Perfumery Notes

An anatomy of rose

"Would Jove appoint some flower to reign In matchless beauty on the plain The rose (mankind will agree) The rose, the Queen of Flowers should be."

This poem, by the Greek poet Sappho, written over 2,500 years ago, is only an indication of the kind of admiration that has been bestowed on the rose over the centuries. Roses have been used in religious ceremonies by various peoples throughout the ages. The rosary, or string of prayers, was first made by stringing rose hips together. Rose hips, very high in vitamin C, are used for making jam that is both tasty and nutritious. Of course, the rose has long been a symbol of romance. Few will doubt that a single rose can capture the heart of any woman, young or old.

However, these bits of trivia, while interesting, are only small facets of the natural wonder of the flower. Its beauty can only be half appreciated by the eye. Its fragrant scent has pleased the nose of man and woman since long before recorded history and long before they knew they had an olfactory epithelium. For roses have been around for quite a long time. The oldest fossil imprint, found in Colorado, dates back about 40 million years.¹

There are over 13,000 identifiable varieties of roses.² The best known and most popular are hybrid tea roses. These are the result of cross breeding for size and color without specific regard to odor. In fact, while appearance and color may have been improved, the fragrance of the hybrid tea rose is often poor, or in the worst cases nonexistent. Two other varieties of roses have gained prominence with perfumers. They are *Rosa Centifolia* (rose of 100 petals) and *Rosa Damascena*.

The essences of these roses are enjoyed by millions. Most may never be aware of this, because rose complexes are skillfully blended into numerous perfumes Felix Buccellato Alpine Aromatics International Inc. Metuchen, NJ

and cosmetic preparations throughout the world. Rose is probably the most popular single floral fragrance used in the fragrance industry. It is not always used as a background or hidden in a blend of balsam and spice. It is often boldly stated and used as a main theme in perfumes like *Joy*, introduced by Jean Patou in 1935. It has been and will continue to be reintroduced again and again along with new notes as in *First*, by Van Cleef and Arpels in 1977. There is no end to the variety of blends yet to be discovered using a rose body.

It should come as no surprise, then, that a young apprentice perfumer's first task may be to examine and study a rose and try to duplicate its beautiful fragrance. Chemists throughout the world have carefully dissected and analyzed this essence; the valuable information available in the literature is a logical place to begin.

A basic rose formula is available in Guenther's treatise on essential oils.³ While this simple formula will smell similar to rose, it will not possess the vibrant vitality of a true rose with all its power and diffusion. Since the publication of this formula in 1952, great technical strides have been made and many additional chemicals have been identified in rose. Some of these chemicals are very well known; others are not widely publicized.

Two types of rose oils are commercially available. Rose otto, which is a steam distillation, does not represent the correct proportion of ingredients as they exist in the flower. For that, one had best look to an analysis of rose absolute, which is an alcoholic extract. The percentages of chemicals in the alcohol extract will be closer to those found in the actual flower.

Table 1 shows an analysis of rose absolute Maroc,*

^{*}Unpublished work in progress, by F. Buccellato, Alpine Aromatics International, Inc., 1979.

Perfumery Notes-Rose

compared with Bulgarian and Turkish rose otto types. $^{\rm 4}$

As can be seen, the percentages differ drastically. This is due to the high solubility of phenylethyl alcohol in water. Once the phenylethyl alcohol is removed, by steam distillation process, the percentages of the trace ingredients increase and provide an attar or otto type rose oil which can be more conveniently analyzed.

Examination of constituents

It is not enough to be able to recognize the odors of phenylethyl alcohol and geraniol. Each item must be studied for its properties and its qualities should be examined from an analytical point of view as well as undergo an organoleptic evaluation at the intended level of usage. This is extremely important for low level constituents. In this way one will develop a feeling for the performance of the various ingredients.

For example, a compound like cis-3-hexenal at full strength is quite harsh but when diluted this aldehyde has a very lovely, fresh green and leafy aroma providing a natural "greenery" effect to a composition.

It may help to organize the characters of rose and list them in table fashion, and list under them the chemicals that contribute to that character (Table II). It should be kept in mind that these are individual interpretations and the reader may find different characters. This is not always a clear cut decision. Many chemicals have more than one side to their character, and there is always the possibility of controversy as to what the character of a chemical is.

