Chapter II

Nomenclature of Organic Compounds

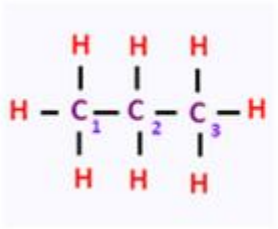
I/ FORMULAS OF ORGANIC COMPOUNDS

1. Molecular formula

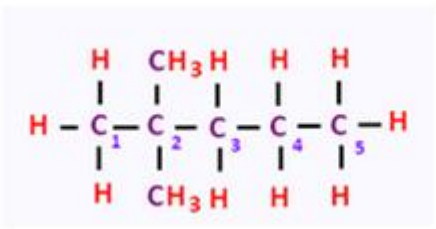
Every organic compound has a corresponding gross formula, for example (Cx Hy Oz) if the compound contains three types of elements C, H, and O. But the same gross formula generally has several bodies called isomers.

2. Developed formula

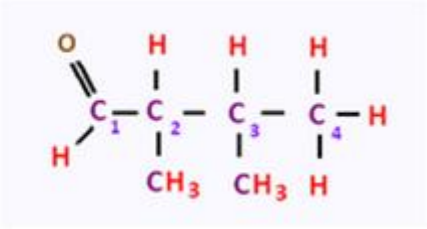
It represents the order of arrangement of the atoms, but not their actual orientation in space.



Propane



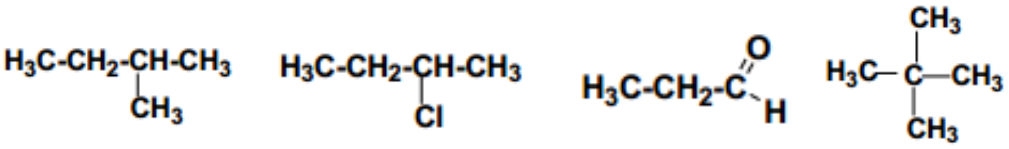
2, 2-dimethylpentane



2, 3-dimethylbutanal

3. Semi-developed formula

Allows to group with each carbon the number of hydrogen linked.



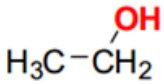
4. Topological formula

II/ NOMENCLATURE IN ORGANIC CHEMISTRY

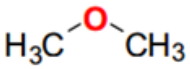
The nomenclature allows one to find the name of a molecule knowing its structure and to determine the structure of a molecule knowing its name. Generally, the names of organic compounds

derive from the names of saturated aliphatic hydrocarbons (alkanes) and obey the ***I.U.P.A.C*** rule ***« International Union of Pure and Applied Chemistry ».***

Example : **C_2H_6O**



Ethanol



dimethylether

For the same gross formula, two developed formulas (***two isomers***) were found.

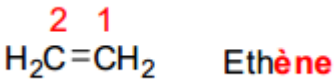
1. Alkanes

Saturated hydrocarbons are alkanes with the general molecular formula C_nH_{2n+2}. In these compounds, the carbon atoms exhibit a tetrahedral geometry (SP^3 hybridization). The names of linear alkanes are presented in the table below:

Number of carbons (n)	Name	Formula (C_nH_{2n+2})	Number of carbons (n)	Name	Formula (C_nH_{2n+2})
1	Methane	CH_4	12	Dodecane	$C_{12}H_{26}$
2	Ethane	C_2H_6	13	Tridecane	$C_{13}H_{28}$
3	Propane	C_3H_8	14	Tetradecane	$C_{14}H_{30}$
4	Butane	C_4H_{10}	15	Pentadecane	$C_{15}H_{32}$
5	Pentane	C_5H_{12}	16	Hexadecane	$C_{16}H_{34}$
6	Hexane	C_6H_{14}	17	Heptadecane	$C_{17}H_{36}$
7	Heptane	C_7H_{16}	18	Octadecane	$C_{18}H_{38}$
8	Octane	C_8H_{18}	19	Nonadecane	$C_{19}H_{40}$
9	Nonane	C_9H_{20}	20	Icosane	$C_{20}H_{42}$
10	Decane	$C_{10}H_{22}$	30	Triacontane	$C_{30}H_{62}$
11	Undecane	$C_{11}H_{24}$	40	Tetracontane	$C_{40}H_{82}$

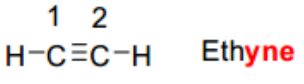
- **Alkenes (olefins)**

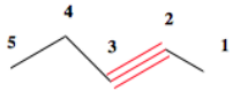
These are unsaturated hydrocarbons, which contain a double bond in their structures. The general formula for alkenes is C_nH_{2n}.



