occur in nearly all other green parts of plants. Colorless liquid with the characteristic odor of freshly cut grass. A stereospecific synthesis for *cis*-3-hexen-1-ol starts with the ethylation of sodium acetylide to 1-butyne, which is reacted with ethylene

oxide to 3-hexyn-1-ol. Selective hydrogenation of the triple bond in the presence of palladium catalysts yields *cis*-3-hexen-1-ol.
Leaf alcohol is used to obtain natural green top notes in perfumes and flavors. In addition, it is the starting material in the synthesis of 2-*trans*-6-*cis*-nonadien-1-ol and 2-*trans*-6-*cis*-nonadien-1-al.

1-Octen-3-ol
$CH_3(CH_2)_4CH(OH)CH=CH_2$, $C_8H_{16}O$, M 128.21, $bp_{946\,mbar}$ 175 – 175.2 °C, d_4^{20} 0.8383, n_D^{20} 1.4378.
May occur in the optically active form. Occurs in, among others, lavender oil and is a steam-volatile component of champignons. 1-Octen-3-ol is a liquid with an intense mushroom and forest-earthy odor. It can be prepared by the Grignard reaction of vinylmagnesium bromide and *n*-hexanal. It is used in lavender compositions and in mushroom aromas.

10-Undecen-1-ol
$CH_2=CH(CH_2)_8CH_2OH$, $C_{11}H_{22}O$, M 170.29, $bp_{21\,mbar}$ 133 °C, d_4^{15} 0.8495, n_D^{20} 1.4500.
Has not been found in nature yet. Colorless liquid, with a fatty-green, slightly citrus-like odor. Can be synthesized from 10-undecylenic acid. 10-Undecen-1-ol is used to give flower perfumes a fresh lift.

2-*trans*-6-*cis*-Nonadien-1-ol, "violet leaf alcohol"
$CH_3CH_2CH=CHCH_2CH_2CH=CHCH_2OH$, $C_9H_{16}O$, M 140.22, $bp_{15\,mbar}$ 96 – 100 °C, d_4^{25} 0.8622, n_D^{25} 1.4631.
Occurs, *inter alia*, in cucumber oil, violet leaf and violet blossom oil. The colorless liquid possesses an intense, heavy-fatty, green odor, reminiscent of violet leaves.
Starting material for synthetic 2-*trans*-6-*cis*-nonadien-1-ol is *cis*-3-hexen-1-ol, which is converted via its halide into the corresponding Grignard reagent. The Grignard reagent is reacted with acrolein to 1,6-nonadien-3-ol, which is converted into 2-*trans*-6-*cis*-nonadien-1-ol by allylic rearrangement.
Nonadienol is a powerful fragrance substance. It is used in extrait perfumery for creating refined violet odors, and to impart interesting notes to other blossom compositions. In aroma compositions it is used for fresh-green cucumber notes.

2.1.3 Aldehydes and acetals

Aliphatic aldehydes are among the most important components in perfumery.
Although the lower fatty aldehydes $C_2 – C_7$ occur widely in nature, they are – with the exception of *n*-hexanal – used relatively little in fragrance and flavor compositions due to their volatility and unpleasant odor characteristics. Fatty aldehydes $C_8 – C_{13}$, however, are used, singly or in combination, in nearly all perfume types and also in aromas. Their odor becomes weaker with increasing molecular mass, so that aldehydes $>C_{13}$ are less interesting perfumistically.

In addition to the straight-chain saturated aldehydes a number of branched-chain and unsaturated aliphatic aldehydes are important as fragrance and flavoring materials. The doubly unsaturated 2-*trans*-6-*cis*-nonadienal, "violet leaf aldehyde", the dominant component of cucumber aroma, is one of the most potent fragrance and flavoring substances and is, therefore, used in very small amounts only.

Acetals derived from aliphatic aldehydes have odor characteristics which resemble those of the aldehydes but are less pronounced. They contribute to the aroma of alcoholic beverages, but can often not be used in flavoring compositions because they are insufficiently stable. Since they are resistent to alkali, a number of them (*e. g.* heptanal dimethyl acetal, octanal dimethyl acetal) are occasionally incorporated into soap perfumes.