For example, citronellol, while floral, has somewhat of a fatty waxy character. While phenylethyl alcohol provides without a doubt the main body and character

Compounds Pulgarian 1 Turkish 1 Turkish 2 Rose Absolute ethanol 1.43 5.14 0.38 pentanal 0.07 0.05 0.38 alpha-pinene 0.73 0.50 0.04 alpha-pinene 0.03 0.02 0.01 0.01 beta-pinene 0.03 0.22 0.01 camphene and heptanal 0.14 0.07 0.01 heptanol 0.02 0.01 hexta actate 0.01 0.01 octanal 0.05 0.02 0.02 octanol 0.07 0.01 0.02 inalool 2.18 0.54 0.95 0.40 octanol 0.07 0.01 0.02 inalool 2.18 0.54 0.95 0.40 octanol 0.07 0.33			Relative p	ercentage	
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citronellol 33.40 45.04 28.20 8.77 nerol 5.90 3.60 6.62 2.52 geraniol and neral 18.47 11.87 26.33 5.18 geranial and carvone 0.72 0.57 0.87 $$ citronellyl acetate 0.53 0.72 0.51 0.23 neryl acetate 0.06 0.04 0.09 0.10 cinnamaldehyde and C_{15} paraffin 0.21 0.30 0.50 $$ geranyl acetate 1.60 1.23 1.10 0.38 eugenol and trans-beta-damascenone 1.20 1.19 1.01 0.89 methyl eugenol and C_{16} paraffin 2.37 3.26 1.42 $$ C_{17} paraffin and C_{17} olefin 1.90 1.80 2.44 $$ C_{15} paraffin and C_{18} olefin 0.30 0.25 0.67 $$ trans-trans-farnesol 0.87 0.36 1.61 1.30 C_{19} paraffin and C_{19} olefin 14.51 13.06 16.17 2.73 C_{20} paraffin and C_{20} olefin 1.07 0.85 0.86 $$ C_{21} paraffin and C_{21} olefin 4.28 3.30 3.87 1.75 C_{22} paraffin 0.90 0.60 0.49 $$ C_{23} paraffin 0.90 0.60 0.49 $$ C_{24} paraffin 0.07 0.03 $$ $ C_{24}$ paraffin 0.07 0.03 $$ $-$ <td>phenylethyl alcohol, decanal and terpinen-4-ol</td> <td>1,45</td> <td>1.88</td> <td>2,58</td> <td>74.06</td>	phenylethyl alcohol, decanal and terpinen-4-ol	1,45	1.88	2,58	74.06
nerol 5.90 3.60 6.62 2.52 geraniol and neral 18.47 11.87 26.33 5.18 geranial and carvone 0.72 0.57 0.87 $$ citronellyl acetate 0.53 0.72 0.51 0.23 neryl acetate 0.06 0.04 0.09 0.10 cinnamaldehyde and C_{15} paraffin 0.21 0.30 0.50 $$ geranyl acetate 1.60 1.23 1.10 0.38 eugenol and trans-beta-damascenone 1.20 1.19 1.01 0.89 methyl eugenol and C_{16} paraffin 2.37 3.26 1.42 $$ C_{17} paraffin and C_{17} olefin 1.90 1.80 2.44 $$ C_{15} paraffin and C_{18} olefin 0.30 0.25 0.67 $$ trans-trans-farnesol 0.87 0.36 1.61 1.30 C_{19} paraffin and C_{19} olefin 14.51 13.06 16.17 2.73 C_{20} paraffin and C_{21} olefin 1.07 0.85 0.86 $$ C_{21} paraffin and C_{21} olefin 4.28 3.30 3.87 1.75 C_{22} paraffin 0.90 0.60 0.49 $$ C_{24} paraffin 0.90 0.60 0.49 $$ C_{24} paraffin 0.90 0.60 0.49 $$ C_{24} paraffin 0.07 0.03 $$ $ C_{24}$ paraffin 0.90 0.00 $$ $ C_{2$	citronellol	33.40	45.04	28.20	8.77
geraniol and neral18.4711.8726.335.18geranial and carvone 0.72 0.57 0.87 citronellyl acetate 0.53 0.72 0.51 0.23 neryl acetate 0.06 0.04 0.09 0.10 cinnamaldehyde and C ₁₅ paraffin 0.21 0.30 0.50 geranyl acetate 1.60 1.23 1.10 0.38 eugenol and trans-beta-damascenone 1.20 1.19 1.01 0.89 methyl eugenol and C ₁₆ paraffin 2.37 3.26 1.42 C ₁₇ paraffin and C ₁₇ olefin 1.90 1.80 2.44 C ₁₅ paraffin and C ₁₈ olefin 0.30 0.25 0.67 trans-trans-farnesol 0.87 0.36 1.61 1.30 C ₁₉ paraffin and C ₁₉ olefin 14.51 13.06 16.17 2.73 C ₂₀ paraffin and C ₂₁ olefin 4.28 3.30 3.87 1.75 C ₂₂ paraffin 0.90 0.60 0.49 C ₂₄ paraffin 0.90 0.60 0.49 C ₂₄ paraffin 0.07 0.03 0.02	nerol	5.90	3.60	6.62	2.52
