International Union of Pure and Applied Chemistry (IUPAC) Nomenclature https://iupac.org/

Naming Molecules by Following the Rules

Getting Started...

 You first have to identify the "family" that your molecule belongs to...

• So, check for functional groups...

• If there are none, then your molecule is simply an alkane...

The Three Basic Parts

 The name for any organic molecule consists of three basic parts:

Prefixes-Parent-Suffix

• Each part of the name has a purpose.

Basic Part - Suffixes

 Suffixes on the end of the name of an organic molecule tell you what major family the molecule belongs to

• The suffix for an alkane is "-ane"

Basic Part - the Parent

 The "parent" part of the name tells you how many carbons are there in the main chain of the molecule

• The main chain of the molecule is defined for alkanes as being the longest chain in the molecule

 CH_4

- The parent is named based on the number of carbons
- 1 carbon = "meth"
- So a one-carbon alkane is called methane

2 carbons = "eth"

• So a two carbon alkane is called ethane.

CH_3CH_3

- 3 carbons = "prop"
- So a three carbon alkane is called propane.

$CH_3CH_2CH_3$

4 carbons = "but"

So a four carbon alkane is called butane.

$CH_3CH_2CH_2CH_3$

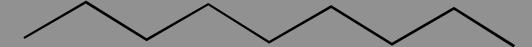
And now the rest...

- 5 carbons = "pent"
- 6 carbons = "hex"
- 7 carbons = "hept"
- 8 carbons = "oct"
- 9 carbons = "non"
- 10 carbons = "dec"

 So be mindful and name the following alkane (shown as both condensed formula and a skeletal structure)

$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$

or

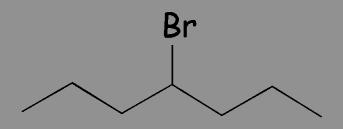


Answer?

- That's right!
- nine carbons + alkane family = NONANE
- One more thing Should you have two or more chains that are the same length, the parent is the one with the most prefixes...
- But We need to talk Prefixes first... we'll come back to this...

Here we go - the Prefixes

- Prefixes are the bits and pieces that are attached to the main chain (parent) of the molecule.
- An example of a prefix might be a halide attached to the main chain as in:



Prefixes - the Halides

- The family called alkyl halides does not have a suffix.
- Halides are always named as prefixes.
- Fluorine is called "fluoro"
- Chlorine is called "chloro"
- Bromine is called "bromo"
- Iodine is called "iodo"

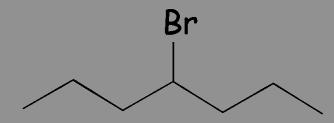
Putting together a name...

- The rules for IUPAC nomenclature include:
- Step 1: Find the main chain
- Step 2: Number the main chain
- Step 3: Identify all prefixes and their position numbers
- Step 4: Write the full name:

Prefixes-Parent-Suffix

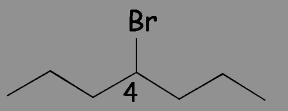
Now let's take a look:

• Follow the rules... Name this molecule...



Find the main chain...

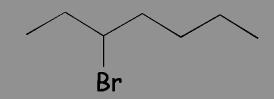
 The longest chain in this molecule has seven carbons... and only a halide (which is always named as a prefix).



• This will be 4-bromoheptane

What would you do different ..?

How would you name this one?



• 3-bromoheptane

More Prefixes

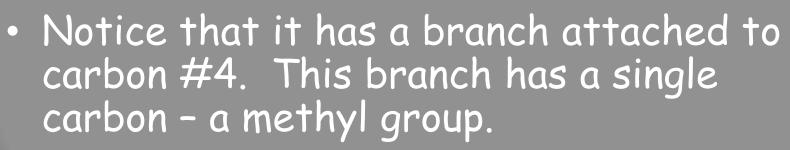
- The most common prefixes we have in organic molecules are those little fragments of carbon pieces attached to the main chains.
- The carbon fragments are called "alkyl groups". They all end in "-yl" to indicate they are fragments of a bigger molecule.

Alkyl Groups

- Alkyl groups are named similarly to alkanes, based on the number of carbons in the fragment.
- A fragment of methane, CH_4 , would be CH_3 -
- This fragment is called "methyl" where "meth" stands for one carbon and "yl" stands for fragment (alkyl group).

Methyl Group

• The molecule shown here has a 7-carbon main chain.



4-methylheptane is the name of this compound.

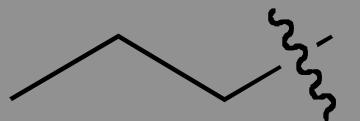
Ethyl Groups

 A two-carbon alkane is called ethane, CH₃CH₃. The corresponding two-carbon fragment is always CH₃CH₂-, which is called "ethyl".

4-ethylheptane is the name for this one.

Propyl Groups

- There are two possible three-carbon alkyl groups to form from propane, $CH_3CH_2CH_3$.
- The straight chain version: CH₃CH₂CH₂which is called "propyl" or "n-propyl" (where n stands for "normal" or straight-chained)

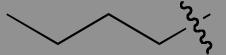


Isopropyl Groups

- There are two possible three-carbon alkyl groups to form from propane, $CH_3CH_2CH_3$.
- The other possibility is to form the fragment on the central carbon: CH₃CHCH₃, which is called "isopropyl" or "propane-2-yl"

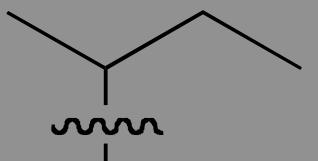
Butyl Groups

- There are four possible four-carbon alkyl groups to form from butane, $CH_3CH_2CH_2CH_3$.
- One possibility is to form the fragment on one of the end carbons: CH₃CH₂CH₂CH₂-, which is called "butyl" or "n-butyl"



Sec-Butyl Groups

 The other possibility is to form the fragment one of the central carbons: CH₃CHCH₂CH₃, which is called "sec-butyl" or "butane-2-yl". [Note that the carbon second from the left only has three bonds - so that's where its bonding to the main chain]

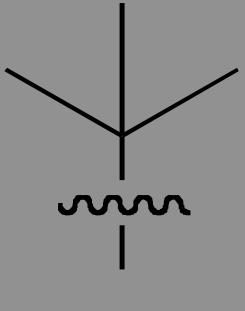


Isobutyl Groups

- There are two other possible four-carbon alkyl groups to form from isobutane, $(CH_3)_3CH$.
- One is formed as a fragment on one of the three symmetrical end carbons: (CH₃)₂CH(CH₂)-, which is called "isobutyl"
 - or "(2-methyl)propyl"

Tert-butyl Groups

 The other is formed as a fragment on the one central carbon, (CH₃)₃C-, which is called "tert-butyl"



What alkyl groups do you see?

 There's two groups attached to the ring below. What are they?

- The group in red has two carbons and is an ethyl group.
- The group in blue has four carbons. Three in a row and the extra attached at the middle carbon. Its an isobutyl group.

What alkyl groups do you see?

There's two groups attached to the ring below. What are they?

- The group in red has three carbons attached at the middle carbon and is an isopropyl group.
- The group in blue has four carbons, in a row, attached at one of the middle carbons. It's a sec-butyl group.

More about Prefixes...

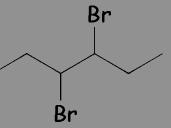
- Every prefix needs a position number...
- And prefixes are always alphabetized by their first letter:
 - Methyl is an "m"
 - Ethyl is an "e"
 - Propyl is a "p"
 - Isopropyl is an "i"
 - Sec-butyl is a "b"... (Say what??)

Alphabetizing Prefixes...

- Sec-butyl and tert-butyl both have a descriptive prefix that tells you the structure of those alkyl groups... (the prefix has a prefix!)
- When alphabetizing, we do NOT use these descriptive prefixes (like sec- or tert-) to alphabetize...

Continuing with Prefixes...

- If you have multiples of the same prefixes, like two bromines in the same molecule, you COULD name them separately or you could combine them into a single prefix name and include "di-" in front to indicate TWO of them.
- 3,4-dibromohexane!



Continuing with Prefixes...

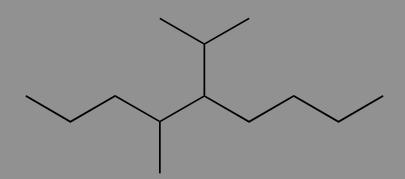
- Di-, tri- and tetra- are more prefixes for the prefixes.
- Remember when alphabetizing for names, prefixes are never alphabetized using a "prefix" like di- or sec-.

– Sec-butyl is a "b"

– Dimethyl is a "m"

Name the following molecule:

 Keeping all of the rules in mind, what would you name this molecule:

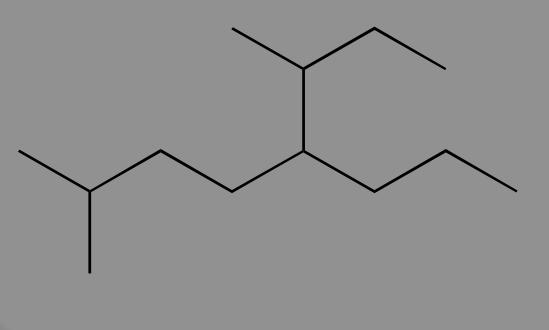


And the answer is ...?

- Longest chain: nine carbons
- Number: left to right (hit that first branch on #4)
- Group on #4 is methyl.
- Group on #5 is isopropyl.
- Alphabetize!
- 4-methyl-5-(propan-2-yl)-nonane.

About that main chain again...

 Recall that we said if you had two chains of the same length, the parent is the one with the most branches. Which is the parent in this example?



