Making Sense (and Scents) of Aroma Chemical Names

A semi-contrarian system for understanding the relationships among aromas

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There are said to be 40,000 named odorous chemicals. To learn the odors of a good portion of these would take a lifetime. So here I will introduce a system that structures the understanding of the relationship of odors to one another and helps break down the problem of remembering a large number of chemical names and smells into a few logical steps. First, consider this quote from R. Harper et al.:[1]

> *Olfaction is undoubtedly a chemical sense; an odour is in all cases the end result of a process which is initiated by the interaction of volatile molecules (i.e. chemical substances) with the olfactory epithelium. The stimulus may, as in the case of the most common odours, such as from foods or perfumes, be a complex mixture of chemical species, or it may be essentially a single chemical substance such as ammonia. In addition the "odour" may be complicated by stimulation of pain or other receptors which are not located in the olfactory epithelium and which account for pungency, coolness and other non-olfactory sensations. These are nevertheless integrated with the true odour response to form an overall pattern which is recognised as a particular odour. However, excepting tumours, lesions or other interface with higher centres of the brain, including hallucinations, there is, to our knowledge, no case on record of an odour response, which cannot be explained as being initiated by the molecules of chemical substances. Hence, as odour perception is the result of, and only of, a chemical initiating stimulus, it is reasonable to attempt to classify odours in terms of known chemical structures."*

I will now introduce a system that helps classify odors of chemicals in such a way that will allow one to group and cross-index them according to structure and odor. When one sees the name of a chemical for the first time, one will already have a good idea of what that material will smell like. No, not *precisely*, but enough to know that if someone presents the completely wrong material, it will be obvious. Within a few hours of practice with the system, one should: 1) Have a good idea of what odor to expect from a named but previously unknown chemical; and 2) When looking for an elusive odor to complete a project, have a good idea of what chemical identities/structures to look for.

What Factors Make a Molecule Smell?

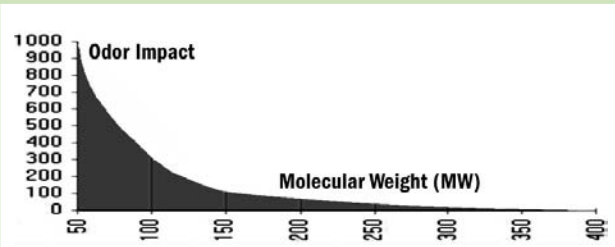
The truth is that no one knows exactly how the sense of smell works. There are two main theories: the shape theory, proposed by John Amoore, in which an odor molecule fits a specific shaped receptor site on the olfactory epithelium like a key fitting into a lock, and the vibrational theory, proposed by Luca Turin, in which the vibration of bonds between atoms in a molecule is detected by receptors on the olfactory epithelium. I suggest that even though the majority of research chemists in the field favor the shape theory, the truth probably lies in a combination of the two factors. Size and shape of the molecule determines whether the molecule is volatile and accessible to the receptors of the olfactory epithelium and that the vibrational energy supplies the mechanism of excitation or detection by the receptors. But here we will use the experiential results that most perfumers and aroma chemists know, about similarities in smells between groups of aroma chemicals, yet don't really make public knowledge. This approach suggests that a specific molecular body (e.g. a benzene ring) adds its specific odor character, but that this odor character is then modified by functional groups on the same molecule that also have their own specific odor character. So the smell of a whole molecule, rather like a gourmet dish, is a product of each part, which play off one another to produce the unique characteristic smell.

In essence, one might think of it like genetics: Both of the parents of a molecule—the body structure and functional groups—add their characteristics to the mix and the resultant overall smell is the sum of the individual components. Yes, sometimes the results are surprising, as with any offspring, but the apple doesn't usually fall too far from the tree. It is true that some of this goes against current thought on the subject by some aroma chemical chemists who believe there is no way to predict what a new chemical structure will smell like. I suggest that these chemists in fact have a very good idea of the expected smell from years of experience, although they may never have verbalized it. This system is simply taking that experience and putting it down into a few logical steps.