geranial and carvone 0.72 0.57 0.87 $$ citronellyl acetate 0.53 0.72 0.51 0.23 neryl acetate 0.06 0.04 0.09 0.10 cinnamaldehyde and C_{15} paraffin 0.21 0.30 0.50 $$ geranyl acetate 1.60 1.23 1.10 0.38 eugenol and trans-beta-damascenone 1.20 1.19 1.01 0.89 methyl eugenol and C_{16} paraffin 2.37 3.26 1.42 $$ C_{17} paraffin and C_{17} olefin 1.90 1.80 2.44 $$ C_{15} paraffin and C_{18} olefin 0.30 0.25 0.67 $$ trans-trans-farnesol 0.87 0.36 1.61 1.30 C_{19} paraffin and C_{19} olefin 14.51 13.06 16.17 2.73 C_{20} paraffin and C_{21} olefin 1.07 0.85 0.86 $$ C_{21} paraffin and C_{21} olefin 4.28 3.30 3.87 1.75 C_{22} paraffin 0.90 0.60 0.49 $$ C_{23} paraffin 0.90 0.60 0.49 $$ C_{24} paraffin 0.07 0.03 0.02 $$	geraniol and peral	18.47	11.87	26.33	5.18
citronellyl acetate 0.53 0.72 0.51 0.23 neryl acetate 0.06 0.04 0.09 0.10 cinnamaldehyde and C_{15} paraffin 0.21 0.30 0.50 $$ geranyl acetate 1.60 1.23 1.10 0.38 eugenol and trans-beta-damascenone 1.20 1.19 1.01 0.89 methyl eugenol and C_{16} paraffin 2.37 3.26 1.42 $$ C_{17} paraffin and C_{17} olefin 1.90 1.80 2.44 $$ C_{15} paraffin and C_{18} olefin 0.30 0.25 0.67 $$ trans-trans-farnesol 0.87 0.36 1.61 1.30 C_{19} paraffin and C_{20} olefin 1.07 0.85 0.86 $$ C_{20} paraffin and C_{21} olefin 4.28 3.30 3.87 1.75 C_{22} paraffin 0.90 0.60 0.49 $$ C_{23} paraffin 0.90 0.60 0.49 $$ C_{24} paraffin 0.90 0.60 <	geranial and carvone	0.72	0.57	0.87	
neryl acetate 0.06 0.04 0.09 0.10 cinnamaldehyde and C_{15} paraffin 0.21 0.30 0.50 geranyl acetate 1.60 1.23 1.10 0.38 eugenol and trans-beta-damascenone 1.20 1.19 1.01 0.89 methyl eugenol and C_{16} paraffin 2.37 3.26 1.42 C ₁₇ paraffin and C_{17} olefin 1.90 1.80 2.44 C ₁₅ paraffin and C_{18} olefin 0.30 0.25 0.67 trans-trans-farnesol 0.87 0.36 1.61 1.30 C ₁₉ paraffin and C_{19} olefin 14.51 13.06 16.17 2.73 C ₂₀ paraffin and C_{21} olefin 1.42 3.30 3.87 1.75 C ₂₁ paraffin and C_{21} olefin 4.28 3.30 3.87 1.75 C ₂₂ paraffin 0.90 0.60 0.49 C ₂₃ paraffin 0.90 0.60 0.49 C ₂₄ paraffin 0.94 0.03	citronelly acetate	0.53	0.72	0.51	0.23
cinnamaldehyde and C_{15} paraffin 0.21 0.30 0.50 geranyl acetate 1.60 1.23 1.10 0.38 eugenol and trans-beta-damascenone 1.20 1.19 1.01 0.89 methyl eugenol and C_{16} paraffin 2.37 3.26 1.42 C ₁₇ paraffin and C_{17} olefin 1.90 1.80 2.44 C ₁₅ paraffin and C_{17} olefin 0.30 0.25 0.67 trans-trans-farnesol 0.87 0.36 1.61 1.30 C ₁₉ paraffin and C_{19} olefin 14.51 13.06 16.17 2.73 C ₂₀ paraffin and C_{20} olefin 1.07 0.85 0.86 C ₂₁ paraffin and C_{21} olefin 4.28 3.30 3.87 1.75 C ₂₂ paraffin 0.10 0.13 0.46 C ₂₃ paraffin 0.90 0.60 0.49 C ₂₄ paraffin 0.94 0.03	nervl acetate	0.06	0.94	0.09	0.10
geranyl acetate 1.60 1.23 1.10 0.38 eugenol and trans-beta-damascenone 1.20 1.19 1.01 0.89 methyl eugenol and C_{16} paraffin 2.37 3.26 1.42 C_{17} paraffin and C_{17} olefin 1.90 1.80 2.44 C_{15} paraffin and C_{18} olefin 0.30 0.25 0.67 trans-trans-farnesol 0.87 0.36 1.61 1.30 C_{19} paraffin and C_{19} olefin 14.51 13.06 16.17 2.73 C_{20} paraffin and C_{20} olefin 1.07 0.85 0.86 C_{21} paraffin and C_{21} olefin 4.28 3.30 3.87 1.75 C_{22} paraffin 0.10 0.13 0.46 C_{23} paraffin 0.90 0.60 0.49 C_{24} paraffin 0.04 0.03	cinnamaldehyde and C ₁ , paraffin	0.21	0.30	0.50	