Fatty aldehydes are generally produced by dehydrogenation of alcohols in the presence of suitable catalysts [4a]. The alcohols are often available cheaply and in good purity. Manufacturing aldehydes via the oxo process is less suitable since the products obtained are often not pure enough for flavor and perfume purposes.

Specific syntheses for those branched-chain and unsaturated aldehydes which are important in perfumery and flavoring techniques are mentioned under the individual compounds.

n-Hexanal, caproaldehyde

$CH_3(CH_2)_4CHO$, $C_6H_{12}O$, M 100.16, $bp_{1013\,mbar}$ 128 °C, d_4^{20} 0.8139, n_D^{20} 1.4039.

Occurs, *inter alia*, in apple and strawberry aroma as well as in orange and lemon oil. It is a colorless liquid, with a fatty-green odor, in low concentrations reminiscent of unripe fruits.

n-Hexanal is used in fruit flavors and, in high dilution, in perfumery for obtaining fruity notes.

n-Octanal, capryl aldehyde

$CH_3(CH_2)_6CHO$, $C_8H_{16}O$, M 128.21, $bp_{1013\,mbar}$ 171 °C, d_4^{20} 0.8211, n_D^{20} 1.4217.

Occurs in, among others, several citrus oils, for example, orange oil. It is a colorless liquid with a pungent odor, citrus-like in dilution.

It is used in perfumery in low concentrations in Eaux de Cologne and in artificial citrus oils.

n-Nonanal, pelargonaldehyde

$CH_3(CH_2)_7CHO$, $C_9H_{18}O$, M 142.24, $bp_{1013\,mbar}$ 190 – 192 °C, d_4^{20} 0.8264, n_D^{20} 1.4273.

Occurs in, among others, citrus oils and also in rose oils. Colorless liquid with a fatty-rose-like odor. It is used in floral compositions, in particular in those with rose characteristics.

n-Decanal, capraldehyde

$CH_3(CH_2)_8CHO$, $C_{10}H_{20}O$, M 156.27, $bp_{1013\,mbar}$ 208 – 209 °C, d_4^{15} 0.830, n_D^{20} 1.4287.

Is a component of many essential oils, for example of neroli oil as well as of various citrus peel oils. It is a colorless liquid with a strong odor, reminiscent of orange peel, changing toward a fresh citrus odor upon dilution.

n-Decanal is used in low concentrations in blossom fragrances; particularly used to create citrus nuances and in the production of artificial citrus oils.

n-Undecanal

$CH_3(CH_2)_9CHO$, $C_{11}H_{22}O$, *M* 170.29, $bp_{24\,mbar}$ 117 °C, d_4^{23} 0.8251, n_D^{20} 1.4325.
Occurs, *inter alia*, in citrus oils. Colorless liquid, possessing a flowery-waxy odor with aspects of freshness. *n*-Undecanal is the prototype of the perfumery aldehydes and is widely used in perfume compositions for imparting the "aldehydic note".

n-Dodecanal, lauraldehyde

$CH_3(CH_2)_{10}CHO$, $C_{12}H_{24}O$, *M* 184.32, $bp_{133\,mbar}$ 185 °C, d_4^{15} 0.8352, n_D^{20} 1.4350.
Colorless liquid with a waxy odor, in high dilution it is reminiscent of violet. Dodecanal occurs in several citrus oils, and has been found in small amounts in the essential oil of a number of *Pinus* species. It is used in perfumery in conifer fragrances with fatty-waxy notes, but also in many other odor types.
It is added to aron.a comppsitions for obtaining citrus notes.

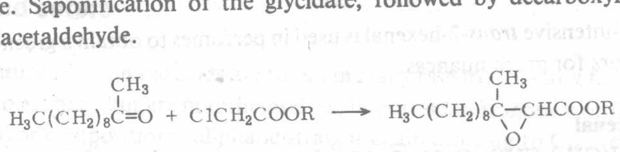
n-Tridecanal

$CH_3(CH_2)_{11}CHO$, $C_{13}H_{26}O$, *M* 198.34, $bp_{13\,mbar}$ 128 °C, d_4^{18} 0.8356, n_D^{18} 1.4384.
Occurs in, among others, lemon oil and has been identified as a volatile constituent of cucumber. Colorless liquid, having a fatty-waxy, slightly citrus-like odor. Addition of tridecanal to fragrance compositions imparts fresh nuances in the topnote as well as in the dry out.