Where's the Parent?

 There are two options: Option 1 is highlighted in red:

• Option 2 is highlighted in blue:

And the winner is...

The red one has two branches:

• The blue one has three branches:

The blue one is the parent.Write that name...

Finally... the name...

- Eight carbons in main chain. Octane.
- Number left to right (first branch on #2!)

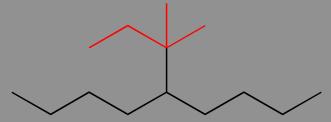
6

5

- Three alkyl groups attached:
- 2-methyl
- 5-propyl
- 6-methyl
- Simplify prefixes by using 2,6-dimethyl
- Full name: 2,6-dimethyl-5-propyloctare.

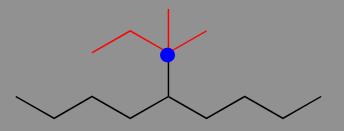
The last kind of alkyl groups -Complex Branches

 Complex branches are those that have no simple name, yet they still need to be named.

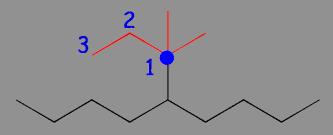


Identify the complex branch and its point of attachment.

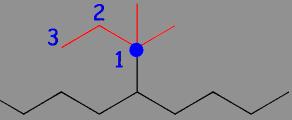
• Find the point of attachment inside the complex branch itself, first.



 Number the longest branch of that complex branch, starting from the point of attachment, #1. In this case, propyl is the miniature parent.



- Identify the prefixes on that little miniature parent (in this case, the propyl chain) of the complex branch, and their position numbers.
- In this example, there are two methyls attached to #1.



- Write the full name, placing the complex branch inside brackets. This complex branch is attached to #5 of the original main chain so:
- 5-[1,1-dimethylpropyl]nonane is the name.

Now: Cyclic Compounds

- When naming cyclic compounds, first determine if the ring is the parent, or not.
- If the ring has more carbons than any of the alkyl groups attached, the ring is the parent.
- If not, the ring becomes a cycloalkyl group and is a prefix for the main chain.

Cyclic Compounds - Parent?

• In this example, the ring has four carbons and the chain has eight.

- The chain is the parent and the ring is a prefix.
- The ring is a cyclobutyl group on #1.
- 1-cyclobutyloctane.

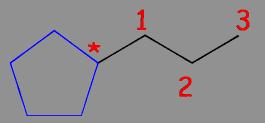
Cyclic Compounds

• In this example, the ring has five carbons and the alkyl group has three.

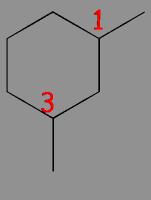
- The five-carbon ring is the parent and is called cyclopentane.
- The one alkyl group will be on #1 (of course - that #1 isn't even needed!)
- Propylcyclopentane is the name.

Cyclic Compounds

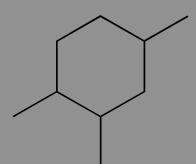
- Word of caution: don't double dip... its really easy to double count the carbon (*) that the alkyl group is attached to.
- Alkyl groups are only those BEYOND the ring carbons. Thus, this is a propyl group not a butyl group.



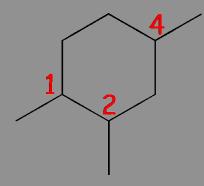
- When a ring has multiple groups, the rule for numbering is: "Number around the ring so as to arrive at the lowest possible sum of the position numbers".
- The sum in this molecule is 1 + 3 = 4.



How about this one?

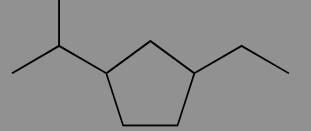


Lowest possible sum?

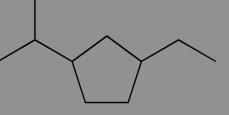


• 1 + 2 + 4 = 7

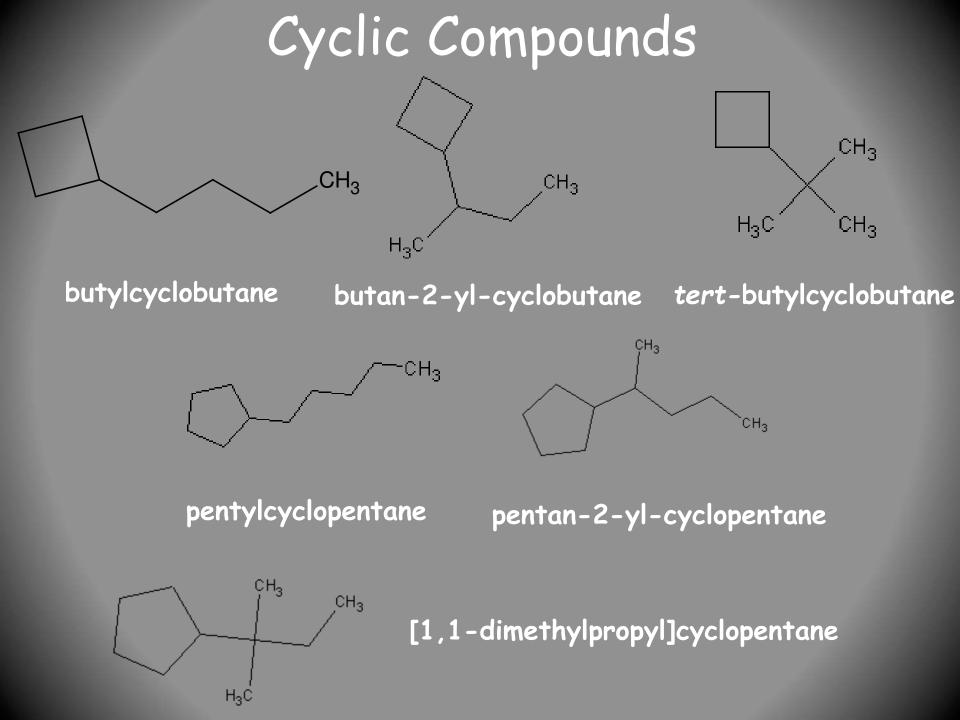
- If you have two possibilities for lowest possible sum, THEN (and only then) you should alphabetize to prioritize your groups.
- What about this one?



- Two possible "lowest sums" of 4, where the groups must be on carbons #1 and #3.
- Prioritize by alphabetizing the ethyl will be #1 and the isopropyl will be #3.



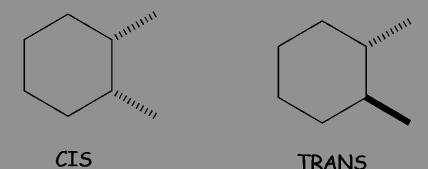
Name? 1-ethyl-3-(propan-2-yl)cyclopentane



Cyclic Compounds - Two groups

- Last comment when you have two groups attached to a molecule, they can potentially either both face up (or down) in the same direction (CIS) or one faces up and the other faces down (TRANS)
- We use wedges to indicate "up" or towards you and dashes for "down" or away.

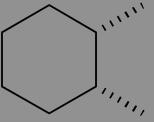
Cyclic Compounds - Two groups



 The molecule on the left has two methyl groups facing down (CIS) and the one on the right has one down and one up (TRANS).

Cyclic Compounds - Two groups

 Incorporating that into the name: Place the term "cis" or "trans" in the beginning of the name, before the first prefix



• Name? *cis*-1,2-dimethylcyclohexane

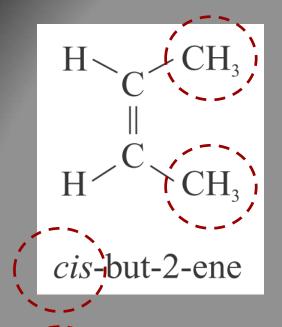
Alkenes $(C_n H_{2n})$

One C=C double bond

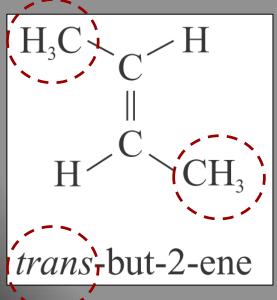
More reactive than alkanes due to weaker $\boldsymbol{\pi}$ bond

→ <u>unsaturated</u> hydrocarbons

NOT contain the maximum possible number of hydrogen atoms per molecule



Both substituent groups are on the same side w.r.t. the axis of the C=C double bond



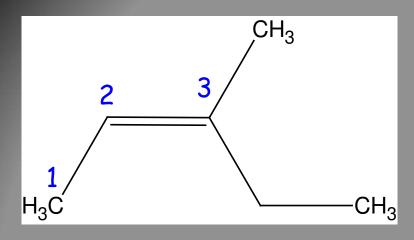
Both substituent groups are on the opposite sides w.r.t. the axis of the C=C double bond

E/Z notation

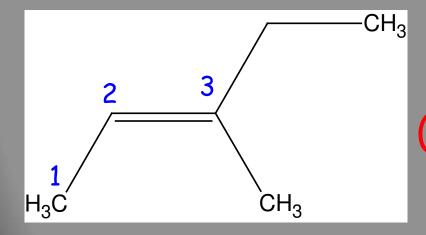
If there are three or four different groups attached to the C atoms of C=C double bond then E/Z notation is used rather than the cis/trans notation

