

PERFUMES

1. Introduction

Perfumes are mixtures created for use in a wide variety of applications, ranging from expensive couturier perfumes to cosmetics, personal grooming products, laundry products, household cleaning products, and many others. They are created from a palette of several thousand materials, most of which are manufactured by chemical processing methods. Until late in the nineteenth century, fragrances were derived exclusively from natural sources, which put a limitation on where and how they could be used. The large increase in the use of perfumes since then would not have been possible without chemical progress that allowed the synthesis and commercial production of many new odorants. As a result, fragrances, once a luxury, have been incorporated routinely into a great number of products in daily use.

1.1. Historical Background. The use of fragrance, deeply rooted in human experience, predates written history. The earliest evidence of such activity is archaeological, found in the tombs of the First Dynasty Egyptian Kings (5100–3500 BC). Small alabaster vases found along with personal grooming tools are taken as an indication of the use of perfumes and cosmetics. Such vases found in the tomb of King Tutankhamen (1350 BC) in 1926 contained some oily material which had remained elusively fragrant. Analytical methods used at that time were able to indicate only that the material appeared to be made mostly of animal fat and some sort of balsamic substance. Early indications of perfume-making, dating back to 3000 BC, have been found in the former Mesopotamia. Extraction pots for herbal and fragrance preparations found there may have been the world's oldest distillation apparatus.

The ancients used fragrances for a variety of reasons. Perfumes were offerings to the gods, probably in the form of incense; and they were used for aesthetic purposes as part of personal grooming in daily life. Their use in Egyptian embalming rituals may well have been an early example of odor masking. It has been suggested that priests were the first perfumers. There are many Old Testament references to perfume (“anointing with oils”), beginning mainly in the book of Exodus. Thus it seems likely that the ancient Hebrews learned to use fragrance from the Egyptians.

Among the earliest writings on compounded perfumes, ie, deliberately created mixtures rather than simple extracts, are those of the Greek, Theophrastus, from 370 BC. He even referred to the use of oil bases to make perfumes long-lasting, something that remains a challenge to the modern perfumer. Although such writings typically focus on Western history, there are ancient writings and artifactual evidence from India and China indicating that the use of perfumes and cosmetics developed independently in those areas, where fragrance use is traditional in the cultures.

By the thirteenth century AD, essential oils were being produced along with medicinal and herbal preparations in pharmacies. Around this time improvements in distillation techniques were made, in particular the development of the alembic apparatus, which would eventually establish the characteristic qualities of such materials. As a result, many of the essential oils in use today are derived from those produced in the sixteenth and seventeenth centuries in

terms of odor character, even though production methods have continued to evolve. The current practice of aroma therapy is an indication of this common root of medicinal and fragrance chemistry.

During the middle of the nineteenth century, chemists began to investigate the compositions of natural fragrance and flavor materials. As the science developed, it became possible to identify and then synthesize many specific chemicals. This was followed by the use of chemicals as perfume ingredients, first as materials isolated from essential oils and then as synthetically produced naturals such as vanillin and coumarin [91-64-5]. Late in the nineteenth century, it was discovered that synthetic materials that are unrelated to natural chemicals could have great value as perfume ingredients; nitro musks and the ionones were among the first such materials found. Since that time, synthetic chemicals have grown steadily in numbers and total use compared with materials of natural origin.

2. Creation of Perfumes

Perfumes are usually considered in two broad categories, as either fine or functional (household product) fragrances. Fine fragrances include perfumes, colognes, men's colognes, aftershaves, and fragrances for cosmetic products. For the purposes of this article, functional products include all personal and household cleaning products that are perfumed, such as bar soaps, detergents of various types, fabric softeners, bleach formulations and air fresheners. The technical and economic requirements for various kinds of perfumes differ widely and are taken into account during their creation. Creation of a successful fragrance can be a lengthy, painstaking, and costly process. The investment in each fragrance that reaches the marketplace is quite substantial. For these reasons, fragrance formulas are held as trade secrets. Patent protection is generally not suitable for this type of intellectual property because most perfume components are in the public domain; it is the unique combination of ingredients that affords competitive advantage. The formulas are significant assets of the companies that produce them and are therefore protected by elaborate security arrangements.

The creation of perfumes is a commercial art practiced in the medium of odoriferous substances; it is highly specialized and individualistic. A wide variety of ingredients, numbering in the thousands and varying greatly in chemical composition, is available to perfumers. The choice of ingredients can be based on aesthetic or technical grounds, depending on the intended use of the perfume. Often a fragrance creation begins with a concept inspired by an existing perfume, a newly available ingredient, or a newly appreciated odor facet of an existing material. The perfumer creates an accord based on the inspiring note. The new accord may be used in conjunction with an existing fragrance base, or a new composition may be composed around the original theme. Computer-assisted design methods are utilized by perfumers to help with formulation changes and to keep track of the large material base available to them.

The performance of a fragrance over time in its intended application is an important consideration. A traditional view holds that perfumes can be viewed as

a blends with a top note continuing into a middle and on to an end note. This is clearly an oversimplification, since it all components of a fragrance would be expected to reach the nose simultaneously, but in differing amounts depending upon volatility. Thus what is perceived is a blend whose character will depend upon such factors as odor threshold and impact (dose vs response) for each ingredient. Over time, the more volatile ingredients (traditionally the top note) will be dissipated to the point where they contribute less and less to the overall impression. The rate at which this happens is a function of the overall matrix in which the ingredients sit as well as individual component properties. The perfumer must smooth the odor profile of a formula so that there are no discontinuities in odor impact as the different components evaporate. The amount of an ingredient in a fragrance formulation can vary widely, from 10–20% for some materials to trace levels (parts per million) for others. The cost of an ingredient or its odor strength can be a limitation on its use.

Perfumes and ingredients are evaluated initially by a simple “bioassay”: smelling them from paper strips or blotters, and from the various media in which they may be used (eg, soap bars, laundry detergent, etc.). This apparently straightforward exercise is made extremely complex by the ability of human beings to perceive hundreds of thousands of different odor nuances, by individual differences in odor perception, and by differences in the way individuals describe odors. The phenomenon of fatiguing or adaptation to odors is also a complicating factor, which is often not taken into account. The simple criterion of a material smelling good or pleasant is entirely inadequate to determine its value as an odorant. In fact, some materials, both of natural and synthetic origin, smell rather unpleasant by themselves and yet are important in perfumery. Even after years of experience in the hands of many perfumers, new ways to use a particular fragrance ingredient can be discovered and become the basis of a new fragrance type.

Odor perception and description are highly subjective in nature. Nevertheless, there is a generally agreed-upon odor vocabulary that is used to characterize individual ingredients and finished fragrances. Table 1 shows some commonly used odor descriptors grouped into six general classifications (1).

3. Fine Fragrances

Fine fragrances must work on the skin and blend with body odor. They must be pleasant, diffusive, substantive (long-lasting), and have the quality of genuine beauty as well as signature characteristics that distinguish them from each other. For most fine fragrances, the perfumes are themselves the products. They are sold to the consumer at various concentrations in alcoholic or aqueous–alcoholic solutions, depending on the type of application intended. For example, women’s perfumes are typically 20–35% fragrance oil in 95% ethanol. Women’s colognes are offered in the range of 15–22% fragrance oil, whereas men’s colognes and aftershaves are usually in the range of 2–12%. Additional water is incorporated into the more dilute forms. The creation of fine fragrances allows for the highest degree of freedom in terms of ingredient choice and economics. Consequently, fine fragrances often set trends that eventually find their way

into other kinds of products. Perfumes can be grouped into broad odor categories in an attempt to show their relationships to each other and sometimes indicate the progress of creative evolution as new fragrances are built on the foundations laid by older ones. Following are a number of fine fragrances grouped by a widely used classification scheme (1).

3.1. Women's Fragrances. *Straight Floral.* The straight floral family contains a large and popular group of flowery odors, most of them easily recognizable.

<i>Carnation</i>	<i>Muguet</i>
Bellodgia (Caron 1927)	Diorissimo (Dior 1956)
Spellbound (Lauder 1992)	Sunflower (Arden 1993)
<i>Jasmine</i>	Diamonds & Sapphires (Arden 1993)
Honeysuckle (Avon 1963)	<i>Tuberose</i>
Dior Dior (Dior 1976)	Fracas (Piguet 1945)
Chevrefeuille (Rocher 1976)	
<i>Rose</i>	
Tea Rose (Workshop 1972)	
Evelyn Rose (Crabtree & Evelyn 1993)	

Floral Bouquet. In the floral bouquet family, fantasy accords are blended into the floral. They have distinct notes that distinguish one perfume from another.

<i>Tuberose</i>	<i>Rose, jasmin, muguet</i>
White Shoulders (Evyan 1939)	Joy (Patou 1930)
Chloe (Lagerfeld 1975)	First (Van Cleef & Arpels 1977)
Amarige (Givenchy 1992)	White Linen (Lauder 1978)
<i>Floral, green</i>	<i>Spicy carnation</i>
Fidji (Laroche 1966)	L'Air du Temps (Ricci 1948)
Norell (Revlon 1969)	Paris (Yves Saint Laurent 1984)
Charlie (Revlon 1973)	Eternity (Calvin Klein 1988)
<i>Woody</i>	<i>Blends</i>
Aromatics Elixir (Lauder 1992)	Beautiful (Lauder 1986)
White Diamonds (Arden 1991)	Eternity (Klein 1988)
Tommy Girl (Hilfiger 1996)	Pleasures (Lauder 1995)
Romance (Lauren 1998)	Happy (Lauder 1999)
Musk	
Tresor (Lancome 1999)	
Glo-Jlo (Coty 2002)	

Aldehydic Floral. This is an important family of fragrances, the typical odor of which is the class odor of aldehydes. Aldehydes, which are present in small quantities in nature, have an peculiar brilliance. Although they have sharp, slightly fruity and grassy odors alone, they blend beautifully and unexpectedly in florals.

<i>Floral, aldehydic</i>	<i>Woody, mossy, peach</i>
Chanel No. 5 (Chanel 1921)	Madame Rochas (Rochas 1960)
L'Interdit (Givenchy 1957)	Calandre (Paco Rabanne 1970)
Delicious (Gayle Hayman 1993)	Infini (Caron 1970)
	Nude (Bill Blass 1990)

Oriental. In these perfumes, a mossy, woody, and spicy accord combines with the sweetness of vanilla or balsam and is accented with animalic notes such as amber, civet or musk. The most important floral accords used in this family are rose and jasmine.

