PHARMACEUTICAL ORGANIC CHEMISTRY-II- BP301T

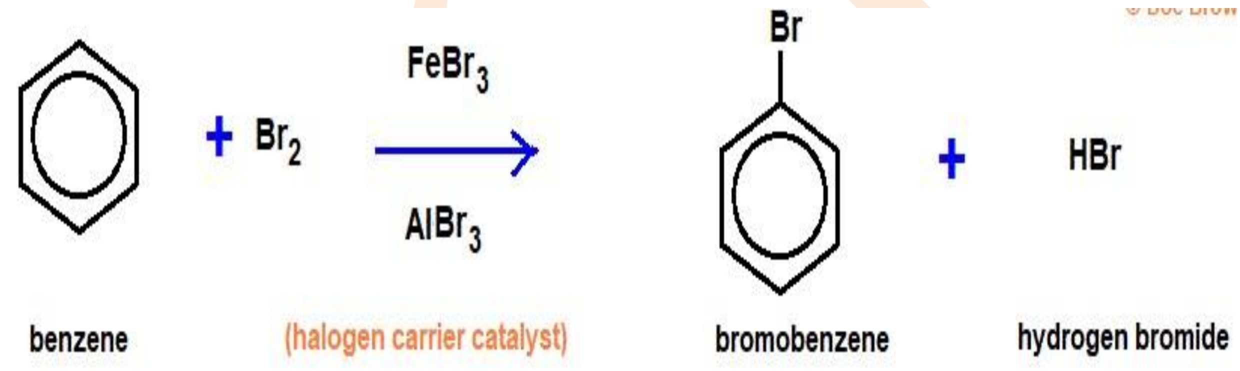
UNIT: 1 Benzene and its derivatives

CLASS:2

TOPIC: Structure of Benzene

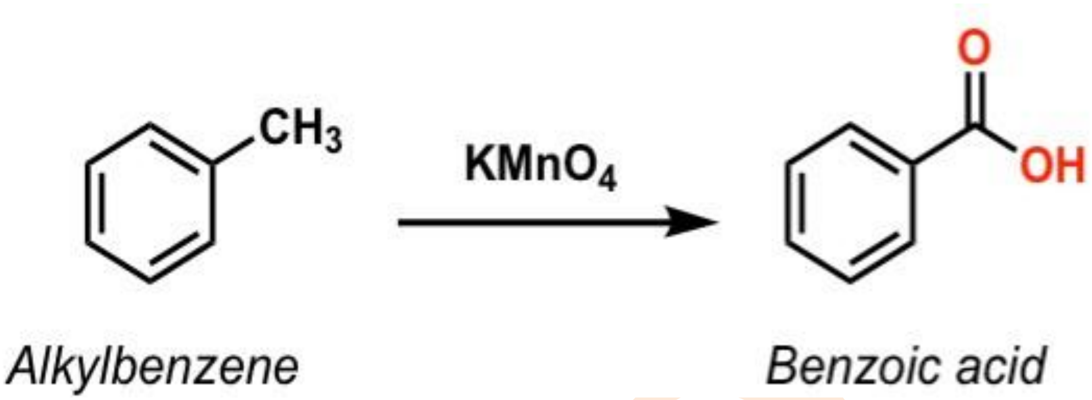
Bromination of benzene:

The bromination of benzene is an example of an electrophilic aromatic substitution reaction. In this reaction, the electrophile (bromine) forms a sigma bond to the benzene ring, yielding an intermediate. Then, a proton is removed from the intermediate to form a substituted benzene ring.



Benzene with $KmnO_4$:

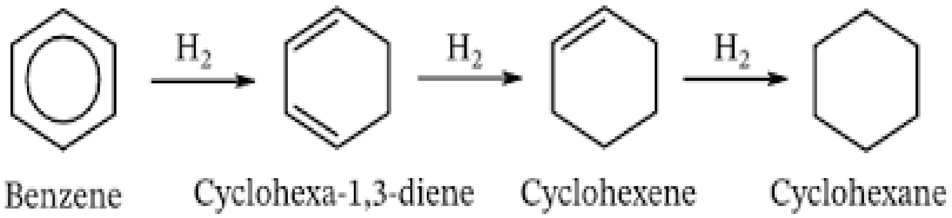
Alkyl benzenes when treated with KMnO4 undergo oxidation to give benzoic acid. The $KMnO_4$ acts as an oxidizing agent. Oxidation Reaction refers to a reaction in which either the addition of Oxygen takes place or the removal of Hydrogen takes place.



