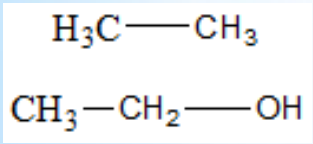
Classification and Nomenclature of Organic Compounds

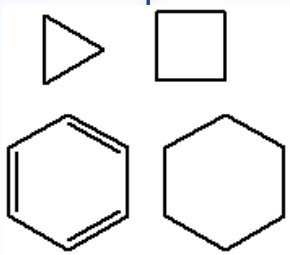
Classification

Organic Compounds

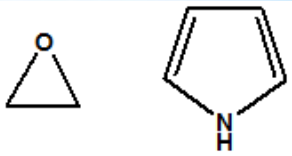
Open chain or acyclic or aliphatic compounds



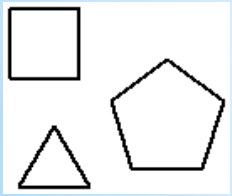
Carbocyclic compounds



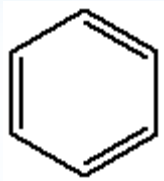
Heterocyclic compound



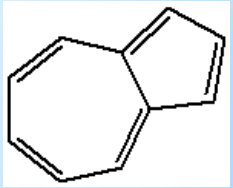
Alicyclic compound



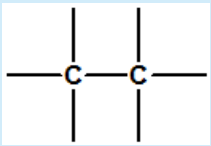
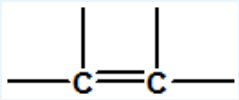
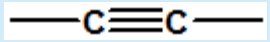
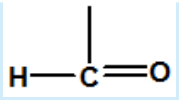
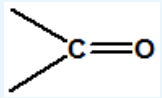
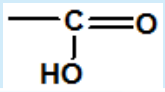
Benzenoid aromatic compound

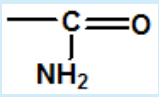
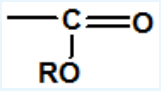
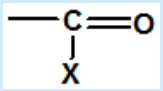
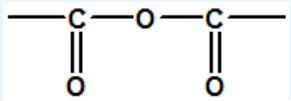
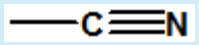
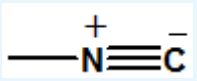
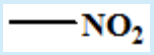
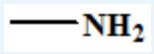
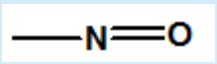
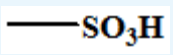


Non-Benzenoid aromatic compound



Functional group and classification of organic compound

Name of the function	Graphic formula	Class name of the compounds G-General I- IUPAC
Carbon-carbon single bond		Paraffin (G) Alkane (I)
Carbon-carbon double bond		Olefin (G) Alkene (I)
Carbon-carbon triple bond		Acetylene (G) Alkyne (I)
Halo		Alkyl halide (G) Haloalkane (I)
Hydroxyl	-OH	Alcohol (G) Alkanol (I)
Ether	-O-	Ether (G) Alkoxyalkane (I)
Aldehyde		Aldehyde (G) Alkanal (I)
Ketone		Ketone (G) Alkanone (I)
Carboxyl		Carboxylic acid (G) Alkanonic acid (I)

Name of the function	Graphic formula	Class name of the compounds G-General I- IUPAC
Acid amide		Acid amide (G) Alkanamide (I)
Ester		Ester (G) Alkyl alkanoate (I)
Acid halide		Acid halide (G) Alkanoyl halide (I)
Acid anhydride		Acid anhydride (G) Alkanoic anhydride (I)
Cyano		Alkyl cyanide (G) Alkanenitrile (I)
Isocyano		Alkyl isocyanide (G) Alkylcarbylamine (I)
Nitro		Nitroalkane (G & I)
Amino		Alkylamine (G) Alkanamine (I)
Nitroso		Nitrosoalkane (G & I)
Sulphonic acid		Alkanesulphonic acid (G & I)
Mercapto	-SH	Thioalcohol (G) Alkanethiols (I)

Nomenclature of Organic Compounds

1. Common naming system

Alkane

- **The total number of C atoms in the compound is counted and this is indicated by-**

