

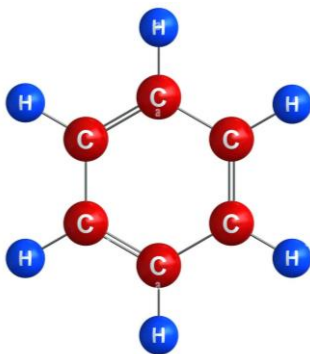
BENZENE AND ITS DERIVATIVES

INTRODUCTION:-

DEFINATION

Benzene and all those compounds which resemble benzene in their chemical behavior are termed as aromatic. Benzene is an aromatic compound having molecular formulae C_6H_6 .

It contains 6 carbon atoms and 6 hydrogen atoms and three conjugate double bonds. Aromatic compounds having one or more benzene rings in their molecule are called benzenoid compounds. For e.g. benzene, toluene, phenol, etc.

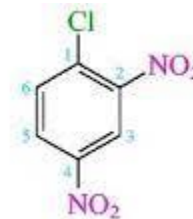
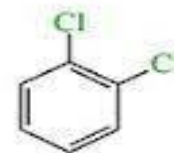
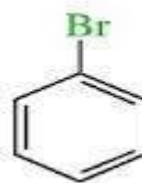


Molecular formula of benzene- C_6H_6

Molecular mass- 78.11 g/m

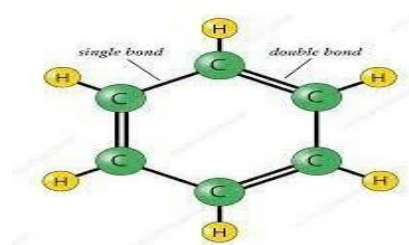
NOMENCLATURE OF DERIVATIVES OF BENZENE

Monosubstituted benzene derivative	Disubstituted benzene derivative	Polysubstituted benzene derivative
------------------------------------	----------------------------------	------------------------------------



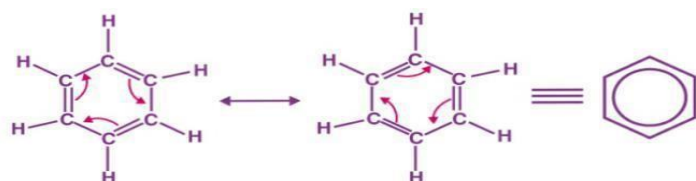
KEKULES STRUCTURE OF BENZENE

In 1865 August Kekulé suggested an answer to the dilemma regarding the structure of benzene. He proposed that, in benzene



RESONANCE STRUCTURE OF BENZENE

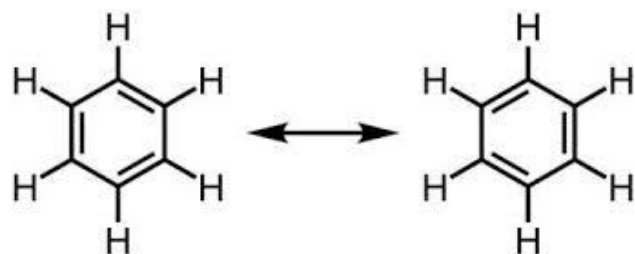
The oscillating double bonds in the benzene ring are explained with the help of resonance structures as per valence bond



theory. One of the two sp^2 hybridized orbitals of one atom

overlaps with the sp^2 orbital of adjacent carbon atom forming six C-C sigma bonds. Other left sp^2 hybridized orbitals combine with s orbital of hydrogen to form six C-H sigma bonds.

HUCKEL'S RULE



in an **aromatic** system can be determined by the following algorithm:

$$N=4n+2 \quad (17.5.1) \quad (17.5.1) \quad N=4n+2$$

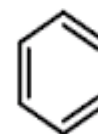
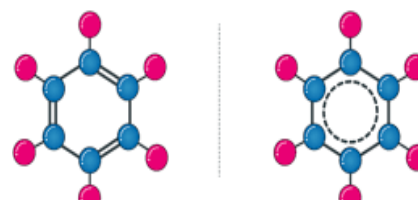
where n is an integer.