<i>Oriental</i>	<i>Orange flower spice</i>
Youth Dew (Lauder 1953)	Après L'Ondée (Guerlain 1906)
Opium (YSL 1977)	L'Origan (Coty 1909)
Cinnabar (Lauder 1978)	Private Collection (Lauder 1973)
<i>Sweet vanilla</i>	Oscar de la Renta (de la Renta 1977)
Emeraude (Coty 1921)	J'ai Osé (Laroche 1978)
Shalimar (Guerlain 1925)	Chloé Narcisse (Parfums International Ltd. 1992)
Exclamation (Coty 1988)	Volupté (Oscar de la Renta 1992)
Tresor (Lancome 1991)	

Chypre. The fragrances of this large and important group are warm, mossy, and long-lasting, having rose, jasmine, and animal notes. By blending different accords in the chypre (moss) base, a large new fragrance group is created. Accords that blend well are fruity, green galbanum, aldehydic, and leathery in character.

<i>Chypre</i>	<i>Amber woody</i>
Chypre (Coty 1917)	Halston (Halston 1975)
Parure (Guerlain 1975)	Red (Giorgio 1989)
<i>Oriental</i>	<i>Chypre peach</i>
Pavilion (Lauder 1978)	Mitsouko (Guerlain 1919)
Mystère de Rochas (Rochas 1978)	Femme (Rochas 1945)
<i>Woody amber</i>	Diorella (Dior 1972)
Bandit (Piguet 1944)	Champagne (YSL 1993)
Cabocharde (Grés 1958)	<i>Chypre aldehydic</i>
Diva (Ungaro 1961)	Crêpe de Chine (Millot 1928)
Ungaro (Ungaro 1977)	White Diamonds (Arden 1992)
<i>Chypre patchouli aldehydic green</i>	
Miss Dior (Dior 1947)	
Givenchy III (Givenchy 1970)	
Ysatis (Givenchy 1985)	

Woody. The perfumer has available many different woody fragrance materials, both natural and synthetic. Naturals such as sandalwood, vetiver, cedar, and patchouli often form the bases of these fragrances. They combine in harmony with sweet notes, florals, and animal accords.

<i>Orris</i>	<i>Patchouli</i>
Chamade (Guerlain 1970)	Shocking (Schiaperelli 1935)
Chanel No. 19 (Chanel 1971)	Clinique Aromatics (Lauder 1971)
Calvin Klein (Klein 1978)	Polo (Lauren 1978)
Safari (Ralph Lauren 1990)	Knowing (Lauder 1988)

Green. This group is characterized by leafy or grassy topnotes. It has taken a long time to gain widespread acceptance, although among perfumers, green notes have always enjoyed great popularity.

Vent Vert (Balmain 1945)	Lauren (Lauren 1978)
Aliage (Lauder 1972)	Escape (Calvin Klein 1991)
Cristalle (Chanel 1974)	L'eau D'Issey (1992)

Citrus. This blend has always been popular and in the 1980s experienced a revival in which citrus was blended with florals and sweet notes.

Jean Marie Farina (Roger & Gallet 1806)	Quartz (Molyneux 1977)
Ô De Lancôme (Lancôme 1975)	Calyx (Lauder 1986)
Ck-One (Klein 1994)	Tommy Hilfiger (Hilfiger 1995)

Musk. Even though the musk trend began as a counterculture fashion, these accords have become widely accepted.

Musk Oil (Caswell-Massey 1950)	Wild Musk (Coty 1993)
Musk Oil (Jovan 1972)	

Leather. Fragrances of this group can always be recognized by their warm, leathery tobacco notes.

Tabac Blond (Caron 1919)	Donna Karan (Donna Karan Beauty Co. 1993)
Cuir de Russe (Chanel 1924)	

3.2. Men's Fragrances. Early in the twentieth century, men's fragrances were expected to have a masculine direction, such as tobacco, leather, fougere, or aspects of citrus. This is no longer true, however; since the 1970s, men's perfumes have become less conservative and have allowed much more creative use of rich woody, ambery, and green notes.

Green. A relatively easily recognizable group having grassy or leafy characteristics, the green family is increasingly popular, but is still regarded as rather exclusive.

<i>Green</i>	<i>Herbal</i>
Old Spice Herbal (Shulton 1974)	Grey Flannel (Beene 1975)
	Devin (Lauder 1977)
	Fahrenheit (Dior 1989)

Citrus. This is a popular fragrance group noted for its refreshing brisk quality. Lemon, lime, orange, and bergamot are important ingredients. These oils combine well with lavender and amber accords.

<i>Lavender</i>	<i>Pine</i>
English Lavender (Yardley 1770)	Pino Silvestre (Vidal 1948)
Pour un Homme (Caron 1934)	Aqua di Silva (Victor 1948)
Eternity (Klein 1988)	<i>Floral</i>
Coolwater (Davidoff 1991)	Eau Sauvage (Dior 1966)
Pleasures (Lauder 1995)	Bravas (Shiseido 1969)
Curve (Claiborne 1996)	
<i>Woody</i>	
Polo Sport (Lauren 1994)	
Acqua Di Gio (L'oreal 1996)	

Fougere. This family has a typically accepted masculine note reminiscent of fern, tonka, and moss.

Fougere Royal (Houbigant 1822)	Moustache (Rochas 1949)
Jicky (Guerlain 1889)	Drakkar Noir (Guy Laroche 1984)

Canoe. This is one of the most popular fragrance families dating back to the 1940s. Also liked by women, it has a typical unisex note.

Canoe (Dana 1935)	Brut (Faberge 1964)
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Spice. This is an easily recognizable fragrance that has a strong, spicy character, typified by Old Spice (Shulton 1937).

Wood. This group of fragrances is well appreciated by men. It owes its character to woody naturals, such as vetivert and patchouli, but has become more complex over the years owing to the use of a large variety of new woody aroma chemicals that gave their own signature to the later fragrances in the group.

<i>Amber</i>	<i>Patchouli</i>
Halston Z-14 (Halston 1976)	Aramis 900 (Lauder 1970)
Yatagan (Caron 1976)	Monsieur Jovan (Jovan 1975)
Adventurer (Bauer 1993)	Polo (Ralph Lauren 1978)
<i>Sandalwood</i>	Egoiste (Chanel 1991)
Arden for Men (Arden 1955)	Polo Blue (Lauren 2002)
YSL (YSL 1971)	
Safari (Lauren 1992)	

Musk. Musk notes, combined with previously accepted accords, have made this a popular group.

Musk for Men (Yardley 1971)	Old Spice Musk for Men (Shulton 1974)
Musk for Men (Jovan 1973)	Royal Copenhagen Musk (Swank 1975)

Leather. A more or less leathery character is typical of this group.

Knize Ten (Caswell-Massey 1927)	Bel Ami (Hermes 1987)
Ted (Lapidus 1978)	

Oriental. Sweet, balsamic notes are typical for this group.

Habit Rouge (Guerlain 1964)	Lagerfeld (Lagerfeld 1978)
Pierre Cardin (Cardin 1972)	
Obsession (Klein 1986)	

Chypre. This is an extremely popular group that was well received at the end of the 1940s. It is not exclusively masculine since many women's perfumes have been used as models for fragrances in this family. This group represents creativity at its best and shows how well a basic chypre accord can blend with new themes.

Zizanie (Fragonard 1932)	Givenchy Gentlemen (Givenchy 1971)
Royal Copenhagen (Swank 1971)	Aramis (Lauder 1965)
Paco (Paco Rabanne 1973)	
Revlon Pour Homme (Revlon 1977)	
Azzaro (Azzaro 1978)	

4. Functional Fragrances

Perfumes for functional products are used in different ways than are fine fragrances. The most obvious difference is that functional fragrances are incorporated into a variety of media in relatively small amounts. Perfuming of cleaning products may have begun with efforts to cover the undesirable odors that accompanied the rendering of tallow to make soap. Although consumers have come to enjoy pleasant-smelling personal and household cleaning products, the covering of malodors in the product bases is still a significant challenge to the perfumer (see ODOR MODIFICATION). Product bases may also contain ingredients that react with certain perfume ingredients to alter or destroy their odors, or to cause discoloration problems. The creation of fragrances for functional products is dominated from the outset by the nature and economics of the product to be fragrancd. Aroma chemicals have important advantages over essential oils and other naturals in functional applications because the former are much better characterized in terms of chemical type and reactivity. A knowledge of the chemical properties of fragrance materials is of great value to the functional products perfumer. However, it has been found rather difficult to make precise predictions of material stabilities because product bases are frequently changing and their complete compositions are generally not revealed. Therefore, a certain amount of empirical testing is necessary. The following are brief descriptions

of the fragrance requirements for a number of household products and the perfumery approaches used for them.

4.1. Detergent Fragrances. There is a great variety of laundry detergent formulations on the market, and new ones are introduced every year. The incorporation of bleaching agents into laundry products and the advent of highly concentrated detergents present new and increasingly difficult challenges to the perfumer. Several factors play important roles. Most critical are chemical stability of the fragrance material in detergent and the rate of evaporation from the sales package. Also important is the performance in the product's end use, ie, in the wash water and on the laundered cloth. To some degree, these factors can be predicted from chemical principles and physical properties, but testing of individual materials under use conditions is also important. Chemical stability can be checked by incorporating the fragrance material in the detergent base packed in a closed container and subjecting it to accelerated aging, eg, 40°C for one month. Storage tests in cardboard containers under controlled, standardized temperature and humidity give a good picture of both chemical and evaporative performance. The country of destination is important in determining stability test conditions. Clearly the customer requirements for laundry detergents in Canada are different from those in Brazil.

Detergent fragrances must be particularly powerful and effective because they are incorporated into the final product at rather low levels. Typical detergent powders can contain as little as 0.3% fragrance, although this may be higher in concentrated products. The fragrance should cover undesirable odors in the product itself and those resulting from soils in the wash solution. It should also reinforce the performance of the laundry product by imparting a pleasant scent to the clean and dried fabrics. This is one of the greatest challenges in perfume creation, because detergents are designed to remove odorous, oily materials. The number of ingredients sufficiently substantive to provide residual fragrance on cloth is fairly small, among them Galaxolide, Lyrall, Lilial, and Ambroxan are used.