  Meth- 1 C, Eth- 2 C, Prop- 3 C, But- 4 C,

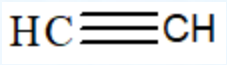
  Pent- 5 C, Hex- 6 C, Hept- 7 C, Oct- 8 C, Non- 9 C

- **To that syllable, add -ane at the end of the name.**
- **The prefix n- is added to the name if all the carbons are in a straight chain.**
- **The prefix iso- is added to the name in case of branched alkane.**
- **The prefix neo- is added if alkane contains tert-butyl group.**

Alkene

- **The total number of carbon atoms is counted and the name of the corresponding alkane is determined.**
- **The suffix 'ylene' is added to the prefix.**

Alkyne

- The simplest member has its common name acetylene, 

Alkyl halide

- They are named according to the names of the alkyl groups they contain; a space is left between the name of the alkyl group and the word ‘halide’.

Nitroalkane

- The name ‘nitro’ is added prior to the name of the alkane.

Ether

- Simple alkyl ethers are named as dialkyl ethers.
- Mixed ethers are named by writing the names of the two hydrocarbon groups separately in an increasing order of complexity, a space is left and then the word ether is written

Alcohol

- First writes the name of the alkyl group and then alcohol.

Carboxylic acid

- They are named based on their source.
- To name carboxylic acid, the last syllable of the Latin name of the source is dropped and add to it ‘ic acid’

Structural formula	English name of the source	Latin synonym	Name of the carboxylic acid
HCOOH	Ant	L. Formica	Formic acid
CH_3COOH	Vineger	L. Acetum	Acetic acid
CH_3CH_2COOH	First fat	Gr. Proto Pion	Propionic acid
$CH_3CH_2CH_2COOH$	Butter	L. Butyrun	Butyric acid
$CH_3(CH_2)_3COOH$	Valerian root	Gr. Valerian	Valeric acid

Aldehydes

- The common name of the aldehyde is derived from the common name of the corresponding acid.
- The ‘ic acid’ ending of the acid is dropped and ‘aldehyde’ is added to the remainder.

Ketones

- The common name of the ketone is also derived from the common name of the corresponding acid.
- The ‘ic acid’ ending of the acid is dropped and ‘one’ is added to the remainder.
- In case of mixed ketone, the names of the different hydrocarbon groups are named separately in an increasing order of complexity before the word ‘ketone’.

Esters

- The hydrocarbon part attached to the oxygen is named first, a space is left and then the common name of the acid is written with the ‘ic acid’ ending changed to ‘ate’.

Acid halide

- The ‘ic acid’ ending of the acid is replaced by ‘yl halide’

Acid anhydride

- The ‘acid’ ending of the parent acid is replaced by ‘anhydride’

Acid amide

- The ‘ic acid’ ending of the acid is replaced by ‘amide’

Carbonitrile

- The ‘ic acid’ ending of the parent acid is replaced by ‘onitrile’

Amine

- The amines have one word common name which are obtained by combining the name of each hydrocarbon group on the N atom with the suffix ‘amine’

Nitroso compound

- **They are named as ‘nitrosoalkane’.**

Thioalcohol

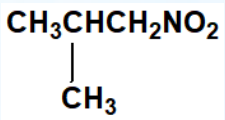
- **They are named according to the name of the hydrocarbon group attached to it, followed by ‘thioalcohol’.**

Sulphonic acid

- **They are named according to the name of the hydrocarbon group joined by ‘sulphonic acid’.**

2. IUPAC system of nomenclature

The IUPAC name of a compound consists of a base name with or without a prefix. The base name consists of (i) root or stem and (ii) prefix or suffix.

E.g. 

2-methyl-1-nitropropane

Here base name is nitropropane - propane is the root and nitro is the prefix of the base name.

IUPAC rules-

1. If the base name of a compound is the name of an actual compound, the prefix is joined to the base name. E.g. Nitropropane; but if the base name is not at all a name of an actual compound, then a space is left in between the base name and prefix. E.g. Methyl ethanoate.
2. To choose the base name of a compound, one should choose the parent part of the molecule. The parent part consists of a parent carbon chain and the most important functional group.
3. The nature of the base chain and the number of the carbon atoms present in it provide the root for the base name.