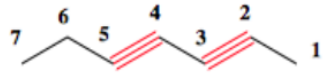
- **Alkynes**

These compounds contain a triple bond in their structures. The general formula for alkynes is C_nH_{2n-2}.



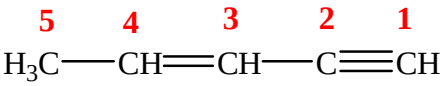


pent-2-yne

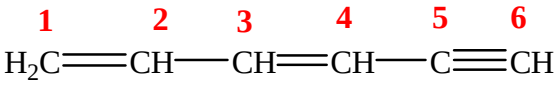


hepta-2, 4-diyne

- **Alkenynes**



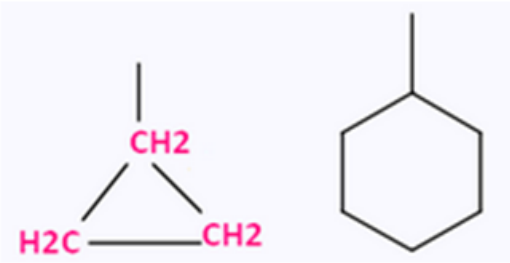
Pent-3-en-1-yne



Hexa-1,3-dien-5-yne

- **Saturated monocyclic hydrocarbons**

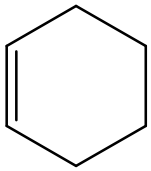
Cyclopropane **Cyclohexane**



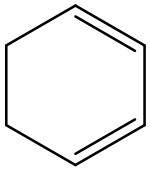
Cyclopropyl **Cyclohexyl**

The names of the radicals (cyclopropyl and cyclohexyl) are obtained by replacing the suffix "ane" with "yl"

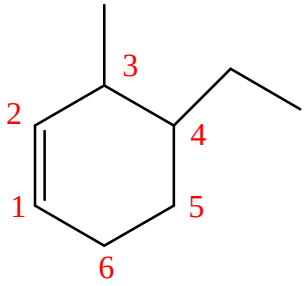
- **Unsaturated monocyclic hydrocarbons**



cyclohexene
cyclohex-1-ene



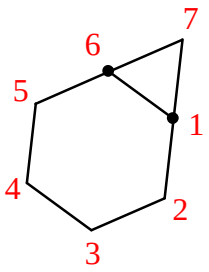
cyclohexa-1, 3-diene

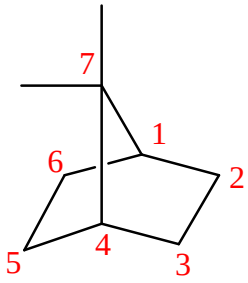


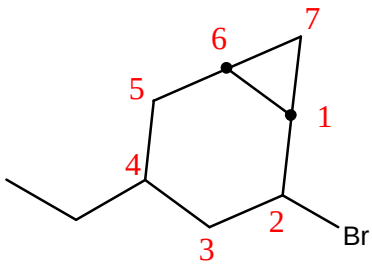
4-Ethyl-3-methylcyclohexene
4-Ethyl-3-methylcyclohex-1-ene

- **Bicyclic alkanes**

The saturated bicyclic hydrocarbons are named after the linear saturated hydrocarbon with the same number of carbon atoms, preceded by the prefix **bicyclo**.



