SNS COLLEGE OF PHARMACY AND HEALTH SCIENCES

Affiliated To The Tamil Nadu Dr. MGR Medical University, Chennai

Approved by Pharmacy Council of India, New Delhi.

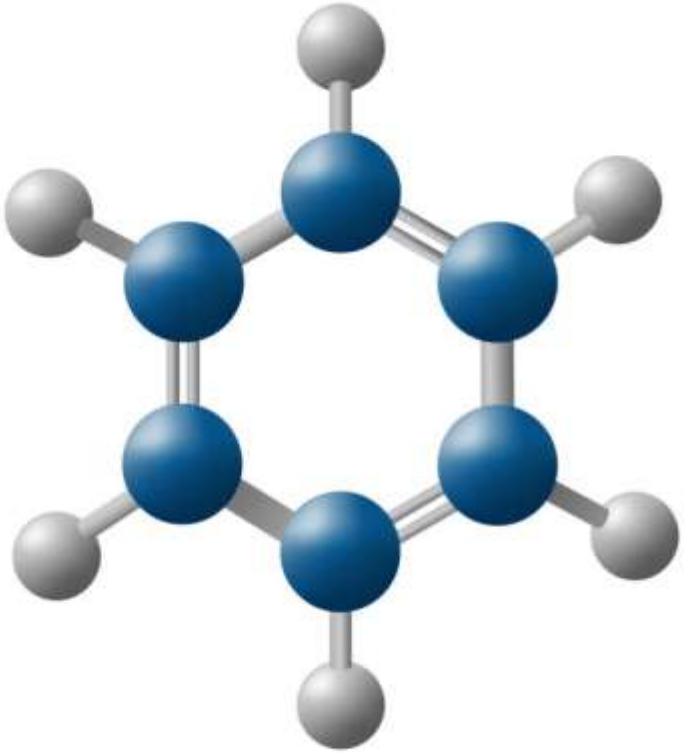
Coimbatore -641035

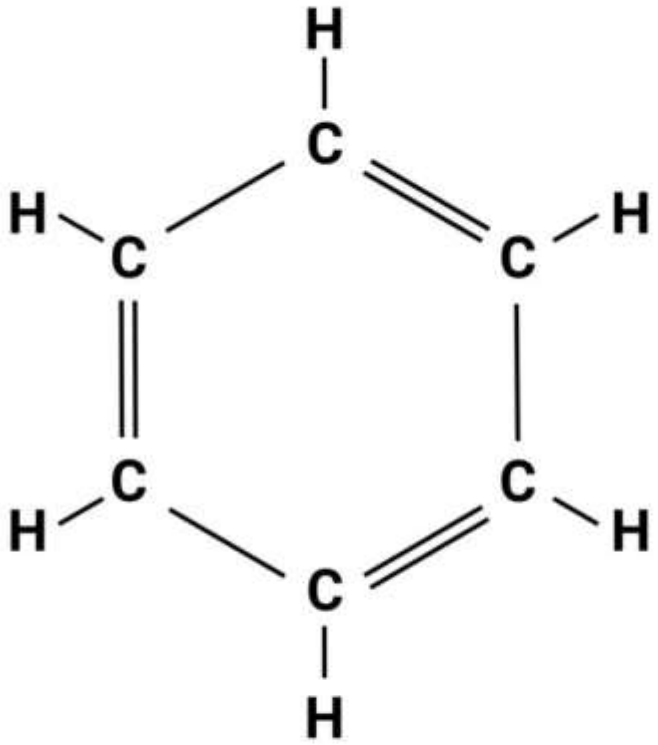
COURSE NAME : PHARMACEUTICAL ORGANIC CHEMISTRY-2(BP 706 T)