General rules for this-

(a) In case of a open chain compound, the base chain is a straight carbon chain. The root for the base name is derived from the name of the alkane corresponding to this chain. In deriving the

root, the name ending of the alkane i.e. ane is changed or not depends on the nature of the function present on the parent part.

(b) In case of alicyclic compound, the root is derived from the name of the cycloalkane that constitutes the compound.

(c) The base chain of aromatic benzenoid compounds may contain a benzene or naphthalene or anthracene or biphenyl ring etc. The root for the base name of such compound is derived from the name of the ring it has.

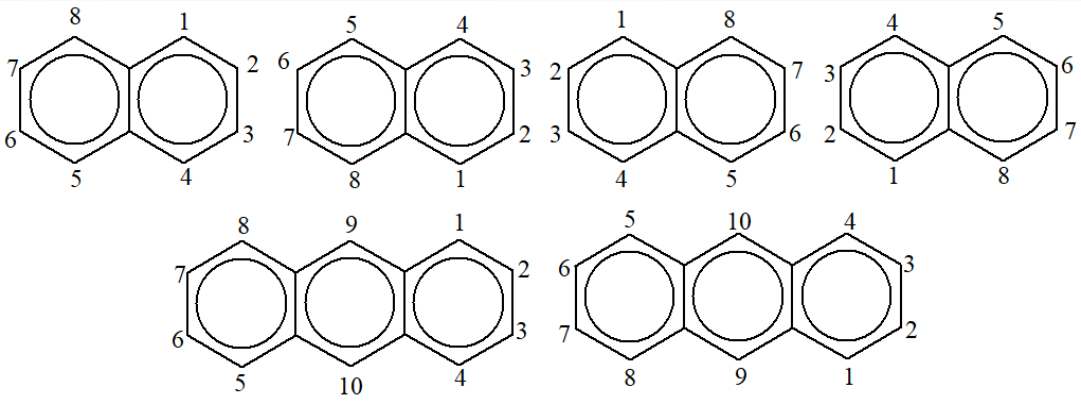
(d) The roots for the heterocyclic compounds are derived from their parent rings.

4. The suffix or prefix is placed after or before the root respectively to construct the base name.
5. Each of the carbon atoms in the base carbon chain is numbered sequentially.
6. The method of numbering is different for different types of chains-

(a) In case of open chain compounds, the numbering on the Cs of the base chain is done from the end of the carbon that will give the lowest number to the primary functional group. If the primary function is equidistant from both the ends, then the numbering starts from that end of the carbon which gives lowest sum of the numbers for those carbons which carry the substituents.

(b) In case of alicyclic compounds consisting of one ring and also for benzene derivatives, the numbering starts from that carbon which carries the primary substituent and to that direction which gives the lowest sum of the substituents.

(c) In case of polynuclear compounds, special numbering system is adopted. 'The lowest sum rule' is followed if there are substituents in the ring.



(d) A heterocyclic compound is numbered from the heteroatom.

4. Knowing the locant of the primary function, it is joined to the base name by a hyphen.

(a) If the position of the primary function on the base chain is unique, its locant is not indicated.
E.g. Keto group

(b) If the primary function is a part of the base chain and if the C atom of the function is numbered 1, then the locant of the primary function is not shown in its name.

This case arises when the primary function is -CHO, -COOH, -$CONH_2$, -COX etc.

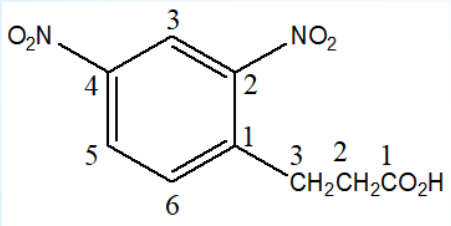
8. The names of the function other than primary and those of branches are denoted by prefixes to the base name. This rule has exceptions- (i) double bond, (ii) triple bond, (iii) two or more identical functions.

(a) Branches are always indicated by prefixes. To indicate a branch or function as a prefix, its locant is prefixed to its name by a hyphen and the combined part is joined to the base name.

(b) If the base name bears the locant of the primary function, the prefix is joined to the base name by a hyphen.