Benzene with Water:

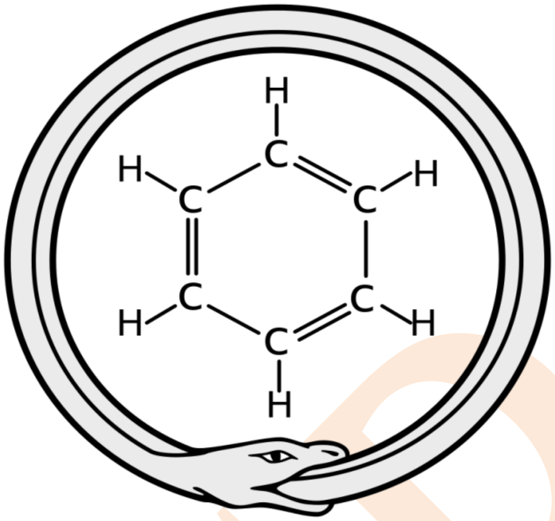
Benzene is insoluble in water according to the reasons mentioned below: Benzene is a symmetrical compound and thus it has zero dipole moment and is non-polar, while water is a polar compound possessing dipole moment, therefore, due to variable polarity, benzene and water cannot mix.

Benzene is reacting with 3 molecules of hydrogen to form Cyclo Hexane



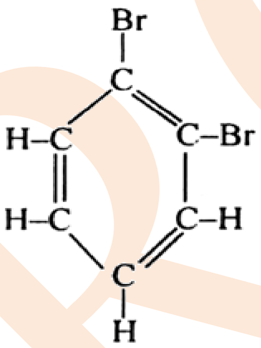
Kekule structure of benzene:

Kekules most famous work was on the structure of benzene. In 1865 Kekules published a paper in French suggesting that the structure contained a six-member ring of carbon atoms with alternating single and double bonds.

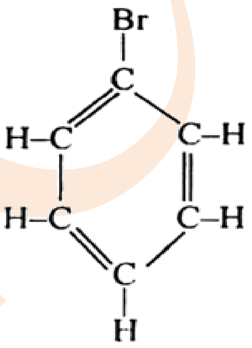


Objections:

Kekule's structure does not explain the extra ordinary stable nature of benzene molecule and its lack of reactivity towards addition reactions, resistance towards oxidation. Equivalence of all the carbon-carbon bond lengths in benzene.



(I)
(Presence of double bond between two adjacent carbon atoms)



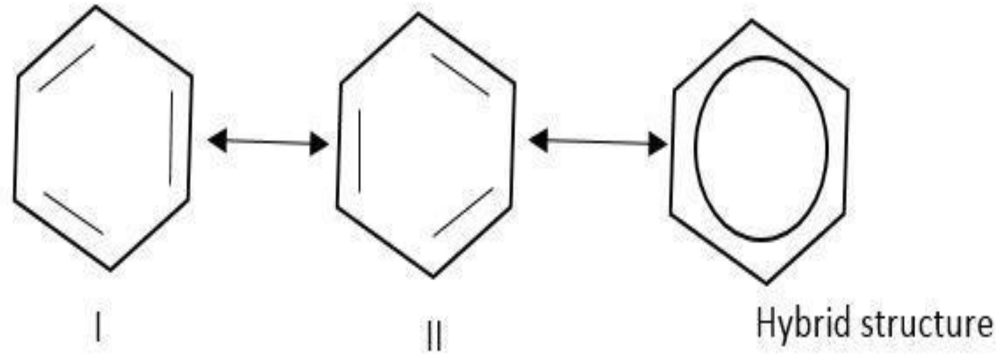
(II)
(Presence of single bond between two adjacent carbon atoms)

Resonance:

The phenomenon in which two or more structures can be written for a substance which involves identical position of atom is known as resonance.

The actual structure of the molecule is said to be resonance hybrid of various possible alternative structures.

The benzene molecule is stabilized by resonance, the pi electrons are delocalized around the ring structure. This delocalization causes each carbon-carbon bond to have a bond order of 1.5, implying that they are stronger than regular C-C sigma bonds.



S.NO	Bond	Bond Length
1	C-C	1.54 A^{o}
2	C=C	1.34 A^{o}
3	Benzene	1.40 A^{o}

<u>Molecular orbital structure of benzene:</u>

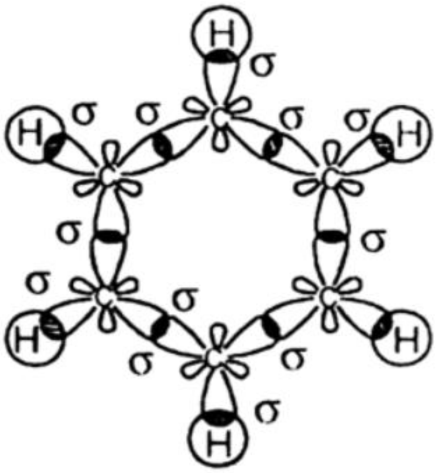
The structure of benzene is best described in terms of molecular orbital theory.

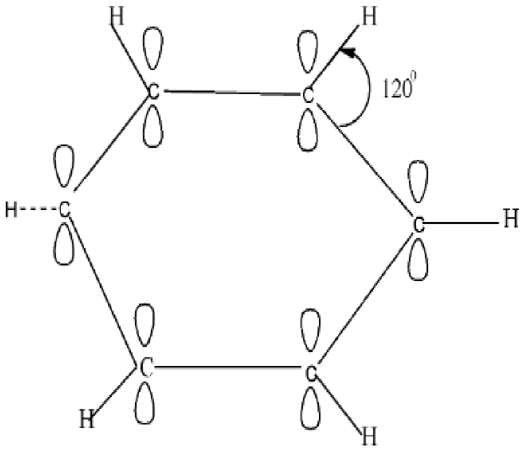
All 6 carbons in benzene SPd hybridization. The SP^{2} hybrid orbital overlap with each other and with S orbital of the 6 hydrogen atoms to form C-C and C-H bonds.