B.PHARM III SEM / II YEAR

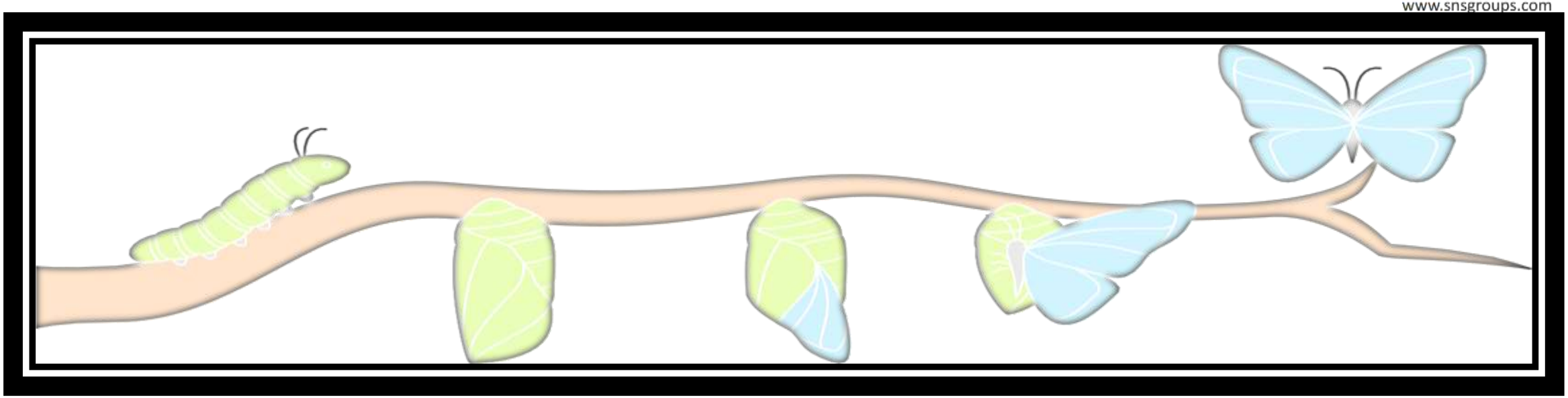
TOPIC : BENZENE AND ITS PROPERTIES

STRUCTURE OF BENZENE





Benzene : C_6H_6



Initial Knowledge

Basic understanding of benzene

Structure & Properties

Learn benzene's structure and properties

Reaction Mechanisms

Grasp benzene's reaction mechanisms

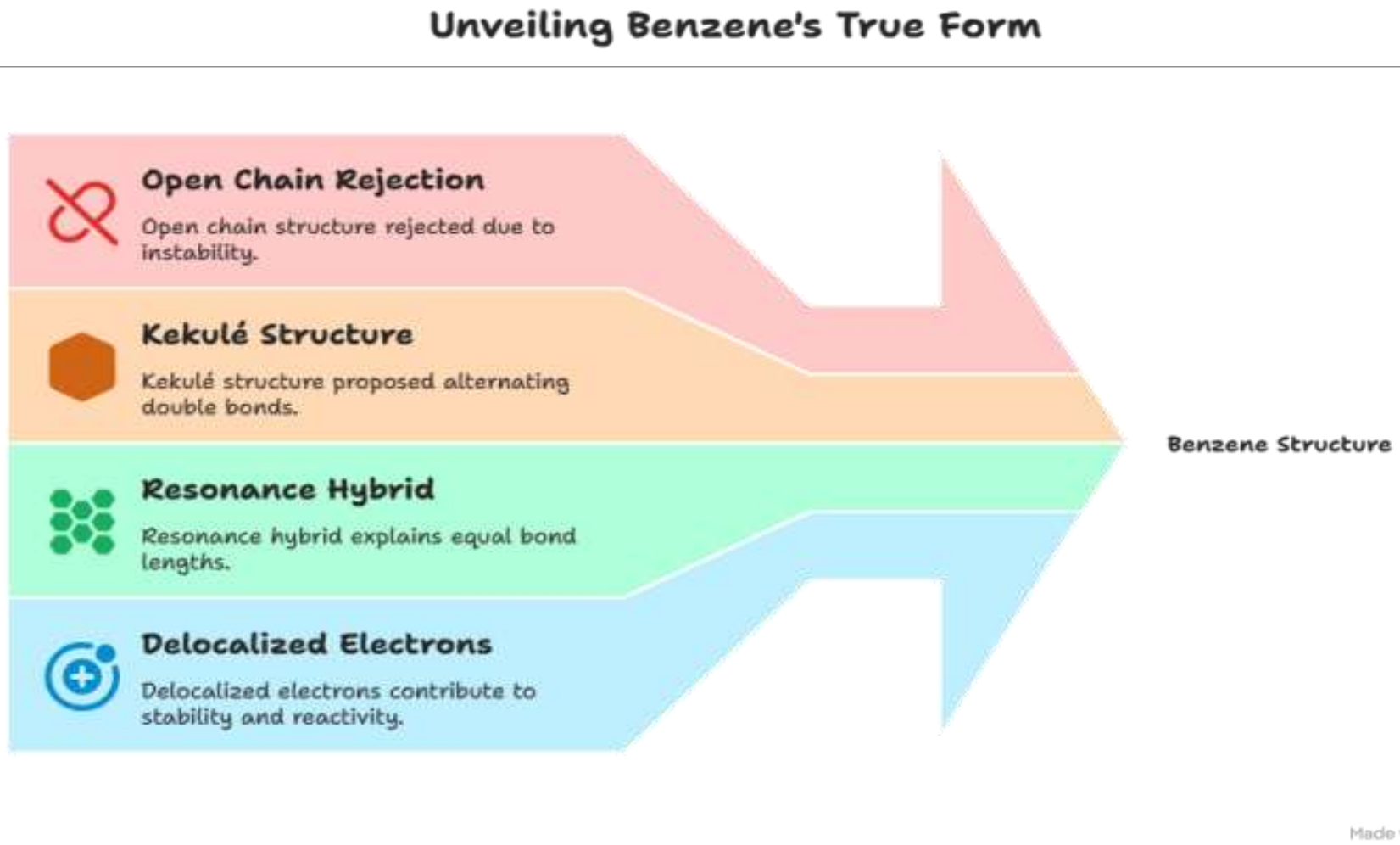
Applications

Appreciate benzene's diverse applications

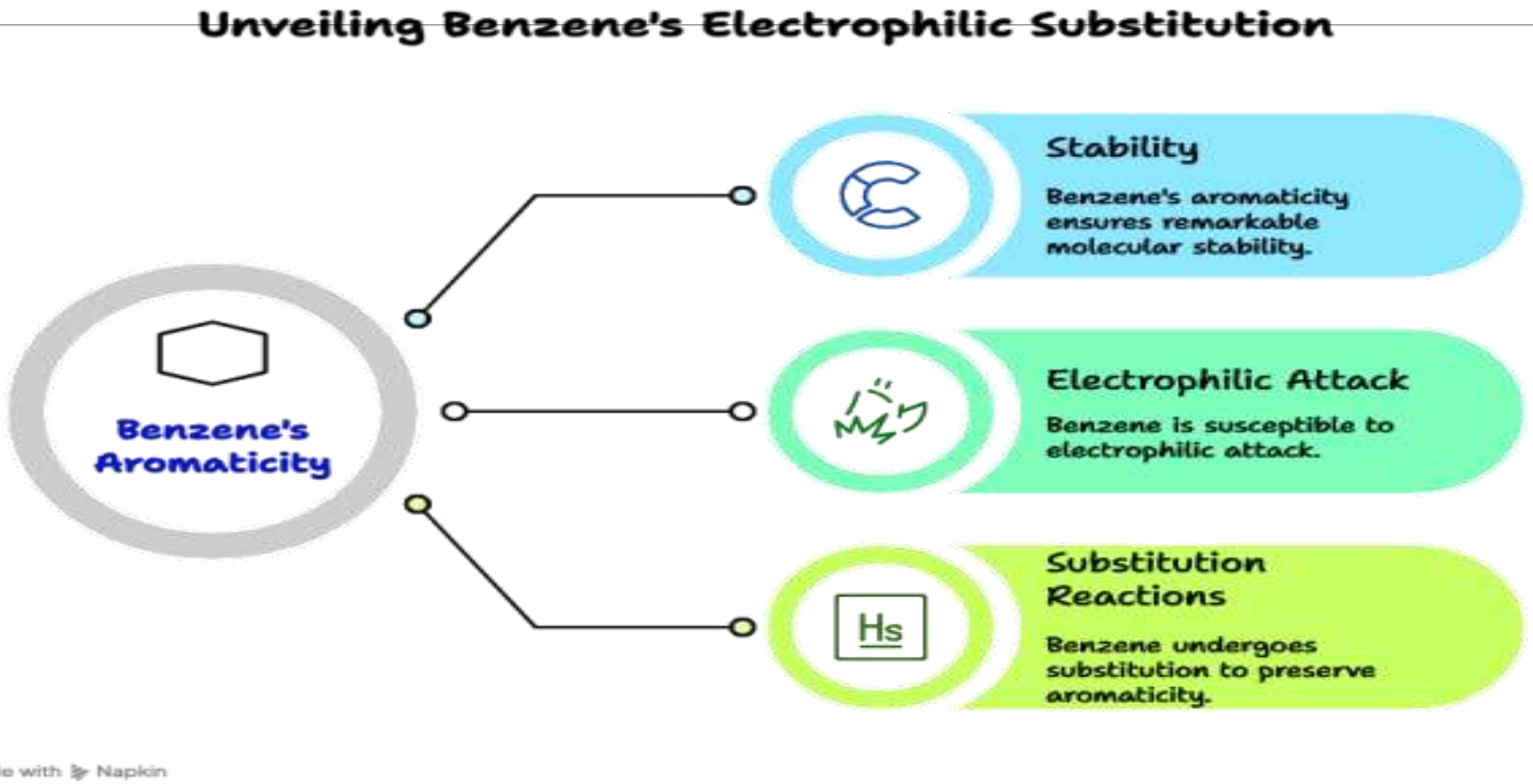
Deep Understanding

Comprehensive knowledge of benzene

MINDMAP OF BENZENE



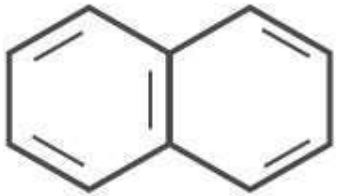