4.2. Soap Fragrances. The function of soap is to clean; however, the fragrance, at a dosage of 1–2%, plays a large role in the perceived quality and effectiveness of the soap bar. Aesthetically, a beauty soap requires a different type of fragrance from a deodorant soap or a freshness bar. The odor types can be single florals or complicated perfumes in which fine fragrances have been the models for the soap creation. Besides the aesthetic quality of the soap fragrance, there are a number of technical complications that arise: limitations on cost, odor quality and other characteristics of the soap base, the presence of additives, and the high pH of most soaps (often between 9.5 and 11.0) which may lead to hydrolysis or discoloration problems. The main ingredients in bar soaps are derived from a variety of sources, ie, animal and vegetable fats as well as synthetics, which result in differing demands on fragrance performance. In addition to predicting the performance and stability of individual ingredients, in many cases a large number of materials may be tested individually in the soap base. As with detergents, the test conditions may vary according to the requirements of the customer and the country where the soap is to be marketed. For example, the soap bar in a typical package may be stored in an oven at 40°C for one month or in a glass jar at 60°C for seven days. The performance of each material in

the soap base at room temperature, stability after accelerated tests, and coloration or possible discoloration in light and at elevated temperatures are determined. Armed with this information for a large number of ingredients and creative ideas, the perfumer can optimize the soap fragrance with respect to both esthetics and performance. As the fragrance is developed it too is subjected to stability tests to insure that the blend will hold up well over storage and use conditions.

4.3. Liquid Fabric Softeners. The principal functions of fabric softeners are to minimize the problem of static electricity and to keep fabrics soft (see ANTISTATIC AGENTS). In these laundry additives, the fragrance must reinforce the sense of softness that is the desired result of their use. This is an example of psychological factors impinging on the perfumer's art, since it is not at all clear what is the odor of "softness".

Most fabric softeners have a pH of about 3.5, which limits to some extent the materials that can be used in the fragrances. For example, acetals cannot be used because they break down and cause malodor problems; in addition, there is the likelihood of discoloration from Schiff bases (imines formed from aldehydes and methyl anthranilate), certain natural extracts (eg, oakmosses) and a few specialty chemicals. Testing of fragrance materials in product bases is done under accelerated aging conditions (eg, 40°C in plastic bottles) to check for odor stability and discoloration.

A special requirement of perfumes for fabric softeners is the ability to leave a residual of odor on fabric after line or machine drying. Substantivity of different fragrance materials can be determined through empirical testing or by analytical methods. Increasing the percentage of substantive materials in the fragrance does not guarantee of a good fabric softener fragrance. This is because substantive materials must not only blend into the fragrance type (which must blend well with or mask odors from the product base), but they must also leave a pleasant and desirable residual odor after rinsing. The information gained through testing, however, can help the perfumer choose the right fragrance type and include a fair amount of substantive materials.

4.4. Tumble-Dryer Softeners. In these products, which are designed for machine drying, the carrier, in the form of a nonwoven fabric, a foamed plastic, or a cotton string, contains the active softener ingredients and the fragrance. The fragrance partly disappears with the hot drying air and is partly absorbed into the fabrics. Testing for this application requires many drying cycles to obtain performance data on a range of individual fragrance materials. Aesthetically, the fragrance should support a sense of softness and caring for fine laundry.

4.5. Bleach Products. Many marketed bleach products, especially those containing hypochlorite, are still unperfumed. This is understandable because hypochlorite bleaches impose severe limitations on the fragrance materials that can be used due to their oxidizing power and high pH of 12.5. The same factors also limit the solubilizers that can be used. These problems place severe limitations on the materials that can be used to perfume bleach products. However, through knowledge of the chemical properties of available aroma chemicals and the selective development of new ones, fragrances for bleaches can be created to support the powerful cleaning properties of such products.

4.6. Shampoo Perfumes. The stability of perfume in shampoo is usually not a problem because shampoo pH is near neutral; it is only when special additives are used that stability and performance tests may be required. However, in some cases the addition of perfume can affect properties of the shampoo such as viscosity. Testing is therefore often necessary to identify interactions that can negatively affect the product. The fragrance is often called upon to support the concept and image of the product, eg, in herbal or balsam shampoos. Fragrance dosages are generally 0.5–1.0% for normal shampoos, but can be up to 1.5% when a particularly strong odor and residual effect are desired.

4.7. Deodorants and Antiperspirants. Deodorants are often made in sticks or lotions. Sticks are mainly alcoholic or glycolic soap gels. Fragrances for these products have stability requirements similar to soap fragrances, and must also withstand the relatively high temperatures ($\sim 60^{\circ}\text{C}$) encountered during manufacture. Depending on the formulation of the lotion, existing fragrances may have to be modified. Traditional deodorants use bacteriostats to help lower body odor. Antiperspirants usually contain aluminum or zirconium salts that can reduce the pH to about 2.3, which makes acid-sensitive fragrance materials unsuitable for this application; as might be expected, coloration can also be a problem, especially in some modern products that are sold as clear gels or colorless lotions.

Deodorant and antiperspirant fragrances must be long-lasting in order to help maintain a pleasant body odor for as long as possible. With increasing trends to “naturalness”, a certain amount of fresh sweat odor may be acceptable. In a modern approach to deodorants, the body odor is used as an animal accord that blends well with the rest of the fragrance. Thus the perfumer attempts to create a fragrance that smells good both in its original form and with the addition of the body odor as it develops.

4.8. Talcs and Powders. In the perfuming of talcum powders and face powders, stability is the most important factor (see also COSMETICS). Even the finest talc contains alkaline impurities that can cause decomposition and discoloration of fragrance ingredients. In addition, the fragrance is spread thinly around the microscopic talc particles, accelerating oxidative reactions. For this reason, many aldehydes and unsaturated terpenes fare poorly and vanish completely as odor contributors. Systematic screening programs are often necessary to obtain a list of stable fragrance raw materials for these applications.

4.9. Environmental Fragrances. This area is a growing outlet for fragrances. Examples of products in this category are air fresheners, which include sprays and products that disperse fragrance from various media, such as paper wicks and plastics, and candles. The last of these is the fastest growing segment. These applications do not place severe restrictions on the materials used in fragrances, but for candles, solubility, release rates and effects of the perfume on the medium can be critical. Solid fragrance ingredients that are relatively polar, may precipitate from the candle formulation causing undesired opacity. Also, in rare cases, high amounts of some materials may cause softening or even affect burning. As the fragrance is created, attention must be paid to the initial odor of the candle, accelerated aging at somewhat elevated temperatures and the fragrance released from the molten wax pool on burning.

5. Perfume Ingredients

The classical materials of perfumery are natural products. These are mostly of vegetative origin, with some obtained from animal secretions. Just about any part of a plant can be used, including flowers, fruits, leaves, twigs, roots, and wood, depending on the amount and quality of essence it contains. Perfume materials of animal origin include tincture of tonquin musk, civet gum, and beaver castoreum. Such materials have been or are being replaced by synthetic substitutes for environmental, political, or economic reasons. Even though synthetics continue to grow and have displaced naturals in overall usage, the latter are deeply rooted in the art of perfumery and so remain extremely valuable in perfume creation; in addition, naturals provide the odor reference points by which synthetics are often judged or described.

5.1. Natural Products. Various methods have been and continue to be employed to obtain useful materials from various parts of plants. Essences from plants are obtained by distillation (often with steam), direct expression (pressing), collection of exudates, enfleurage (extraction with fats or oils), and solvent extraction. Solvents used include typical chemical solvents such as alcohols and hydrocarbons. Liquid (supercritical) carbon dioxide has come into commercial use in the 1990s as an extractant to produce perfume materials. Generally the extracts produced this way are of very good quality, but differ from those traditionally produced. For this reason, they usually cannot replace the older products in existing perfumes, but they may become part of the palette for new creations.

The principal forms of natural perfume ingredients are defined below; the methods used to prepare them are described in somewhat general terms because they vary for each product and supplier. This is a part of the industry that is governed as much by art as by science.

Concretes. Concretes are produced by extraction of flowers, leaves, or roots, usually with hydrocarbon solvents. After removal of the solvent by distillation, the concrete is obtained as a thick, waxy residue. Such materials are used in some fine fragrances, but the waxes they contain can give rise to solubility problems. For this reason, concretes are often dissolved in alcohol to make tinctures, or in other low-odor diluents. Production of concretes, especially flower concretes, usually takes place where the botanicals are grown since the odors of such materials deteriorate rapidly after harvesting.

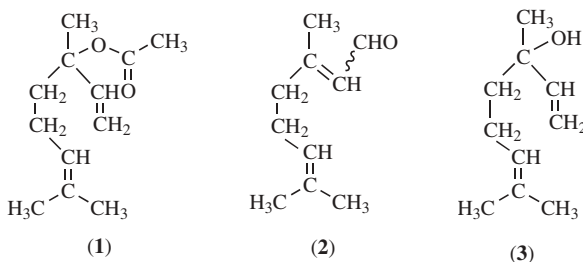
Absolutes. Absolutes are prepared from concretes by further processing to remove materials that can cause solubility problems in perfumes. This is done by dissolution in alcohol, filtering, and removal of the solvent, ultimately at reduced pressures. The resulting products are viscous, oily materials which may be diluted with low-odor substances such as diethyl phthalate.

Concretes and absolutes, both obtained by total extraction of the plant material and not subject to any form of distillation other than solvent removal, are complex mixtures containing many chemical types over a wide molecular weight range. In some cases, the volatile materials comprise only a very small part of the total. Yet these products have powerful odors and contribute in important ways to the perfumes in which they are used.

Essential Oils. Essential oils are produced by distillation of flowers, leaves, stems, wood, herbs, roots, etc. Distillations can be done directly or with steam. The technique used depends mostly on the desired constituents of the starting material. Particular care must be taken in such operations so that undesired odors are not introduced as a result of pyrolytic reactions. This is a unique aspect of distillation processing in the flavor and fragrance industry. In some cases, essential oils are obtained by direct expression of certain fruits, particular of the citrus family. These materials may be used as such or as distillation fractions from them (see OILS, ESSENTIAL).

5.2. Naturally Derived Materials. The following are descriptions of some of the most important naturally-derived materials in use. Importance in this context is defined in terms of total value, which may derive from expensive, low volume materials with great aesthetic value to relatively inexpensive and widely-used products. In some cases, the oils are distilled to provide individual chemicals for use as such or as chemical intermediates. Materials produced in this way from a given natural source are usually not interchangeable with those from other naturals or synthetics. This may be due to optical isomerism, which can have a significant effect on odor, or to trace impurities.

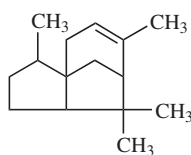
Bergamot. Bergamot oil is produced by cold expression from peels of fruits from the small citrus tree, *Citrus bergamia*. The fruits themselves are inedible and of little value. Bergamot is grown mainly in southern Italy and northern and western Africa. The oil is used to impart a sweet freshness to perfumes. Its largest chemical constituent, to the extent of 35–40%, is linalyl acetate [115-95-7] (1), with a much smaller amount of citral [5392-40-5] (2) as an important odor contributor.