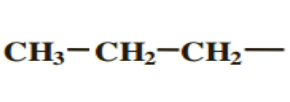




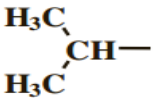
Bicyclo [4,1,0]heptane 7,7-dimethylbicyclo [2,2,1]heptane 2-bromo-4-ethylbicyclo [4,1,0]heptanes

- **Alkyl groups**

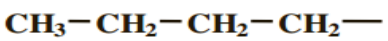
For branched alkanes, it is necessary to indicate the position and nature of the alkyl groups. The name of an **alkyl group** (radical) is derived from that of the corresponding **alkane** by replacing the ending "**ane**" with "**yl**". **For Example**: **methyl, ethyl, propyl, butyl**…



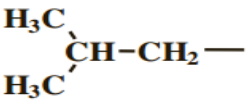
n-propyl



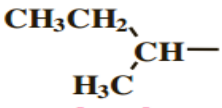
iso-propyl



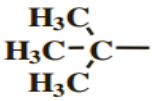
n-butyl



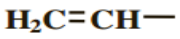
iso-butyl



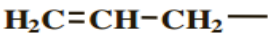
sec-butyl



tert-butyl

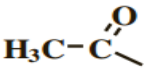


vinyl

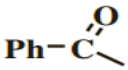


alkyl

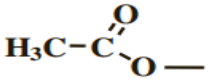
benzyl



acetyl



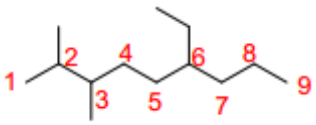
benzoyl



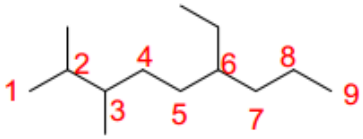
acetate

2. Nomenclature rule applied to alkanes (C_nH_{2n+2})

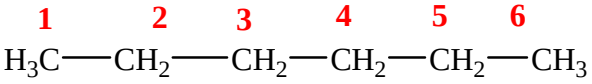
1. Find the longest carbon chain
2. Number the carbons by having the lowest numerical combination. (1st number must be the smallest possible for the 1st group).



3. Match alphabetical order with numbering (alphabetical order takes priority).
4. Write the carbon number of the chain that carries the front group, separated by a hyphen.
5. Use the prefixes **di-**, **tri-**, **tetra-**, penta-, **hexa-**, **…..** for the identical group on the string (multiplicity).



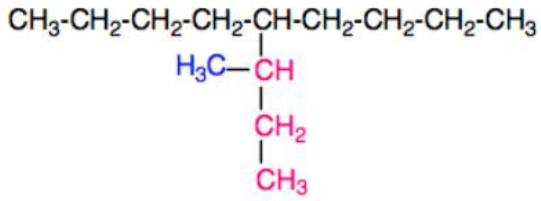
6-ethyl-2,3-dimethylnonane



2,4-dimethylhexane

6. A comma (,) is placed between two numbers. A hyphen is placed between a letter and a number.
7. End the name with the name of the linear alkane corresponding to the longest chain.

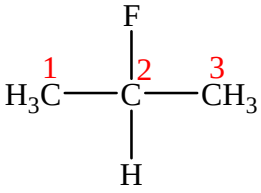
Example:



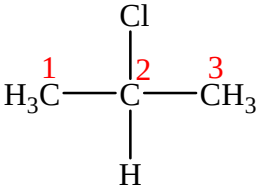
5-(1-methylpropyle)nonane

3. Simple-function compounds

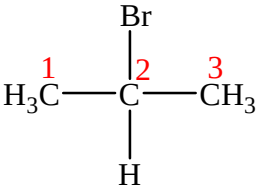
a. Halogenure derivatives



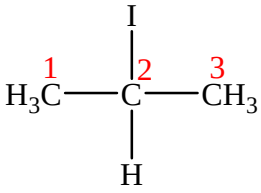
2-fluoropropane



2-chloropropane

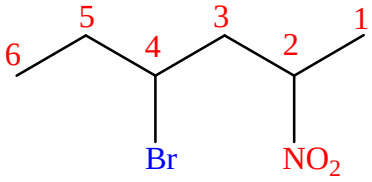


2-bromopropane



2-iodopropane

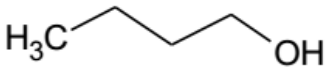
b. Nitro group (-NO_2)



4-Bromo-2-nitrohexane

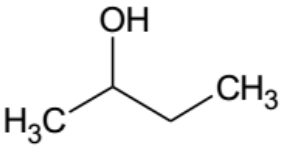
c. Alcohols (ol)

There are three classes of alcohols: **primary**, **secondary** and **tertiary alcohols**.



