

How to name organic compounds using the IUPAC rules

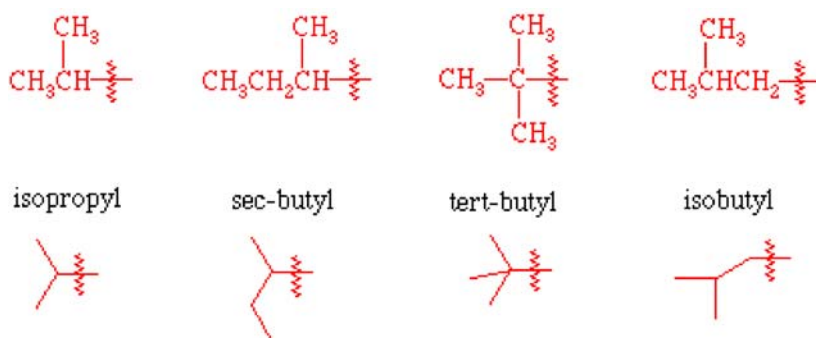
In order to name organic compounds you must first memorize a few basic names. These names are listed within the discussion of naming alkanes. In general, the base part of the name reflects the **number** of carbons in what you have assigned to be the **parent chain**. The **suffix** of the name reflects the type(s) of functional group(s) present on (or within) the parent chain. Other groups which are attached to the parent chain are called **substituents**.

- **Alkanes - saturated hydrocarbons**

The names of the straight chain saturated hydrocarbons for up to a 12 carbon chain are shown below. The names of the substituents formed by the removal of one hydrogen from the end of the chain is obtained by changing the suffix **-ane** to **-yl**.

Number of Carbons	Name
1	methane
2	ethane
3	propane
4	butane
5	pentane
6	hexane
7	heptane
8	octane
9	nonane
10	decane
11	undecane
12	dodecane

There are a few common branched substituents which you should memorize. These are shown below.



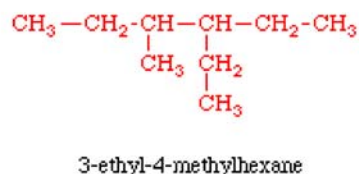
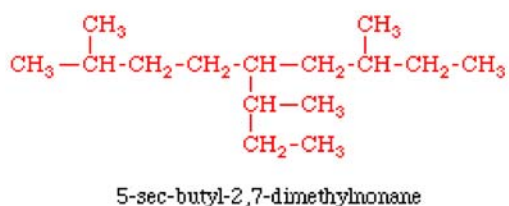
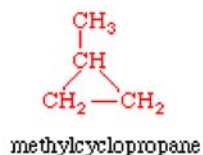
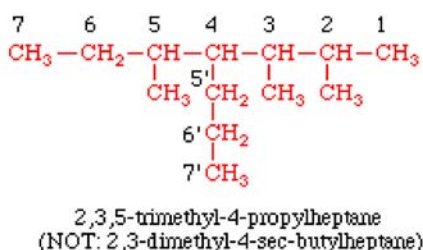
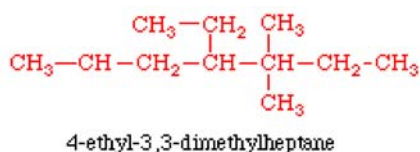
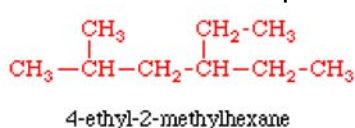
Here is a simple list of rules to follow. Some examples are given at the end of the list.

1. Identify the longest carbon chain. This chain is called the parent chain.
2. Identify all of the substituents (groups appending from the parent chain).