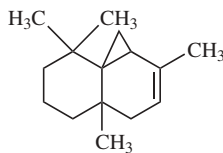
Bois de Rose. Bois de rose oil is obtained by steam distillation of wood chips from South American rosewood trees, *Aniba rosaeodora*. The tree, a wild evergreen, grows mainly in the Amazon basin. The oil is used as obtained in perfumery for its sweet, woody-floral odor and as a source of linalool [78-70-6] (3), which it contains to the extent of 70%. Linalool distilled from bois de rose oil is used directly in perfumery and for conversion to esters, eg, the acetate (1).

Cedarwood. Many varieties of cedarwood oil are obtained from different parts of the world. They are produced mainly by steam distillation of chipped heartwood, but some are produced by solvent extraction. The oils, which vary significantly in chemical composition, are used in perfumes as such, but the main uses are as distillation fractions and chemical derivatives. For the latter purposes the most used oils, which are similar in composition, come from China (*Cupressus funebris*) and from Texas in the United States (*Juniperus mexicana*).

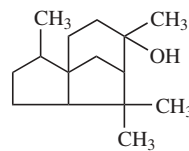
The principal constituents of these oils are cedrene [11028-42-5] (4), thujopsene [470-40-6] (5), and cedrol [77-53-2] (6). The first two of these are obtained together by distillation and used mostly in the form of acetylated derivatives. Cedrol is used as such and, to a greater extent, as its acetate ester.



(4)

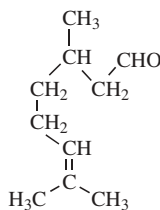


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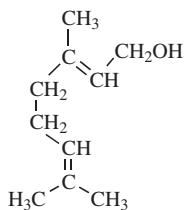


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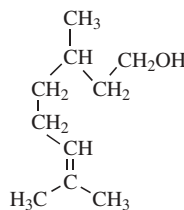
Citronella. Citronella oil is produced in Ceylon, China, Java, and Brazil by steam distillation of similar, but not identical, grasses. The main constituents of the oil are citronellal [106-23-0] (7), geraniol [624-15-7] (8), and citronellol [106-22-9] (9). The Javanese and, more recently, the Chinese oils have emerged as the most used materials in this family because they contain larger amounts of the desired aldehyde and alcohols. Citronellal, which should comprise 50–60% of a good quality oil, is mainly of the dextrorotatory form. It is desirable both as a perfume ingredient in its own right and for chemical conversion to hydroxycitronellal [107-75-5] (10), a long-lasting muguet odorant.



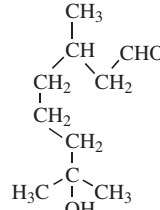
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(8)

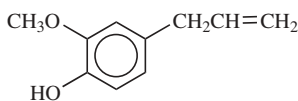


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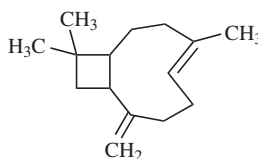


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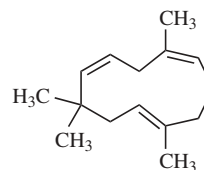
Clove Leaf Oil. Clove leaf oil is produced mainly in Madagascar and Indonesia. It is obtained by distillation of leaves and twigs of the *Eugenia caryophyllata*. The material from Madagascar is considered of superior quality to those from the other areas, because its eugenol [97-53-0] (11) content is in the ranges 82–92%; in Indonesia, the eugenol content is somewhat lower, 78–86%. Eugenol from this source is used as a chemical raw material for conversion to several derivatives, the most important of which is isoeugenol. The sesquiterpene section contains mainly caryophyllene [13877-93-5] (12), along with some humulene [6753-98-6] (13).



(11)

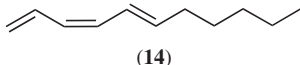


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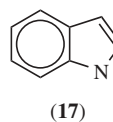
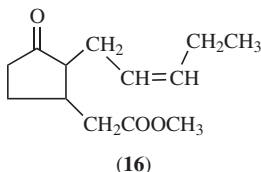
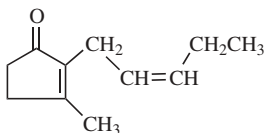
(13)

Galbanum. Galbanum gum is an exudate collected from large umbelliferous plants of the *Ferula* species, which grow wild in the Middle East. The gum is extracted with alcohol to produce a resinoid or steam-distilled to produce an oil. The odor of galbanum blends excellently with lilac fragrances. In modern perfumery, it is used to give a greenish top note. Galbanum oil and resinoid are complex mixtures from which many materials have been identified. Of these, a group of isomeric 1,3,5-undecatrienes has been identified as key odor contributors, in particular the 3(*E*),5(*Z*)-isomer [51447-08-6] (**11**).



Geranium. Various perfume ingredients are produced from geranium, *Pelargonium graveolens*, in many parts of the world. These include a concrete from Morocco and an absolute produced from it. The most important geranium product by far is geranium bourbon, an oil produced by steam distillation of pelargonium leaves and branches. It originated from the island of Reunion in the Indian Ocean; however, most current production is from China and Egypt. In addition to its direct use in perfumes, geranium oil is fractionally distilled to provide, among other products, rhodinol, which is comprised mainly of *l*-citronellol (**9**), although this by no means accounts for all of its fine odor quality. Rhodinol is highly desirable for fine perfumery applications, in particular as a base for rose, muguet, and other floral fragrances.

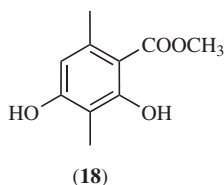
Jasmine. Jasmine is one of the most precious florals used in perfumery. The concrete of jasmine is produced by hydrocarbon extraction of flowers from *Jasminum officinale* (var. *Grandiflorum*). The concrete is then converted to absolute by alcoholic extraction, filtration and solvent removal. It is produced in many countries, the most important of which is India, followed by Egypt. Jasmine products are rather expensive and are produced in relatively small amounts compared with other materials. However, jasmine is particularly important in perfume creation for its great power and aesthetic qualities. Four of the principal odor contributors to jasmine are *cis*-jasnone [488-10-8] (**15**), methyl jasmonate [91905-97-4] (**16**), benzyl acetate [140-11-4], and indole [120-72-9] (**17**).



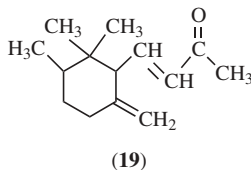
Lavandin. Lavandin oil is produced from *Lavandula hybrida*, a plant species of recent origin, unknown until the late 1920s. It is a hybrid of two common lavenders, *Lavandula officinalis* and *Lavandula latifolia*. Lavandin is cultivated mainly in southern France and has become one of the most produced and used natural perfumery materials. The flowering tops of the shrub are used to produce a concrete, an absolute, and a steam-distilled oil; the last is by far the

most used. Low cost and refreshing odor quality allow lavandin to be employed in a wide variety of perfume applications and at high concentrations. Chemically it is comprised of 30–32% linalool (**3**) and linalyl acetate (**1**), along with numerous other substances, mostly terpenic.

Oakmoss or Mousse de Chene. Oakmoss, *Evernia prunastri*, is a lichen that grows mostly on oak and spruce trees. It is collected mostly in the Czech Republic, Croatia, and Morocco. A cheaper quality, which is also called tree moss or mousse d'arbre, grows on spruce and pine trees. Oakmoss is worked into a variety of products, including a concrete, resinoid, and absolute, the last of which is the most used. Materials of this type are typically green in color and are thus limited in some functional perfumes. Decolorization techniques can be applied but some loss of odor quality occurs. Small amounts of oakmoss absolute are remarkably effective in perfumery for imparting a long-lasting, typically sweet mossy note. They are used in the most expensive perfume products and blend well with other oriental or flowery notes. The main odor constituent of oakmoss is the ester methyl 2,4-dihydroxy-3,6-dimethylbenzoate [115-10-6] (**18**).

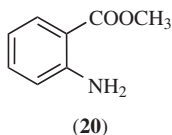


Orris. Orris is produced from rhizomes of *Iris pallida* and *Iris germanica*. The plants are found and cultivated mostly in Italy, but also in Morocco and China. It is used in perfumery as an absolute, a steam-distilled essential oil, and a concrete. The last material, which is a low melting solid (due to a high content of myristic acid), is by far the most used. Orris has a violet-like odor useful in fine perfumes, luxury soaps, and fragrances for powders and other cosmetic products. Its most important odor contributors are the irones, of which the most important isomer is γ -irone [79-68-5] (**19**).

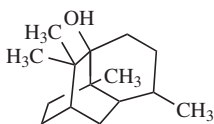


Orange Flower. Extraction of freshly picked flowers of the bitter orange tree, *Citrus aurantium* (subspecies *amara*), for the production of concrete is carried out mainly in Morocco and Tunisia. Most of this material is processed further to give orange flower absolute, one of the most important absolutes used in perfumes after rose and jasmine. It is highly valued, even when used at low levels, for its long-lasting, rich, warm, yet delicate and fresh floralcy. The material is a complex mixture, to which methyl anthranilate [134-20-3], linalool

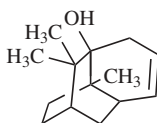
(3), methyl jasmonate (16), and indole (17) are important odor contributors.



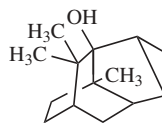
Patchouli. Patchouli oil is produced by steam distillation of the dry leaves of *Pogostemon cablin*, a shrub-like plant that originated in the Philippines and Indonesia. Most production is done in Indonesia. Patchouli oil has a wonderfully rich odor profile which is described as warm, sweet, herbaceous, spicy, woody, and balsamic. It is relatively inexpensive for a natural product and is usually available in abundance. For these reasons, patchouli oil is very widely used in many kinds of perfumes. Its main odor-donating constituents are polycyclic alcohols. The best known of these, patchouli alcohol [5986-55-0] (21), is present in the oil to the extent of about 30%. However, it is believed that norpatchoulénol [41429-52-1] (22) and nortetrapatchoulol [62731-84-4] (23), which are present in smaller amounts (0.5–1%), are more important as odor contributors.



(21)



(22)

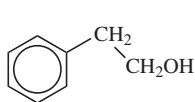


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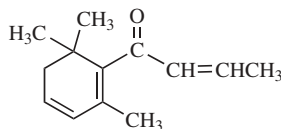
Petitgrain. Petitgrain oils are produced by steam distillation of leaves and twigs of the bitter orange tree, *Citrus aurantium*, the same species used to produce orange flower oil. The so-called biogarde oil is produced from the true bitter orange tree grown in southern France, Italy, Spain, and northern Africa. Petitgrain Paraguay, by far the most used material of this type, is produced from the bitter-sour variety in South America. The odor of these oils is fresh, bitter, and floral, with woody undertones. They are used widely in perfumery, particularly in citrus colognes and floral bouquet perfumes. In addition, the oils, mainly the Paraguay version, are redistilled to give a useful terpeneless oil. (This is a term applied to various essential oils indicating that most of the terpenic hydrocarbons have been removed). Oxygenated terpenes remain as important odor contributors. The most significant odor constituents of petitgrain oils are linalyl acetate (1), linalool (3), methyl anthranilate (7), geraniol (8), and its corresponding **Z** isomer, nerol [106-25-2].