Molecular Weight

The smaller the molecules of an aroma chemical are, the stronger its odor impact tends to be. As the molecule

Odor impact tends to reduce with increasing molecular weight (not to scale) **F-1**



increases in size, its odor impact tends to decrease and its odor life on a smelling strip increases. The largest molecules that are known to have smells have molecular weights (MW) not exceeding 400 (**see F-1**). Odor impact refers to the odor impact compared to linalool (odor impact of 100) as a reference material.

Solubility

A material's solubility in water seems to be inversely proportional to its odor impact. This means that soluble molecules have very little odor; the more insoluble they are, the stronger their smell tends to be. A molecule with a hydroxyl/alcohol group (OH group, oxygen and hydrogen), like water (H_2O), demonstrates a softer odor compared to its equivalent aldehyde (H-C=O) or insoluble esters.

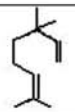
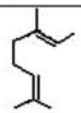
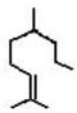
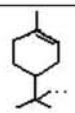
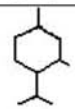
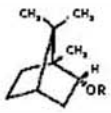
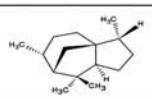
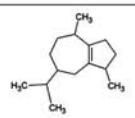
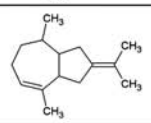
Body (R-): Molecular Structure of the Body of the Aroma Chemical

The body of a molecule is the core structure on which the functional groups are attached. These are usually rendered in diagrams, using lines with each corner representing a carbon atom saturated with hydrogen atoms. As many might know, a carbon atom has four valences, links that can connect to other atoms; hydrogen has one, oxygen has two. Short straight (aliphatic) radicals (one to five

Molecular structure of the body of aroma chemicals and resulting odors* **F-2**

Body				
Straight chain bodies Alkanes-saturated 				
Name	**Carbons**	**Formula**	**MW**	**Odor contribution**
Methyl	C_1	CH_3	15	Harsh chemical (dry)
Ethyl	C_2	$CH_3\ CH_2$	29	Fresh
Propyl	C_3	$CH_3\ (CH_2)_2$	43	Sweet-fresh
Butyl	C_4	$CH_3\ (CH_2)_3$	57	Fruity
Pentyl, amyl, valeryl	C_5	$CH_3\ (CH_2)_4$	71	Fruity-wine
Hexyl	C_6	$CH_3\ (CH_2)_5$	85	Green
Heptyl	C_7	$CH_3\ (CH_2)_6$	99	Green-oily
Octyl	C_8	$CH_3\ (CH_2)_7$	113	Hard citrus-sharp (lime-lemon)
Nonyl	C_9	$CH_3\ (CH_2)_8$	127	Citrus-fatty (lemon-orange)
Decyl	C_{10}	$CH_3\ (CH_2)_9$	141	Fatty-citrus (orange-tangerine)
Undecyl	C_{11}	$CH_3\ (CH_2)_{10}$	155	Fatty note (roselike)
Dodecyl/lauryl	C_{12}	$CH_3\ (CH_2)_{11}$	169	Fatty-rancid/soapy

**Alkenes—unsaturated molecules:* These molecules feature two carbon atoms in a molecule link with double $H_2C{=}CH_2$ or even triple HC≡CH bonds. Molecules with unsaturated bonds in the body tend to be more diffusive, sweeter and stronger than the equivalent saturated molecules. The nomenclature to indicate a chemical is unsaturated is the presence of an "e" in the name—hexene instead of hexane; the second "e" in undecylenic, as opposed to undecylic; or the suffixes "diene" or "triene."