- Number the carbons of the parent chain from the end that gives the substituents the lowest numbers. When comparing a series of numbers, the series that is the "lowest" is the one which contains the lowest number at the occasion of the first difference. If two or more side chains are in equivalent positions, assign the lowest number to the one which will come first in the name.
- If the same substituent occurs more than once, the location of each point on which the substituent occurs is given. In addition, the number of times the substituent group occurs is indicated by a prefix (di, tri, tetra, etc.).
- If there are two or more different substituents they are listed in alphabetical order using the base name (ignore the prefixes). The only prefix which **is** used when putting the substituents in alphabetical order is **iso** as in isopropyl or isobutyl. The prefixes sec- and tert- are not used in determining alphabetical order except when compared with each other.
- If chains of equal length are competing for selection as the parent chain, then the choice goes in series to:
 - the chain which has the greatest number of side chains.
 - the chain whose substituents have the lowest- numbers.
 - the chain having the greatest number of carbon atoms in the smaller side chain.
 - the chain having the least branched side chains.
- A cyclic (ring) hydrocarbon is designated by the prefix **cyclo-** which appears directly in front of the base name.

In summary, the name of the compound is written out with the substituents in alphabetical order followed by the base name (derived from the number of carbons in the parent chain). Commas are used between numbers and dashes are used between letters and numbers. There are **no** spaces in the name.

Here are some examples:

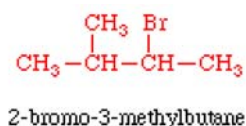
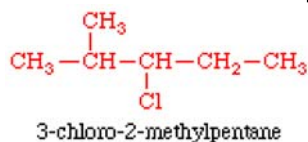


- Alkyl halides

The halogen is treated as a substituent on an alkane chain. The halo-substituent is considered of equal rank with an alkyl substituent in the numbering of the parent chain. The halogens are represented as follows:

F	fluoro-
Cl	chloro-
Br	bromo-
I	iodo-

Here are some examples:



- Alkenes and Alkynes - unsaturated hydrocarbons

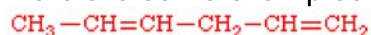
Double bonds in hydrocarbons are indicated by replacing the suffix **-ane** with **-ene**. If there is more than one double bond, the suffix is expanded to include a prefix that indicates the number of double bonds present (**-adiene**, **-atriene**, etc.). Triple bonds are named in a similar way using the suffix **-yne**. The position of the multiple bond(s) within the parent chain is(are) indicated by placing the number(s) of the first carbon of the multiple bond(s) directly in front of the base name.

Here is an important list of rules to follow:

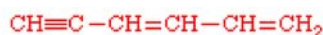
- The parent chain is numbered so that the multiple bonds have the lowest numbers (double and triple bonds have priority over alkyl and halo substituents).
- When both double and triple bonds are present, numbers as low as possible are given to double and triple bonds even though this may at times give "-yne" a lower number than "-ene". When there is a choice in numbering, the double bonds are given the lowest numbers.
- When both double and triple bonds are present, the -en suffix follows the parent chain directly and the -yne suffix follows the -en suffix (notice that the e is left off, -en instead of -ene). The location of the double bond(s) is(are) indicated before the parent name as before, and the location of the triple bond(s) is(are) indicated between the -en and -yne suffixes. See below for examples.
- For a branched unsaturated acyclic hydrocarbon, the parent chain is the longest carbon chain that contains the **maximum number of double and triple bonds**. If there are two or more chains competing for selection as the parent chain (chain with the most multiple bonds), the choice goes to (1) the chain with the greatest number of carbon atoms, (2) the # of carbon atoms being equal, the chain containing the maximum number of double bonds.
- If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at

the first point of difference.

Here are some examples:



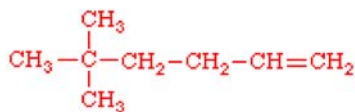
1,4-hexadiene



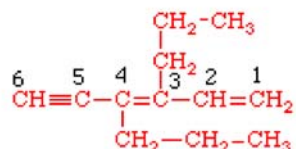
1,3-hexadien-5-yne



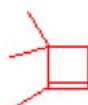
3-penten-1-yne



5,5-dimethyl-1-hexene



3,4-dipropyl-1,3-hexadien-5-yne

1,4,4-trimethylcyclobutene
(NOT: 2,3,3-trimethylcyclobutene)