ELECTROPHILIC AROMATIC SUBSTITUTION OF BENZENE



STRUCTURE OF BENZENE

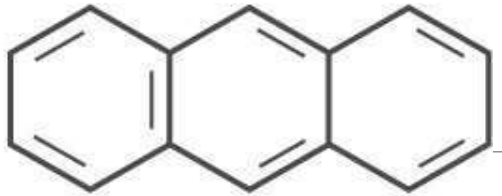
Benzene

n = 1
(4 x 1 + 2) = 6π
Electrons



Naphthalene

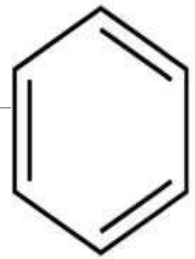
n = 2
(4 x 2 + 2) = 10π
Electrons



Anthracene

n =3
(4 x 3 + 2) = 14π
Electrons

Benzene



Since benzene has 6 pi electrons:

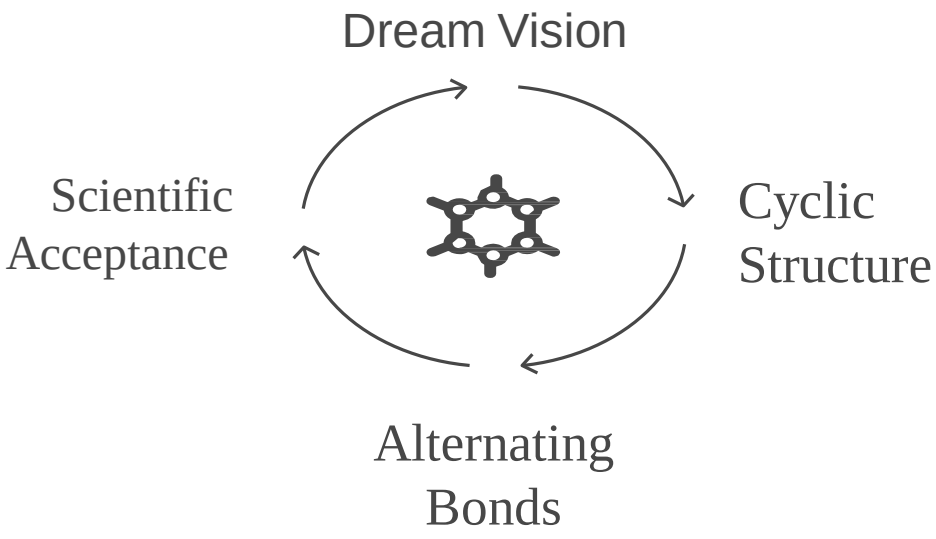
4n + 2 = 6
Find n:

4n + 2 = 6
4n = 6-2
4n = 4
n = 1 ←

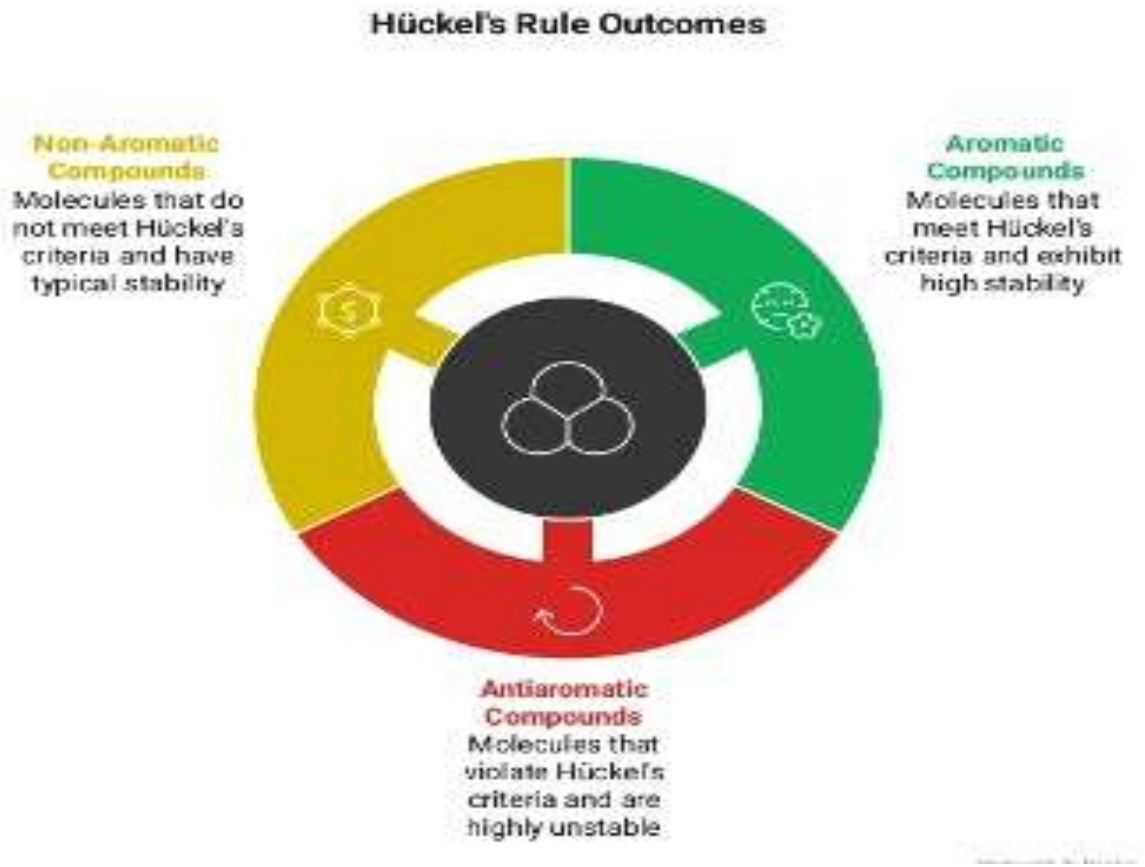
An aromatic compound follows Huckel's rule if n is equal to zero or a positive whole number.