E (Entgegen) = "in opposition to" \rightarrow *trans Z* (*Zusammen*) = "together" \rightarrow *cis*

http://en.wikipedia.org/wiki/Cahn-Ingold-Prelog_priority_rule



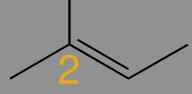
(2Z)-3-methylpent-2-ene



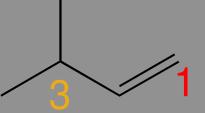
(2E)-3-methylpent-2-ene



2-methylbut-1-ene



2-methylbut-2-ene



3-methylbut-1-ene

Functional group has a higher priority than branches

Alkynes (C_nH_{2n-2})

One $C \equiv C$ triple bond Reactive (unsaturated) due to weak π bonds First member is ethyne (acetylene), C_2H_2

Cycloalkenes and alkadienes have the same general formula as alkynes

Naming alkenes and alkynes

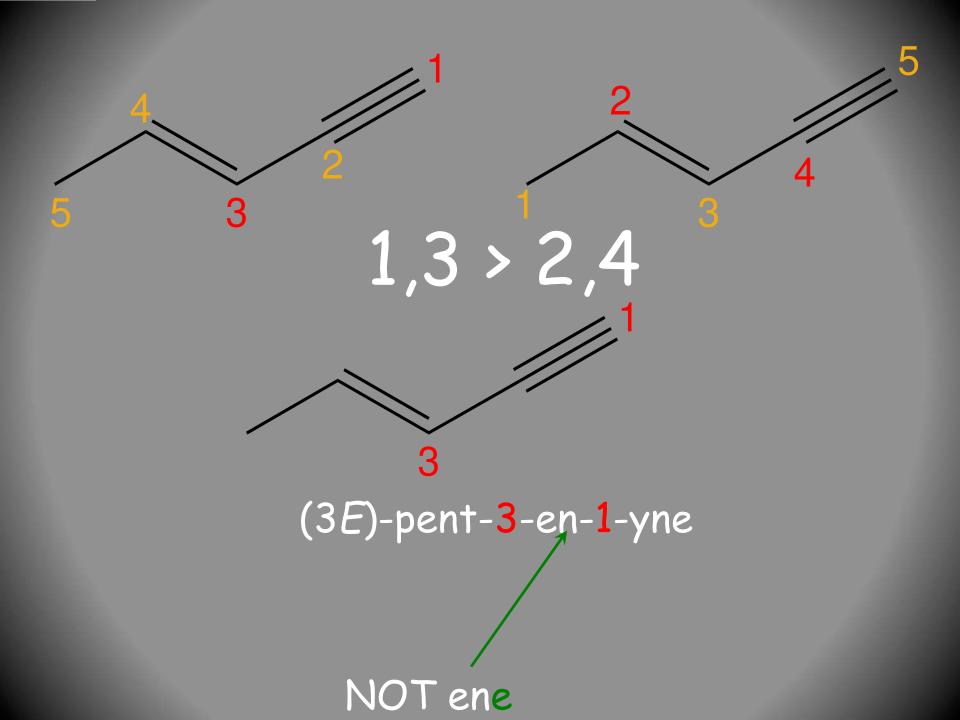
the 'longest' carbon chain need NOT be the one that contains the multiple bond.

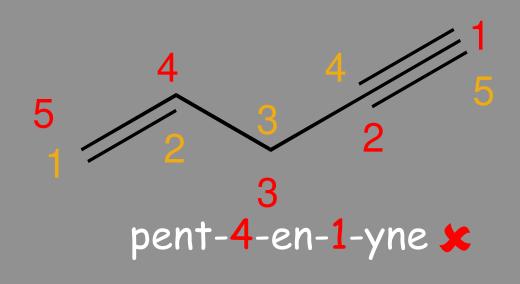
2-ethylpent-1-ene x

3-methylenehexane ✓

methylene

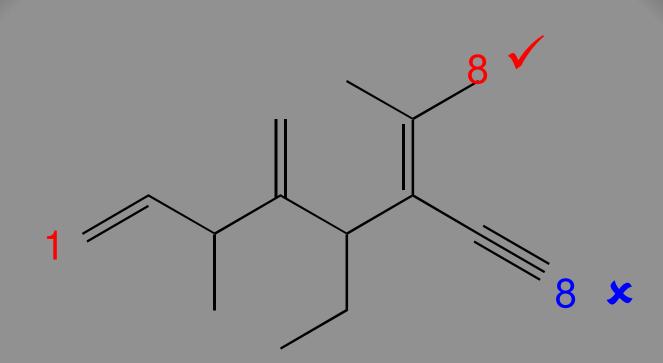
3





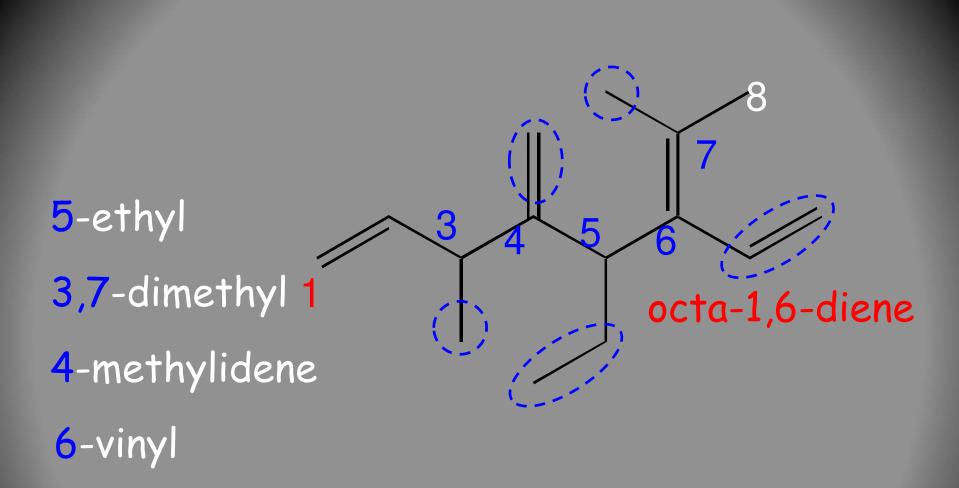
pent-1-en-4-yne 🧹

If the same set of numbers is obtained by counting in either direction, the number is assigned in alphabetical order.



diene has a higher priority than enyne

If the envne chain is longer, envne > diene The length of C chain is more important !

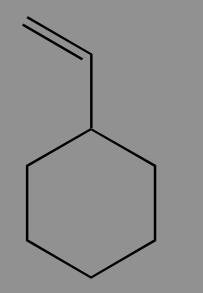


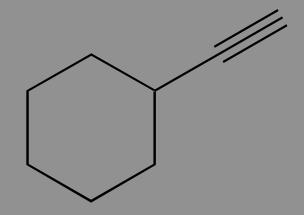
5-ethyl-3,7-dimethyl-4-methylidene-6-vinylocta-1,6-diene

Common cycloalkanes

Name	Molecular Formula	Structural Formula
cyclopropane	$C_{3}H_{6}$	$H_2 \subset I_{CH_2}^{CH_2}$ or \subset
cyclobutane	C_4H_8	$\begin{array}{c c} H_2 C - C H_2 \\ I I \\ H_2 C - C H_2 \end{array} \text{ or } \Box$
cyclopentane	C ₅ H ₁₀	H_2C CH_2 or H_2C H_2C H_2C H_2C H_2 H_2C H_2 H_2C H_2 H_2C H_2 H_2C H_2 H_2C H_2 H_2C H_2
cyclohexane	C ₆ H ₁₂	$H_{2}C$ $H_{2}C$ $H_{2}C$ $H_{2}C$ $H_{2}C$ $H_{2}C$ H_{2} H_{2} H_{2} H_{2} H_{2} H_{2} H_{2} H_{2} H_{2}

In naming hydrocarbons, cyclic structures always have higher priority than C=C, C=C.

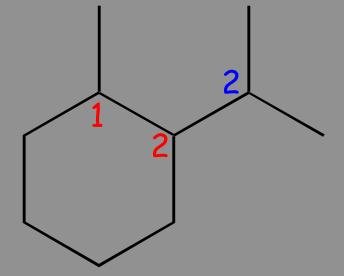




ethenylcyclohexane

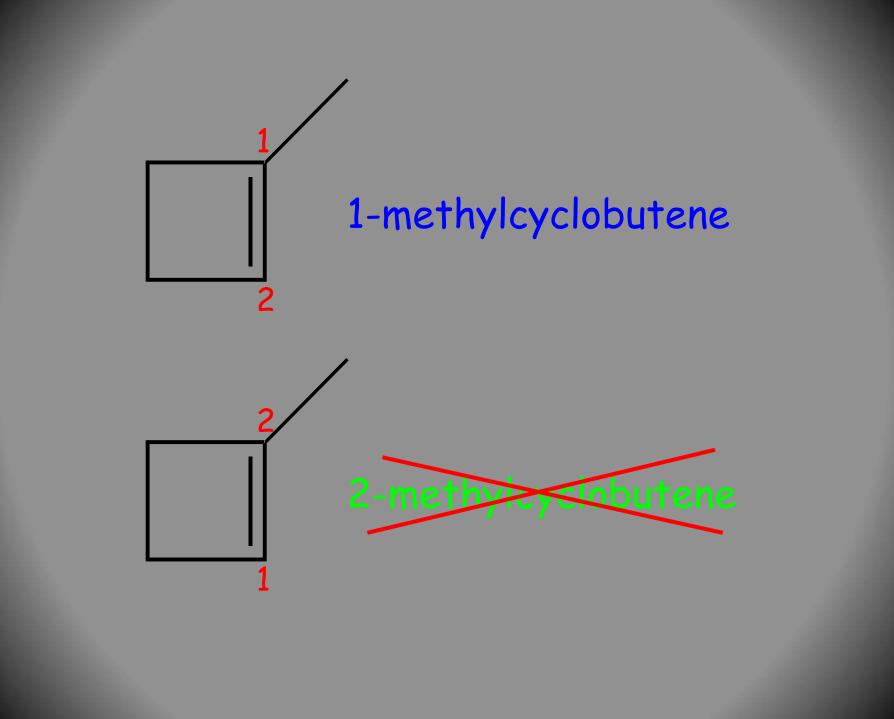
ethynylcyclohexane

In naming cyclic hydrocarbons, the side branches are numbered in alphabetical order.



