IUPAC NAMING

IUPAC nomenclature uses the ***longest continuous*** chain of carbon atoms to determine the basic ***root name*** of the compound. The root name is then modified due to the presence of different ***functional groups*** which replace hydrogen or carbon atoms in the parent sturcture.

There are a number of different ways to modify the root name to indicate the functional groups present.

- **Substitutive** : (most common) : the highest priority ***functional group*** modifies the suffix of the ***root name***, while all other groups, or ***substituents***, are added as prefixes to the ***root name***.
- **Functional group** : names the compound based on the highest priority functional group, *i.e.* as an alcohol, ketone, alkyl halide, *etc*.
- **Replacement** : used to indicate when an atom, usually carbon, is replaced by another atom.
- **Conjunctive** : used to combine named subunits (*i.e*. cyclohexanecarboxylic acid).
- **Common** or **trivial** : due to widespread use, some compunds with simple names have been adopted into basic IUPAC nomenclature.

These pages focus primarily on the **substitutive** and **functional group** nomenclature but also include examples of all systems in cases where the name is generated by a combination of methods.

Remember:

- that organic molecules can in general be either chains (also known as acyclic) or cyclic or a combination of both. In most cases this doesn't make a difference. The general rules for cyclic systems will be developed for cycloalkanes and can be applied to other scenarios.
- molecules are not restricted to a single functional group, they can have several functional groups. A common example are amino acids which have both an amine and a carboxylic acid present.

Basic rules

The **IUPAC systematic name** of an organic compound can be constructed based on a series of steps and rules:

- Indentification of the **principle functional group** and **substituents**
- Indentification of the **longest continuous chain** containing the principle functional group.
- Assign **locants** (*i.e*. numbering) to the **principle functional group** and **substituents**.

The steps and rules are *summarised* below, more details are provided as the cases are encountered.

Principle Functional group	• The **principle functional group** is used to define the class the compound belongs to *e.g.* an alcohol, ROH • The **principle functional group** is the **highest priority functional group**. • The **principle functional group** is usually given the **lowest locant possible**.
Longest chain	• The **longest continuous chain** containing the **principle functional group** defines the **root name**. • Other groups attached to this chain are called **substituents**. • If there are two chains of equal length, then the choice that gives the simplest **substituents** is chosen.
Numbering (*i.e.* assigning locants)	• The numbers that define the positions of the principle functional group and substituents are called **locants**. • Compounds are numbered from one end of the **longest continuous chain**. • The locants are assigned such that the **principle functional group** gets the **lowest possible locant**. • If this results in a "tie" then the **first point of difference rule** is applied so that the first time a difference in numbering occurs, then the method that gives the lower number at this first difference is used. • In the event that there is no first point of difference then **alphabetisation** is used.

What's in a name?

The IUPAC name of an organic molecule is assembled from components that describe various features of the molecule.

Functional group suffix
This is added to the end of the name based on the **principle functional group**.

Root
This defines the number of atoms (usually carbon atoms) in the **longest continuous chain** that contains the principle functional group.

Substituent prefix
Any groups other than the principle functional group are **substituents** and are added to the beginning of the name in **alphabetical order**.

Multiplier
If a group occurs more than once, a simple **multiplier** (*e.g.* di, tri, tetra, *etc*.) is used to indicate how many times it occurs.

Locants

Locants are numbers (or occasionally letters *e.g.* N-) that define the position of the **principle functional group** and **substituents**. Typically there needs to be a locant for each functional groups and each substituent. The 1993 modifications requires that the locant for the principle functional group is placed before the functional group suffix, *e.g.* pentan-2-ol, see below.

The basic structure of the IUPAC name is shown schematically below :

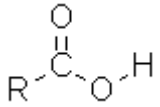
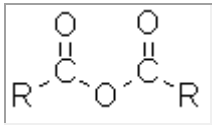
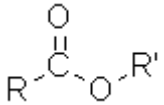
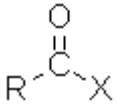
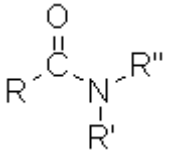
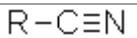
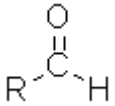
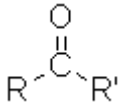
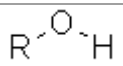
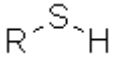
Functional Group Name	**Formula**	**Suffix** (when highest precedence)	**Prefix** (when lower precedence)
carboxyl	-COOH	-oic acid	carboxy-
aldehyde	-CHO	-al	formyl-
ketone	-CO-	-one	oxo-
alcohol	-OH	-ol	hydroxy-
amine	$-NH_2$	-amine	amino-
ether	-OR	none	alkoxy-
alkene	C=C	-ene	en-
alkyne	$C \equiv C$	-yne	yn-