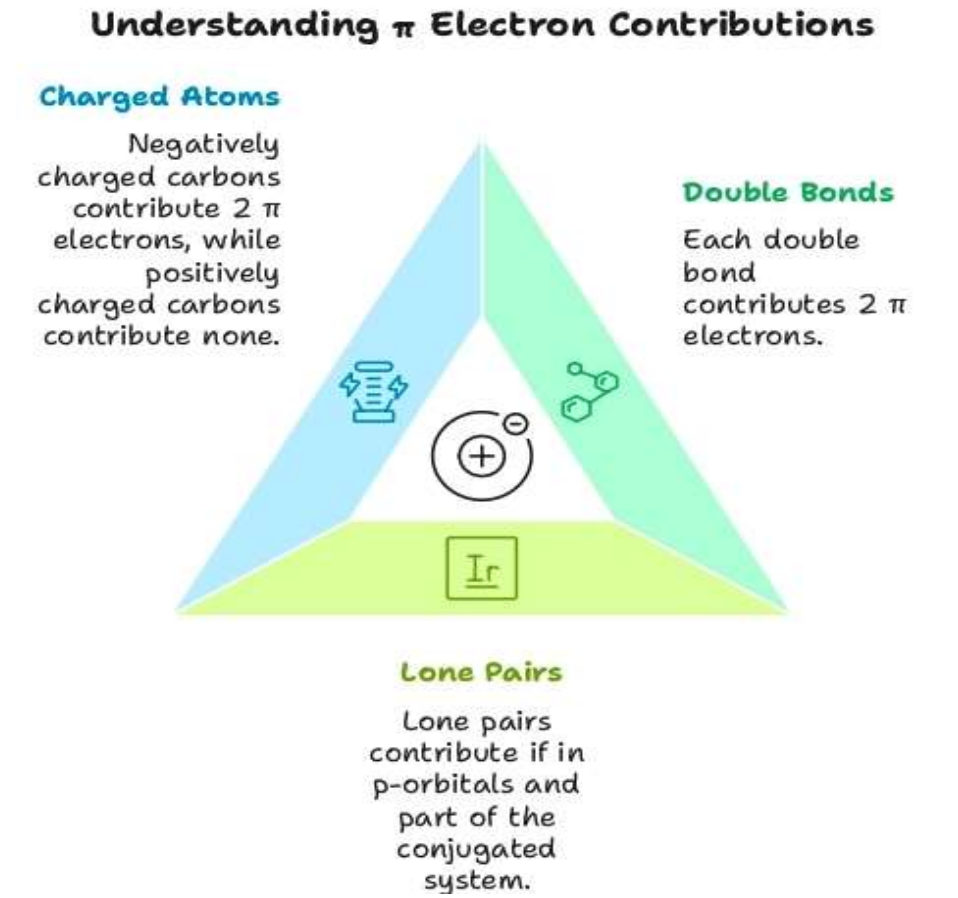
Benzene is aromatic

KEKULE'S DISCOVERY CYCLE-BENZENE



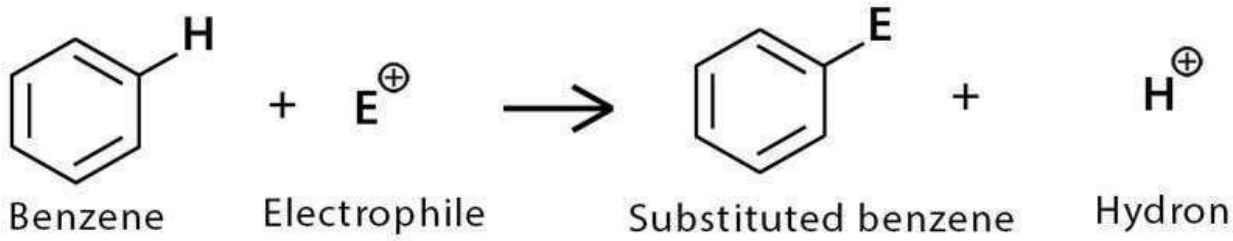
HUCKEL'S RULE OF AROMATICITY

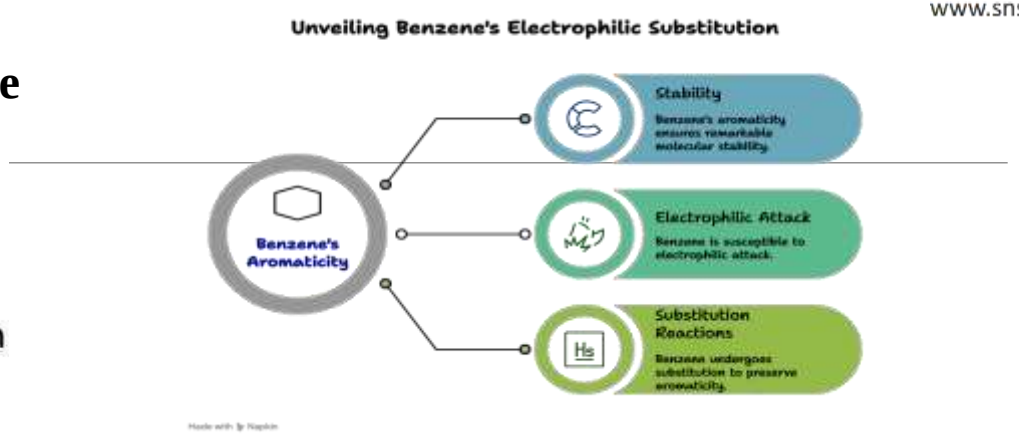




ELECTROPHILIC AROMATIC SUBSTITUTION

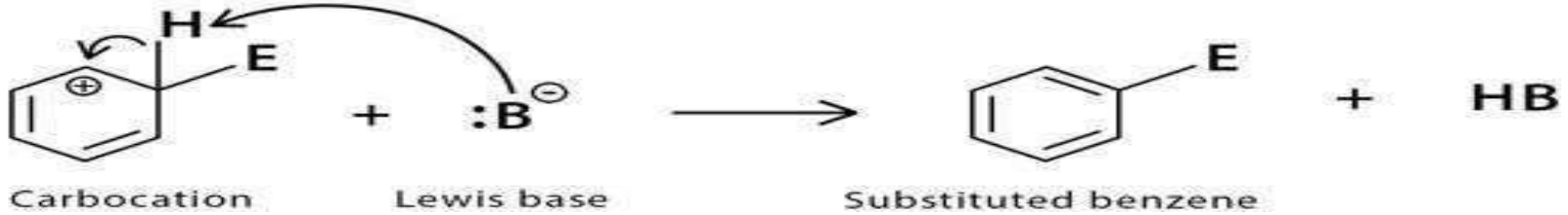
Mechanism of Electrophilic Aromatic Substitution of Benzene