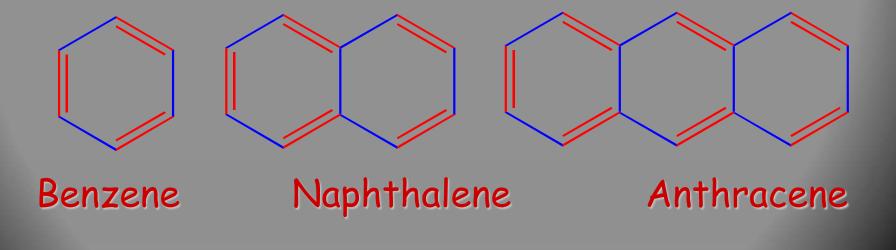
1-methyl 2-(propan-2-yl)

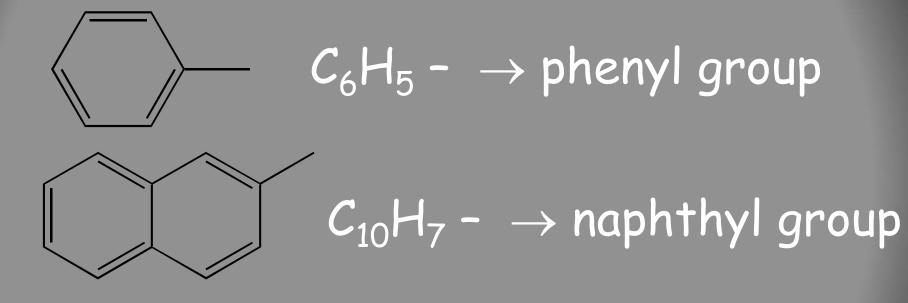
1-methyl-2-(propan-2-yl)cyclohexane



Aromatic hydrocarbons

Extra stability (aromaticity) due to delocalization of π electrons Also called arenes

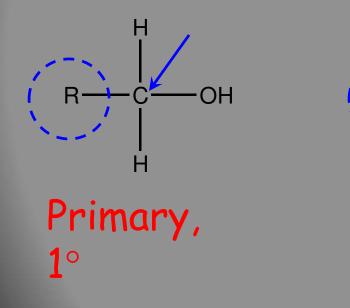


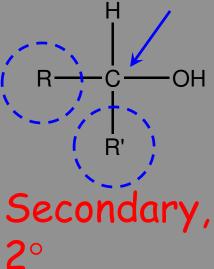


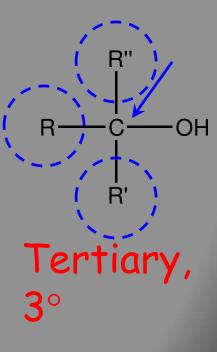
Both are aryl groups

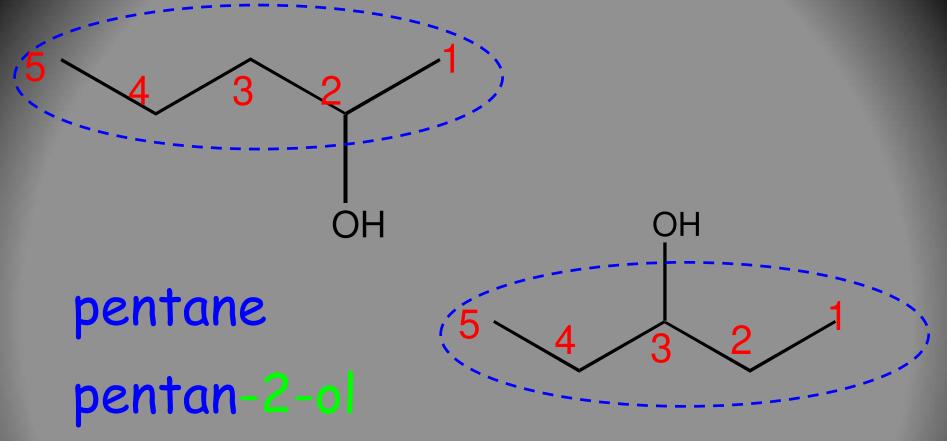
Alkanols (alcohols)

General formula : C_nH_{2n+1}OH (acyclic) Three classes :

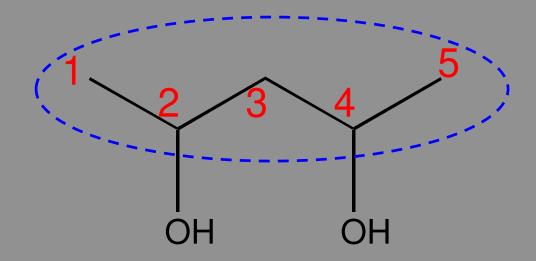








pentane pentan-3-0



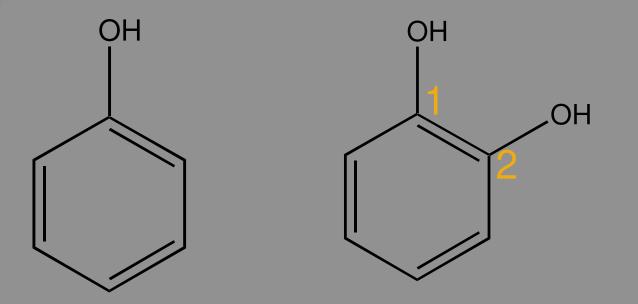
pentane

pentane-2,4-diol / / 'e' is retained in diol

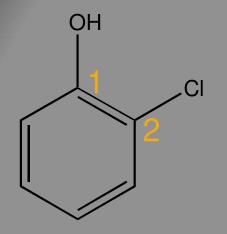
Phenols

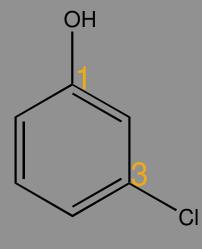
Derived from aromatic hydrocarbons Contain one or more -OH groups attached to an aryl group

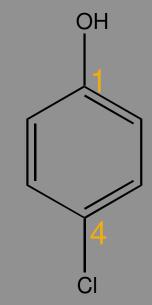




phenol 2-hydroxyphenol Benzene-1,2-diol







2-chlorophenol o-chlorophenol

 $o \rightarrow ortho$

3-chlorophenol m-chlorophenol

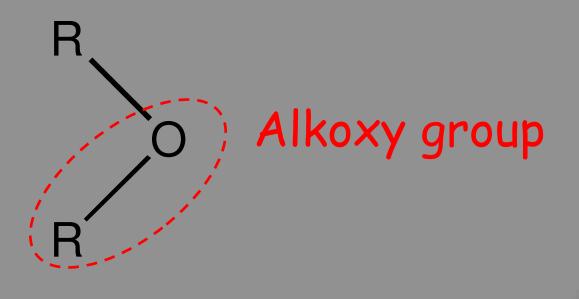
 $m \rightarrow meta$

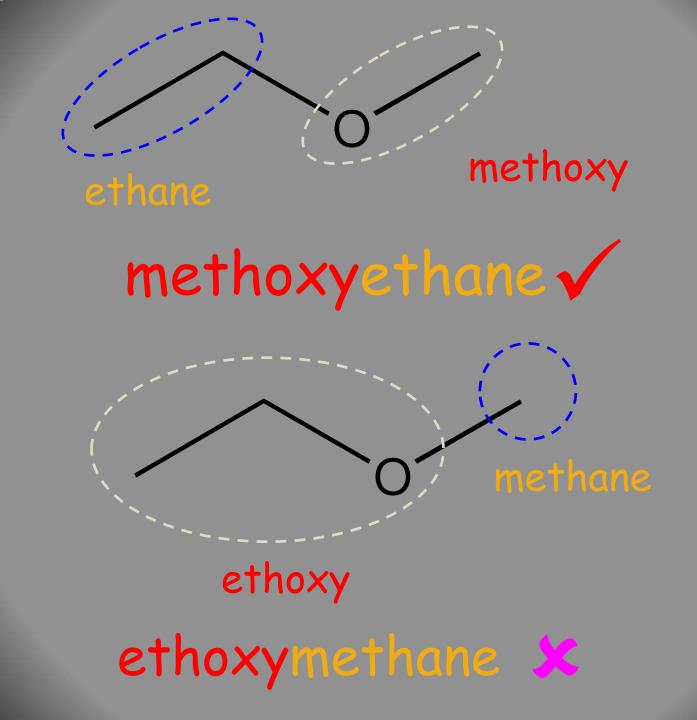
4-chlorophenol p-chlorophenol

 $p \rightarrow para$



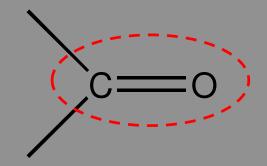
Contain the oxy, -O-, group or alkoxy, R-O- group