Benzene has a planar hexagonal structure in which all the carbon atoms are sp2 hybridized, and all the carbon-carbon bonds are equal in length. As shown below, the remaining cyclic array of six p-orbital's (one on each carbon) overlap to generate six molecular orbitals, three bonding and three anti bonding.

Since the sigma bond result from the overlap of the planar SP^{2} orbital.

All carbon and hydrogen atoms in benzene lie in same plane all sigma bonds in benzene lie in one plane and all bond angles are 120^{0}

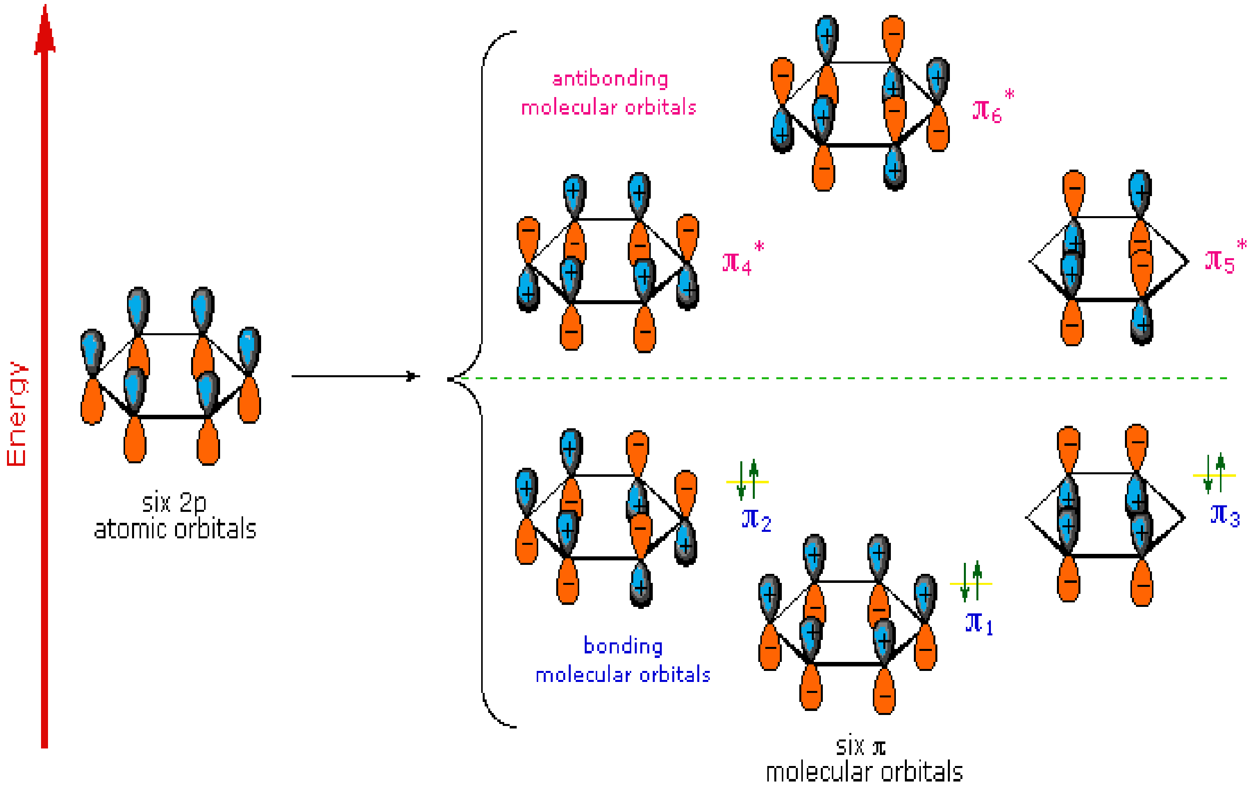




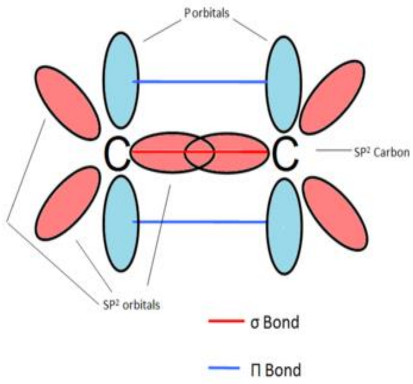
Also each carbon atom in benzene possesses a UN hybridised P-Orbital containing one electron.

These P orbitals are perpendicular to the plane of sigma bonds.

The lateral overlap of these P-Orbital's produce a ∏ molecular orbital containing 6 electrons. One half of this ∏ molecular orbital lies above and the other half of lies below the plane of sigma bonds.



Delocalisation of pi molecular orbitals is formed by the overlap of p-orbital.



All carbons in benzene have a p-orbital on their structure.