9. If there are two or more substituents, each of them is to be combined with its locant and then the combined parts are arranged either alphabetically or in order of increasing complexity and joined to each other by hyphens. The last combined part is joined to the base name without hyphen if the base name does not have any locant.

10. If a substituent on a base chain contains substituent groups, the substituent is called compound substituent. The substituted groups of a compound substituent are to be located; to do this numbering within the compound substituent is done and it starts from the point of the attachment of the substituent which is attached to the base chain is given number 1 and lowest sum rule is followed.



3-(2,4-dinitrophenyl) propanoic acid

A sequential procedure to name an organic compound-

- Select the parent part of the molecule.
- Select the base carbon chain and determine the root for the base name.
- Determine the primary function and decide the suffix or prefix to the root for constructing the base name.
- Number the carbons of the base carbon chain.
- Represent the base name with the locant of the primary function if necessary.
- Decide whether the IUPAC name of the given compound will be a one word name or not.
- Decide the name of the prefixes to the base name.
- Combine each of the prefixes with its locant.
- Assemble the prefixes with locants in the alphabetical order.
- Join the combined prefix to the base name and this will give the full IUPAC name.

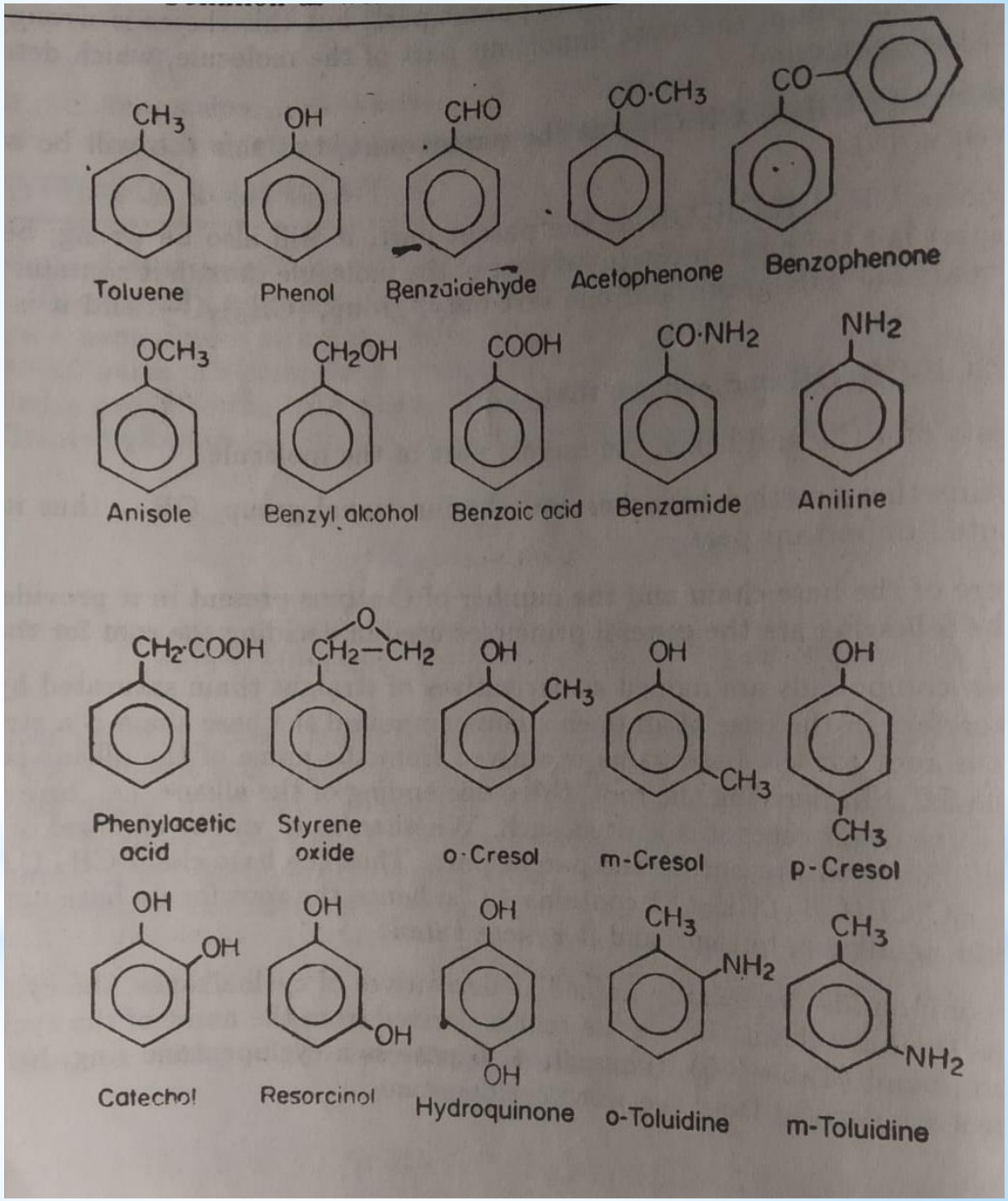
Table 1: List of some functions with prefixes and suffixes