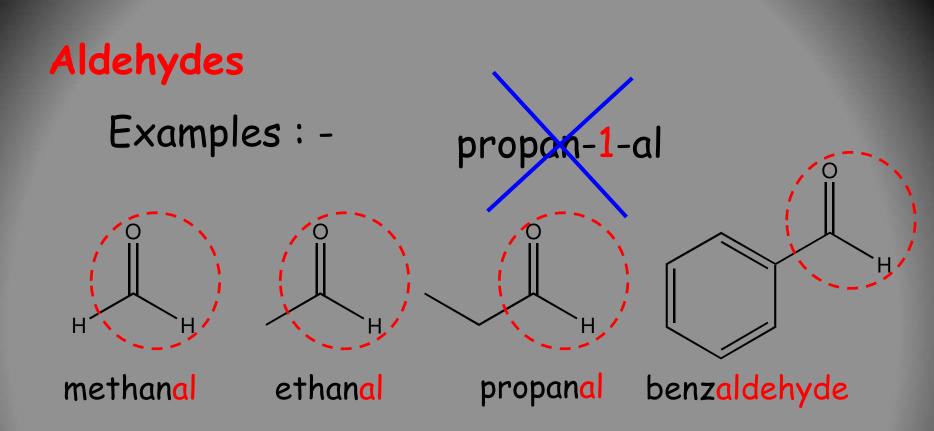




Carbonyl compounds

Organic compounds with the carbonyl group

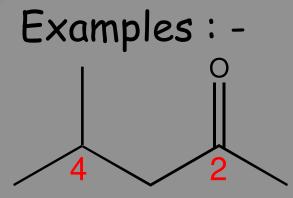


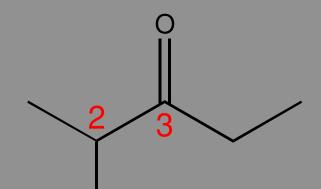


The aldehye group, -CHO, always occupies the terminal position

 \Rightarrow No need to specify its position

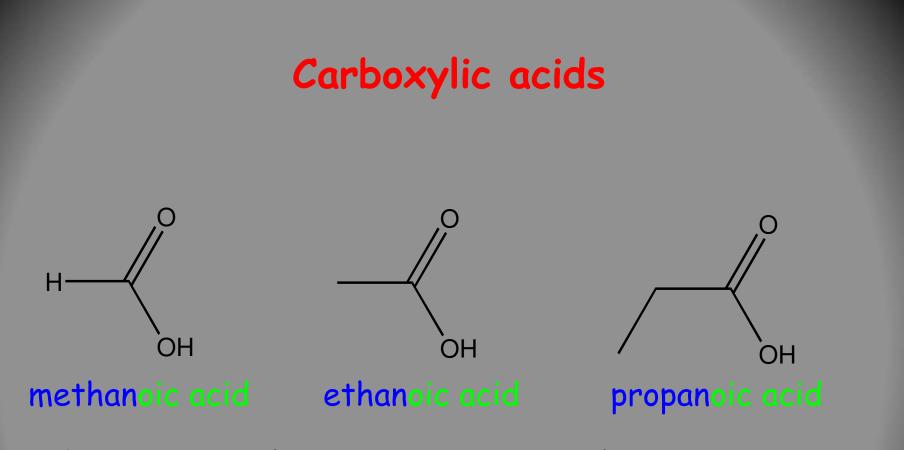






4-methylpentan-2-one 2-methylpentan-3-one 3^{2}

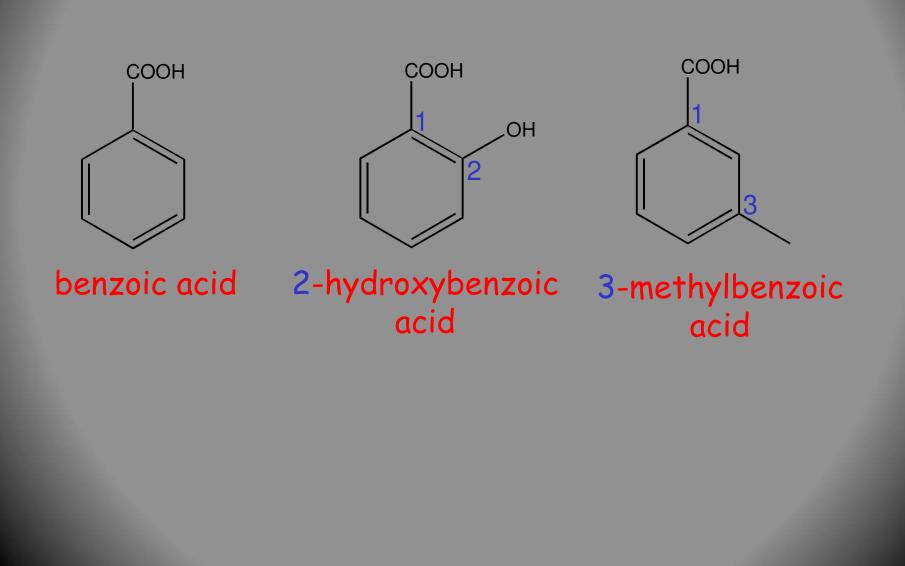
pentane-2,3-dione pentane-2,4-dione



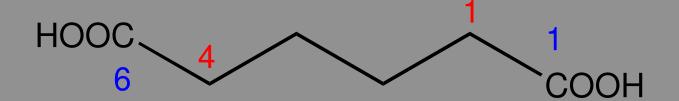
The carboxyl group, -COOH, always occupies the terminal position