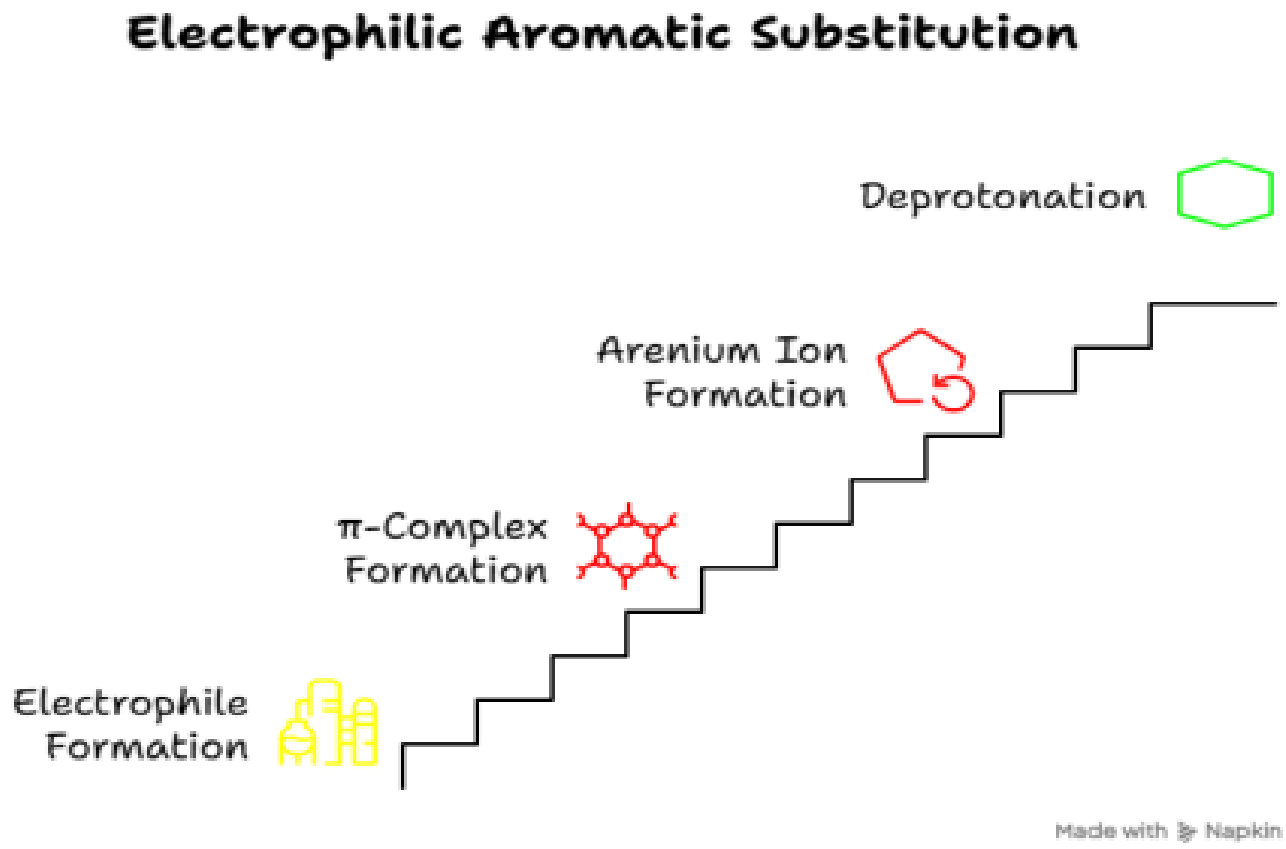
Step 1: Electrophilic attack on a pi bond of benzene by an electrophile to form a carbocation