Table 3.11 List of some functions with pre... (the order is followed up to $-\overset{|}{N}-$ group)

Graphic formula of the function	Name of the function	Prefix	Suffix	The process of forming* base names of acyclic compounds
$\overset{+}{N}R_3, \overset{+}{S}R_2$, etc.	Ammonium Sulphonium		-onium (halide, sulphide)	*Tryalkyl ammoniam*
OOH		hydroperoxyl	Hydroperoxide	
$-C(=O)-OH$	Carboxyl	Carboxy	oic acid or carboxylic acid	*Alkanoic* acid *Alkanecarboxylic* acid
$-SO_2OH$	Sulphonic acid	Sulpho	sulphonic acid	*Alkane*sulphonic acid
$-C(=O)-OR$	Ester	Alkoxycarbonyl* Alkyl	carbalkoxylate ...oate	*Alkane*carbalkoxylate **Alkyl** *alkano*ate
$-C(=O)-X$	Carbonyl halide	Haloformyl	oyl halide carbonyl halide	*Alkano*yl halide *Alkane*carbonyl halide
$-C(=O)-NH_2$	Amido	Carbamoyl	amide carboxamide	*Alkan*amide *Alkane*carboxamide
$-C\equiv N$	Carbonitrile	Cyano	nitrile	*Alkane*nitrile
$-\overset{+}{N}\equiv\overset{-}{C}$	Isonitrile	Isocyanide	carbylamine	*Alkyl*carbylamine
$-C(=O)-H$	Formyl	Formyl, oxo, aldo	al carboxaldehyde	*Alkan*al *Alkane*carboxaldehyde
$C(=O)C$	Keto	Oxo or Keto	one	*Alkan*one
$-OH$	Hydroxyl	Hydroxy	ol	*Alkan*ol
$-SH$	Mercapto	Mercapto	thiol	*Alkane*thiol
$-N-$	Amino	Amino	amine	*Alkan*amine *Alkyl*amine
$RO-$	Ether linkage	Alkoxy	alkane	**Alkoxy** *alkane* *Alkyl* ether
RSO_2-	Alkyl Sulphonyl	Alkyl Sulphonyl	sulphone	*Alkane*sulphone

Graphic formula of the function	Name of the function	Prefix	Suffix	The process of forming* base names of acyclic compounds
$C=C$	double bend	...	ene	*Alk*ene
$C\equiv C$	Triple bond	...	yne	*Alk*yne
$-Cl$	Chloro	Chloro	...	**Chloro***alkane*
$-Br$	Bromo	Bromo	...	**Bromo***alkane*
$-I$	Iodo	Iodo	...	**Iodo***alkane*
$-N=N-$	Azo	Azo	...	**Azo***alkane*
$-NO_2$	Nitro	Nitro	...	**Nitro***alkane*
$-NO$	Nitroso	Nitroso	...	**Nitroso***alkane*

Common as well as IUPAC names of some aromatic compounds



In cases of molecules with multiple functional groups, the functional group with highest priority will be the one which gives suffix to the name of the molecule.

Functional group priorities from highest to lowest:

-COOH, -SO_3H, -COOR, -COCl, -$CONH_2$ or -$CONR_2$, -CN, -CHO, -C=O, OH, SH, NH_2, NR_2, alkyne, alkene