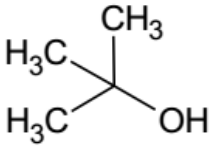
Butan-1-ol

(**Primary alcohol**)



Butan-2-ol

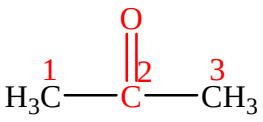
(**Secondary alcohol**)



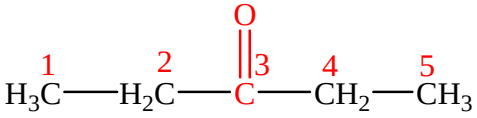
2-Methylpropan-2-ol

(**Tertiary alcohol**)

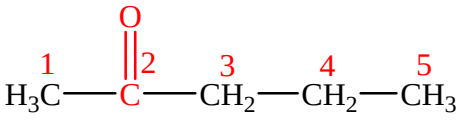
d. Ketone (one)



Propanone (acetone ; dimethylketone)

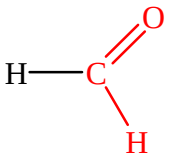


pentan-3-one



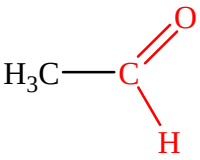
pentan-2-one

e. Aldehyde (al)

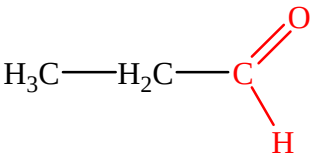


methanal (Formaldehyde)

(Formic Aldehyde)

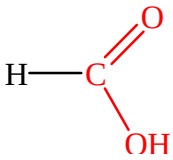


ethanal



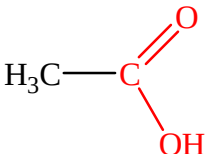
propanal

f. Carboxylic Acid (……oic acid)



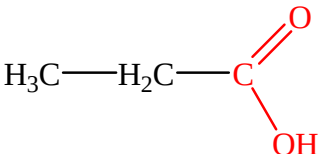
Methanoic acid

Formic acid



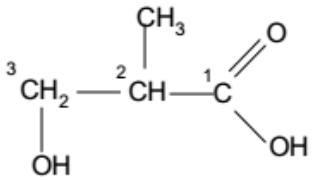
Ethanoic acid

Acetic acid

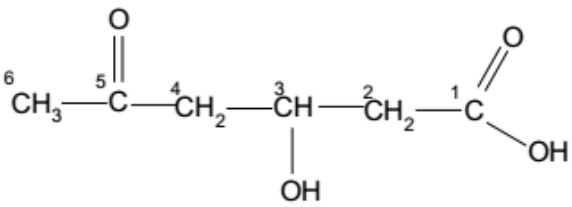


Propanoic acid

Propionic acid (Ethylformic acid)

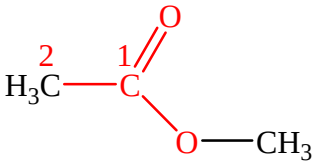


3-hydroxy-2-methylpropanoic acid

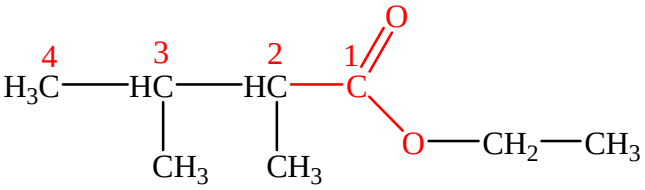


3-hydroxy-5-oxohexanoic acid

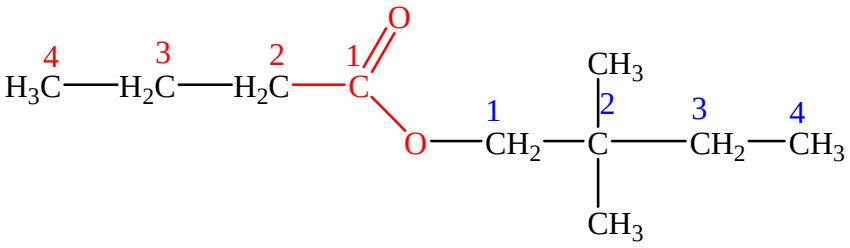
g. Ester (Alkyl ….oate)