Rose. Rose is one of the most important florals in perfumery, the most valuable derivatives of which are produced from *Rosa damascena*, which is grown principally in Bulgaria, but also in Russia, Turkey, Syria, India, and Morocco. The concrete, absolute, and steam-distilled essential oil (rose otto) are particularly valuable perfume ingredients. Careful handling and processing of freshly picked flowers are required to produce materials of warm, deeply floral, and rich odor quality. They are complex mixtures of which citronellol (9), geraniol (8), phenethyl alcohol [60-12-8] (24), and β -damascenone [23726-93-4] (25)

(trace component) are important odor constituents.

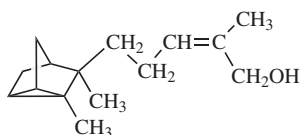


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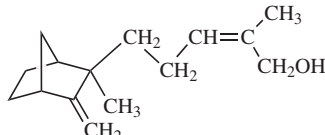


(25)

Sandalwood. Sandalwood is one of the oldest materials in fragrance use. Its oil is produced by steam distillation of coarsely ground wood and roots of *Santalum album*, a comparatively small, slow-growing tree. Its world production is concentrated in India and Indonesia, the latter being of less preferred quality. In order to obtain a good oil and high yield, only trees that are over 30 years in age are used. This limits the supply of the oil and makes it expensive. Although sandalwood oil is still valuable in some fine fragrance applications, much of the sandalwood odor of perfumes produced since the 1980s is a result of the excellent synthetic materials that have been introduced. The main odor contributors to sandalwood oil are alpha-santalol [115-71-9] **(26)** and beta-santalol [77-42-9] **(27)**.

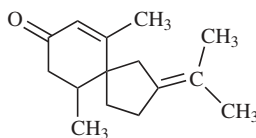


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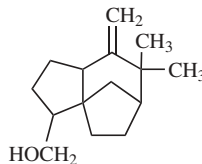


(27)

Vetivert. Vetivert oil is steam-distilled from cleaned, dried, and chopped rootlets of *Vetiveria zizanioides*, a tall perennial grass normally grown for up to 20 months prior to harvesting. Most production of this material is in Haiti, Indonesia, Reunion, and, of a poorer quality, in China. The oil has a heavy woody-earthly odor and an undertone of precious wood. It is used as such, as distillation sections, and is treated with acetic anhydride to produce a mixture known as vetivert acetate. β -Vetivone [18444-79-6] **(28)** is probably the main odor contributor to this essential oil, along with a number of lower keyed vetiverols, a chemically interesting example of which is [16223-63-5] **(29)**.



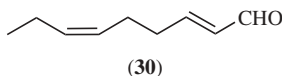
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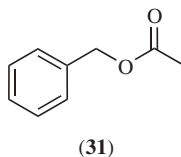
(29)

Violet Leaf. Violet leaf absolute is produced by the usual extraction methods from *Viola odorata* (var. *Victoria*). It is grown mainly in the south of France and Egypt. Although this material is not produced in large amounts, it is quite

valuable in perfumery for its powerful green leafy and floral character, an odor that belongs to many floral bouquets. The principal odorant in violet leaf absolute is 2-*trans*-6-*cis*-nonadienal [557-48-2] (**30**).



Ylang-Ylang. Flowers from the cultivated *Cananga odorata* tree, grown mostly in the Comoro islands and Madagascar, are the starting material for the concrete, absolute, and steam-distilled oil of ylang-ylang. The essential oil is the most important of these products. As with other florals, the flowers of ylang-ylang must be handled carefully and quickly to produce materials of high odor quality. The oil has a powerful floral and intensely sweet odor as well as some spicy and balsamic character. It is a valuable component of many different floral- and oriental-type perfumes. Benzyl acetate (**31**) is the largest component (~30%) of the oil but is responsible for only a small part of its odor profile, which is the result of numerous minor constituents.



5.3. Aroma Chemicals. The use of aroma chemicals in perfumery has been growing since they were first introduced. A number of practical advantages account for this trend. Probably foremost among them is that the growing use of fragrance in the world outstripped the ability to produce enough natural materials, particularly the aesthetically important concretes and absolutes. Increasing world population and the need for food-farming have displaced some of the land area and labor required for production of perfume ingredients. Naturals, especially those produced from flowers, have become more and more expensive due to limited supply and rising labor costs. Some essential oils, particularly those derived from slow-growing trees such as sandalwood, have also been limited in supply for environmental or political reasons. Quality control of synthetics is straightforward compared with naturals because the raw material and product compositions are much less complex. Also, synthetics are not subject to variation in quality and supply due to growing conditions.

Aroma chemicals have grown to be such a major part of the fragrance industry because of their availability at relatively low costs. This has been possible because synthetic fragrance materials are produced from a wide variety of starting materials, from both petrochemical and renewable sources. The most important renewable source is turpentine, followed at some distance by cedarwood oil. The most produced synthetics as of 2005 reached worldwide production levels on the order of ten thousand tons per year, but most are produced in much smaller amounts. In general, batch-manufacturing is used, although there are exceptions, usually for chemical reasons rather than economic ones. Thus, synthetic

fragrance ingredients are specialty chemicals and as such do not usually place heavy demands on available feedstocks.

Aroma chemicals are not limited to any particular functional group, but some are more common than others. The majority of materials contains a single oxygenated functional group, although there are also important materials containing two and even three. Most of these are manufactured by syntheses of one to four chemical steps; some of the starting materials are isolated by distillation from abundant natural sources, eg, cedarwood and clove leaf oils. Some hydrocarbons are important fragrance ingredients, as well as several sulfur or nitrogen-containing materials, but the latter two classes are generally used in very small amounts to provide special nuances. The molecular weight range is roughly from 100–300, and most of the materials have from 10–18 carbon atoms per molecule. There are no simple rules for chemically defining a good odorant. Table 2 and Figure 1 present a number of widely used aroma chemicals by chemical type.

Aroma chemicals are used in perfumes over a wide range of concentrations. The importance of a material to the overall creation should not be judged only by the amount used. Some very minor components impart essential character that may be the key to the commercial success of a perfume. Thus it is characteristic of chemical manufacturing in the fragrance industry that many different materials are produced over a wide range of production volumes. Larger fragrance companies often attempt to simplify their product lines by giving up production of some low-volume products. However, the demands for novelty and richness in perfume creation mitigate against these efforts. It is reasonable to assume that manufacturers of aroma chemicals will continue to produce wide ranges of materials.

6. Manufacture and Quality Control

Perfumes are manufactured by blending ingredients as called for by the created formulations. Most ingredients are oily liquids; however, some are solids and therefore mixing must allow for dissolution and thorough blending. During this operation, some protection from air oxidation is advisable for safety reasons and to assure the quality of the finished product. Depending on the final application, perfumes may be produced in batches of several kilograms to several tons. Because individual ingredients are used over wide concentration ranges, precise weighing of small and large quantities is required.

6.1. Quality Control. Reproducible production of perfumes requires careful quality control of all materials used as well as the compounding process itself. The use of analytical tools has increased over the years with their availability, but there can be no substitute for organoleptic evaluation. The human nose is far more sensitive than any analytical instrument for certain materials, yet it is also quite limited as a quantitative tool and is subject to fatigue. There are also well-documented examples of specific anosmias in individuals, ie, inability to smell certain odor types, somewhat analogous to colorblindness.

In a modern fragrance company, there can be several thousand ingredients, either manufactured or purchased, in inventory for perfume compounding.

Maintaining quality control by odor evaluation requires much organization, skill, and experience. Standard target samples of each ingredient and each finished fragrance must be kept on hand and properly stored for comparison with each new batch or shipment. Experienced odor evaluators usually make the necessary odor comparisons; various systems are employed throughout the industry.

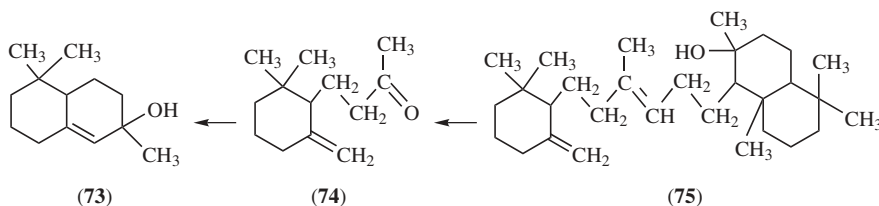
The techniques of analytical chemistry have been applied in the fragrance industry for as long as they have been available. Ingredients have long been characterized by wet chemical methods, color tests, distillation, and bulk analytical methods such as density and refractive index. These were as limited in value for fragrance materials as for other areas of organic chemistry; however, they can be helpful in maintaining consistency. The rise of more specific instrumentation during the middle of the twentieth century brought great changes in the ability to test and standardize materials. Gas-liquid chromatography (glc) is particularly applicable to analysis of fragrances and fragrance materials. Refinements in the instrumentation of glc, especially capillary columns, have made welcome additions to quality-control laboratories. Nevertheless, odor quality cannot be ensured by even the best analytical techniques. The fragrance industry therefore relies on both odor evaluation and analytical methods for control of ingredient and product quality.

7. Research

7.1. Analytical Chemistry. Research in the fragrance industry is rooted in the chemistry of natural products. Chemists have long analyzed essential oils and other fragrant materials derived from nature in order to determine their compositions and in particular to identify the odoriferous principles. This has produced a wealth of synthetic targets, many of which have become important aroma chemicals. Analysis of naturals has also been used to allow the preparation of synthetic reconstitutions or duplications, which can have great commercial importance if a material is in short supply or becomes very expensive. Duplications also allow important natural odor notes to be used in functional perfumery where supply or discoloration problems can arise.

There have been moves since the 1980s to replace natural materials of animal origin. This has occurred for humanitarian or economic reasons. One of the first and best known perfume ingredients to be eliminated from use was tincture of ambergris. The starting material for this was ambergris, a principal by-product of the whaling industry. Its use was therefore eliminated as part of international efforts to preserve whale populations. Tincture of ambergris has been replaced by formulas that include the most important contributors to ambergris odor, namely, α -ambrinol [41199-19-3] (**73**) and dihydro- γ -ionone [13720-12-2] (**74**). These are believed to form via oxidation and cyclization from the principal

component, ambrein [473-03-0] (**75**) (2).