Pinene, limonene, cymene, myrcene, sabinene, ocimene terpinolene,	C_{10}	$C_{10}H_{16}$	136	Volatile fresh but bland chemical notes. Each has specific characteristics but will be left out here for brevity.
Terpene body C_{10}				
Linalyl	C_{10}		137	Fresh light chemical floral (the alcohol is linalool.
Geranyl	C_{10}		137	Rose metallic, slightly green (the alcohol is geraniol).
Citronellyl	C_{10}		139	Rich red rosy, or the background of lily of the valley (the alcohol is citronellol).
Cyclic terpene ester body C_{10}				
Terpinyl	C_{10}		137	Harsh chemical pine floral (the alcohol is terpineol).
Menthyl	C_{10}		139	Cool fresh light chemical (the alcohol is menthol).
Bornyl (bicyclic C_{10})	C_{10}		137	Herbal, cool, chemical, metallic (the alcohol is borneol).
Sesquiterpene structures C_{15}				
Caryophyllene, longifolene, santalene	C_{15}	$C_{15}H_{26}$	206	Soft bland woody notes. Each has specific characteristics, but will be left out here for brevity.
Sesquiterpene body C_{15}				
Cedryl	C_{15}		205	Soft, woody (the alcohol is cedrol).
Guaiyl	C_{15}		205	Rich woody.
Vetiveryl	C_{15}		203	Softer, velvet woody (the alcohol is vetiverol).
Aromatic body				
Phenyl	C_6		77	Medicinal (the alcohol is phenol).
Benzyl	C_7		91	Heavy aromatic (the alcohol is benzyl alcohol).

carbon atoms long) lead to light, fresh smells; medium chains (six to seven or eight to 10 carbons) to green notes and to citrus, respectively; and longer chains (11 to 13 carbons) to fatty notes. Radicals seem to continue to display similar odor effects common to esters with the same radical (i.e. geraniol, geranyl acetate and geranyl butyrate all have rosy metallic characters; see **F-2, F-3**).

Meanwhile, one should check for some specific structures that are common to aroma chemicals used in perfumery and that have distinctive odor characteristics (**F-4**).

Functional Groups

These are the active groups such as alcohols (R-OH), aldehydes (R-CHO) and esters (R-COOH) and have by far the biggest effect on the odor of a molecule. The functional groups are like the arms and legs on the molecule's body and therefore tend to interact more with the environment and noses. There is some indication that the vibrational qualities of these groups may be responsible for the odor. The active groups on molecules—alcohols, aldehydes, acetates, butyrates, etc.—show specific odor characteristics that can be detected irrespective of the radical of the molecule they are on (e.g. amyl acetate, benzyl acetate, geranyl acetate—all have a sour-fruitiness when compared with their alcohols). For functional groups, see **F-5**.

Isomers

As readers may know, isomers are chemicals with molecules made up from the same elements and numbers of atoms in a different arrangement and with the same molecular weight. The functional groups and the carbon chains are positioned differently, thus forming different structures. Where these are markedly different, they are listed under radicals and special structures. If the differences are small, e.g. n- or iso- isomers, they may not have a drastic effect on the odor, perhaps making it more or less fresh or fruity for example, but generally the effect is little more than a basic structural change. One may need to concern oneself with these when getting closer to a target smell, but for the purpose of keeping this system manageable, it can be disregarded for the time being. The point is *not* that isomers have the same smells as each other, but that they do share clear similarities despite the oft-quoted example of leavo-carvone (spearmint) and dextro-darvone (dill). A reminder of common terms used:

- **n-** normal
- ***cis-*** same side
- **l-leavo** (left)
- **iso-** isomer
- ***trans-*** opposite
- **d-dextro** (right)
- **1,2,3,4,5,6,** etc.: indicate the position of functional groups (the arms of a molecule)
- **α-, β-, γ-, δ-** : indicate position relative to a functional group
- ortho, para, tertiary: indicate positions on a benzene ring body

One should note that the isomer terms are not normally used when indexing chemicals alphabetically, so *cis*-3-hexenol is usually indexed under H for hexenol. Below are some examples to illustrate how this system can be used practically.

Making Sense of Material Names

Assuming one has never smelled the chemical phenyl ethyl isobutyrate, what is the prediction of its odor?

- **Factor 1. MW:** Phenyl ethyl (105) isobutyrate (87) MW = 192 ; this is a medium-sized molecule.
- **Factor 2. Solubility:** Without testing one can guess—no hydroxyl groups, so probably insoluble in water.
- **Factor 3. Body:** Phenyl = medicinal; ethyl = fresh.
- **Factor 4. Specific structures:** Phenyl ethyl = rose floral.
- **Factor 5. Functional groups:** Butyrate = fruity, buttery-sour.

