CHM 102

Classification of organic compounds:-

Organic compounds constitute about 90% of all compounds. It is necessary to classify them into categories. Depending upon the arrangement of carbon atoms in their structure, organic compounds are broadly categorized into

(1) Acyclic or open chain compounds
(2) Cyclic or closed chain compounds

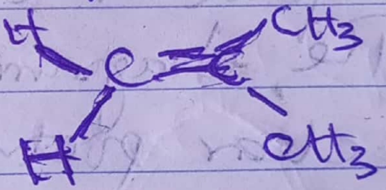
The diagram below ~~shows~~ give a clear picture about the classification organic compounds.

- Organic Compounds
  - Cyclic or closed chain
    - Homocyclic or Carbocyclic compounds
      - Alicyclic compounds
      - Aromatic compounds
        - Benzenoid compounds
        - Non-benzenoid compounds
    - Heterocyclic compounds
  - Acyclic or open chain

(1) Acyclic or open chain compounds

The carbon atoms are present in the form of an open chain. This chain may either be a straight chain or a branched chain. They are initially known as Aliphatic compounds because they were derived from either animal or vegetable fats.

Examples are n-propane $CH_3-CH_2-CH_3$ with is a straight chain compound and Isobutylene which is a branched chain compound



2 Cyclic or Closed Chain Compounds

They are marked by the presence of one or more closed chains or ring of atoms in their structure. Depending on whether there is a presence of any other atom apart from carbon in the construction of the ring, they are further classified as:

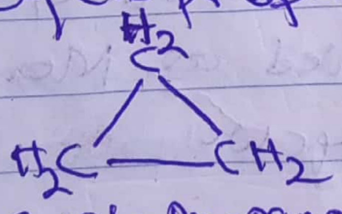
(i) Homocyclic or Carbocyclic compounds

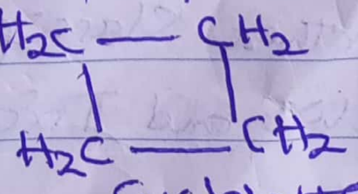
(ii) Heterocyclic Compounds.

Homocyclic or Carbocyclic compounds
The rings in these compounds are entirely made up of Carbon atoms. No other atom is present in the ring skeleton. They are further divided into two sub-classes:

(a) Alicyclic compounds
(b) Aromatic compounds

~~Aromatic~~ Alicyclic Compounds
Their name is attributed to their resemblance to Aliphatic compounds in their properties. Examples are Cyclopropane, Cyclobutane etc.


cyclopropane


Cyclobutane

Aromatic Compounds
These are cyclic unsaturated

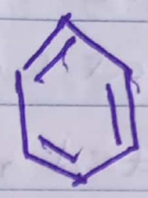
Compounds. Their name was derive from the Greek word Aroma which means "fragrant smell" since most of these compounds bear a pleasant smell. These are further classified into two types

(1) Benzenoid Aromatic ~~com~~ Compounds
(2) Non- Benzenoid Aromatic compounds

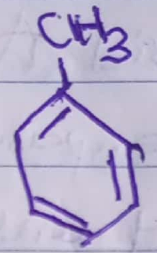
Benzenoid Aromatic Compounds
They are Characterized by the presence of one or more fused ~~or~~ isolated benzene rings as well as their derivatives in their structure. Depending upon the number of benzene rings that are fused together in their structure, they can be further classified as Monocyclic, Bicyclic, and Tricyclic

Monocyclic compounds
They are characterized by the presence of a single benzene ring to

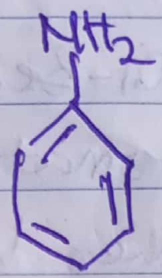
which other groups are attached. Examples are benzene, toluene, Aniline, ortho-xylene, meta-xylene, para-xylene.