Most natural perfume ingredients, especially some of the most valuable ones, are complex mixtures. Advances in the techniques of separation and identification have been quickly adopted and applied in order to examine the compositions of natural substances in ever greater depth (3). Gas-liquid chromatography is the essential tool for the investigation of fragrant materials because such materials must exhibit some degree of volatility in order to be perceived. The fused-silica capillary columns, which became widely available in the 1990s, are a mainstay of analytical research. In order to obtain chemical structural information on the hundreds of materials that may be present in a complex mixture, gas chromatography is coupled with mass spectrometry (gc-ms). Advances in computer methods for acquiring, sorting, and interpreting molecular fragmentation data from gc-ms runs make it possible to perform in-depth analyses with remarkable speed.

For those components that are not readily identified from their mass spectra alone, gas chromatography coupled with infrared spectroscopy (gc-ir) has been applied. In these instruments, the infrared spectra are acquired in the vapor phase by Fourier transform methodology. Those components that resist identification by these methods must be isolated and analyzed by nuclear magnetic resonance (nmr). Instruments that utilize superconducting magnets and Fourier transform data acquisition, because of their small sample requirements and large resolving power, have allowed natural product chemists to identify many important and interesting materials.

Headspace analysis techniques have also been used to investigate fragrant materials and have produced fascinating technical and commercial results. Initially, purge and trap techniques were used to capture volatiles, often with cryo-focusing onto the head of the gc column. Later on solid phase microextraction (SPME) (4), which had initially been developed for environmental analyses, was applied for headspace studies of natural fragrance materials. This method utilizes a fiber of absorbent polymer to concentrate the substances of interest. The fiber is sufficiently narrow that it can be used to inject the "extracts" directly into a gc or gc/ms instrument. Although these headspace techniques are quite convenient, they also have significant limitations in that they are skewed toward analysis of more volatile components and do not allow for the use of identification techniques other than gc/ms and gc/ir.

At first, such methods were used to investigate the top notes, ie, the most volatile part, of essential oils and other naturals. This was done in order to allow more complete reconstitution of naturals using synthetic ingredients. It was then found that these techniques could be applied directly to flowers and other parts of

plants. This avoids the heating and other processing involved in producing natural extracts, so that duplications based on these results differ significantly from the older standard products. It also allows the duplication or imitation of flowers, herbs, fruits, etc, which do not produce satisfactory extracts either because they do not contain sufficient fragrant oil or because they produce undesirable odors during the extraction processes.

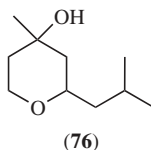
It was also found that flowers and other plant parts can be analyzed using head space techniques without removing them from the living plant (5). Significant differences in the volatile compositions of live and picked flowers have been noted, as exemplified for jasmine flowers in Table 3. The reasons for these remarkable differences are not known.

7.2. Synthesis. Exploratory research has produced a wide variety of odorants based on natural structures, chemicals analogous to naturals, and synthetic materials derived from available raw materials and economical processing. As in most areas of the chemical industry, the search for new and useful substances is made difficult by the many materials that have been patented and successfully commercialized (6). In the search for new aroma chemicals, many new materials are prepared for screening each year. Chemists who perform this work are involved in a creative exercise that takes its direction from the commercial sector in terms of desirable odor types and specific performance needs. Because of economic limitations, considerations of raw material costs and available processing methods may play a role early in the exploratory work.

Initial evaluations of chemicals produced for screening are performed by smelling them from paper blotters. However, more information is necessary given the time and expense required to commercialize a new chemical. No matter how pleasant or desirable a potential odorant appears to be, its performance must be studied and compared with available ingredients in experimental fragrances. A material may fail to live up to the promise of its initial odor evaluation for a number of reasons. It is not at all uncommon for the odor character of a chemical disappear in a formulation or skew the overall odor in an undesirable way. Some materials are found to be hard to work with in that their odors stick out and cannot be blended well. Because perfumery is an individualistic art, it is important to have more than one perfumer work with a material of interest and to have it tried in several different fragrance types. Aroma chemicals must be stable in use if their desirable odor properties are to reach the consumer. Therefore, testing in functional product applications is an important part of the evaluation process. Other properties that can be important for new aroma chemicals are substantivity on skin and cloth, and the ability to mask certain malodors.

In recent years synthetic research has been significantly influenced by safety and environmental factors. For example, hydroxy citronellal (**10**), which is a long-appreciated muguet odorant, was found to have some allergenic properties and hence its use has been restricted. Research and development efforts led to the introduction of Florol (**76**), which offers similar odor and performance. It must be noted that direct substitutions of one odorant for another across a wide range of applications is rarely if ever achieved - for esthetic or performance reasons. However, what may be lost in one sense may be gained in another. In this example, Florol, not having an aldehyde functional group, offers superior

stability and is therefore more widely applicable than the material it was intended to replace.



The appearance of nitro and polycyclic musks in the environment (7) led to a search for materials of similar odor that would be more readily biodegradable. In fact these findings sensitized the industry to environmental issues in general. Most of the research done in this area involved macrocyclic ketones and lactones. An example is the unsaturated macrocyclic lactone oxacyclohexadecen-2-one (77), which is marketed as Globalide[®] and Habanolide[®] (8). The search continues and has been expanded to include non-macrocyclic materials (9).

7.3. Structure–Odor Correlations and Olfactory Receptors. The issue of structure–odor correlation is one that continues to fascinate and frustrate fragrance chemists. In certain odor areas, particularly for musk (10) and amber (1) odors, much work has been done and some correlations have been made. In these areas, chemical structures are rather well-defined and many are rigid in nature, thus simplifying conformational questions. Much careful synthetic work has been done in conjunction with some of these studies. It has been shown that odor strength and character can be exquisitely sensitive to very small structural changes in some, but not all, cases. This applies to stereochemical and chiral differences (11) as well as other simple changes such as adding, removing, or changing the position of a methyl group. Computer methods have been applied by using such techniques as molecular modeling, pattern recognition, and molecular orbital calculations in attempts to correlate various molecular properties with odor quality. These efforts cannot be generalized over a range of odor types and are quite limited in predictive value.

The sense of smell is a chemical sense in that the molecules of an odorant must come in contact with some sorts of receptors, which are located on the outside of neurons in the olfactory epithelium. The pathway of neuronal signals to the brain via the olfactory bulb has been known for some time, but until the early 1990s little was understood about the mechanisms of odor recognition and signal transduction. However, by using the techniques of modern biochemistry, important findings were made and the beginnings of important insights emerged (12,13).

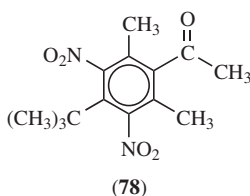
Olfactory receptors have been a subject of great interest (14). Much that has been postulated was done by analogy to the sense of sight in which there are a limited number of receptor types and, as a consequence, only three primary colors. Thus attempts have been made to recognize primary odors that can combine to produce all of the odors that can be perceived. Evidence for this includes rough correlations of odors with chemical structural types and the existence in some individuals having specific anosmias. Cross-adaptation studies, in which exposure to one odorant temporarily reduces the perception of a chemically related one, also fit into this hypothetical framework. Implicit in this theory is the

idea that there is a small number of well-defined odor receptors, so that eventually the shape and charge distribution of a specific receptor can be learned and the kinds of molecular structures for a specified odor can be deduced.

Research in olfaction was revolutionized by the finding in of Buck and Axel in 1991 of a large family of mammalian genes which code for as many as 1000 olfactory receptors (15). The receptors are proteins that cross the cell membranes of olfactory neurons seven times and are related to other types of sensory receptors. For a number of years, a direct proof that these proteins were indeed olfactory receptors was lacking. This was provided in 1998 by Firestein et. al, who were able to make electrical activity measurements on a single modified receptor showing differing responses to a variety of odorants (16). Another important finding was that a given receptor responds to a variety of odorants (but not all) and a given odorant activates a variety of receptors (17). Thus we have a combinatorial scheme of odor perception.

These findings are consistent with smell being a primitive sense, more acute in lower animals that have smaller brains. In fact it has been shown that in higher mammals fewer of the genes are expressed as functional receptors, nevertheless it appears that even humans have 300–400 different odor receptors. Thus it is reasonable to assume that the signal leaving the nose contains most of the information needed by the brain to recognize an odor. It can be seen from Table 2 that most odorants used in perfumes are rather nonpolar and therefore likely to have weak, hydrophobic, and fleeting interactions with receptor proteins.

Under this scenario, it is not at all clear if the characterization of a single receptor or several receptors would be helpful in predicting the odor caused by a given chemical entity. Many structure–odor researchers in the past have looked for similarities in the structures of rather disparate chemicals having similar odors, for example the musk odorants cyclopentadecanone (also known as Exaltone) [502-72-7] (**44**), Galaxolide[®] [1222-05-5] (**64**), and musk ketone [81-14-1] (**78**). The new theory suggests that there may be more than one combination of receptors that can produce a given type of odor perception, or more than one way to stimulate a given combination of receptors. Chemists working in this area have begun to take these new findings into account (18). It remains to be seen what impact this will have on the future of fragrance chemical research.

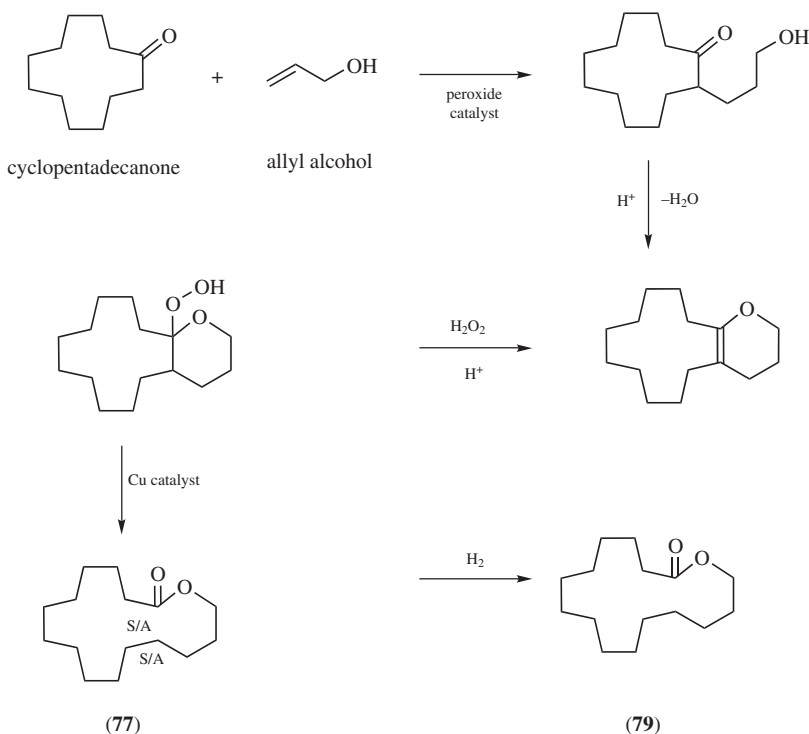
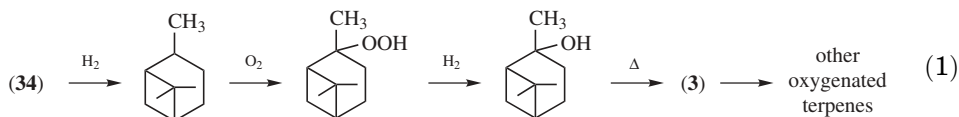


For more information on the fascinating field of olfactory research, the reader is referred to various recent review articles (19–22).