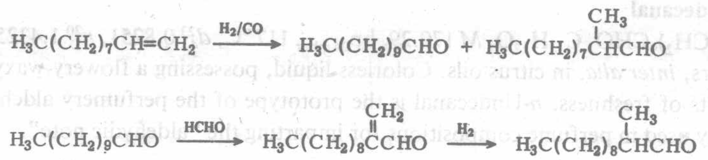
2-Methylundecanal, methylnonylacetaldehyde

$CH_3(CH_2)_8CH(CH_3)CHO$, $C_{12}H_{24}O$, *M* 184.32, $bp_{13\,mbar}$ 114 °C, d_4^{15} 0.830, n_D^{20} 1.4321.
Has not been found in nature. Colorless liquid, with an odor markedly different from that of the isomeric *n*-dodecanal. It has a fatty odor with incense and ambergris notes.
There are two technical routes to 2-methylundecanal:

(a) Methyl nonyl ketone is converted into its glycidate by reaction with an alkyl chloroacetate. Saponification of the glycidate, followed by decarboxylation, yields methylnonylacetaldehyde.

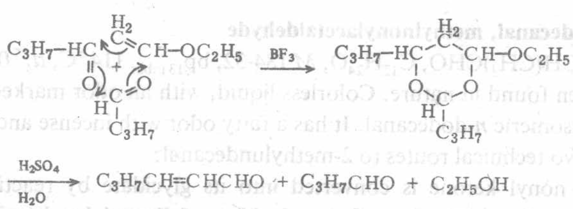


(b) The second synthesis makes use of the conversion of *n*-undecanal into 2-methyleneundecanal by reaction with formaldehyde in the presence of catalytic amounts of amines [5]. Hydrogenation of 2-methyleneundecanal yields methylnonylacetaldehyde. A convenient process starts from 1-decene: hydroformylation gives a mixture of, predominantly, *n*-undecanal and 2-methyldecanal. Reaction of the crude product with formaldehyde in the presence of di-*n*-butylamine yields a mixture containing over 50% 2-methyleneundecanal. After hydrogenation of the double bond, pure methylnonylacetaldehyde is separated from by-products by fractional distillation [6].



In comparison with the other fatty aldehydes, 2-methylundecanal is used in perfumery in rather large amounts for conifer notes, in particular fir impressions, but frequently also in phantasy compositions.

***trans*-2-Hexenal, "leaf aldehyde"**
$CH_3CH_2CH_2CH=CHCHO$, $C_6H_{10}O$, *M* 98.14, $bp_{1013\,mbar}$ 146–147 °C, d_4^{20} 0.8491, n_D^{20} 1.4480.
The simplest straight-chain unsaturated aldehyde of interest for perfumes and flavors. It occurs in essential oils obtained from green leaves of many plant species.
trans-2-Hexenal is a colorless, sharp herbal-green smelling liquid with a slight acrolein-like pungency. Upon dilution, however, it smells pleasantly green apple-like. The aldehyde can be synthesized from butanal, by reaction with vinyl ethyl ether in the presence of boron trifluoride, followed by hydrolysis of the reaction product with dilute sulfuric acid [7].



The odor-intensive *trans*-2-hexenal is used in perfumes to obtain a green leaf note, and in fruit flavors for green nuances.

10-Undecenal
$CH_2=CH(CH_2)_8CHO$, $C_{11}H_{20}O$, *M* 168.28, $bp_{4\,mbar}$ 103 °C, d_4^{21} 0.8496, n_D^{21} 1.4464.
Has not yet been found in nature. Colorless liquid with a fatty-green, slightly metallic, at the same time heavy-flowery odor. The aldehyde can be synthesized from undecylenic acid, for example by hydrogenation of the acid chloride (Rosenmund reduction) or by reaction with formic acid in the vapor phase in the presence of titanium dioxide.
In perfumery, 10-undecenal is one of the aldehydes essential for creating the "aldehydic note".