The number of π electrons in an **antiaromatic** system can be determined by the following algorithm:

$$N=4n \quad (17.5.2) \quad (17.5.2) \quad N=4n$$

where n is an integer.

If a compound does not have a continuous ring of conjugated p orbitals in a planar conformation, then it is nonaromatic



Aromatic

6 π electrons - $n = 1$, $4n+2 = 6$

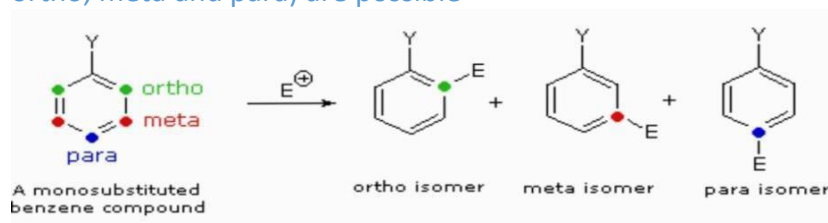
Satisfies the **Hückel's rule**

In 1931,

German chemist and physicist Erich Hückel proposed a theory to help determine if a planar ring molecule would have aromatic properties.

SUBSTITUENTS AN EFFECT OF SUBSTITUENTS ON REACTIVITY AND ORIENTATION OF MONO SUBSTITUED BENZENE

Benzene has 6 hydrogen which all are equal. If they replace 2 or 3 substituents, then it's give a di and poly substituted derivative. when mono substituent benzene is converted into di-substituted in derivative, then three isomers (it's known as ortho, meta and para) are possible



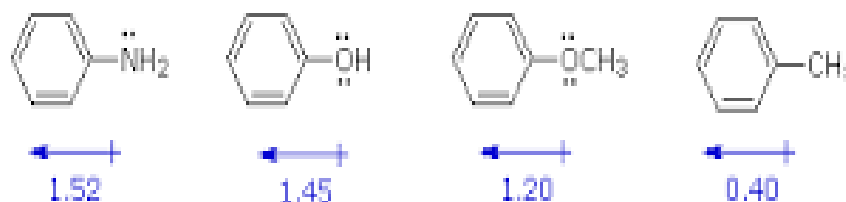
On the basis of directive influence of groups, all the groups can be divided into following two classes:

A) Ortho-para directing groups: These groups direct the incoming groups to the ortho and para positions. For example, Alkyl(R), phenyl(-C₆H₅), Halogen (-Cl, -Br F I), hydroxyl(-OH), amino(-NH₂) etc.

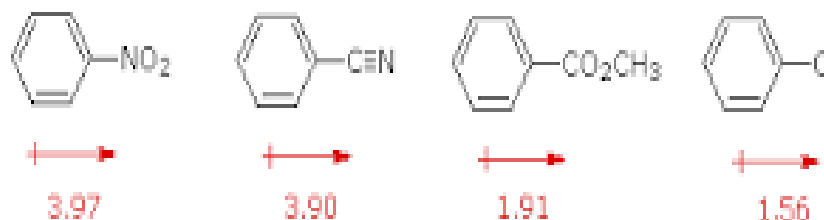
B) Meta directing groups: this groups direct the incoming groups to the meta position. For example: trialkyl ammonium ion (N+R₃), nitro(NO₂), Cyano(-CN), aldehyde (-CHO), Carboxylic (-COOH). etc

Effect of substituents on reactivity: ortho and para directing groups (except alkyl and phenyl) contains one or more pair of electrons on the atom this electrons interact with the π -electrons of the Benzene and increase the electron density.