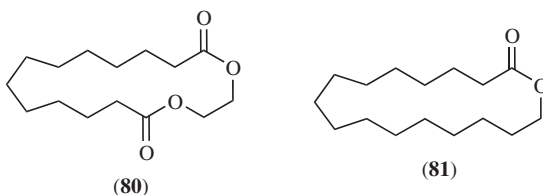
7.4. Process Research and Development. In the fragrance industry, as in other parts of the chemical industry, chemical processing costs must be consistent with values of the materials produced. It is a common fallacy, probably

inferred from the costs of couturier perfumes, that fragrance ingredients are expensive. This is true for certain natural materials produced laboriously from flowers, but is certainly not the case for the vast majority of aroma chemicals in use. The costs of most large-volume (roughly >50t/yr) aroma chemicals are quite competitive. Consequently, the fragrance industry has invested much effort in process research and development. In addition to looking for ways to improve yields and throughputs, significant changes have taken place in the scale of manufacture, the equipment used, and the manufacturing operations themselves. As these changes occur, maintaining product quality is a critical concern.

In several important cases, new synthetic strategies have been developed into new production schemes. An outstanding example of this is the production of an entire family of terpene derivatives from α -pinene (**34a**), the major component of most turpentine, via linalool (**3**) (23). Many of these materials had been produced from β -pinene (**34b**), a lesser component of turpentine, via pyrolysis to myrcene and further chemical processing. The newer method offers greater manufacturing flexibility and better economics, and is environmentally friendly in that catalytic air oxidation is used to introduce functionality.



It was mentioned above that the industry has carrying out synthetic research to find alternatives to the nitro and polycyclic musks. Another approach to this problem is the investigation of known macrocyclic ketones and lactones (24) in search of more efficient processes that could be practiced on larger scales than had previously been contemplated. Some of the materials that have received this sort of attention are muskalactone (79) (25), cyclopentadecanone (44), hexadecanolide (80) (26) as well as the dilactone ethylene brassylate (81) and its lower homolog prepared from dodecanedioic acid. Reaction scheme shows some of the chemistry that has been developed in connection with the new chemical, oxacyclohexadecen-2-one (77) and muskalactone (79).



In addition to large-scale process work, there is also effort expended in providing synthetic methods for producing small amounts (<100kg/yr) of materials needed for replacement of naturals that are being discontinued or in short supply. Examples are ambrinol (73) and dihydro- γ -ionone (74) for the replacement of ambergris. More recently, tincture of tonquin musk has been replaced by using, among other materials, mixtures of macrocyclic ketones and alcohols which have been found in the natural substance.

Most aroma chemicals are relatively high boiling (80–160°C at 0.4 kPa = 3 mm Hg) liquids and therefore are subject to purification by vacuum distillation. Because small amounts of decomposition may lead to unacceptable odor contamination, thermal stability of products and by-products is an issue. Important advances have been made in distillation techniques and equipment to allow routine production of 5000 kg or larger batches of various products. In order to make optimal use of equipment and to standardize conditions for distillations and reactions, computer control has been instituted. This is particularly well suited to the multipurpose batch operations encountered in most aroma chemical plants. In some instances, on-line analytical capability is being developed to work in conjunction with computer controls.

7.5. Physiological and Psychological Effects of Fragrance. The sense of smell is much more important for the preservation of life for most animals than it is for human beings. It is critical, among other things, to feeding, safety, recognition of individuals, and reproduction. As humans evolved, the importance and acuity of the sense of smell decreased, though it still can have powerful effects on humans, such as the stimulation of memory. Considerable research effort has been and continues to be made to evaluate the role of fragrance in human behavior.

Some efforts to determine physiological effects have focused on peripheral measurements such as pulse rate, blood pressure, and galvanic skin response. Pleasant odors have little or no effect on these functions, whereas unpleasant odors can produce alarm reactions. Brain waves, measured by electroencephalography

(eeg), are one area where physiological changes have been observed upon exposure to fragrances (28). Odors have been shown to evoke event-related potentials (ERPs) in the brain. These vary with the pleasantness of the odor and whether or not an odor is also a trigeminal stimulus. Odors also affect the brain's spontaneous eeg and ERPs to visual stimuli, which indicates that they have the potential to influence the brain's processing of information. This line of research is quite new, however, and much more work remains before brain mechanisms of olfaction can be addressed.

Faced with the limits of physiological measurements in determining the effects of fragrance on humans, researchers have turned to psychological measurements and produced some interesting results (29). Such methods as monitoring behavior and various types of self-reporting (eg, questionnaire) before and after exposure to many odor types have been used; requiring subjects to relate odors to various kinds of images has also been fruitful. The results indicate that odors have small priming effects on mood and can affect behavior in predictable ways. Pleasant odors tend to improve mood. For example, several studies have shown that pleasant odors, compared to unpleasant ones, elicit more happy memories, enhance creative performance, and result in more positive evaluations (photographs or computer images) of people. Social psychological studies have examined the effects of odors on simulated negotiations; subjects exposed to pleasant odors were more cooperative and less prone to confrontational approaches. Thus, by studying and quantifying the effects of fragrance and fragrance ingredients on mood, it may be possible to add a new dimension to the performance of perfumes.

8. Economic Aspects

Attempts to estimate worldwide merchant sales of fragrances are complicated by various factors. There are many suppliers; all of the principal ones are also engaged in flavor business and most are also producers, to differing degrees, of aroma chemicals and natural ingredients (used for both flavors and fragrances). Further, the ingredients are used internally and sold throughout the industry (see FLAVORS). The industry has enjoyed fairly rapid growth rates, 3–6%, but figures from year to year can be highly distorted by relative currency changes.

For purposes of this discussion, only the value to the fragrance supplier is considered. Retail sales of fine perfumes would give substantially higher numbers. According to SRI Consulting (29), worldwide sales of flavors and fragrances in 2003 were \$16,300 million, of which 43% was flavor compositions, 27% compounded fragrances, 13% aroma chemicals, and 17% was for natural ingredients, which may be used in either flavors or fragrances. IAL Consultants estimated that in 1999 fragrances comprised 51% of F & F market. Thus it appears that the worldwide fragrance market in 2003 was approximately \$8,200 million. Of this total, toiletries and cosmetics were approximately 25% with soaps and detergents at 24%(30).

Worldwide fragrance and ingredient sales for 1990 were projected at \$5,650 million, of which compounded fragrances were \$2,800 million, aroma chemicals \$1,500 million and natural ingredients \$1,350 million (31). A breakdown of

product types where perfumes are used as determined for 1987 is as follows: women's and men's fragrances (perfumes, colognes, etc), at 26% of the market share; cosmetics and toiletries, at 26%; soaps (including toilet soaps), as well as laundry and dishwashing products, at 34%; and cleaning, disinfecting, and polishing products, air fresheners, and industrial products, at 14% (31).

9. Safety, Regulatory, and Environmental Aspects of the Industry

The fragrance industry has a long record of safety, largely on account of the nature and sources of its ingredients, and how its products are used. The approach to product safety, used successfully for many years, is based on individual ingredients rather than finished perfumes. Far more testing of fragrance formulations would be required than is done for ingredients because the rate of new fragrance creation is high. By examining individual ingredients and setting appropriate limits on their use, it is possible to ensure the safety of fragrances as they are created. This approach is accepted by relevant governmental agencies around the world, such as the U.S. Food and Drug Administration.

The industry supports the International Fragrance Association (IFRA) that strengthens scientific criteria and develops guidelines for the safe and environmentally sound use of fragrances. IFRA is composed of two arms governed by the IFRA Executive Committee: a scientific arm, the Research Institute for Fragrance Materials (RIFM), and a Communications arm (IFRA). The Research Institute for Fragrance Materials (RIFM) is an internationally recognized scientific organization that collects, generates, and disseminates information on the safety of perfume ingredients. This information may originate from published or unpublished sources, or through RIFM's ongoing research program. The findings are reviewed by an independent expert panel of academicians and published in peer-reviewed journals such as *Food & Chemical Toxicology*. The activities of RIFM are harmonized with those of the International Fragrance Association (IFRA). IFRA, whose members come from various national associations of fragrance manufacturers (eg, from the Netherlands, France, Germany, United States, and Japan), is concerned with all aspects of safety evaluation and regulation in the industry, into which it has introduced self-regulatory discipline. Its primary function is the formulation and continuous updating of the Code of Practice for the Fragrance Industry. The Code provides guidelines on manufacturing practices, as well as toxicological methodology, safety assessments and standards on the safe usage of fragrance materials. These guidelines and standards have been followed by the fragrance industry since the early 1970s.

Fragrances must comply with all applicable regulations and legislation that address occupational and consumer health, safety, and environmental concerns. Many countries have adopted chemical substance inventories in order to monitor use and evaluate exposure potential and consequences. For most fragrance applications, all ingredients must be on these lists. New substances must be subjected to premanufacturing or premarketing notification (PMN). PMN requirements vary by country and by the predicted volumes of production, and/or import; they require assessments of environmental and human health-related properties, and reporting of the results to designated governmental authorities.

Perfumes are also impacted by legislation that regulates specific products which may contain fragrances; such legislation includes the U.S. Food, Drug and Cosmetic Act and the European Community Cosmetic Directive. Under the latter regulation, a list of fragrance ingredients is being added to the European Community Cosmetic Ingredient Inventory to assist regulators and health officials in evaluating the safety of such products. An example of environmental legislation that may affect fragrance use requires the reduction of the atmospheric release of volatile organic chemicals (VOCs) from consumer products and other sources. However, because fragrances are recognized as unique, essential components of consumer products, and generally used at low levels, they are given specific exemptions from most VOC regulations.

In recent years the finding of several, relatively persistent aroma chemicals in river water at trace levels has led to an examination of this aspect of fragrance usage as well as environmental safety and fate by RIFM and IFRA. Studies have been carried out to determine biodegradability, bioaccumulation and biotoxicity for several materials of particular concern including two ingredients in the polycyclic musk group. Thus the industry is gaining experience with environmental risk assessment that is being applied mainly to the highest volume aroma chemicals. Although the chemical structural factors used to predict the environmental fate of the polycyclic musks would indicate these materials to be potentially persistent and bioaccumulative, actual experimental data have indicated that they are not (32). This area is under continued scrutiny by RIFM.

