STRUCTURE OF BENZENE

DR.JESY.E.J.

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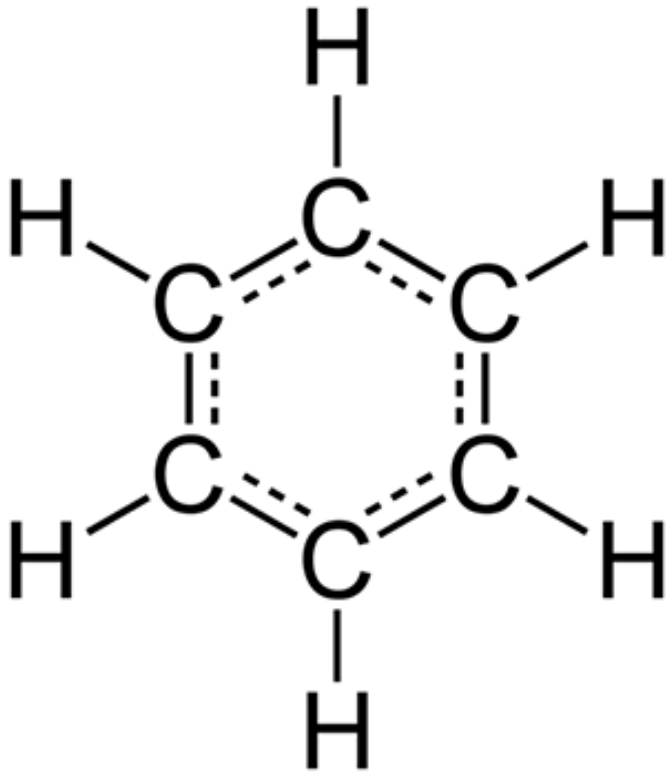
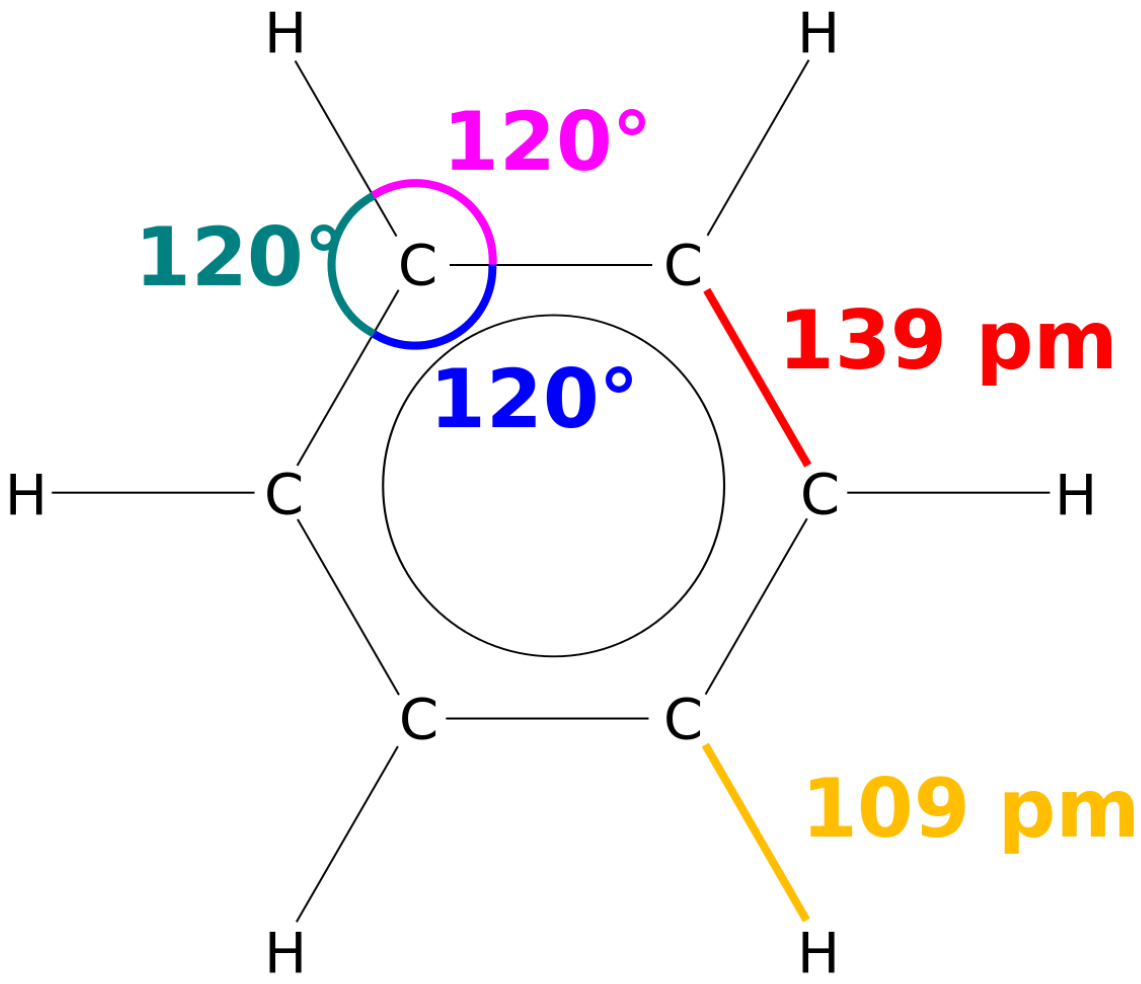
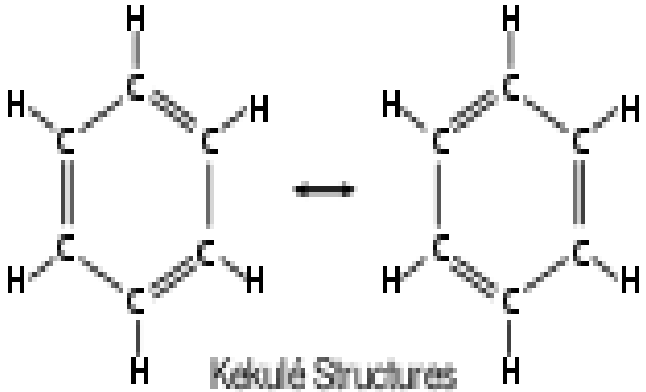