One must remember that the functional group tends to have a bigger effect on the smell compared to the body. So, phenyl ethyl isobutyrate, it can be reasoned, should have a fruity, buttery, sour, floral, rose note. Steffen Arctander describes the material's odor as "refreshing fruity-rosy odor, more fruity than rosy … moderate to poor tenacity."[2] He also notes that it finds use in flavors including cheese.

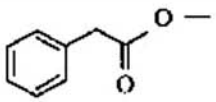
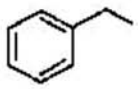
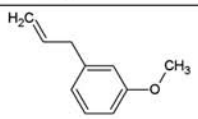
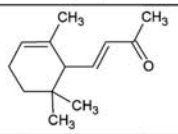
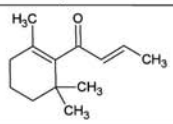
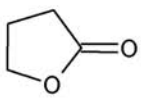
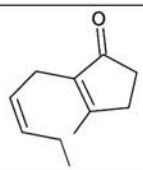
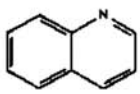
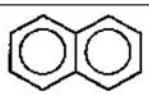
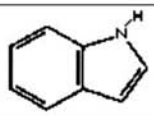
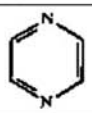
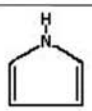
Up next is phenyl ethyl alcohol.

- **Factor 1.** phenyl ethyl (105), alcohol (17) MW = 122; a smaller molecule more volatile higher impact
- **Factor 2.** Solubility = the alcohol group imparts water solubility; therefore, the impact will be low.
- **Factor 3.** Phenyl = medicinal; ethyl = fresh (same as the isobutyrate).
- **Factor 4.** Phenyl ethyl = rose floral (same as the iso butyrate).
- **Factor 5.** Alcohol = mild floral.

Phenyl ethyl alcohol should be a mild floral rose, probably quite weak compared to the butyrate. Arctander notes that this material is mild and warm, with a rose-honeylike odor of moderate to poor tenacity.[2] Poorer grades, he adds, impart earthy, green grassy notes due to impurities.

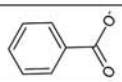
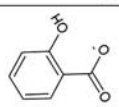
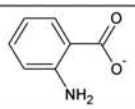
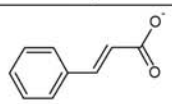
Now, one can consider the creation of a jasmine perfume. At the moment one's formula contains benzyl acetate, it feels about right, but the benzyl acetate one is using is a bit harsh. The perfumer may want to find a similar odor, but smoother. If one looks at alternative functional groups, the answer is easy to find. Benzyl alcohol will give a milder floral note, benzyl propionate slightly fruitier. Benzyl benzoate will last longer and may be a good fixative.

When looking for a green note for an orchid perfume, one may find that *cis*-3-hexenol is too volatile and disappears in the top note. The formulator can research the alternative functional groups for the alcohol (indicated by the "ol" on the end of the hexenol). Bearing in mind that one is formulating an orchid perfume, a salicylate

Some specific structures				
.....Phenyl Acetate	C_8		137	honey (this is more like a functional group)
Phenyl Ethyl.....	C_8		105	rose floral (the alcohol is Phenyl Ethyl Alcohol)
Eugenyl	C_{10}		163	spicy - clove, carnation (the alcohol is Eugenol)
Ionone	C_{13}		192	alpha- violet, fresh woody beta- violet, fruity woody
Damascone (isomer of ionone)	C_{13}		192	alpha- sweet rosy fruity, diffusive beta- fruity (berry), diffusive
Lactone (....ide) Note: gamma = 4 carbon ring delta = 5 carbon ring	C_8 C_9 C_{10} C_{11} C_{12} C_{15}		142 156 170 184 198 240	C_8- coconut C_9- coconut/prune C_{10}- oily peach C_{11}- heavy oily peach C_{12}- increasingly oily peach C_{15}- macrocyclic – musk
Jasmone	C_{11}		164	heavy jasmine
Quinolene	C_9		129	velvety animalic mossy tobacco herbaceous
Napthyl	C_{10}		128	naphthalene – harsh sweet narcotic heavy orange flower
Indole	C_8		117	harsh heavy narcotic jasmine warm floral fecal
Pyrazine	C_4		80	nutty, cooked notes
Thiazole	C_3		86	cooked sulphur notes (e.g.. meat, vegetable)
Pyrrole	C_4		66	cooked notes

