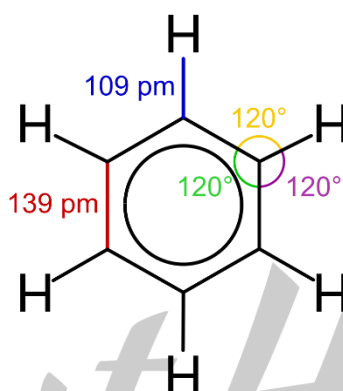


Benzene and Its Derivatives

Benzene and its derivatives

- **Benzene (C₆H₆)** is a simple aromatic hydrocarbon, characterized by a six-carbon ring with alternating single and double bonds.
- The molecule is planar, with each carbon atom bonded to two other carbons and a hydrogen atom.
- Due to the presence of resonance structures, the electrons in the π -bonds are delocalized, which results in the ring having a high degree of stability.
- Benzene and its derivatives form a crucial part of organic chemistry, with applications in many industries.



Derivatives of Benzene

- Benzene derivatives are compounds in which one or more hydrogen atoms have been replaced by other atoms or functional groups.

Some common derivatives include:

1. Phenol (C₆H₅OH)

- **Functional Group:** Hydroxyl group (-OH)
- **Uses:** Antiseptic, disinfectant, precursor to various resins and plastics.

2. Toluene (C₆H₅CH₃)

- **Functional Group:** Methyl group (-CH₃)
- **Uses:** Solvent, fuel additive, starting material for synthesizing other chemicals.

3. Aniline (C₆H₅NH₂)

- **Functional Group:** Amino group (-NH₂)
- **Uses:** Production of dyes, rubber chemicals, and pharmaceuticals.

4. Nitrobenzene (C₆H₅NO₂)

- **Functional Group:** Nitro group (-NO₂)

- **Uses:** Precursor for the synthesis of aniline and other chemicals.

5. Styrene (C₆H₅CH=CH₂)

- **Functional Group:** Vinyl group (-CH=CH₂)
- **Uses:** Production of polystyrene and other plastics.

6. Xylene (C₆H₄(CH₃)₂)

- **Functional Group:** Two methyl groups (-CH₃)
- **Uses:** Solvent, starting material for the production of polyester fibers and other chemicals.

7. Halo benzenes (C₆H₅X)

- **Functional Group:** Halogen atom (X = F, Cl, Br, I)
- **Uses:** Solvents, intermediates in chemical synthesis, production of pesticides and pharmaceuticals.

Evidence in the Derivation of the Structure of Benzene

- The structure of benzene has been the subject of extensive research since its discovery in 1825 by Michael Faraday.

Various evidences:

1. Analytical Evidence

- **Molecular Formula:**
 - Determined as C₆H₆ through combustion analysis, indicating high unsaturation.
- **X-ray Crystallography:**
 - Showed benzene is planar with equidistant carbon atoms, suggesting a hexagonal ring structure.

2. Synthetic Evidence

- **Aromatic Character:**
 - Benzene derivatives displayed aromatic properties, indicating the essential benzene ring structure.
- **Electrophilic Aromatic Substitution:**
 - Benzene undergoes substitution rather than addition reactions, indicating delocalized π-electrons.

3. Other Evidence

- **Kekulé's Proposal:**

- In 1865, proposed a hexagonal structure with alternating single and double bonds, but it couldn't explain benzene's stability.
- **Resonance:**
 - In 1931, Linus Pauling suggested benzene is a resonance hybrid with delocalized π -electrons, explaining its unique stability.
- **Heats of Hydrogenation:**
 - Found to be less than expected for three isolated double bonds, supporting delocalized π -electrons and enhanced stability.

Orbital Picture of Benzene

- Benzene (C_6H_6) is a planar, cyclic molecule with six carbon atoms arranged in a hexagonal ring.
- Each carbon atom in benzene is sp^2 hybridized, meaning each carbon atom forms three sigma (σ) bonds: two with adjacent carbon atoms and one with a hydrogen atom.
- This leaves one unhybridized p orbital on each carbon atom.

Types of bonds in benzene:

1. Sigma Bonds (σ Bonds):

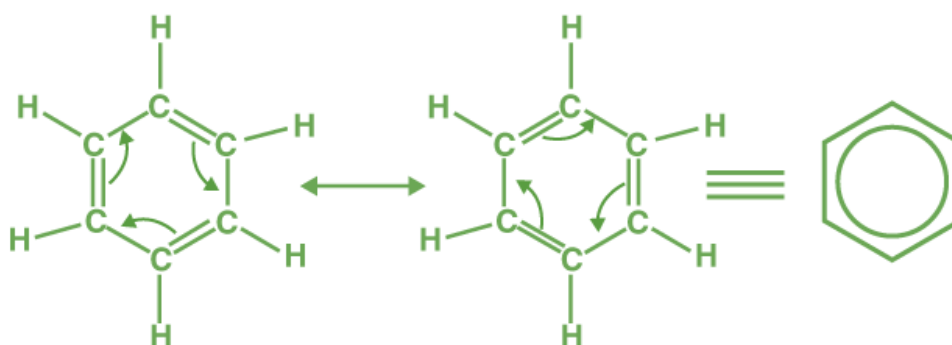
- These are the single bonds formed by the overlap of sp^2 hybrid orbitals from each carbon atom with its neighbours and with hydrogen atoms.

2. Pi Bonds (π Bonds):

- The unhybridized p orbitals, which are perpendicular to the plane of the benzene ring, overlap side-by-side above and below the plane of the ring to form a continuous π electron cloud.
- This delocalization of electrons results in π bonds that are spread equally over all six carbon atoms.

Resonance in Benzene

- Benzene exhibits resonance, a phenomenon where the actual electronic structure is a hybrid of two or more contributing structures.





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