In addition to the observation of fragrance materials in the environment, several materials including the polycyclic musks and the nitromusks have been found at extremely low levels (parts per billion) in human milk. This is most likely the result of several factors: extensive use of certain aroma chemicals in cosmetics fragrances, hydrophobicity, which allows partitioning into adipose tissues, and slow removal. The latter two factors allow for the secretion of trace amounts in the fatty portion of milk. These findings have led to new testing and assessment of fragrance materials for mutagenicity and teratogenicity. In general the safety of fragrance materials with respect to these concerns is being demonstrated (32).

Evaluation of the safe use of perfumes is an ongoing process. It is conducted mainly through self-disciplinary efforts of the fragrance industry and involves continuing investigation of the safety of new and existing ingredients. The manufacture and use of perfumes must comply with the growing body of environmental and human health-related regulations worldwide and must meet the rigorous standards set forth by the industry as well as the many legislative requirements throughout the world.

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Table 1. **Perfumery Descriptions**

Floral		Citrus	Woody	Green	Fruity	Oriental
carnation	lilac	bergamot	cedar	basil	apple	spicy
chrysanthemum	lily	grapefruit	fir	cucumber	apricot	amber
gardenia	marigold	lemon	hickory	grass	banana	oakmoss
honeysuckle	muguet	lime	patchouli	parsley	black currant	musk
hyacinth	narcissus	mandarin	pine	rhubarb	cherry	woody
iris	orange flower	orange	sandal	string bean	fig	
jasmine	rose	tangerine	vetivert	violet	grape	
jonquil	violet	verbena		watercress	melon	
lavender	mimosa				peach	
					pineapple	
					prune	
					raspberry	
					strawberry	

Table 2. **Typical Aroma Chemicals by Functional Group**

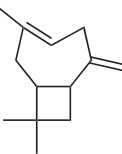
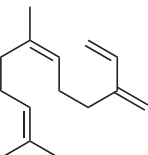
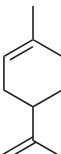
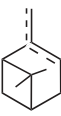
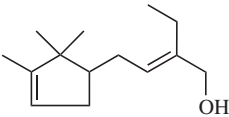
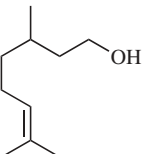
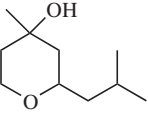
Name [CAS Registry number]	Structure	Odor Type
<i>A. Hydrocarbons</i>		
caryophyllene [13877-93-5]	 (12)	woody, spicy (cloves)
β -farnesene [18794-84-8]	 (32)	mild, sweet, warm
limonene [138-86-3]	 (33)	orange, citrus
pinenes (a) alpha [80-56-8](b) beta [127-91-3]	 (34)	piney, woody
<i>B. Alcohols</i>		
Bacdanol [29219-61-6]	 (35)	sandalwood
citronellol [106-22-9]	 (9)	rosy, citrus
Florol [®] [63500-71-0]	 (36)	floral, muguet

Table 2. (Continued)

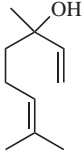
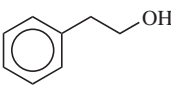
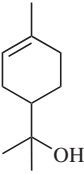
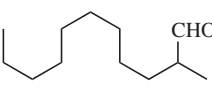
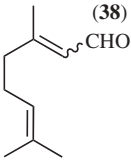
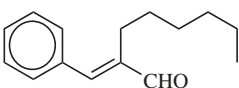
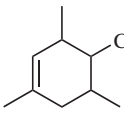
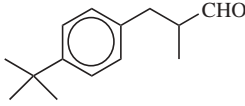
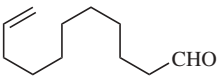
Name [CAS Registry number]	Structure	Odor Type
linalool [78-70-6]	 (3)	floral, citrus
phenethyl alcohol [60-12-8]	 (24)	floral, rosy
terpineol [98-55-5]	 (37)	floral, lilac
<i>C. Aldehydes</i>		
methyl nonyl acetaldehyde [110-41-8]	 (38)	fresh, citrus (orange)
citral [5392-40-5]	 (2)	citrus, lemon
hexyl cinnamic aldehyde [101-86-0]	 (39)	floral, jasmine
isocyclocitral [1423-46-7]	 (40)	floral, carnation
Lilial [80-54-6]	 (41)	floral, muguet
undercylenic aldehyde [112-45-8]	 (42)	citrus, waxy

Table 2. (*Continued*)

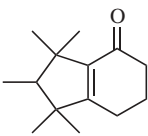
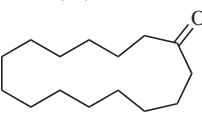
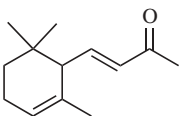
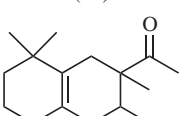
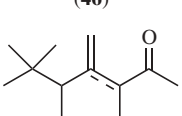
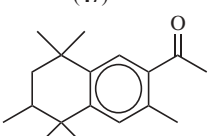
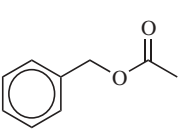
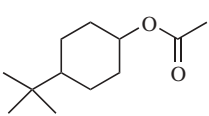
Name [CAS Registry number]	Structure	Odor Type
<i>D. Ketones</i>		
cashmeran [33704-61-9]	 (43)	musky, sweet
cyclopentadecanone [502-72-7]	 (44)	musk
α -ionone [127-41-3]	 (45)	floral, violet
Isocyclemone E [54464-57-2]	 (46)	amber, woody
Koavone [86115-11-9]	 (47)	woody, ambery, floral
Tonalide [21145-77-7] [1506-02-1]	 (48)	musk
<i>E. Esters</i>		
benzyl acetate [140-11-4]	 (49)	floral, jasmine
<i>p</i> - <i>t</i> -butylcyclohexyl acetate <i>cis</i> [10411-92-4] <i>trans</i> [1900-69-2]	 (50)	woody, floral

Table 2. (Continued)

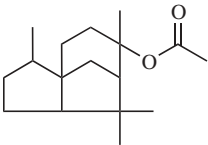
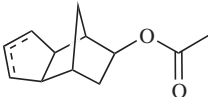
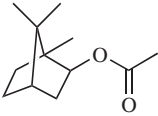
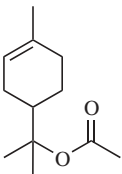
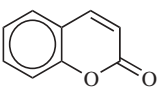
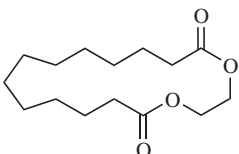
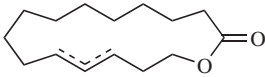
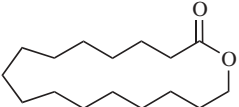
Name [CAS Registry number]	Structure	Odor Type
cedryl acetate [77-54-3]	 (51)	woody, cedar
Cyclacet [5413-60-5] [2500-83-6]	 (52)	green, woody
isobornyl acetate [125-12-2]	 (53)	pine needles
terpinyl acetate [80-26-2]	 (54)	herbaceous, piney
<i>F. Lactones</i>		
coumarin [91-64-5]	 (55)	sweet, hay
ethylene brassylate [105-95-3]	 (56)	musk
Habanolide [®] , Globalide [®] [34902-57-3]	 (57)	musk
hexadecanolide [109-29-5]	 (58)	musk

Table 2. (*Continued*)

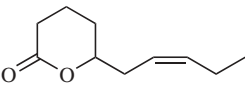
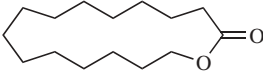
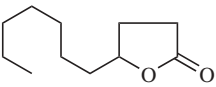
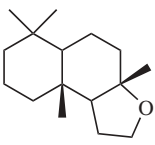
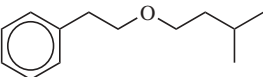
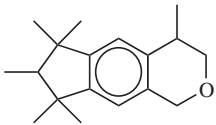
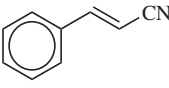
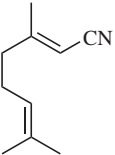
Name [CAS Registry number]	Structure	Odor Type
jasmine lactone [34686-71-0]	 (59)	floral, jasmine
muskalactone [106-02-5]	 (60)	musk
“peach aldehyde” [104-67-6]	 (61)	fruity, peach
<i>G. Ethers</i>		
Ambroxan [3708-00-9]	 (62)	amber, woody
Anther [56011-02-0]	 (63)	floral, hyacinth
Galaxolide [1222-05-5]	 (64)	musk
<i>H. Nitriles</i>		
cinnamonnitrile [4360-47-8]	 (65)	cinnamic, balsamic
geranonitrile [31983-27-4]	 (66)	citrus, lemon

Table 2. (Continued)

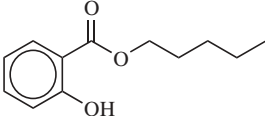
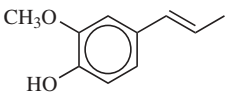
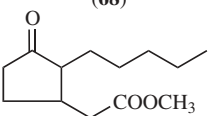
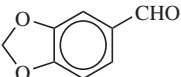
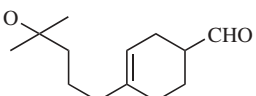
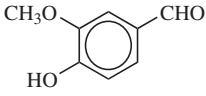
Name [CAS Registry number]	Structure	Odor Type
<i>I. Polyfunctionals</i>		
amyl salicylate [2050-08-0]	 <p>(67)</p>	floral, jasmine
isoeugenol [97-54-1]	 <p>(68)</p>	warm, spicy, floral
Hedione [29852-02-6]	 <p>(69)</p>	jasmin, lemon
heliotropine [120-57-0]	 <p>(70)</p>	sweet, floral
Lylal [31906-04-4]	 <p>(71)</p>	floral muguet
vanillin [121-33-5]	 <p>(72)</p>	sweet, vanilla

Table 3. Head Space Constituents of Jasmine Flowers

Chemical component	Living flower, %	Picked flower, %
6-methyl-5-hepten-2-one	0.2	
<i>cis</i> -3-hexenyl acetate	0.2	
benzyl alcohol		4.0
ocimene (cis and trans)	0.2	1.1
benzyl acetate	60.0	40.0
linalool	3.0	30.0
indole	11.0	2.0
<i>cis</i> -jasmone	3.0	
3,5-dimethyl-2-ethylpyrazine		0.5
methyl jasmonate	0.3	