Predicted smell exercise **T-1**

Aroma chemical name	MW	Soluble	Predicted smell
Phenyl ethyl alcohol	122	Yes	*Rose, mild floral, light (MW), mild (soluble)*
Acetyl isoeugenol			
Aldehyde C10, decyl			10% in DPG
Aldehyde C11, undecyl			10% in DPG
Aldehyde C12, lauryl			10% in DPG
Aldehyde C12, MNA			10% in DPG
Aldehyde C8, octyl			10% in DPG
Aldehyde C9, nonyl			10% in DPG
Amyl acetate			
Amyl salicylate			
Benzyl acetate			
Benzyl alcohol			
Benzyl aldehyde			
Benzyl benzoate			
Benzyl formate			
Benzyl propionate			
Benzyl salicylate			
Butyl acetate			
Butyl salicylate			
Cedryl acetate			
Cinnamic alcohol			
cis-Jasmone			10% in DPG
Citronellol			
Damascone			10% in DPG
Ethyl acetate			
Eugenol			
γ-Decalactone			
γ-Nonalactone			
γ-Octalactone			
γ-Undecalactone			
Geraniol			
Geranyl acetate			
Guaiayl acetate			
Hexyl acetate			
Hexyl salicylate			
Indol			10% in DPG
Ionone			
Isobornyl acetate			
Isopropyl methyl thiazole			
Linalool			
Linalyl acetate			
Menthol			
Methyl anthranilate			
Octanol			
Phenyl ethyl phenyl acetate			
Rose oxide			10% in DPG
Terpineol			
Terpinyl acetate			

...ol Alcohol	-	R-OH	17	Mild, floral (compared to aldehyde and esters).
...al Aldehyde	C1	R-CHO	29	Powerful, chemical.
...one Ketone	-	R=O	16	Brash chemical winey.
Nitrile	C1	R-CN	26	Powerful, chemical, metallic.
Sulphide	-	R-S	32	Gassy, rotten eggs.
Esters (produced from a reaction of an alcohol with an acid, the acid forms the functional group.)				
Formate (from formic acid)	C1	HCOO-R	45	Dry to green woody.
Acetate (from acetic acid)	C2	CH_3COO-R	59	Sour, fruity.
Propionate (from propionic acid)	C3	CH_3CH_2COO-R	73	Fruity, sweet.
Butyrate (from butyric acid)	C4	$CH_3CH_2CH_2COO$-R	87	Fruity-buttery sour.
Valerate (from valeric acid)	C5	$CH_3CH_2CH_2CH_2COO$-R	101	Dairy, fruity-sour.
Benzoate (from benzoic acid)	C7		121	Heavy sweet aromatic.
Salicylate (from salicylic acid)	C7		137	Sweet medicinal (methyl/ethyl) and then flowery herb/orchid.
Anthranilate (from anthranilic acid)	C6		136	Narcotic floral.
Cinnamate (from cinnamic acid)	C9		147	Spicy-cinnamon.

functional group may be appropriate. *cis*-3-Hexenol provides the solution.

Mastering the System

To master this system only takes a few hours, using the techniques listed above. Below are some chemical names with which to get started practicing.

Looking at the chemical name, one should note its molecular weight from adding the MW of each factor; the presence of OH groups with names like hydroxy, alcohol or "ol" on the end of a name; check the names in the factor tables presented in the figures; and check the odor characteristics. In closing, **T-1** presents a useful exercise. In the table, one can fill in the predicted odor of a material *first* before smelling it. One should be sure to smell dilutions for strong materials; this of course will dilute their impact.

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References

1. R Harper, EC Bate Smith and DG Land, *Odour description and odour classification: a multidisciplinary examination*. Churchill, London (1968)
2. S Arctander, *Perfume and Flavor Materials of Natural Origin*. Allured Business Media (1994)