SYSTEM OF NAMING HYDROCARBONS

The names of organic compounds are given in accordance with the International Union of Pure and Applied Chemistry (IUPAC) system of nomenclature. The procedure is as follows:

1. Find and name the longest unbranched, (continuous) carbon chain in the compound, this is taken as the backbone.
2. Number the longest chain from the end that gives the lowest numbers for the substituent groups attached.
3. Name the substituents, and assign numbers
4. Give the positions, (the **locant**), of the substituent groups. If there is more than one substituent group of the same type along the chain, the number of groups of that type is indicated by a prefix: di- (two), tri- (three), tetra- (four), penta- (five), and so forth; and each substituent will need a locant to place it on the chain, even if the substituents are on the same carbon of the chain.
5. Remember to alphabetize substituents.

Hint: *In chemical names, strings of numbers are separated by commas. A hyphen is placed between words and numbers.*

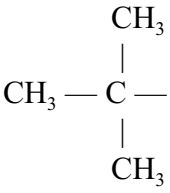
HYDROCARBONS

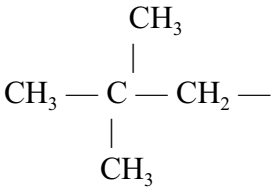
Compounds of carbon and hydrogen are called **hydrocarbons**. The compounds methane, ethane and propane are **alkanes**. They possess only single bonds and have the general formula C_nH_{2n+2}.

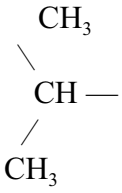
A series of compounds with similar chemical properties, in which members differ from one another by the possession of an additional CH_2 group, is called a **homologous series**. The first twelve members of the unbranched-chain alkane series are given in the table below:

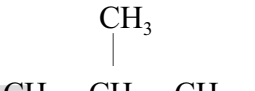
Name	*Formula*
Methane	CH_4
Ethane	C_2H_6
Propane	C_3H_8
Butane	C_4H_{10}
Pentane	C_5H_{12}
Hexane	C_6H_{14}
Heptane	C_7H_{16}
Octane	C_8H_{18}
Nonane	C_9H_{20}
Decane	$C_{10}H_{22}$
Undecane	$C_{11}H_{24}$
Dodecane	$C_{12}H_{26}$

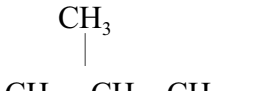
In general, a group that is formed by removing a hydrogen atom from an alkane is called an **alkyl group.** The names for alkyl groups are derived by dropping the *-ane* ending from the name of the parent alkane and adding *-yl*. For example, the groups of atoms CH_{3}—, C_2H_5— and C_nH_{2n+1}— are called methyl, ethyl and alkyl groups.
You should also memorize the following common structures:


t-butyl


neopentyl


isopropyl


sec-butyl


isobutyl

Unsaturated Hydrocarbons

Alkanes are said to be **saturated** hydrocarbons as they contain only single bonds between carbon atoms. Alkenes and alkynes are **unsaturated** hydrocarbons; they contain multiple bonds between carbon atoms.
The homologous series alkenes have the general formula C_nH_{2n}, where as alkynes contain one or more triple bonds and have the general formula C_nH_{2n-2}. Alkanes, alkenes and alkynes are classified as **aliphatic** hydrocarbons. Aliphatic means 'fatty' in Greek, the connection being that fats contain large alkyl groups, e.g. $C_{15}H_{31}$ — .
In naming alkenes and alkynes, the positions of the multiple bonds must be stated. Compounds with more than one multiple bond are named using di-, tri-, etc. to indicate the number of the multiple bond as well as locants to show where they are.
Examples
But-1-ene But-2-ene Buta-1,3-diene 2-methylbut-1-ene pent-1,3-diyne

Note: The existence of geometrical isomerism: .:nomenclature requires cis– and trans– identification in alkenes

Alicylic Hydrocarbons (Cycloalkanes)

Alicylic hydrocarbons contain rings of carbon atoms, they are given the prefix cyclo — . They have the general formula $C_nH_{2n.}$
Examples


cyclopropane cyclobutane cyclohexene


methylcyclohexane 1,2-dimethylcyclohexane

Cycloalkane structures are sometimes drawn as simple polygons in which each corner of the polygon represents a CH_2 group.

Carbon rings containing fewer than five carbon atoms are strained because the C— C— C bond angle in the smaller rings must be less than the 109.5^0 tetrahedral angle. The amount of strain increases as the rings get smaller. In cyclopropane, which has the shape of an equilateral triangle, the angle is only 60^0; this molecule is therefore much more reactive than either propane, or cyclohexane, which has no ring strain.