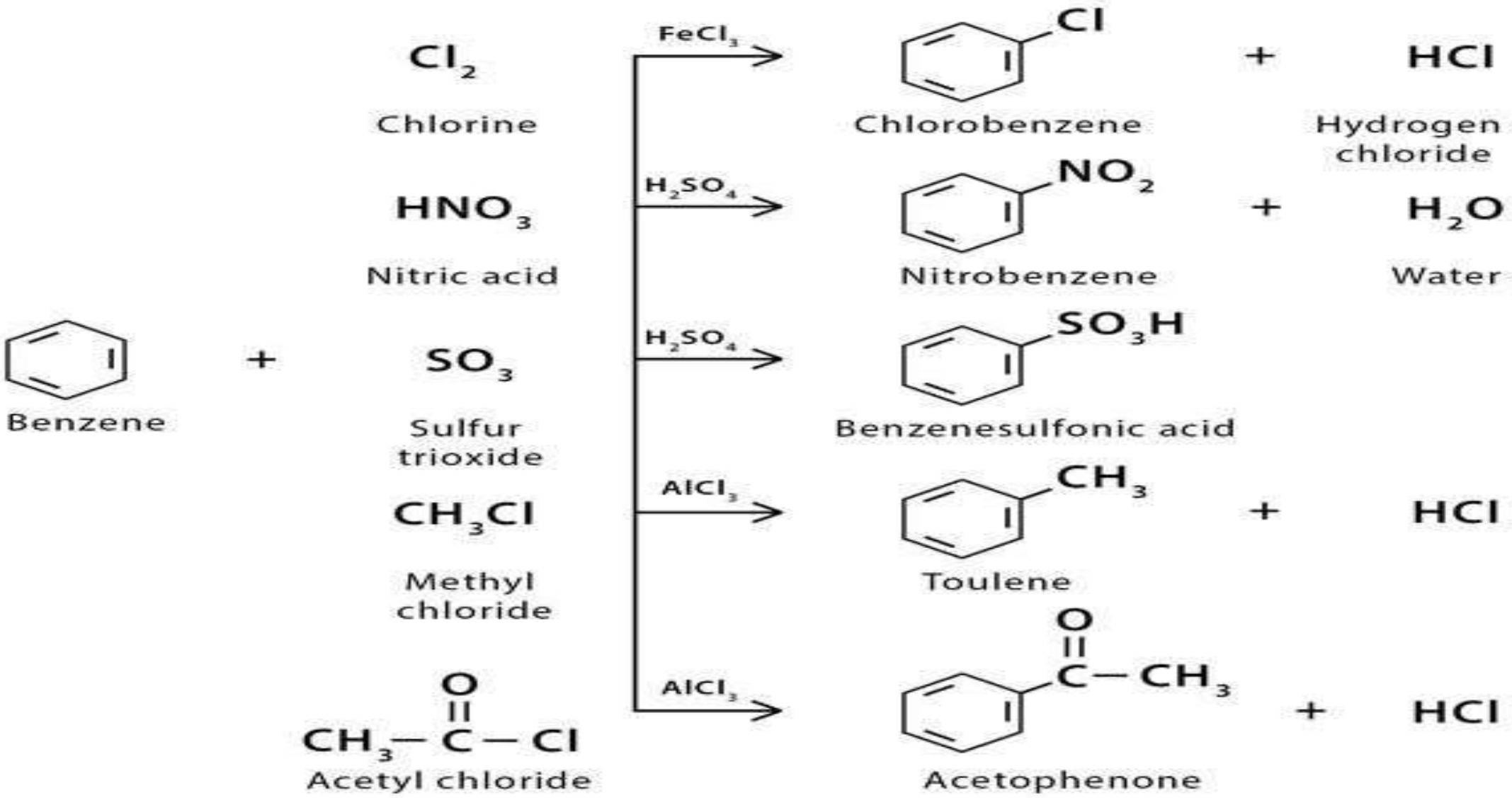
Step 2: Deprotonation of the carbocation to restore its aromacity, resulting in a substituted product



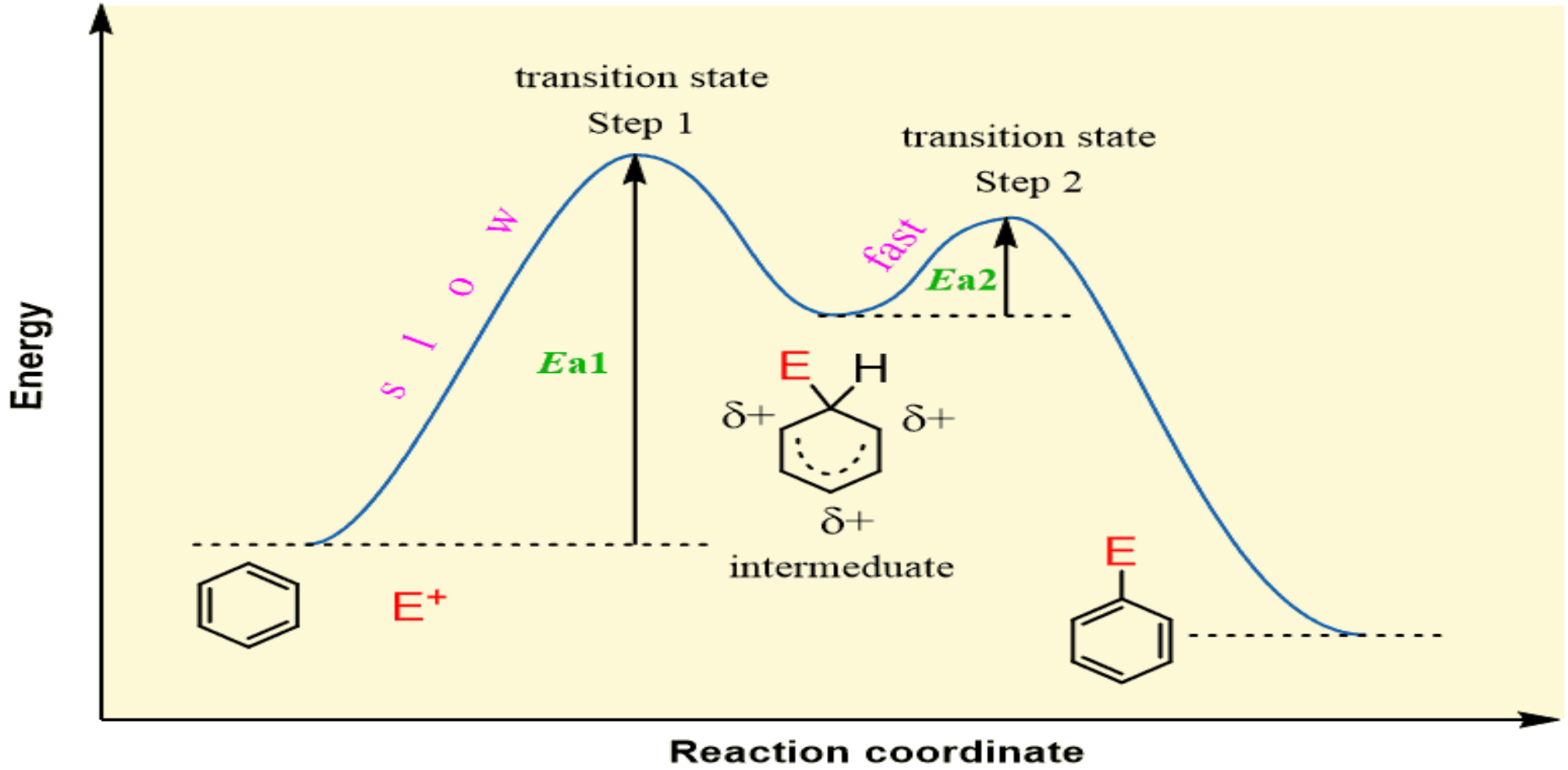
ELECTROPHILIC AROMATIC SUBSTITUTION

AES is the characteristic reaction of benzene, preserving its high aromatic stability.
The mechanism proceeds in two steps: (1) Attack by E+ to form the σ-complex (slow) and (2) Loss of H+ to restore aromaticity (fast).
The σ-complex (arenium ion) is a resonance-stabilized but non-aromatic intermediate.
Key reactions include Nitration, Halogenation, Sulfonation, and Friedel-Crafts (Alkylation and Acylation).
AES reactions are the primary tools used by organic chemists to build complex molecules upon the benzene backbone.