eugenol and trans-beta-damascenone 1.20 1.19 1.01 0.89 methyl eugenol and C_{16} paraffin 2.37 3.26 1.42 C ₁₇ paraffin and C_{17} olefin 1.90 1.80 2.44 C ₁₅ paraffin and C_{18} olefin 0.30 0.25 0.67 trans-trans-farnesol 0.87 0.36 1.61 1.30 C ₁₉ paraffin and C_{19} olefin 14.51 13.06 16.17 2.73 C ₂₀ paraffin and C_{20} olefin 1.07 0.85 0.86 C ₂₁ paraffin and C ₂₁ olefin 4.28 3.30 3.87 1.75 C ₂₂ paraffin 0.10 0.13 0.46 C ₂₃ paraffin 0.90 0.60 0.49 C ₂₄ paraffin 0.04 0.03	geranyl acetate	1.60	1.23	1.10	0.38
methyl eugenol and C_{16} paraffin 2.37 3.26 1.42 C_{17} paraffin and C_{17} olefin 1.90 1.80 2.44 C_{15} paraffin and C_{13} olefin 0.30 0.25 0.67 trans-trans-farnesol 0.87 0.36 1.61 1.30 C_{19} paraffin and C_{19} olefin 14.51 13.06 16.17 2.73 C_{20} paraffin and C_{20} olefin 1.07 0.85 0.86 C_{21} paraffin and C_{21} olefin 4.28 3.30 3.87 1.75 C_{22} paraffin 0.10 0.13 0.46 C_{23} paraffin 0.90 0.60 0.49 C_{24} paraffin 0.04 0.03	eugenol and trans-beta-damascenon	e 1.20	1.19	1.01	0.89
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	methyl eugenol and C ₁₆ paraffin	2,37	3.26	1.42	
C_{15} paraffin and C_{18} olefin 0.30 0.25 0.67 trans-trans-farnesol 0.87 0.36 1.61 1.30 C_{19} paraffin and C_{19} olefin 14.51 13.06 16.17 2.73 C_{20} paraffin and C_{20} olefin 1.07 0.85 0.86 C_{21} paraffin and C_{21} olefin 4.28 3.30 3.87 1.75 C_{22} paraffin 0.10 0.13 0.46 C_{23} paraffin 0.99 0.60 0.49 C_{24} paraffin 0.04 0.03	C_{17} paraffin and C_{17} olefin	1.90	1.80	2.44	
12^{-1} 13^{-1} trans-trans-farnesol 0.87 0.36 1.61 1.30 C_{19} paraffin and C_{19} olefin 14.51 13.06 16.17 2.73 C_{20} paraffin and C_{20} olefin 1.07 0.85 0.86 $$ C_{21} paraffin and C_{21} olefin 4.28 3.30 3.87 1.75 C_{22} paraffin 0.10 0.13 0.46 $$ C_{23} paraffin 0.90 0.60 0.49 $$ C_{24} paraffin 0.04 0.03 $$ $$ C_{24} paraffin 0.07 0.03 0.02 $$	C_{15} paraffin and C_{19} olefin	0.30	0,25	0.67	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	trans-trans-farnesol	0.87	0.36	1,61	1.30
C_{20} paraffin and C_{20} olefin 1.07 0.85 0.86 C_{21} paraffin and C_{21} olefin 4.28 3.30 3.87 1.75 C_{22} paraffin 0.10 0.13 0.46 C_{23} paraffin 0.90 0.60 0.49 C_{24} paraffin 0.04 0.03 C_{24} paraffin 0.07 0.03 0.02	C ₁₉ paraffin and C ₁₉ olefin	14.51	13.06	16.17	2.73
C_{21} paraffin and C_{21} olefin 4.28 3.30 3.87 1.75 C_{22} paraffin 0.10 0.13 0.46 C_{23} paraffin 0.90 0.60 0.49 C_{24} paraffin 0.04 0.03 C_{24} paraffin 0.04 0.03	C_{20} paraffin and C_{20} olefin	1.07	0.85	0.86	
C_{22} paraffin 0.10 0.13 0.46 C_{23} paraffin 0.90 0.60 0.49 C_{24} paraffin 0.04 0.03 C_{24} paraffin 0.07 0.03 0.02	C ₂₁ paraffin and C ₂₁ olefin	4.28	3.30	3.87	1.75
C_{23}^{22} paraffin 0.90 0.60 0.49 C_{24} paraffin 0.04 0.03 C_{24} paraffin 0.07 0.03 0.02	C ₂₂ paraffin	0.10	0.13	0.46	
C_{24} paraffin 0.04 0.03 C_{c-c} paraffin 0.07 0.03 0.02	C ₂₃ paraffin	0.90	0.60	0.49	
Con paraffin 0.07 0.03 0.02	C ₂₀ paraffin	0.04	0.03		
	C ₂₅ paraffin	0.07	0.03	0.02	