Aromatic Hydrocarbons

These are related to benzene, C_6H_6. The first benzene compounds to be isolated had pleasant aromas, and gave this group of hydrocarbons their name. The English language definition of aromatic is "of or having an aroma, smelling sweet or spicy, fragrant or pungent." (The modern chemical definition of aromatic has to do with the cyclic delocalized bonding in a molecule rather than its odour.) Aromatic hydrocarbons are related to benzene, they are called **arenes**.
The group C_6H_5 — is called a **phenyl** group.
Substituted arenes are generally named as derivatives of benzene, so benzene forms the root of the name.
With more than one substituent, locants are used to show where they are attached. The ring is numbered from where the principal group is attached at carbon 1.

Examples

methylbenzene chlorobenzene benzene-1,2-diol 1,2-dimethylbenzene

toluene aniline phenol benzoic acid benzaldehyde (benzenecarbaldehyde)

2-aminobenzenecarbaldehyde 2-nitrophenol Benzenesulphonic acid

methyl benzene
(not: phenylmethane ∵most of its reactions are those of C_6H_6 and not of CH_4)

Phenylethene
(Not: ethenylbenzene ∵main reactions are those of ethene rather than those of benzene)

Functional Groups

The double bond in alkenes and the triple bond in alkynes is responsible for most of the chemical reactions of these compounds. Thus, the multiple bond is referred to as the functional group of the alkenes and the alkynes. The reactions of a homologous series depend on the functional group.

Halogenoalkanes (Haloalkanes)

These have the formula, $C_nH_{2n+1}X$, shortened to RX where R is an alkyl group and X is a halogen. The prefixes fluoro— , chloro— , bromo— , and iodo are used, together with locants where necessary, to indicate the position of the halogen atoms or atoms on the chain or ring.
The prefixes di— , tri– , tetra — , etc. are used as usual to indicate how many atoms of each halogen are present.
When a compound contains two or more different halogens the substituents are given in alphabetical order.

Examples

chloromethane 2-chloro-2-methylpropane 1,1-dichloroethane

3-chloro-2-iodohexane 1,4-dichlorocyclohexane 1-bromoprop-1-ene

Alcohols (Alkanols)

These are compounds with the functional group — OH, a hydroxyl group. They are named by taking the name of the alkane with the same number of carbon atoms and changing the ending from — ane to — anol.
A locant is needed to tell us where on the chain the — OH group is situated. If there is more than one — OH group we use di— , tri —, tetra — , etc. to say how many — OH groups there are. We will also need locants to say where they are.
— OH has priority over a multiple bond when numbering the chain.

Examples
methanol Ethanol propan-1-ol propan-2-ol propane-1,2,3-triol

ethane-1,2-diol 2-hydroxypropanoic acid propane-2,2-diol
(∵– OH is not the principal group,
the – COOH group is.)

Classification of alcohols

Alcohols are classified as primary (1^0), secondary (2^0) or tertiary (3^0) according to how many other groups (R) are bonded to the carbon that has the — OH group.
In a primary alcohol, this carbon has one R group: propan-1-ol

In a secondary alcohol, the — OH group is attached to a carbon with two R groups:

Tertiary alcohols have three R groups attached to the carbon which is bonded to the —OH:

Molecules with two hydroxyl groups are called **diols** (or **glycols**) and are named with the suffix **-diol**. Two numbers are necessary to locate the two functional groups. Diols with hydroxyl groups on adjacent carbons referred to as **vicinal**, and diols with hydroxyl groups on the same carbon are **geminal**. Geminal diols (also called **hydrates**) are not commonly observed because they spontaneously lose water (**dehydrate**) to produce carbonyl compounds.

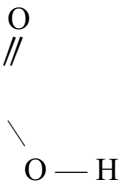
Ethers R — O— R′

These compounds contain two hydrocarbon groups bonded to one oxygen. In the IUPAC system, ethers are named as derivatives of alkanes, and the larger alkyl group is chosen as the backbone. The ether functionality is specified as an **alkoxy-** prefix, indicating the presence of an ether (– oxy), and the corresponding smaller alkyl group (alk—). The chain is numbered to give the ether the lowest position. Common names for ethers are frequently used. They are derived by naming the two alkyl groups in alphabetical order and adding the word ether. The generic term "ether" refers to diethyl ether, a commonly used solvent.

For cyclic ethers, numbering of the ring begins at the oxygen and proceeds to provide the lowest numbers for the substituents. Three -membered rings are termed **oxiranes** by IUPAC, although they are commonly called **epoxides**

methoxyethane oxirane 2-methyloxirane tetrahydrofuran (THF)

Carboxylic Acids (Alkanoic Acids)

The carboxylic acid functional group is 

sometimes written as — COOH or as — CO_2H. Carboxylic acids are named using the suffix — oic acid. The carbon atom of the functional group is counted as part of the carbon chain of the root.. They are named by taking the alkane with the same number of carbon atoms and changing the ending from — ane to — anoic acid
Where there are substituents or side chains on the carbon chain, they are numbered using locants, counting from the carbon of the carboxylic acid as the number one.