 \Rightarrow No need to specify its position

Carboxylic acids



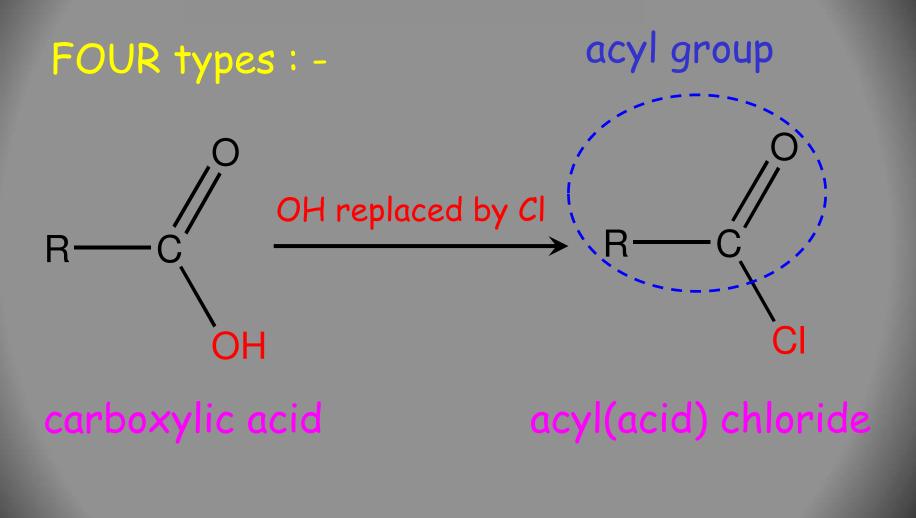
Carboxylic acids

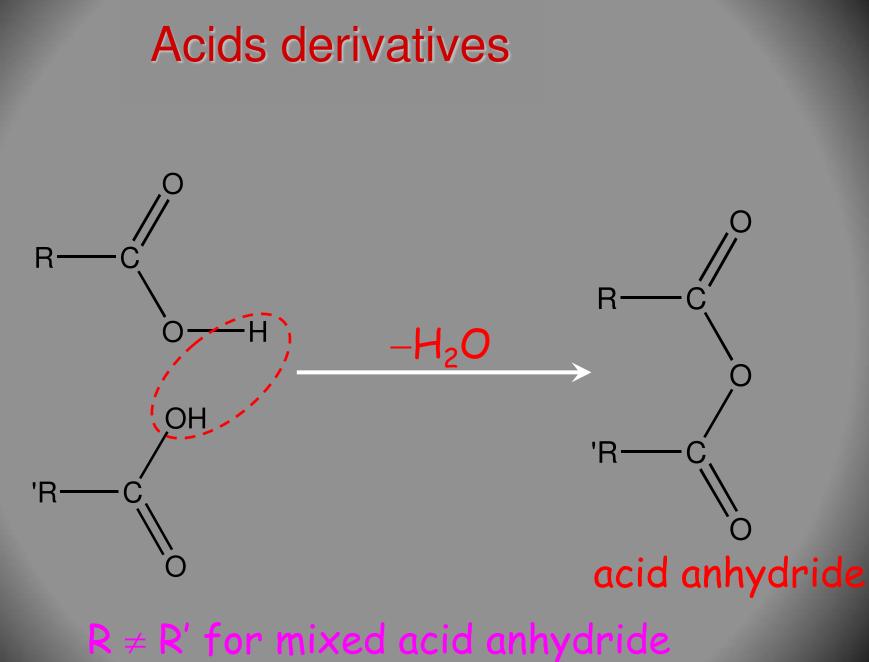


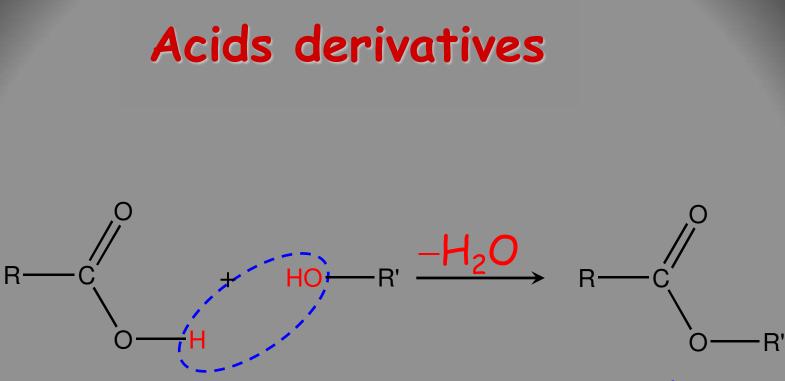
hexanedioic acid 🗸

- hexane-1,6-dioic acid 🗶
- hexane-1,4-dioic acid 🗶

Acids derivatives





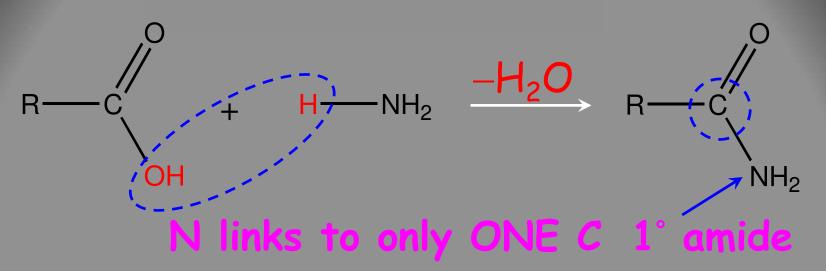


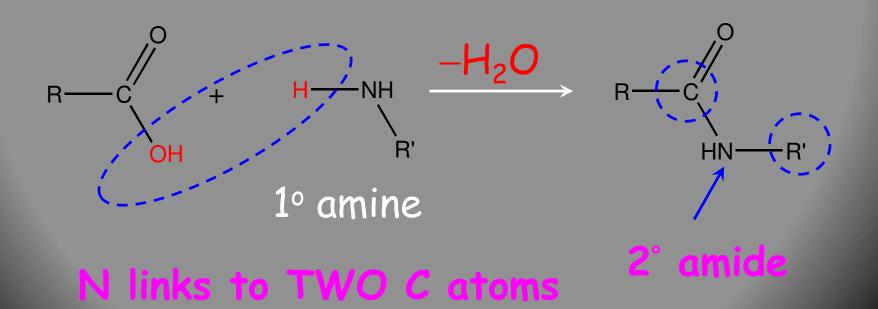
ester

R : alkyl, aryl or H

R' : alkyl or aryl

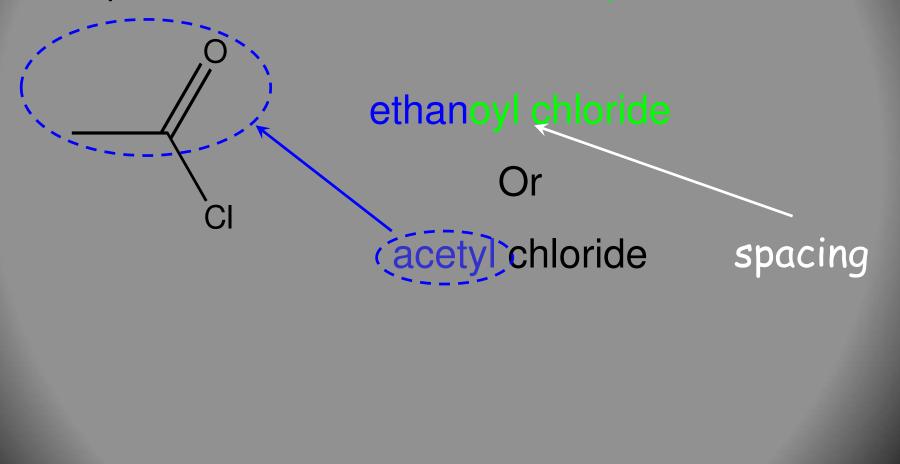
Acids derivatives

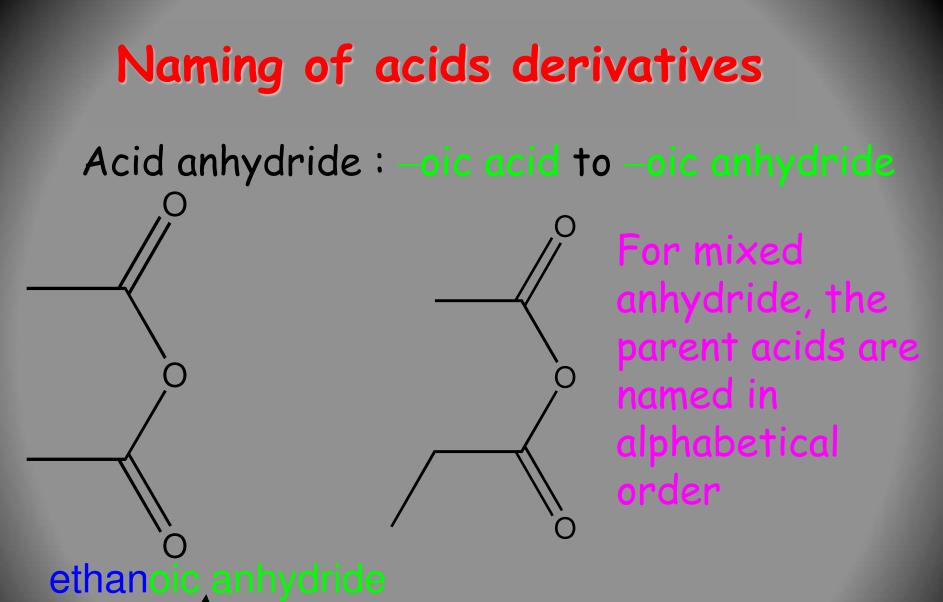




Naming of acids derivatives

Acyl chloride : -oic acid to -oyl chloride

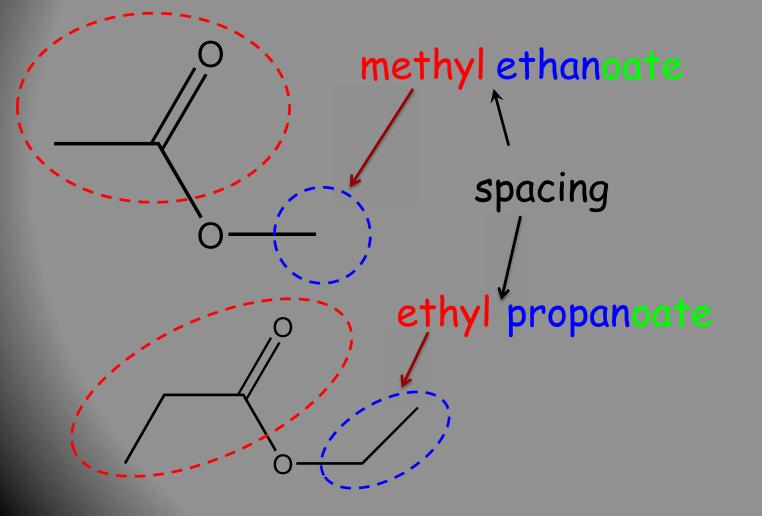


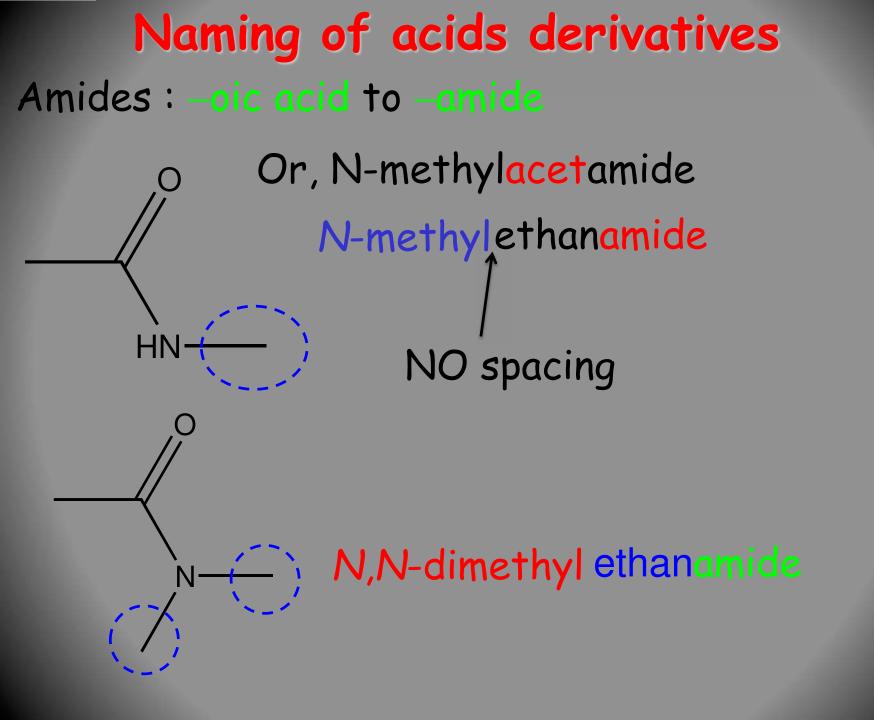


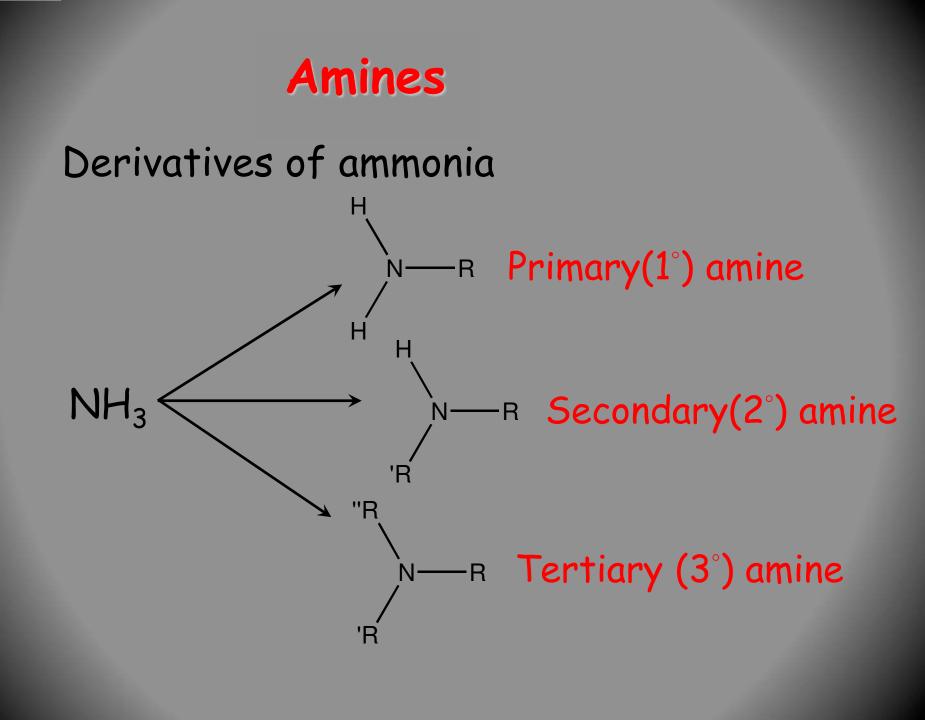
ethanoic propanoic anhydride

spacing

Naming of acids derivatives Ester : -oic acid to -oate preceded by R group of ROH







Amines

Naming amines derived from hydrocarbons

The amino group, is always treated as the principal functional group and expressed as suffix. e replaced by amine

——NH₂ methanamine

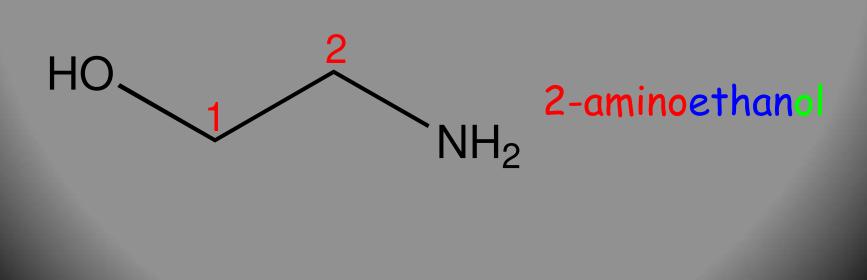
NH₂ ethenamine (ethylenamine)

—NH₂ ethynamine (acetylenamine)

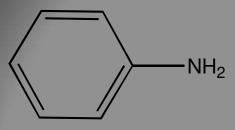
