Organic Chemistry – Who needs it?

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For many of us, organic chemistry is a subject from long ago and far away. For others, it is a topic we have learned on the job, having come from other academic fields into our industry. Regardless of which of the two describes your particular situation, the answer to the question "Who needs it?" is we all do. Organic chemistry employs a language we allows us to clearly and precisely define our products, raw materials and processes used to make them.

I present the following on the functional groups present in many of our raw materials, to hopefully remind, enlighten, amuse and hopefully teach those who will take the time to remember. Also, as was the case in the university, a short quiz will follow at the end!

1. Hydrocarbons

The compounds within the hydrocarbon class all share the structural properties of being non-ringed compounds with only carbon and hydrogen.

There are a variety of ways to classify hydrocarbons.

I. Number of carbon-carbon multiple bonds

1. Alkanes—only single carbon-carbon bonds.

   Dodecane **CH_3-$(CH_2)_{10}$$CH_3$**

2. Alkenes—contain at least one carbon-carbon double bond.

   Internal double bond CH_3-$(CH_2)_8$**CH=CH**-CH_3
   Terminal double bond CH_3-$(CH_2)_9$**$CH=CH_2$**

3. Alkynes—contain at least one carbon-carbon triple bond.

   CH≡CH Acetylene

II. Each type can have branching

A. Linear

1A-Alkane $CH_3\text{-}(CH_2)_{10}CH_3$

2A-Alkene $CH_3\text{-}(CH_2)_7CH{=}CHCH_3$

3A-Alkyne $CH{\equiv}C\text{-}CH_2\text{-}CH_3$

B. Branched

1B-Alkane $CH_3\text{-}(CH_2)_8CHCH_2CH_3$ (with CH_3 branch)

2B-Alkene $CH_3\text{-}(CH_2)_6CHCH{=}CHCH_3$ (with CH_3 branch)

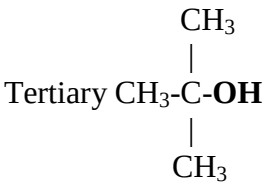
3B-Alkyne $CH{\equiv}C\text{-}CH\text{-}CH_3$ (with CH_3 branch)

2. Alcohols

Alcohols contain a hydroxyl group as well as hydrocarbon groups. Alcohols can be branched or linear, and as such primary, secondary or tertiary.

Primary $CH_3(CH_2)_{10}$**OH**

Secondary $CH_3(CH_2)_9$ CH-**OH**



Tertiary CH_3-C-**OH**

3. Amines

Amines contain an amino group as well as hydrocarbon groups. They can be branched or linear, and as such primary, secondary or tertiary. Additionally they are classified by the number of alkyl groups on the amine.

A. Primary Amines **H_2N**-CH_2CH_2OH
(Also present: hydrocarbon portion and alcohol portion)

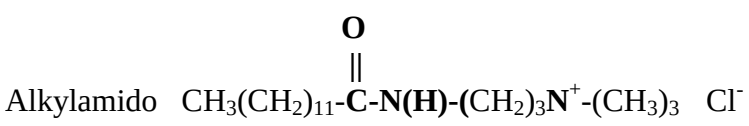
B. Secondary Amines **HN**-$(CH_2CH_2OH)_2$
(Also present: hydrocarbon portion and two alcohol portions)

C. Tertiary Amines **N**-$(CH_2CH_2OH)_3$
(Also present: hydrocarbon portion and three alcohol portions)

4. Quarternary Ammonium Compounds

Quarternary ammonium compounds contain positively charged nitrogen, and are surrounded by four alkyl groups. The alkyl groups can be branched or linear, and as such primary, secondary or tertiary. Additionally, quats are classified as either alkyl or alkyl amido.

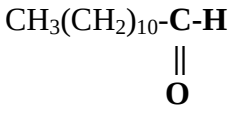
Alkyl $CH_3(CH_2)_{11}$-**N^+**-$(CH_3)_3$ Cl^-



Alkylamido $CH_3(CH_2)_{11}$-**C-N(H)-(**$(CH_2)_3$**N^+**-$(CH_3)_3$ Cl^-

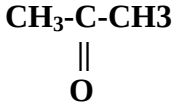
5. Aldehydes

Aldehydes have a carbonyl group with an alkyl group on one side and a hydrogen on the other.



6. Ketones

Ketones have a carbonyl group with an alkyl group on both sides.

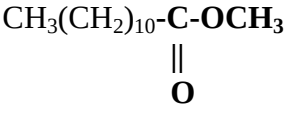


7. Esters

Esters are compounds that contain a carbonyl group (C=O) connected to a alkoxy group (-O-alkyl).

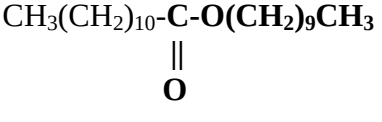
A. Methyl Esters

Methyl esters are a type of simple ester, containing only one ester group in the molecule, but are commonly raw materials containing a carbonyl group and a methoxy group as shown below;



B. Simple fatty Esters

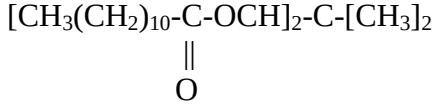
Simple esters contain only one ester group in the molecule.