Table II. Odor characteristics of rose

Floral	Fruity	Woody
Linalool	Hexyl acetate	alpha-Pinene
Phenylethyl alcohol	Geranial	Camphene
Citronellol	Neral	beta-Pinene
Nerol	CitronellyI acetate	Myrcene
Geraniol	Neryl acetate	Floral (Fatty Wax)
Spicy	Geranyl acetate	Heptanol
Pentanal	trans-Damascenone	Octanal
Heptanal	Minty	Octanol
Benzaldehyde	Methyl heptenone	Nonanol
Rose oxide	Carvone	Decanal
Cinnamic aldehyde	Green Leafy	Citronellol
Eugenol	3-Hexenal	Paraffins
Methyl Eugenol	Hexanol	Olofines
	Terpinene-4-ol	Farnesol

of rose, it is possible to create a rose effect without it.

Construction of rose

Starting with a base consisting of 70% phenylethyl alcohol, 10% citronellol, 6% geraniol, and 3% nerol, one can begin by adding the characters that are most obviously missing. At this point, I would like to emphasize that the percentages of components given above are merely a guide to their level in the flower. It is the responsibility of the perfumer through familiarity with the character and performance of each chemical to establish a suitable balance. It is important to remember that all the chemicals in rose are still not known and, as is often the case, the trace constituents play a major role in the odor and performance. Some important trace components are rose oxide, nerol oxide, rose furan, p-menth-1-en-9-al, β -ionone, β -damascone, and β -damascenone.⁵ The three cyclic ethers—rose oxide, nerol oxide, and rose furan—all have unusual characters that contribute more to the spicy character of rose than to its floralcy.