Methyl ethanoate

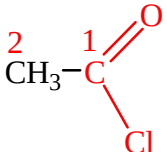


Ethyl 2,3-dimethylbutanoate



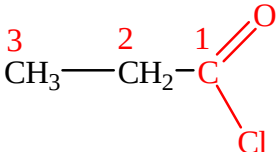
2,2-dimethylbutyl butanoate

h. Acid halogenure (oyl halogenure)

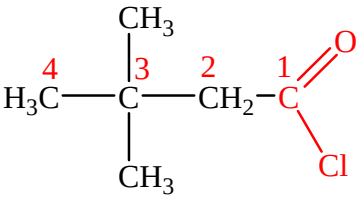


Ethanoyl Chloride

(acetyl Chloride)



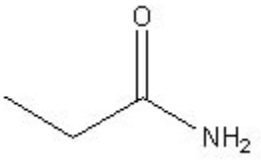
Propanoyl chloride



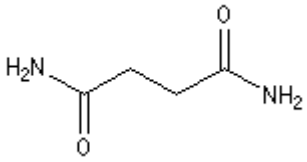
3,3-dimethylbutanoyl chloride

i. Amide (….amide)

Primary N

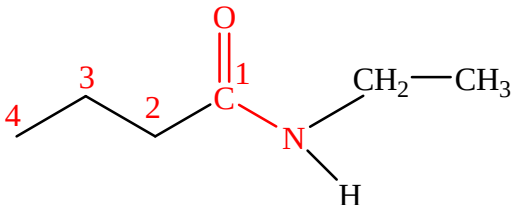


propanamide



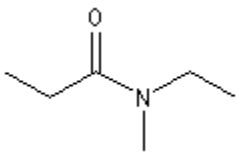
butandiamide

Secondary N

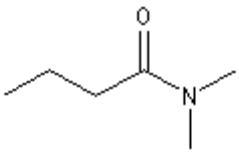


N-ethylbutanamide

Tertiary N

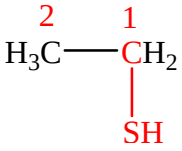


N-ethyl-N-methylpropanamide



N,N-dimethylbutanamide

j. Thiol (…..thiol)



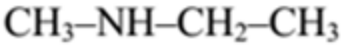
Ethanethiol

k. Amine (…..amine)

✓ Primary amine

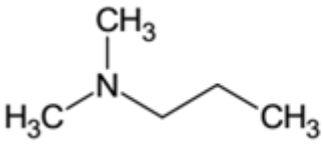
methylamine

✓ Secondary amine

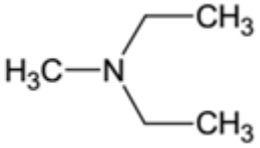


Ethylmethylamine ou bien (N-ethyl-N-methylamine)

✓ Tertiary amine



dimethylpropylamine

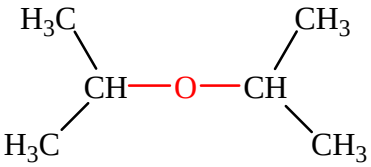


trimethylamine

l. Ether oxide (ether)

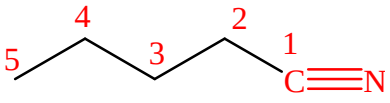
Dimethylether

diethylether

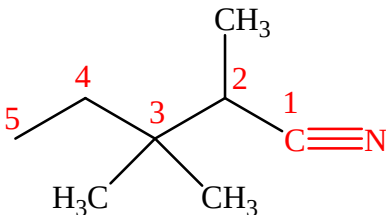


diisopropylether

m. Nitrile (…..nitrile)

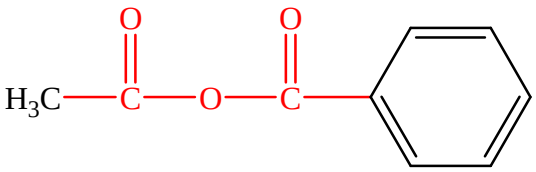


Pantanonitrile

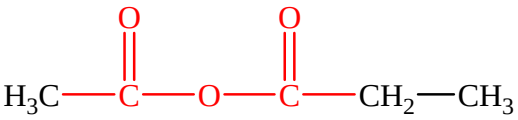


2,3,3-trimethylpantanonitrile

n. Acid anhydride (…….oic anhydride)