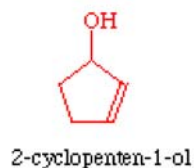
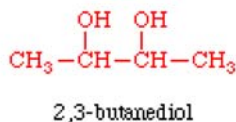
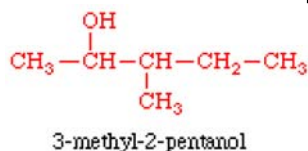
- Alcohols

Alcohols are named by replacing the suffix **-ane** with **-anol**. If there is more than one hydroxyl group (-OH), the suffix is expanded to include a prefix that indicates the number of hydroxyl groups present (**-anediol**, **-anetriol**, etc.). The position of the hydroxyl group(s) on the parent chain is(are) indicated by placing the number(s) corresponding to the location(s) on the parent chain directly in front of the base name (same as alkenes).

Here is an important list of rules to follow:

1. The hydroxyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.
2. When both double bonds and hydroxyl groups are present, the **-en** suffix follows the parent chain directly and the **-ol** suffix follows the **-en** suffix (notice that the e is left off, **-en** instead of **-ene**). The location of the double bond(s) is(are) indicated before the parent name as before, and the location of the hydroxyl group(s) is(are) indicated between the **-en** and **-ol** suffixes. See below for examples. Again, the hydroxyl gets priority in the numbering of the parent chain.
3. If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.

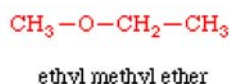
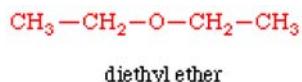
Here are some examples:



- Ethers**

You are only expected to know how to name ethers by their common names. The two alkyl groups attached to the oxygen are put in alphabetical order with spaces between the names and they are followed by the word ether. The prefix di- is used if both alkyl groups are the same.

Here are some examples:



- Aldehydes**

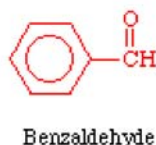
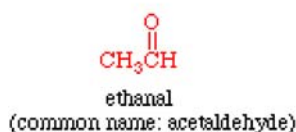
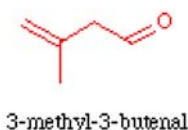
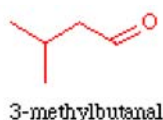
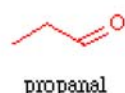
Aldehydes are named by replacing the suffix **-ane** with **-anal**. If there is more than one **-CHO** group, the suffix is expanded to include a prefix that indicates the number of **-CHO** groups present (**-anedial** - there should not be more than 2 of these groups on the parent chain as they must occur at the ends). It is not necessary to indicate the position of the **-CHO** group because this group will be at the end of the parent chain and its carbon is automatically assigned as C-1.

Here is an important list of rules to follow:

1. The carbonyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.
2. When both double bonds and carbonyl groups are present, the **-en** suffix follows the parent chain directly and the **-al** suffix follows the **-en** suffix (notice that the e is left off, **-en** instead of **-ene**). The location of the double bond(s) is(are) indicated before the parent name as before, and the **-al** suffix follows the **-en** suffix directly. Remember it is not necessary to specify the location of the carbonyl group because it will automatically be carbon #1. See below for examples. Again, the carbonyl gets priority in the numbering of the parent chain.
3. There are a couple of common names which are acceptable as IUPAC names. They are shown in the examples at the end of this list but at this point these names will not be accepted by the computer. Eventually they will be accepted.

4. If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.

Here are some examples:



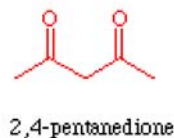
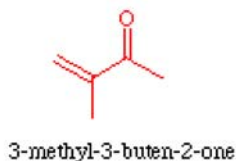
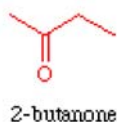
- Ketones**

Ketones are named by replacing the suffix **-ane** with **-anone**. If there is more than one carbonyl group (C=O), the suffix is expanded to include a prefix that indicates the number of carbonyl groups present (**-anedione**, **-anetrione**, etc.). The position of the carbonyl group(s) on the parent chain is(are) indicated by placing the number(s) corresponding to the location(s) on the parent chain directly in front of the base name (same as alkenes).