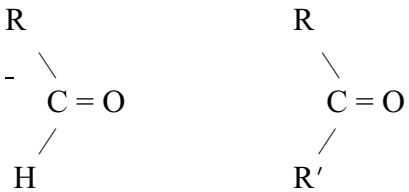
Examples
methanoic acid ethanoic acid pent-2-enoic acid

2-bromopropanoic acid benzoic acid (benzenecarboxylic acid)

When the functional group is attached to a benzene ring, the suffix — carboxylic acid is used and the carbon of the functional group is not counted as part of the root:

benzene-1,4-dicarboxylic acid (terephthalic acid) 3-nitro-benzoic acid

Aldehydes and Ketones (Alkanals and Alkanones)



Aldehyde Ketone

The R group in both aldehydes and ketones may be alkyl or aryl.
Aldehydes are named using the suffix — al where the aldehyde is the principal group and the prefix oxo— when it is not. (Oxoethanoic acid: as the aldehyde is not the principal group, but the acid group is.)

The carbon of the aldehyde functional group is counted as part of the carbon chain of the root. The aldehyde group can only occur at the end of a chain, so locants are not needed

When the ketone is the principal group ketones are named using the suffix — one. When it is not the principal group, it shares with aldehydes the prefix oxo— . It is not possible to confuse yourself, because in ketones the carbonyl group must occur within the chain, however in aldehydes it must come at the end. (2-oxopropanoic acid)

As with aldehydes, the carbon atom of the ketone functional group is counted as part of the root. Locants are not needed in propanone or in butanone because there is no possible ambiguity about the position of the carbonyl group, however, the position of the carbonyl group in all other ketones is indicated by a locant preceding the suffix — one.
Carbons near a carbonyl can be designated as α,(adjacent) or β, γ, etc. (moving farther away from the carbonyl.

Examples

methanal	ethanal	benzenecarbaldehyde	2,2-dichloropropanal
propanone	butanone	cyclohexanone	phenylethanone
pentan-3-one	iodopropanone	tri-iodo-ethanal	phenylethanal

Amines

Amines are derivatives of ammonia. They are classified as primary (1^0), secondary (2^0) or tertiary (3^0) amines according to the number of alkyl or aryl groups attached to the nitrogen atom. Amines are named by replacing the final "e"in the alkane and replacing it using the suffix — amine, secondary and tertiary amines are named as di— and tri— substituted derivatives:

Example

ethanamine	dimethylamine	trimethylamine	phenylamine (aniline)

If the amine is not the principal group, the prefix amino— is used:
Example

aminoethanoic acid 4-aminophenol 4-aminohept-2-en-1-ol

This notation may also be used to distinguish between isomers:

1-aminopropane 2-aminopropane

When there are two or more substituents they are written in alphabetical order:

methylpropylamine

An aromatic amine has the nitrogen atom directly attached to the aromatic ring:
phenylamine 4-methyl-phenylamine

In phenylmethylamine, $(C_6H_5)CH_2NH_2$, (or benzylamine), the nitrogen atom is not directly attached to the ring, thus it is not an aromatic amine; it is a phenyl-substituted alkylamine.

When other alkyl groups are substituted to the nitrogen: these substituents are listed in alphabetical order, where N— indicates the alkyl groups bonded to the nitrogen, rather than the benzene ring:

N-methylphenylamine	N,N-dimethylphenylamine
$C_6H_5NHCH_3$	$C_6H_5N(CH_3)_2$

In quaternary (4^0) ammonium compounds, the nitrogen is tetravalent. They are named as alkyl-substituted ammonium salts:

tetramethylammonium iodide	ethyldimethylpropylammonium bromide
$(CH_3)_4\ N^{+1}I^{-1}$	$(C_2H_5)(CH_3)_2(C_3H_7)N^{+1}Br^{-1}$

Nitriles — C ≡N

This functional group can only occur at the end of a carbon chain. The — C ≡N group is named using the suffix — nitrile when it is the principal group and the prefix cyano— when it is not. When the suffix – nitrile is used, the carbon of the functional group is counted as part of the root:

$CH_3C{\equiv}N$	$CH_3CH_2C{\equiv}N$	2-hydroxypropanenitrile
ethanenitrile	propanenitrile	

Where the — C ≡N is attached to the benzene ring, the carbon of the functional group is not counted as part of the root and the suffix – carbonitrile is used:

(C_6H_5) - C≡N
benzenecarbonitrile

Amide linkage: R — C(=O) — N — R'

where R and R' are alkyl groups, it is the key functional group in the structures of proteins.

Esters R— C(=O) — O — R'

Esters are compounds in which the H atom of a carboxylic acid is replaced by a hydrocarbon (alkyl) group.
Esters are named by using first the group from which the alcohol is derived and then the group from which the acid is derived, and replacing the -oic suffix of the acid name with — oate suffix.