Benzene
+
Cl2
Chlorine
HNO3
Nitric acid
SO3
Sulfur trioxide
CH3Cl
Methyl chloride
CH3—C(=O)—Cl
Acetyl chloride
FeCl3
H2SO4
H2SO4
AlCl3
AlCl3
Cl
Chlorobenzene
+
HCl
Hydrogen chloride
NO2
Nitrobenzene
+
H2O
Water
SO3H
Benzenesulfonic acid
CH3
Toulene
+
HCl
C(=O)—CH3
Acetophenone
+
HCl

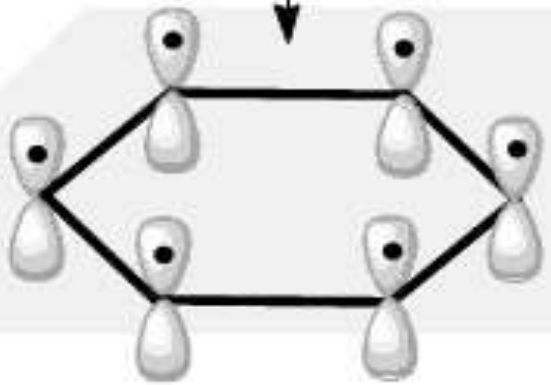
ELECTROPHILIC AROMATIC SUBSTITUTION

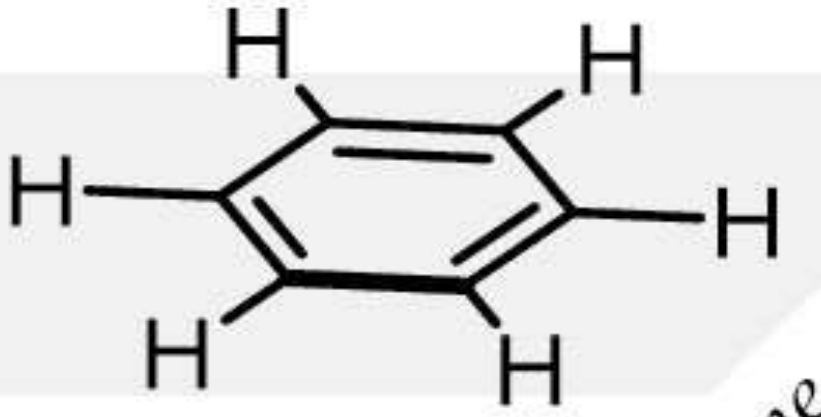


DELOCALISATION OF ELECTRONS

C=C sp^2 carbons

π bond **trigonal planar** geometry





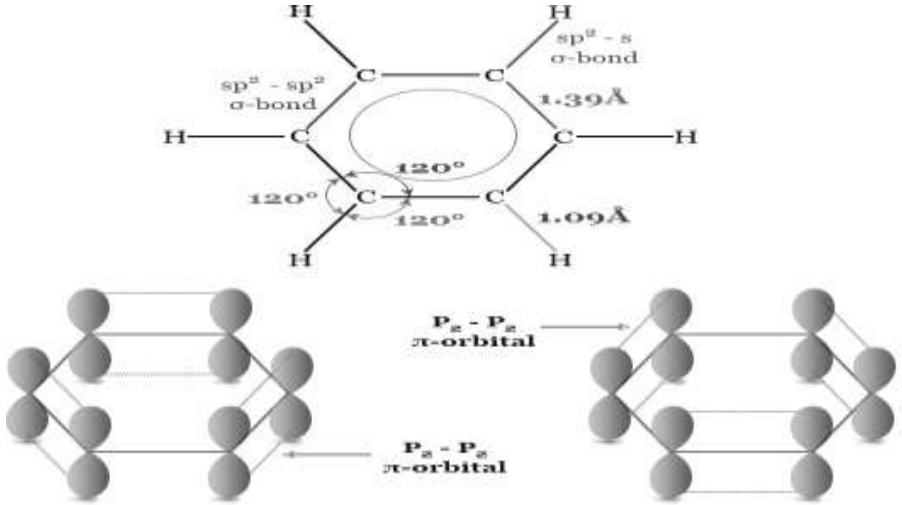
plane of the atoms

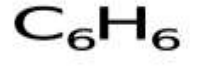
***p* orbitals** - 90° to the plane

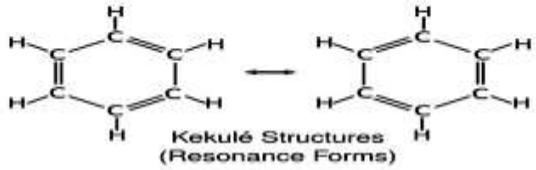
DELOCALISATION OF ELECTRONS

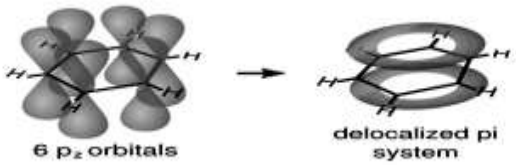
Equivalent carbon-carbon bonds: All carbon-carbon bonds in benzene have identical lengths, intermediate between single and double bonds.

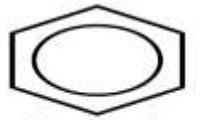
→***Delocalized electrons***: The six electrons involved in the hypothetical double bonds are not localized between specific carbon atoms but are spread out across the entire ring. This delocalization is often represented by a circle within the hexagon.