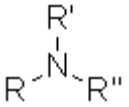
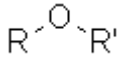
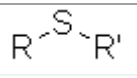
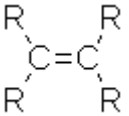
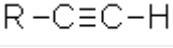
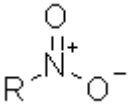
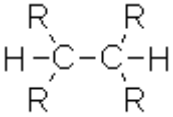
Functional Groups

Here is a list of the more important functional groups **arranged in decreasing priority order** for a nomenclature perspective. Note that aromatic systems (arenes) should also be thought of as a functional group, but they don't fit into the priority order list shown below.

This priority order is important in nomenclature as the higher priority group is the principle functional group and it is typically numbered such that is has the lowest number (the locant).

You need to learn to recognise these functional groups not just for nomenclature but in order to recognise their reactions later.
In each case the fundamental functional group unit is shown, it is this that you need to be able to recognise - pay attention to the atoms involved and the bonding patterns.

Functional Group	Formula	Structure
Carboxylic Acids		
Acid Anhydrides		
Esters		
Acyl Halides		
Amides		
Nitriles		
Aldehydes		
Ketones		
Alcohols		
Thiols		

Amines		
Ethers		
Sulphides		
Alkenes		
Alkynes		
Alkyl Halides		
Nitro		
Alkanes		

Learn how to name amines. An *amine* is a carbon chain with an NH_2 bonded to it. Use the suffix -*amine* and a position number if necessary.
Ex: $CH_3CHNH_2CH_3$ is named 2-propanamine.

Learn how to name amides. An *amide* is a carbon chain with a NH_2 and an oxygen bonded to the last/first carbon. Use the suffix -*amide* (no position number required).
Ex: $CH_3C(=O)NH_2$ is named ethanamide.

Learn how to name esters. An ester is a carbon chain with an oxygen both double and single bonded to one carbon. Name the group without an oxygens (R') first. Then name the R-C(=O)O part using the suffix -anoate.
Ex: $CH_3C(=O)OCH_2CH_2CH_2CH_3$ is named methyl pentanoate.

Learn how to name carboxylic acids. A carboxyl*ic acid* is a carbon chain with an oxygen double bonded and a hydroxide bonded to the last/first carbon. Use the suffix -ano*ic acid*. No position number is required.
Ex: $CH_3CH_2C(=O)OH$ is named propanoic acid.

Learn how to name ketones. A ket*one* is a carbon chain with an oxygen bonded to a middle carbon. Use the suffix -an*one* and use position numbers past propanone.
Ex: $CH_3CH_2CH_2C(=O)CH_3$ is named 2-pentanone.

Learn how to name aldehydes. An *al*dehyde is a carbon chain with an oxygen double bonded to the last/first carbon. Use the appropriate prefix for carbon chain and use the suffix -an*al*. No position number is required.
Ex: $CH_3CH(=O)$ is named ethanal.

Learn how to name ethers, a carbon chain bonded to an oxygen that is bonded to another carbon chain. The shorter of the two chains becomes the first part of the name (use a prefix). Then add "oxy". Then add the longest chain, preffixed with the ending -ane.
Ex: $CH_3OCH_2CH_3$ is named methoxyethane.

The common name is often more commonly used. Name the carbon chains like attached groups. Alphabetize these and place them before the word "ether".
Ex: $CH_3OCH_2CH_3$ is named ethyl methyl ether.

Learn how to name alcohols. An alcoh*ol* is a carbon chain with a hydroxide (OH^-) attached. Name the carbon chain, using the suffix -an*ol*. Place a number in front to indicate what carbon the hydroxide is attached to.
Ex: $CH_3CH_2CH_2(OH)$ is named 1-propanol.

Learn how to name hydrocarbons. *Halo*carbons, organic compounds containing one or more *halo*gens, are named using the same procedure. Take the name of the element attached (chlorine) and replace the -ine with -o (chloro). Use the same group prefixes to describe the amount. Ex: $CF_3CHBrCl$ is named 2-bromo-2-chloro-1,1,1-trifluoroethane.