It may be helpful to think of odors according to their chemical class. For example, if the flower has a particular fruity note, I will examine all the esters (though these are not the only fruity notes in rose), and raise or lower their level until the desired effect is achieved. With regard to the fruity note of rose, it is my opinion that the most important components are β -damascenone and β -damascone. These unusual chemicals have extraordinary diffusivity and character. They lend not only beauty and lift but also a rich long lasting body to a rose formulation. They provide a quality that seems difficult to ascribe to such minute trace constituents. These chemicals, when used in conjunction with the rose alcohol esters and β -ionone will prove to be the crowning touch. The other classes of chemicals all contribute in their own way.

Aldehydes

Aldehydes C5-C9 add brightness, power, and freshness to the blend. However, it is the alkenals and alkadienals that play an extremely important part in

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this class of chemicals. There is only one unsaturated aldehyde reported in this work but there exist many more at unreported trace levels.

Alcohols

The alcohols, of course, include phenylethyl alcohol, eitronellol, nerol, and geraniol. They constitute the main body and character of rose. The other alcohols provide softer, lighter lift to the overall bouquet.

Ketones

The two ketones reported, carvone and methyl heptenone, add a somewhat minty character to the blend.

Hydrocarbons

This group, in general, tends to characterize the soft petal, waxy, fatty effect of the floral body. This class of chemicals, when unsaturated, provides very distinctive notes. The sesquiterpenes are a member of this class and they provide the very long lasting woody and peppery sections of the background of the rose fragrance.

Phenols

This class is not as thoroughly discussed as some others, but its importance should be neither overlooked nor underestimated. While eugenol provides the spicy note in rose, other phenols and derivatives add warmth and a sweet herbaceous character.

Ethers

While I have not elaborated on the presence of ethers in this discussion (methyl eugenol is really eugenol methyl ether), it should be remembered that rose oxide, nerol oxide, and rose furan are all cyclic ethers and play a major part in the odor and performance of the rose fragrance composition.

As mentioned previously, all the chemicals known are not reported here. Some classes such as sulfides, thiazoles, and bifunctional compounds, to name a few, have been left out. There are reportedly 275 compounds known in rose today.⁶ It is certain that more will be discovered in the future as the quest for a beautiful synthetic rose oil proceeds.

While it is my policy to first understand the character and performance of those chemicals naturally occurring in rose, many other commercially available chemicals are used in composing fragrances, for example, various esters of phenylethyl alcohol, citronellol, and geraniol. Many specialtics, such as Damascenia 185 and Dorinia from Firmenich are available and provide interesting notes. Many patents have been assigned to various companies. Listed below are a few that have a specific claim to imparting a rose aroma.

2,4, dimethyl-4, 4a5,9b tetrahydroindeno [1,2-d] -m-dioxin (fig. 1) is claimed to possess a rose odor similar to Rosa damascena.⁷ Methyl and ethyl esters of cyclododecanoic and cycloundecanoic acids have a persistent woody, fruity odor with a rose characteristic.⁸ Acetals of p-menthanediol 3,8 possess a fresh green and rosy odor.⁹ Ethynylation of citronella oil produces an oil having a fresh rose-like odor which is distinguished by its excellent lasting properties.¹⁰ 2-(2-Methyl-1-propenyl)2,4,6-trimethyldihydro-4,5 pyran (fig. 2) imparts an intense top note to rose and enhances the rose note of a perfume blend.¹¹ The relationship of this chemical to rose oxide (fig. 3) and nerol oxide (fig. 4) can readily be seen.



One should remember that the chemicals reported may not always be desirable to use. They may be artifacts of production or analysis. After reviewing the chemicals at one's disposal, one should be able to determine which constituents are characteristic and which are playing only a supporting role. The importance of being intimately familiar with the character and performance of each chemical cannot be overemphasized.

It will take much time and effort to complete the task of creating a beautiful rose, but at the finish you will understand how to achieve any type of rose effect that you desire.

> A rose is a rose, is a rose As far as the nose can tell Whose scent in the hand of a perfumer Is frequently used . . . quite well!

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