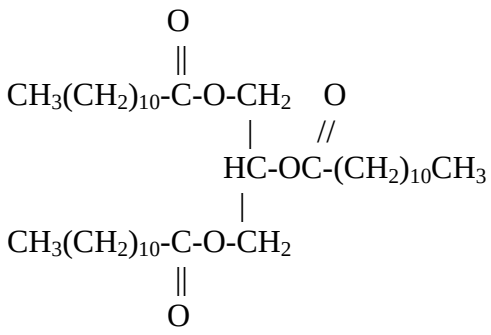
C. Complex Esters

Complex esters, unlike simple esters, contain multiple ester groups in one molecule. There needs to be at least two ester groups to be a complex ester, there can be many more as well. The difference between complex esters and polyesters is that the complex ester are made using one mono functional and one multifunctional reactants. Polyesters are made using two multifunctional reactants.

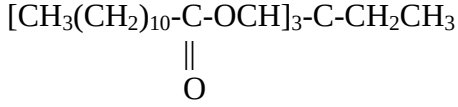
Neopentyl Glycol (2 ester groups)



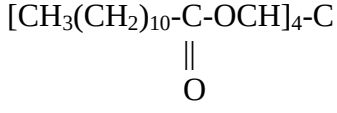
Glyceryl (3 ester groups)



Trimethylol Propane (3 ester groups)

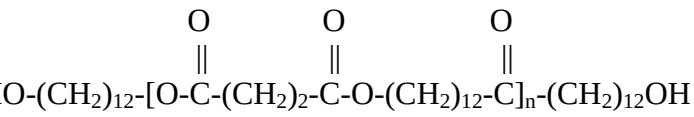


Pentaerythritol (4 ester groups)



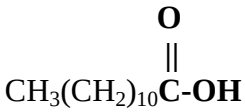
D. Polyesters

Polyesters are a group of polymeric compounds made by the reaction of an acid having at least two carboxyl groups and at least two hydroxyl groups.



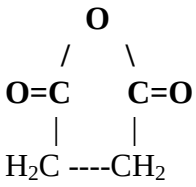
8. Fatty Carboxylic Acids

Fatty carboxylic acids hace a –COOH group.

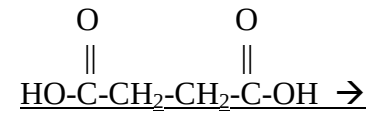


<u>9. Anhydrides</u>

An anhydride is a compound that can be considered as derived from another compound by subtracting the molecules of water. Typical is succinic anhydride.



It can be considered succinc acid, a diacid, from which water is removed;



```
          O
        /   \
    O=C       C=O
      |       |          +   H2O
    H2C ----CH2
```

10. Ethers

Ethers are compounds having a (-H_2C-O-CH_2-) bond.

A. Polyoxyalkylene

i. Polyoxyethylene

$CH_3(CH_2)_{11}$-O-$(CH_2CH_2O)_9H$

ii. Polyoxypropylene

```
CH3(CH2)11-O-(CH2CHO)9H
                   |
                  CH3
```

B. Alkyl Ethers

CH_3-$(CH_2)_{11}OCH_3$

11. Epoxides (also called an oxirane)

Epoxides are three membered rings are containing two carbons and one oxygen. They are very reactive.

```
        O
       / \
CH3-CH-CH2
```

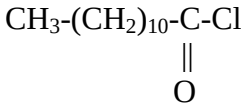
12. Alkyl Halides

Alkyl halides are compounds that contain a carbon-Cl bond.

CH_3-$(CH_2)_{11}$-Cl

13. Acyl Halides

Acyl halides are compounds that contain a  bond.



14. Aromatics

Aromatic groups are six membered ring compounds that have aromaticity. There are three double bonds distributed evenly over the six carbon atoms. This resonance of the double bond provides the compound in which it is contained with very specific characteristics:

- A delocalized conjugated π system, most commonly an arrangement of alternating single and double bonds.
- Coplanar structure, with all the contributing atoms in the same plane.
- Special reactivity in organic reactions such as electrophilic aromatic substitution and nucleophilic aromatic substitution.

within the aromatic family one encounters:

A. Benzenoid—Aromatic ring connected to compound—C_6H_5

B. Phenolic—Phenolic compounds are benzenoid compounds that in addition to the Aromatic ring containing one OH directly on the ring—C_6H_5OH

Although similar to alcohols, phenols have a relatively higher acidic level due to the aromatic ring. Their pK_a is usually around 11. Loss of a positive hydrogen ion (H^+) from the hydroxyl group of a phenol forms a negative phenolate ion. Although employed less frequently than in the past, these materials can be used to make unique products. For example, a phenol can be ethoxylated with one mole of ethylene oxide to produce a relatively pure material, while ethoxylation of decyl alcohol, for example, will yield a very wide distribution. Hydroxyl groups on aromatic rings, unlike those on alkyl groups are acidic due to the effect of the aromatic group.