Here is an important list of rules to follow:

1. The carbonyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.
2. When both double bonds and carbonyl groups are present, the **-en** suffix follows the parent chain directly and the **-one** suffix follows the **-en** suffix (notice that the e is left off, **-en** instead of **-ene**). The location of the double bond(s) is(are) indicated before the parent name as before, and the location of the carbonyl group(s) is(are) indicated between the **-en** and **-one** suffixes. See below for examples. Again, the carbonyl gets priority in the numbering of the parent chain.
3. If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.

Here are some examples:



- **Carboxylic Acids**

Carboxylic acids are named by counting the number of carbons in the longest continuous chain including the carboxyl group and by replacing the suffix **-ane** of the corresponding alkane with **-anoic acid**. If there are two **-COOH** groups, the suffix is expanded to include a prefix that indicates the number of **-COOH** groups present (**-anedioic acid** - there should not be more than 2 of these groups on the parent chain as they must occur at the ends). It is not necessary to indicate the position of the **-COOH** group because this group will be at the end of the parent chain and its carbon is automatically assigned as C-1.

Here is an important list of rules to follow:

1. The carboxyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.
2. If the carboxyl group is attached to a ring the parent ring is named and the suffix **-carboxylic acid** is added.
3. When both double bonds and carboxyl groups are present, the **-en** suffix follows the parent chain directly and the **-oic acid** suffix follows the **-en** suffix (notice that the **e** is left off, **-en** instead of **-ene**). The location of the double bond(s) is(are) indicated before the parent name as before, and the **-oic acid** suffix follows the **-en** suffix directly. Remember it is not necessary to specify the location of the carboxyl group because it will automatically be carbon #1. See below for examples. Again, the carboxyl gets priority in the numbering of the parent chain.
4. There are several common names which are acceptable as IUPAC names. They are shown in the examples at the end of this list **but** at this point these names will **not** be accepted by the computer. Eventually they will be accepted.
5. If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.

Here are some examples:



methanoic acid
(common name: formic acid)



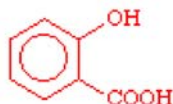
ethanoic acid
(common name: acetic acid)



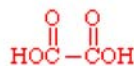
3-methylpentanoic acid



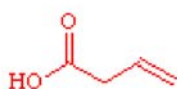
benzoic acid



salicylic acid
(common name)



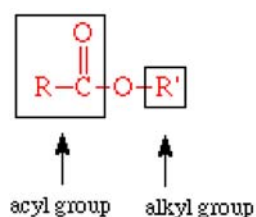
ethanedioic acid
(common name: oxalic acid)



3-butenic acid

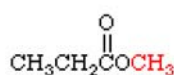
- Esters**

Systematic names of esters are based on the name of the corresponding carboxylic acid. Remember esters look like this:

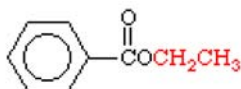


The alkyl group is named like a substituent using the **-yl** ending. This is followed by a space. The acyl portion of the name (what is left over) is named by replacing the **-ic acid** suffix of the corresponding carboxylic acid with **-ate**.

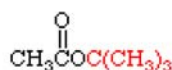
Here are some examples:



methyl propanoate



ethyl benzoate



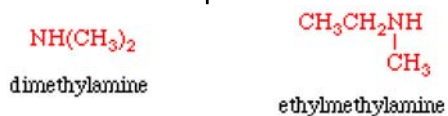
tert-butyl acetate

- Amines**

You are only expected to know how to name amines by their common names. They are named like ethers, the alkyl (R) groups attached to the nitrogen are put in alphabetical order with no spaces between the names and these are followed by the word amine. The prefixes di- and tri- are used if two or three of the alkyl groups are the same.

NOTE: Some books put spaces between the parts of the name, but we will not. Follow the examples.

Here are some examples:



- Summary of functional groups

Functional group	Prefix	Suffix
carboxylic acids	none	-oic acid
aldehydes	none	-al
ketones	none	-one
alcohols	hydroxy-	-ol
amines	amino-	-amine
ethers	alkoxy-	-ether
fluorine	fluoro-	none
chlorine	chloro-	none
bromine	bromo-	none
iodine	iodo-	none