Activating Substituents

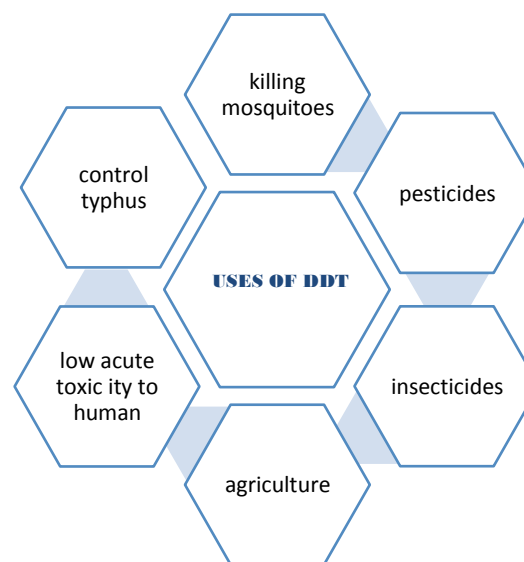
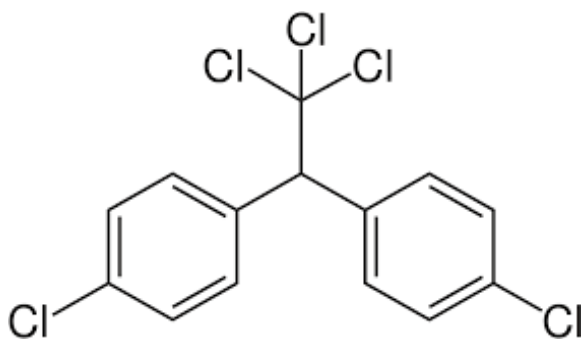


Deactivating Substituents

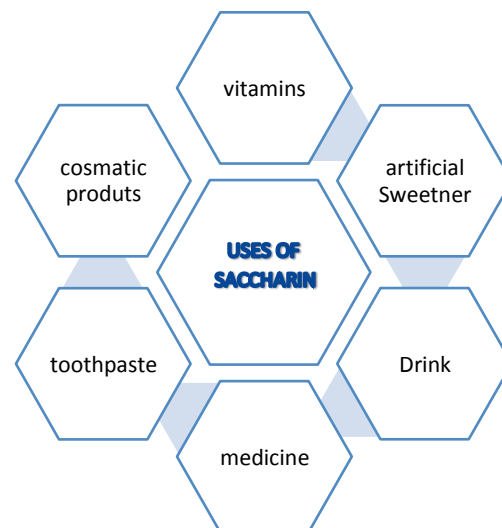
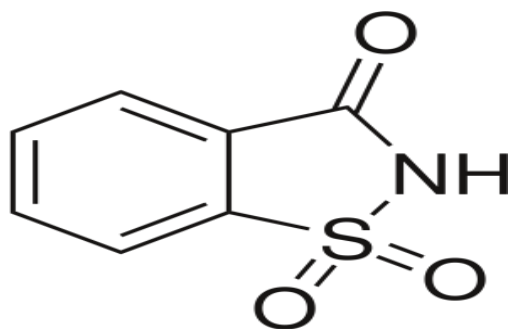


STRUCTURE AND USES

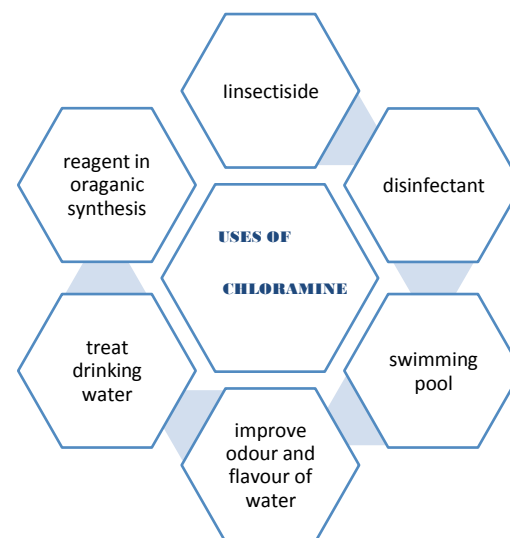
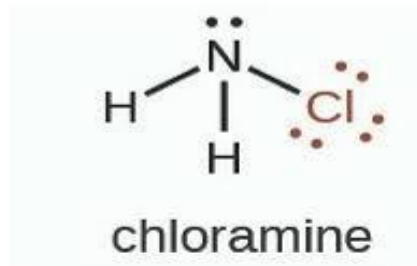
1. Dichlorodiphenyltrichloroethane (DDT)