Amines

Naming amines with functional groups other than C=C, C=C, X- and RO-

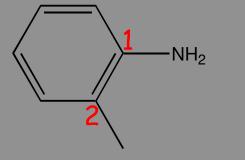
The amino group, is always treated as the substituent and expressed as prefix, amino-



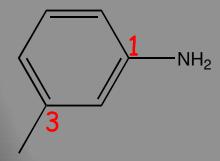




NOT benzenamine phenylamine or aniline



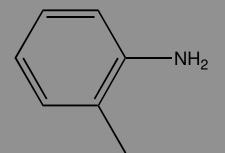
2-methylaniline or o-toluidine



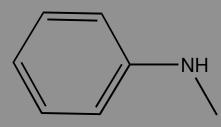
-NH2 **3-methylaniline** or m-toluidine

-NH2 4-methylaniline or p-toluidine

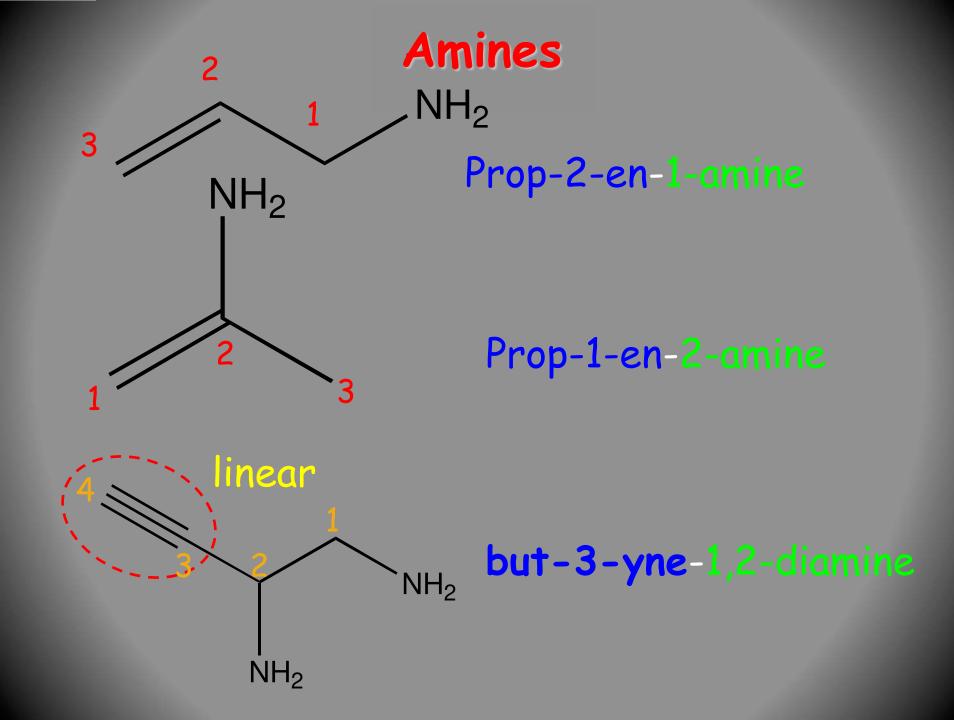


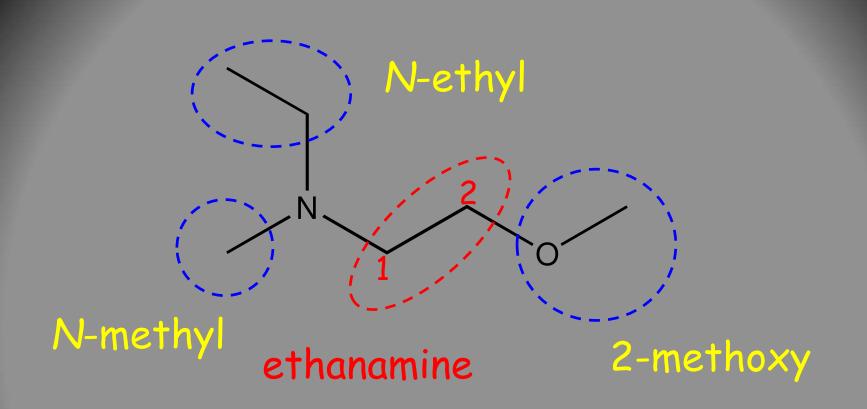


-NH2 **2-**methylaniline

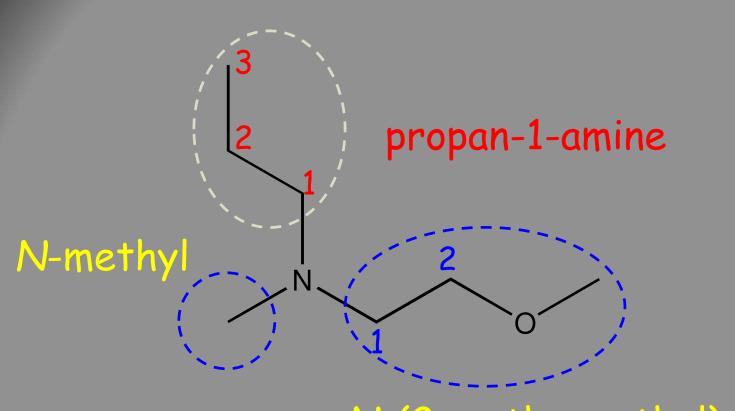


N-methylaniline N-phenylmethanamine





N-ethyl-2-methoxy-N-methylethanamine



N-(2-methoxyethyl)

N-(2-methoxyethyl)-N-methylpropan-1-amine

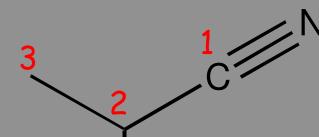
Nitriles

Containing the cyano group, $-C \equiv N$ Naming : -If acting as the principal functional group, it is expressed as the suffix, -nitrile If acting as the substituent, it is expressed as the prefix, cyano-.

Nitriles



ethane**nitrile**

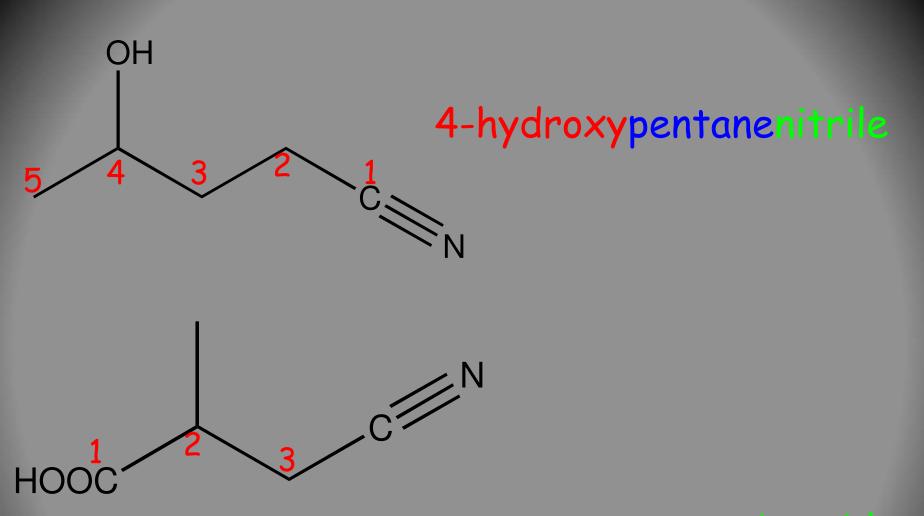


2-methylpropanenitrile

The $-C \equiv N$ group always occupies the terminal position.

