Common Fragrance and Flavor Materials: Preparation and Uses, Fourth, Completely Revised Edition
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ISBNs: 3-527-30364-2 (Hardcover); 3-527-60020-5 (Electronic)

1 Introduction

1.1 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 people 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 survived from pre-Christian times to this day.

Although distillation techniques were improved, particularly 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 currently used by perfumers and flavorists were originally prepared by distillation in pharmacies in the 16th and 17th centuries.

Another important step in the history of natural fragrance materials occurred in the first half of the l9th century, when the production of essential oils was industrialized due to the increased demand for these oils as perfume and flavor ingredients. Around 1850, single organic compounds were also used for the same purposes. This development resulted from the isolation of cinnamaldehyde from cinnamon oil by DUMAS and PÉLIGOT in 1834, and the isolation of benzaldehyde from bitter almond oil by LIEBIG and WÖHLER in 1837. The first synthetic 'aroma oils' were introduced between 1845 and 1850. These consisted of lower molecular mass fatty acid esters of several alcohols and were synthesized by the chemical industry for their fruity odor. Methyl salicylate followed 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, Federal Republic of Germany), a new branch of the chemical industry was founded.

The number of synthetically produced fragrance and flavor chemicals has since expanded continually as a result of the systematic investigation of essential oils and fragrance complexes for odoriferous compounds. Initially, only major components were isolated from natural products; their structure was then elucidated and processes were developed for their isolation or synthesis. With the development of modern analytical techniques, however, it became possible to isolate and identify

characteristic fragrance and flavor substances that occur in the natural products in only trace amounts. The isolation and structure elucidation of these components requires the use of sophisticated chromatographic and spectroscopic techniques. Interesting products can then be synthesized.

1.2 Definition

Fragrance and flavor substances are comparatively strong-smelling organic compounds with characteristic, usually pleasant odors. They are, therefore, used in perfumes and perfumed products, as well as for the flavoring of foods and beverages. Whether a particular product is called a fragrance or a flavor substance depends on whether it is used as a perfume or a flavor. Fragrances and flavors are, like taste substances, chemical messengers, their receptors being the olfactory cells in the nose [1, 2].

1.3 Physiological Importance

Chemical signals are indispensable for the survival of many organisms which use chemoreceptors to find their way, to hunt for and inspect food, to detect enemies and harmful objects, and to find members of the opposite sex (pheromones). These functions are no longer vitally important for humans. The importance of flavor and fragrance substances in humans has evolved to become quantitatively and qualitatively different from that in other mammals; this is because humans depend to a greater extent on acoustic and optical signals for orientation. However, humans have retained the ability to detect odors and human behavior can undoubtedly be affected by fragrances and aromas.

Sensory information obtained from the interaction of fragrance and flavor molecules with olfactory and taste receptors is processed in defined cerebral areas, resulting in perception. During the past 10 years much research has been done concerning sensory perception and results have been published in, e.g., [2–4b].

Although food acceptance in humans is determined mainly by appearance and texture, flavor is nevertheless also important. For example, spices are added to food not for their nutritional value, but for their taste and flavor. Furthermore, aromas that develop during frying and baking enhance the enjoyment of food.

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

1.4 Natural, Nature-identical, and Artificial Products

Natural products are obtained directly from plant or animal sources by physical procedures. *Nature-identical* compounds are produced synthetically, but are chemically identical to their natural counterparts. *Artificial* flavor substances are compounds that have not yet been identified in plant or animal products for human consumption. Alcohols, aldehydes, ketones, esters, and lactones are classes of compounds that are represented most frequently in natural and artificial fragrances.

Nature-identical aroma substances are, with very few exceptions, the only synthetic compounds used in flavors besides natural products. The primary functions of the olfactory and taste receptors, as well as their evolutionary development, may explain why artificial flavor substances are far less important. The majority of compounds used in fragrances are those identified as components of natural products, e.g., constituents of essential oils or resins. The fragrance characteristics of artificial compounds nearly always mimic those of natural products.

1.5 Sensory Properties and Structure

Similarity between odors arises because dissimilar substances or mixtures of compounds may interact with receptors to create similar sensory impressions in the sensory centers of the brain. The group of musk fragrances (comprising macrocyclic ketones and esters as well as aromatic nitro compounds and polycyclic aromatics) are, for example, compounds with similar odors but totally different structures [5, 6]. Small changes in structure (e.g., the introduction of one or more double bonds in aliphatic alcohols or aldehydes) may, however, alter a sensory

impression or intensify an odor by several orders of magnitude. Increasing knowledge of the structure and functioning of olfactory receptors provides a better scientific basis for the correlation of odor and structure in fragrance and flavor substances, and facilitates the more accurate prediction of the odor of still unknown compounds [7–7l].

1.6 Volatility

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 also an important factor. Molecular masses of ca. 200 occur relatively frequently; masses over 300 are an exception.

Since fragrance materials differ in volatility, the odor of a perfume composition changes during evaporation and is divided into the top note, the middle notes or body, and the end note or dry out, which consists mainly of less volatile compounds. Odor perception also depends largely on odor intensity. Therefore, the typical note is not determined only by the most volatile compounds.

In some cases, substances (fixatives) are added to perfumes to prevent the more volatile components from evaporating too rapidly [8].

1.7 Threshold Concentration

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 at which a chemical compound can be distinguished with certainty from a blank under standard conditions.

For the compounds described in Chapter 2, threshold concentrations vary by a factor of 10^6–10^7. This explains why some fragrance and flavor materials 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 actual concentration of the compound and its threshold concentration [9, 9a].

1.8 Odor Description

The odors of single chemical compounds are extremely difficult to describe unequivocally. The odors of complex mixtures are often impossible to describe unless one of the components is so characteristic that it largely determines 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, or hay-like, which relate the fragrances to natural or other known products with similar odors.

A few terms used to describe odors are listed below:

Aldehydic	odor note of the long-chain fatty aldehydes, e.g., fatty-sweaty, ironed laundry, seawater
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 or orange
Earthy	humus-like, reminiscent of humid earth
Fatty	reminiscent of animal fat and tallow
Floral, flowery	generic terms for odors of various flowers
Fruity	generic term for odors of various fruits
Green	typical odor of freshly cut grass and leaves
Herbaceous	noncharacteristic, 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 forests and seaweed
Powdery	note associated with toilet powders (talcum), diffusively sweet
Resinous	aromatic odor of tree exudates
Spicy	generic term for odors of various spices
Waxy	odor resembling that of candle wax
Woody	generic term for the odor of wood, e.g., cedarwood, sandalwood