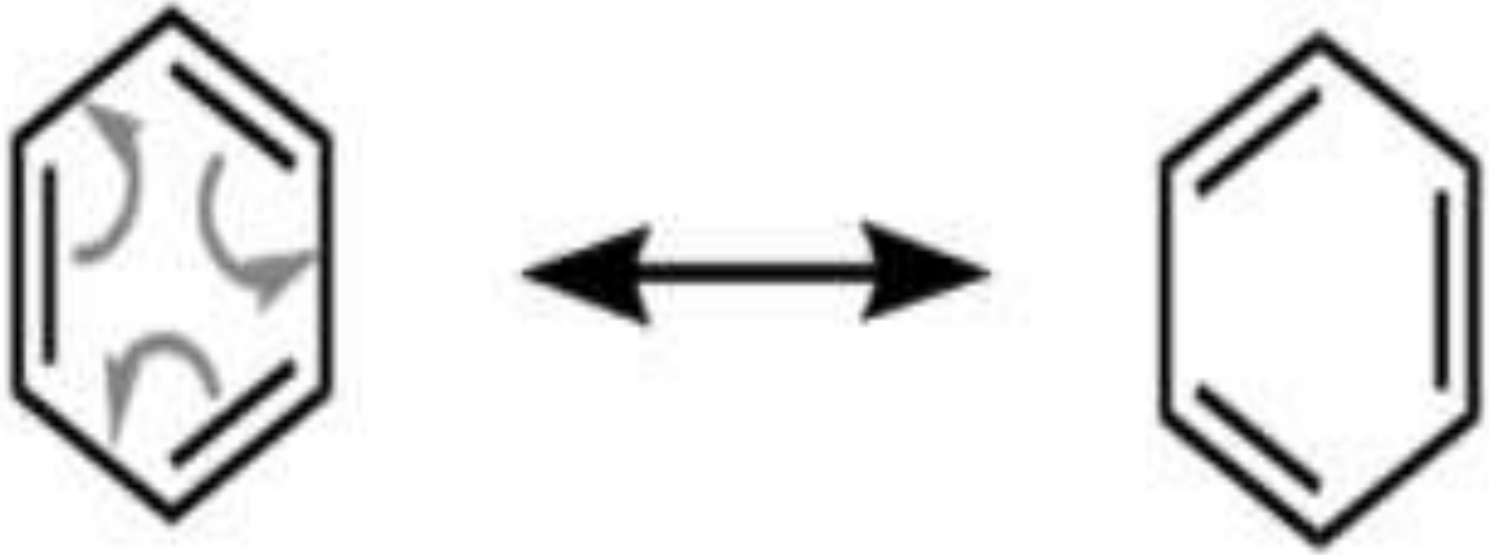






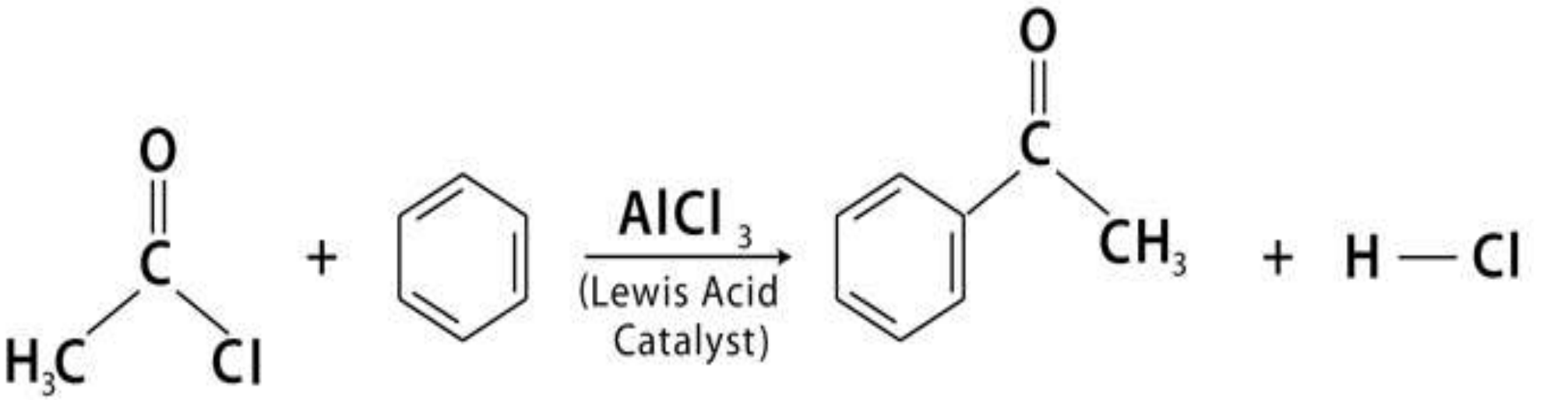






Resonance structures of benzene

Friedel-Crafts Acylation




Intramolecular
Acylation
Aromatic Substrates

CASE STUDY PUZZLE: THE MYSTERY OF THE AROMATIC COMPOUND

Scenario

You are a chemist at ChemSolve Labs, tasked with identifying an unknown aromatic compound and solving a series of chemical mysteries.

Your team has received a sample labeled "Compound X," which is a derivative of benzene (C_6H_6).

Through analytical tests, you know it has a molecular formula of C_6H_5Y, where Y is an unknown substituent.

Additionally, the lab is investigating a set of reactions and compounds related to benzene derivatives used in industry.

Solve the following puzzles to identify Compound X and address the lab's challenges

- **Puzzle 1: Unraveling the Structure of Benzene**

- Your first task is to confirm that Compound X is derived from benzene. The lab provides the following clues about benzene's structure:

  - Elemental analysis confirms a C:H ratio of 1:1.
  - The compound is unusually stable and does not undergo addition reactions like alkenes.
  - Spectroscopic data show all C–C bonds are equal in length (1.39 Å).
  - It follows a rule for aromaticity involving (4n + 2) π-electrons.

- **Questions:**

  1. Based on the clues, propose the structure of benzene and explain why it is stable compared to a hypothetical cyclohexatriene.
  2. What is Huckel's rule, and how does it apply to benzene's aromaticity? Calculate the number of π-electrons in benzene to confirm its aromatic character.
  3. Draw the orbital picture of benzene, describing the hybridization of carbon atoms and the nature of the π-system.

Puzzle 2: Identifying Compound X Through Reactions

To identify the substituent Y in Compound X (C_6H_5Y), you perform a series of electrophilic aromatic substitution reactions on benzene and compare the products to Compound X:

- **Reaction A:** Benzene reacts with a mixture of HNO_3 and H_2SO_4 at 50°C, yielding nitrobenzene.
- **Reaction B:** Benzene reacts with Cl_2 in the presence of $FeCl_3$, forming chlorobenzene.
- **Reaction C:** Benzene reacts with CH_3COCl and $AlCl_3$, producing acetophenone.

REFERENCES

- March's Advanced Organic Chemistry (6th ed.) by Michael B. Smith & Jerry March
- Organic Chemistry (by authors such as L. G. Wade or others) — e.g., the chapter titled "Alkylation and Acylation of Aromatic Rings: The Friedel–Crafts Reaction"
- Friedel–Crafts Reactions (RSC Books monograph, Chapter 10)

•Advances in Friedel–Crafts Acylation Reactions: Catalytic and Green Processes by G. Sartori & R. Maggi

•Khan Academy: Friedel-Crafts Acylation" — an instruction video with mechanism step by step.


thank
BENZENE
you