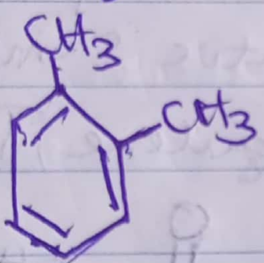
Benzene



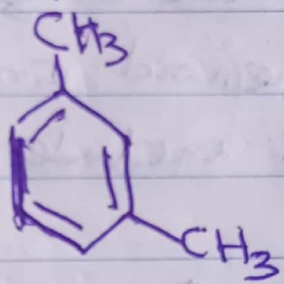
Toluene



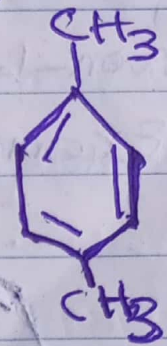
Aniline



ortho-xylene



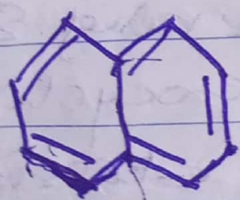
meta-xylene



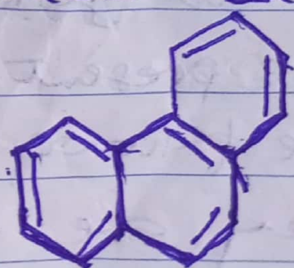
Para-xylene

Bicyclic and Tricyclic Compounds

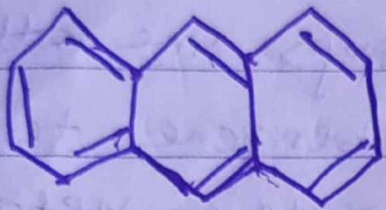
These are characterized by the presence of two or more rings in their Structure. Examples include Naphthalene, Phenanthrene, Anthracene.



Naphthalene



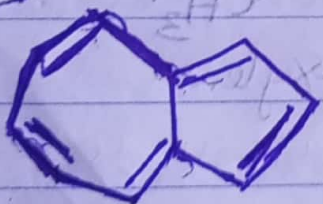
Phenanthrene



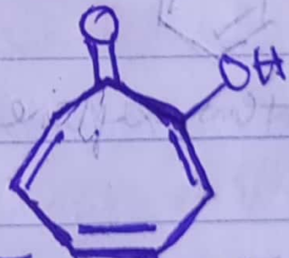
Anthracene

Non-Benzenoid Aromatic Compounds

Aromatic compounds that contain other highly unsaturated rings in place of the benzene ring are called non-benzenoid aromatic compounds. Examples include Azulene, Tropolone etc.



Azulene



Tropolone

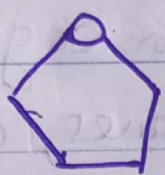
Heterocyclic Compounds

When one or more heteroatoms such as oxygen, nitrogen, sulphur, boron etc are present in the ring such compounds are known as heterocyclic compounds. They are further classified into two types.

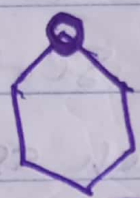
(1) Alicyclic heterocyclic compounds
(2) Aromatic heterocyclic compounds

Alicyclic heterocyclic compounds

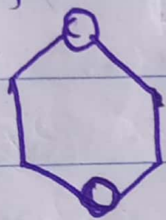
There are aliphatic heterocyclic compounds that contain one or more heteroatoms in their rings.



Tetrahydrofuran



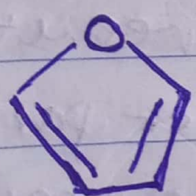
Tetrahydropyran



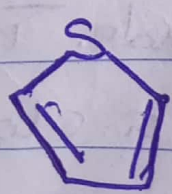
1,4 dioxane

Aromatic heterocyclic compounds

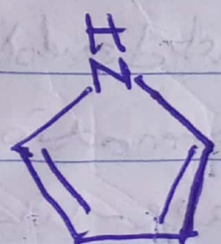
Aromatic heterocyclic compounds are compounds that contain one or more heteroatoms in their ring skeleton.



Furan



Thiophene



Pyrrole

Homologous Series

A group or series of organic compounds in which each member contains the same characteristic functional group and differs from each other by a fixed unit (CH_2) form a homologous series and therefore its members are known as homologous. There are a number of homologous series in organic chemistry such as alkanes, alkenes, alkynes, haloalkanes, alkanols, amines, etc.

Fullerene

Fullerene is an allotrope of carbon whereby its molecules consist of carbon atoms that are connected by single and double bonds. This results in the formation of a closed or partially closed cage-like structure (a mesh consisting of fused rings) that further contain several atoms. The fullerene molecule in this form can either have a hollow sphere, be an ellipsoid, tube, or it can also have many other different shapes and sizes. When the carbon molecules are arranged in a cylindrical form they usually form a tube-like structure known as carbon nanotubes.