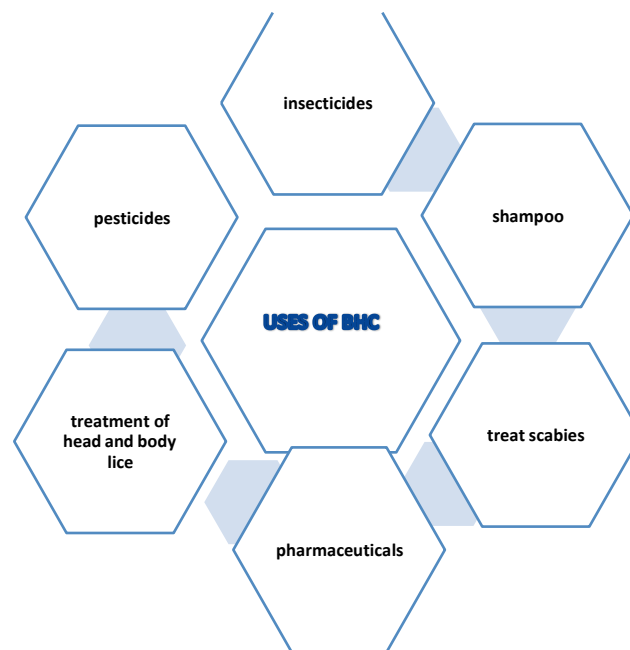
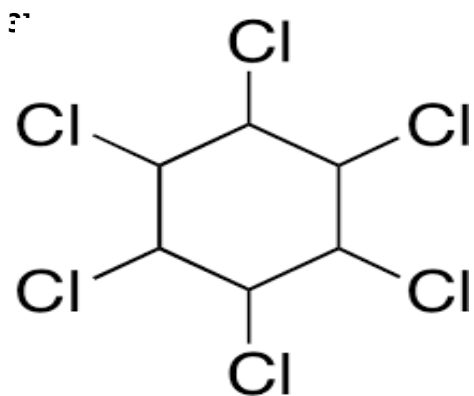
2. SACCHARIN



3. CHLORAMINE



4. Benzene Hexachloride (BHC)



REFERENCES:

1. ARUN BAHL,B.S BAHL(textbook of organic chemistry)S .chand Publications page no-598-617
2. VARUN ARORA,PRAGI ARORA,SAPNA K.SHAH,ARVIND R.UMARKAR(pharmaceutical organic chemistry)PV publication
3. JERRY MARCH (textbook of organic chemistry)wiley inerscience publication page no. 501 to 521
4. <https://chem.libretexts.org/>
5. [https://en.wikipedia.org/wiki/Benzene ups_and_Nomenclature](https://en.wikipedia.org/wiki/Benzene_ups_and_Nomenclature)

PREPARED BY:

1. Nikita Gholap(22)
2. Kaveri Dagale(12)
- 3.Dhanashree Dama(13)
4. Pritam Garbade(19)
5. Divyata Ghagas(20)

GUIDED BY:

Mrs. Chiwadshetti N.S(Asst.Professor
spcop,otur

DEPARTMENT : Pharmaceutical chemistry

SUBJECT : pharmaceutical organic chemistry

TOPIC NAME: Benzene and its Derivitives

ACADEMIC YEAR : 2021-22