Ethanoic and benzoic anydride

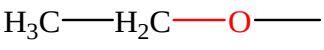


ethanoic and propanoic anydride

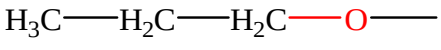
(acetic and propionic anhydride)

Remark

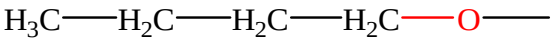
methoxy



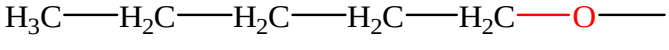
ethoxy



propoxy

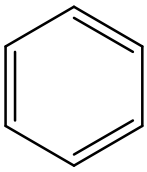


butoxy

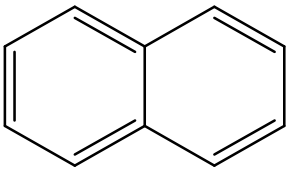


pentyloxy

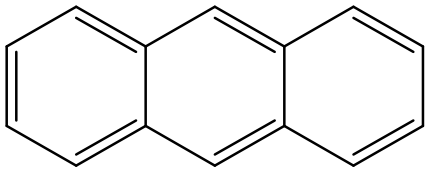
4. Aromatic compounds



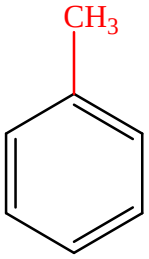
Benzene



Naphtalene

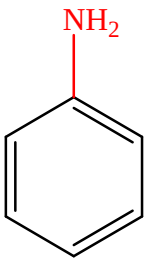


Anthracene



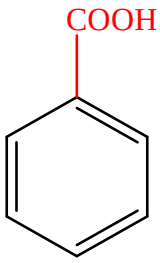
Toluene

(Methylbenzene)



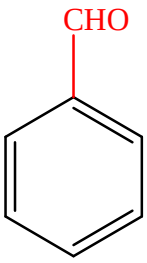
Aniline

phenylamine

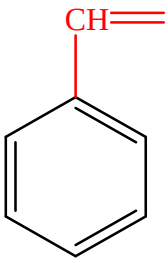


Benzoïque acid

benzene carboxylic acid

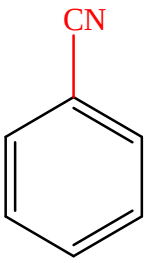


benzaldehyde

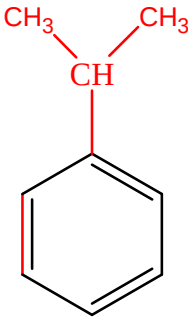


styrene

vinylbenzene

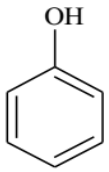


benzonitrile

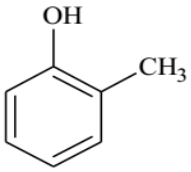


cumène

isopropylbenzene

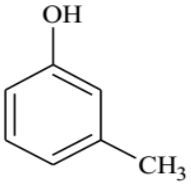


Phenol



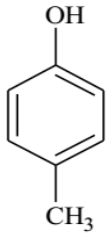
o-Methylphenol

(o-Cresol)



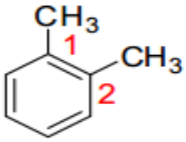
m-Methylphenol

(m-Cresol)



p-Methylphenol

(p-Cresol)