15. Mercaptans

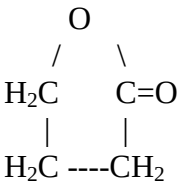
Methyl mercaptan is a colorless gas with a smell like rotten cabbage. Mercaptans, like phenols, are weak acid, with a pKa of ~10.4. This acidic property makes it reactive with ethylene oxide and propylene oxide. If lauryl mercaptan is reacted, an essentially odorless surfactant results.

CH_3-$(CH_2)_{11}$-**SH**

CH_3-$(CH_2)_{11}$-S-$(CH_2CH_2O)_xH$

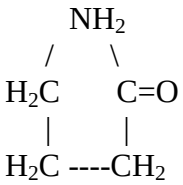
16. Lactones

Lactones are cyclic esters.



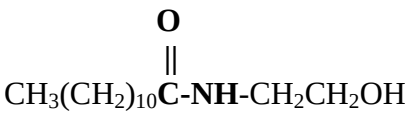
17. Lactams

Lactams are cyclic amides.



18. Amide

Amides are compounds that -C-NH- groups.



Conclusion

All organic compounds are made up of functional groups. These groups render the specific functional attributes in formulation. It is the functionality in formulation that is most important to the usefulness of a compound in cosmetic products. Structure and function are intimately related.

The chemisty of the compounds used in the cosmetic industry all contain one or more of the above functional groups. Once one recognizes the group, the next step is to understand the raw materials used for making that group, then the chemistry used for snthesis. In almost all compounds used in our industry, there is more than one group present in the molecule. In fact very few compounds, particularly if they are surface active do not contain a hydrocarbon group.

Quiz

A. Identify Functional Groups

1. CH_3 -$(CH_2)_{10}$ -C(O)-NH-CH_2 CH_2 OH

2. CH_2 =CH$(CH_2)_8$ -C(O)-O-CH_2 -CH=CH-CH_2 -CH_3

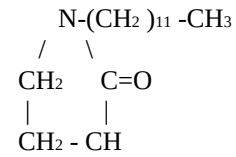
3. CH_2 =CH$(CH_2)_8$ -S-CH_2 CH_2 OCH_2 CH_2 OH

4. CH_3 $(CH_2)_6$ -C(O)H

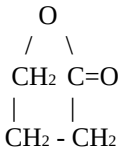
5. CH_3 -$(CH_2)_{10}$ -NH_2

6. H_2 N-$(CH_2)_{10}$ -C(O)OH

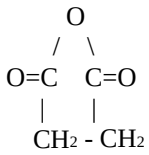
7.



8.



9.



10. CH_3 -$(CH_2)_{10}$ -C(O)-NH-CH_2 CH_2 OCH_2 CH_2 OC(O)-$(CH_2)_{10}$ CH_3

Answers

1. CH_3 -$(CH_2)_{10}$ -C(O)-NH-CH_2 CH_2 OH
   Linear hydrocarbon
   Amide
   Alcohol

2. CH_2 =CH$(CH_2)_8$ -C(O)-O-$(CH_2)_8$ -CH=CH-$(CH_2)_7$ -CH_3
   Terminal hydrocarbon
   Ester
   Internal hydrocarbon

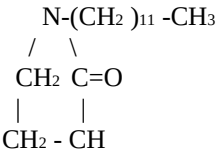
3. CH_2 =CH$(CH_2)_8$ -S-CH_2 CH_2 OCH_2 CH_2 OH
   Terminal hydrocarbon
   Mercaptan
   Ether
   Alcohol

4. CH_3 $(CH_2)_6$ -C(O)H
   Linear hydrocarbon
   Aldehyde

5. CH_3 -$(CH_2)_{10}$ -NH_2
   Linear hydrocarbon
   Primary amine

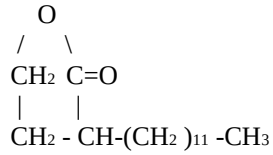
6. H_2 N-$(CH_2)_{10}$ -C(O)OH
   Linear hydrocarbon
   Amine
   Acid

7.



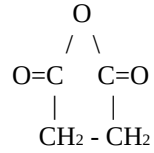
Linear hydrocarbon
Lactam

8.



Linear hydrocarbon
Lactam

9.



Anhydride

10. CH_3 -$(CH_2)_{10}$ -C(O)-NH-CH_2 CH_2 OCH_2 CH_2 OC(O)-$(CH_2)_{10}$ CH_3

Linear hydrocarbon
Amid

Reference

1. O'Lenick, Anthony J and O'Lenick, Thomas G., *Organic Chemistry for Cosmetic Chemists*, Allured Publishing, 2008 p. 1-12. © 2016 Tony O'Lenick used with permission