Course Code : BPHT3001

Course Name: Pharmaceutical Organic

Benzene and its Derivatives

STRUCTURE OF BENZENE-II GALGOTIAS UNIVERSITY

Name of the Faculty: Dr. Kalpana Rahate

Program Name: B.Pharm.

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STRUCTURE OF BENZENE

4. Kekule structure of benzene:

Kekule suggested that benzene consists of a cyclic planar structure of 6 carbons with alternate double and single bonds and one hydrogen attached to each carbon

According to this proposal benzene was simple 1,3,5-cyclohexatriene

Objections to Kekule structure:

a) If Kekule structure was correct there should exist two orthoisomers of dibromobenzene

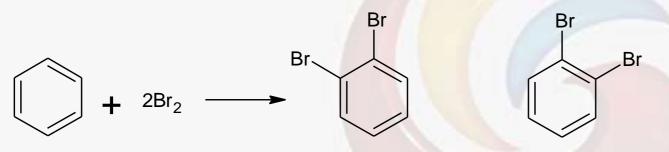
In one isomer the two bromine atoms should be on carbon that are connected by a double bond, while in the other isomer the bromine should be on carbons connected by a single bond.

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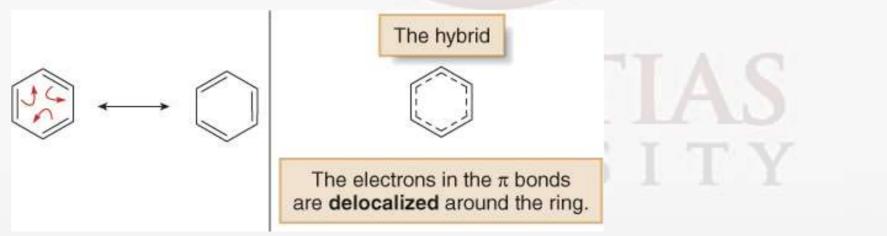
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4. Kekule structure of benzene:

In fact, only one ortho dibromobenzene could be prepared



To overcome this objection Kekule further suggested that benzene was a mixture of two forms in rapid equilibrium



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- 4. Kekule structure of benzene
- b) Kekule's structure failed to explain why benzene with 3 double bonds did not give addition reactions like other alkenes
 e.g. benzene did not react with HBr or Br₂ in CCl₄

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STRUCTURE OF BENZENE

5. Resonance description of benzene

The phenomena in which 2 or more structures can be written for a compound with identical positions of atoms is called **RESONANCE**

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

A double headed arrow between the resonance structure is used to represent the resonance hybrid

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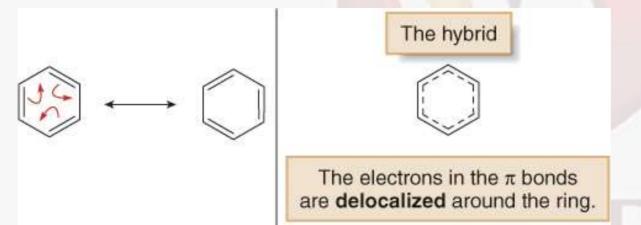
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5. Resonance description of benzene

Thus in case of benzene, Kekule's two structures represent the resonance structures

The actual structure of the molecule may be represented as hybrid of these two resonance structures



All single bonds in the first structure are double bonds in the second structure

The C-C bonds in benzene are neither single bonded nor double bonded, they are something halfway between Name of the Faculty: Dr. Kalpana Rahate Program Name: B.Pharm.

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5. Resonance description of benzene

Spectroscopic measurements show that benzene is planar and all of its C-C bonds are of equal length 1.40A⁰. this value lies in between C-C single bond length 1.54A⁰ and the C-C double bond length 1.34A⁰

Resonance hybrid is more stable than any of its contributing structure for benzene

The stability due to resonance is so great that pi bonds of the molecule will normally resist breaking and this explains lack of reactivity of benzene towards addition

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