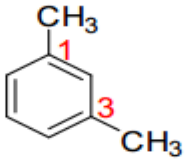


1,2-dimethylbenzene

Ortho-dimethylbenzene

o-methyltoluene

o-xylene

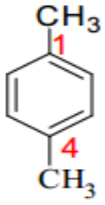


1,3-dimethylbenzene

meta-dimethylbenzene

m-methyltoluene

m-xylene



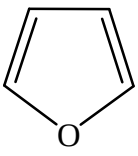
1,4-dimethylbenzene

para-dimethylbenzene

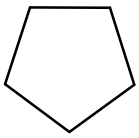
p-methyltoluene

p-xylene

5. Heterocyclic Compounds

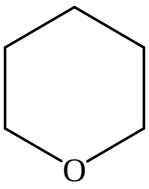


Furane



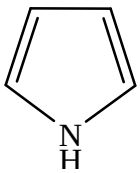
Tetrahydrofurane

THF

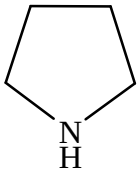


Tetrahydropyrane

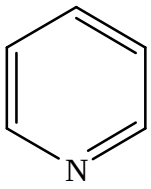
THP



pyrrole



pyrrolidine

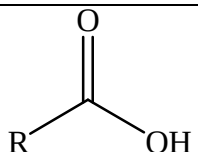
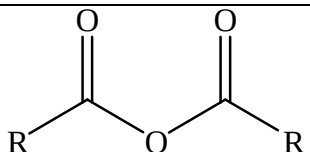
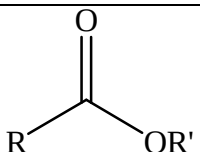
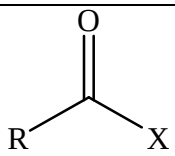
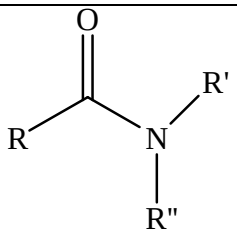
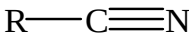
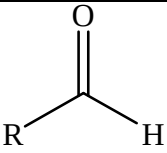
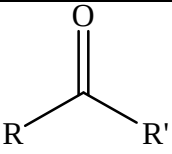
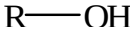
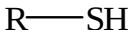
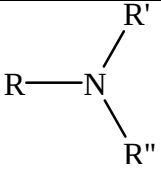
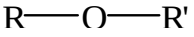
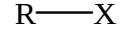


pyridine

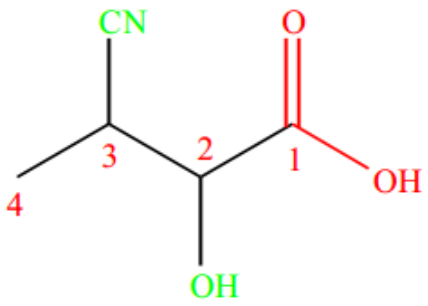
6. Multi-functional compounds

Mixed-function compounds contain different functional groups within the same molecule. The combination of two (or more) functions primarily raises questions of priority among them. The priority functional group is designated by a **suffix**, and the numbering is chosen to assign it the lowest possible index. Other functional groups are indicated by **prefixes**. The groups presented in the Table 2 are arranged in descending order of priority.

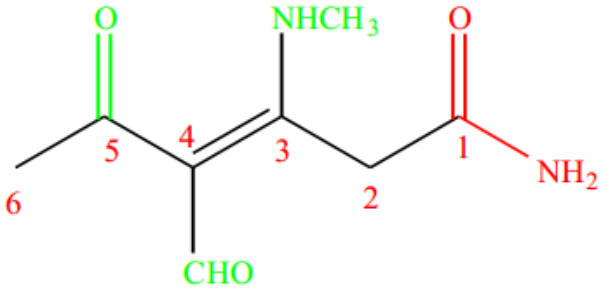
Table 2: Suffixes and prefixes used to denote some important groups.

Fonction	Formula	If the Function is Not Priority (prefix)	If the Function is Priority (suffix)
Carboxylic acid		**Carboxy ……**	**….oic acid**
Acid anhydride		**acyloxy …….**	**….oic anhydride**
Ester		**yloxycarbonyl …….**	***Alkyl ….oate***
Acid halogenure		**Halogenocarbonyl….**	**……oyl halogenure**
Amide		**Alcanamido…..**	**……amide**
Nitrile		**Cyano…..**	**…….nitrile**
Aldehyde		**Formyl……**	**……..al**
Ketone		**Oxo…..**	**……one**
Alcohol		**Hydroxyl…..**	**…..ol**
Thiol		**Mercapto……**	**….thiol**
Amine		**amino…..**	**……amine**
Ether-oxyde		**Alkoxy……**	**…….ether**
Alkyl halogenure		**Halogeno……..**	-

Example:



3-Cyano-2-hydroxybutanoic acid



3-(N-methylamino)-4-formyl-5-oxohex-3-enamide