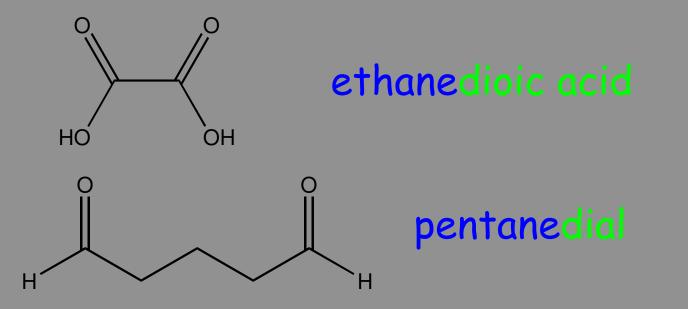
No need to specify its position.

The carbon of the $-C \equiv N$ group is counted as part of the longest carbon chain.



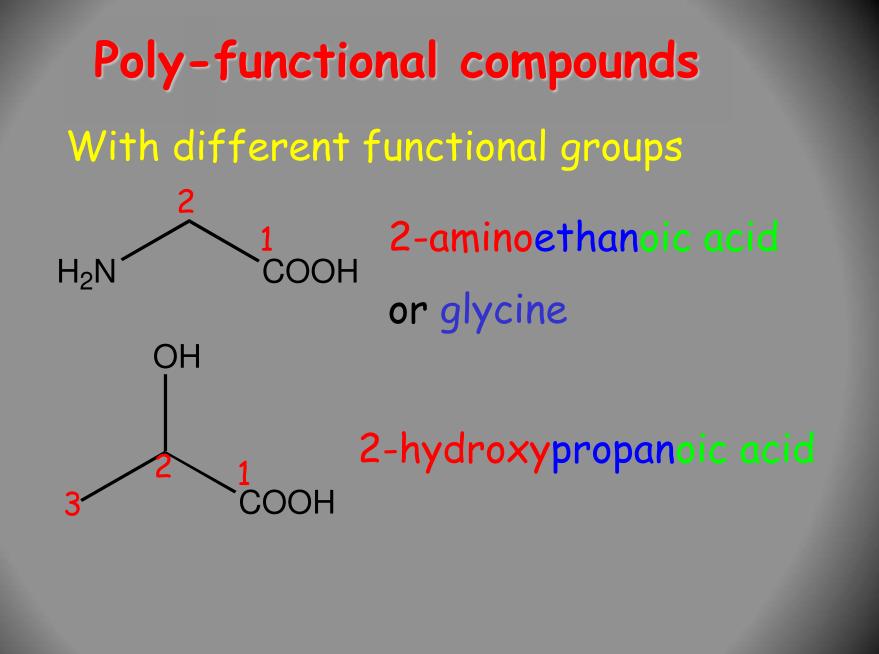
3-cyano-2-methylpropanoic acid

If used as prefix, its carbon is not counted as part of the main carbon chain **Poly-functional compounds** With identical functional groups



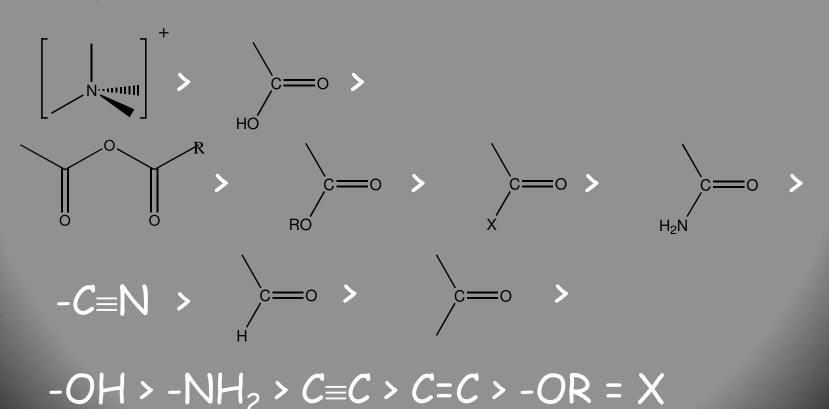
-COOH and -CHO groups always occupy the terminial positions.

No need to specify its position



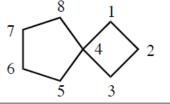
Poly-functional compounds Naming : -

1. The functional group with the highest priority (the principal functional group) is expressed as the suffix.

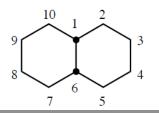


"Bicyclic" compounds are those that contain two rings

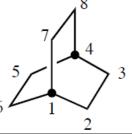
> Two rings with one common atom : spiro ring system



> Two rings with two common atoms : fused ring system

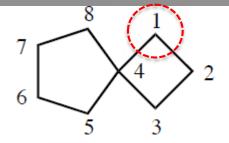


Two rings with more than two common atoms : bridged ring system

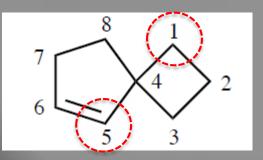


Two rings with one common atom : spiro ring system
 Smaller ring is numbered first and through the common atom other ring is numbered such that all the substituents get lowest number

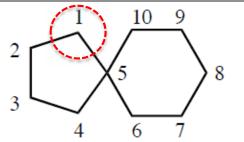
Numbering starts from the first atom after the common atom



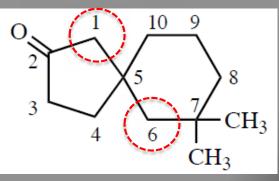
spiro[3.4]octane



spiro[3.4]oct-5-ene



spiro[4.5]decane



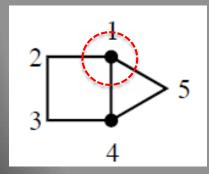
7,7-dimethylspiro[4.5]decan-2-one

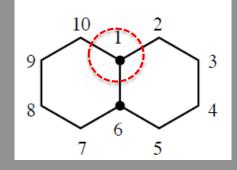
Two rings with two common atom : fused ring system

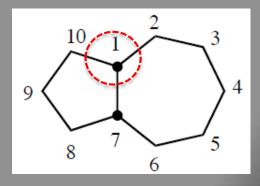
The common atoms are called bridgehead atoms.
 There are three paths between the two bridgehead atoms
 Longer path is numbered first and then the shorter path and then the shorter path

> Numbering starts at a bridgehead.

In case of these systems, the shortest path has direct contact and hence number of atoms between the two bridgehead atoms is 0.





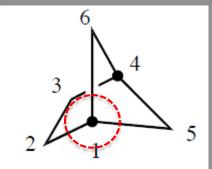


bicyclo[2.1.0]pentane bicyclo

bicyclo[4.4.0]decane

bicyclo[5.3.0]decane

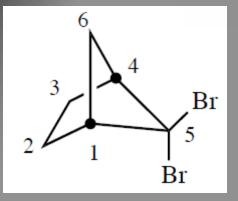
- Two rings with more than two common atom : bridged ring system
- > The common atoms are called bridgehead atoms.
- > There are three paths between the two bridgehead atoms
- Longer path is numbered first and then the shorter path and then the shortest.
- > Numbering starts at a bridgehead.
- In case of these systems, the shortest path does not have direct contact and hence number of atoms between the two bridgehead atoms is variable.

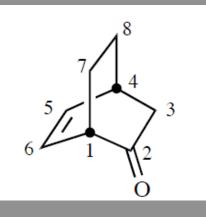


bicyclo[2.1.1]hexane

bicyclo[2.2.2]octane

bicyclo[3.2.1]octane

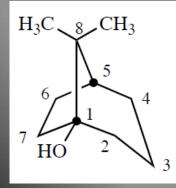






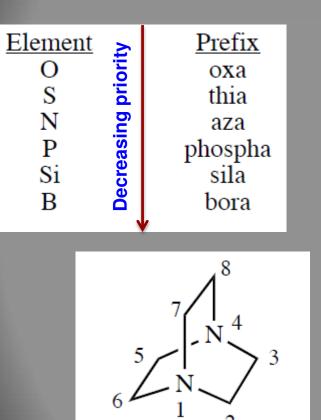
bicyclo[2.2.2]oct-5-en-2-one

8,8-dimethylbicyclo[3.2.1]octan-1-ol

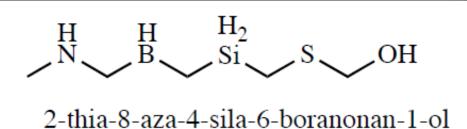


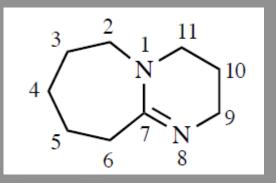
Compounds with hetero-atoms

Compounds with one or more non-C atom present in the main chain are compounds with hetero-atoms



1,4-diaza-bicyclo[2.2.2]octane DABCO Polymerization reaction





1,8-diaza-bicyclo[5.4.0]undec-7-ene DBU Catalyst and complexing agent

Many more to go.....