Structure of Fullerene

Fullerene in their natural form tend to be highly symmetrical. Their structure is quite similar to that of graphite and is made up of sheet of connected hexagonal rings (cage structure). However they have pentagonal and sometimes heptagonal rings which do not allow the sheet to become planar. They are often referred to as buckyballs and buckytubes depending on their shape. Cylindrical fullerene are referred to as nanotubes. In any case, there is an infinite number of fullerenes that can exist. Fullerenes can be C_{60}, C_{70}, C_{80} and C_{90} existing in various forms. This depends largely on the number of carbon atoms present on the molecule.

Properties of Fullerene

a Physical properties of fullerene

(1) its behaviour and structure depend on the temperature. As the temperature is increased fullerene gets converted into C_{70}.

(2) Fullerene structure can change under different pressures.

(3) Fullerene has an ionization enthalpy of 7.61 electron volts.

4 its electron affinity is 2.6 to 2.8 electron volts.

chemical properties

(1) Fullerene are stable, but not totally unreactive.

(2) In chemical reactions, fullerene can act as an electrophile.

(3) it acts as an electron-accepting group and is characterized as an

oxidizing agent.

(4) Fullerenes when doped or crystallized with alkali or alkaline earth metals it showcases superconductivity properties

(5) Fullerene is ferromagnetic

(6) It is soluble in organic solvents such as toluene, chlorobenzene, and 1,2,3-trichloropropane

Types of Fullerene

Fullerenes exist in two major families depending on some distinct properties and application. The two families include the closed buckyballs and the open-ended cylindrical carbon nanotubes.

(1) Buckyball Cluster: These fullerenes are basically unsaturated versions of dodecahedra. These are also some of the smallest members of fullerene group. Its structural formula is C_{20}

(2) Buckminster fullerene: Buckminster-fullerene is the smallest fullerene

molecule. It contains pentagonal and hexagonal rings and no two pentagons will share an edge. Buckminster-fullerene exists in C60 form is the most common in terms of natural occurrence. The structure of buckminsterfullerene is a truncated icosahedron similar to that of a football.

(3) Linked Ball and Chain Dimer: In this type of fullerene, two buckyballs are mainly linked by a carbon chain. There are also other fullerenes such as heterofullerenes which have heteroatoms substituting carbons in cage or tube-shaped structures. There is also metallofullerene whose molecule is composed of a metal atom trapped inside a fullerene cage.

4. Carbon Nanotubes: This type of fullerene has cylindrical or hollow tubes of very small dimensions; they are mostly a few nanometers wide. However, they

can also be micrometre to several millimetres in length. Carbon nanotubes can be both closed and open-ended. As a result of their unique molecular structure, they have some unique macroscopic properties. Some of them include high tensile strength and electrical conductivity, high ductility and heat conductivity including relative chemical inactivity.

Production of Fullerene

Fullerene preparation starts with the production of fullerene-rich soot. The method that was used to produce fullerene involved sending a large electric current between two nearby graphite electrodes in an inert atmosphere. The electric arc that was created vaporized the carbon into a plasma that then cooled into the sooty residue.

Alternatively, the soot can also be produced by laser ablation of graphite or pyrolysis of aromatic hydrocarbons. combustion is the most efficient process that was used. These methods usually resulted in the production of different fullerenes in various mixtures and other forms of carbon. So the fullerenes are then basically extracted from soot using appropriate organic solvents, and the mixture is usually separated by chromatography.

Uses of fullerenes

(1) fullerenes are used in the medical field as light-activated antimicrobial agents.

(2) It is also used in several biomedical applications including the design of high-performance MRI contrast agents, X-ray imaging contrast agents, photodynamic therapy and drug and gene delivery.

(3) Buckminster fullerene is used in drug delivery systems, in lubricants and

as catalyst

(4) it is also used as a conductor

(5) Some types of fullerene can be used as an absorbent for gases

(6) It is used in making cosmetic products.

(7) C_{60} based films are used for photovoltaic applications.

(8) Fullerenes are used in making carbon nanotubes based fabrics and fibres.