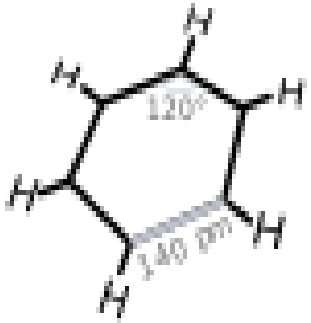

H
H
120°
120°
C
C
139 pm
120°
H
C
C
H
C
C
109 pm
H
H

C_6H_6

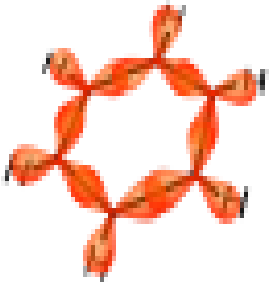
Benzene
Molecular formula



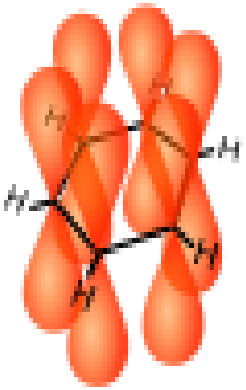
Kekulé Structures
(Resonance Forms)



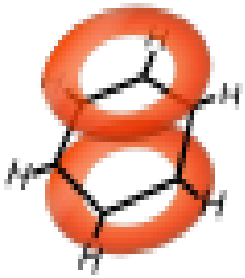
Planar Hexagon
Bond Length 140 pm



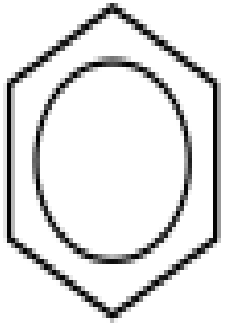
Sigma Bonds
sp^2 Hybridized orbitals



6 p_z orbitals



delocalized pi
system

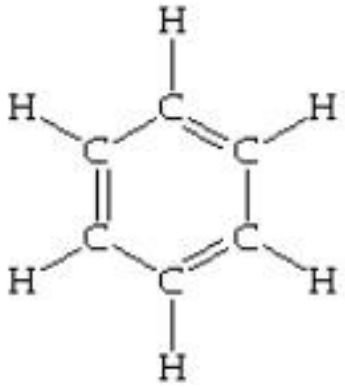


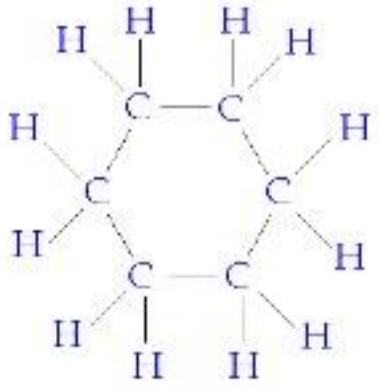
Benzene ring
Simplified depiction

Introduction

Kekulé was the first to suggest a sensible structure for benzene. The carbons are arranged in a hexagon, and he suggested alternating double and single bonds between them. Each carbon atom has a hydrogen attached to it.

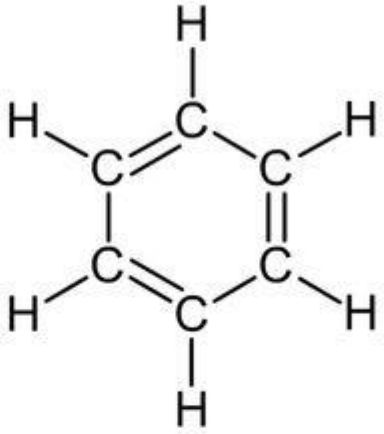
- ***Problems with the chemistry***
- ***Problems with the shape***
- ***Problems with the stability of benzene***

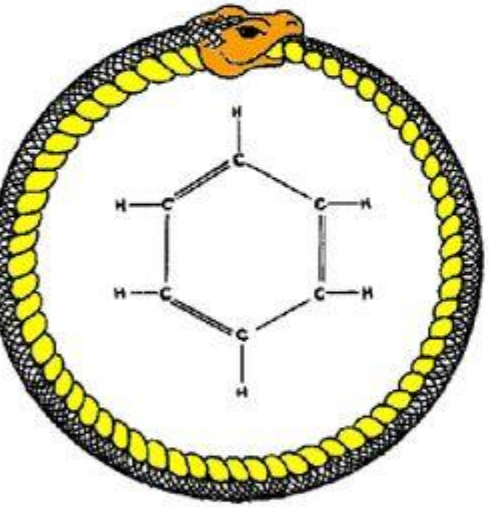




Kekulé structure of benzene

Kekulé proposed a cyclic structure consisting of alternating single and double bonds.





Kekulé's claimed that his inspiration came from a dream of a snake eating its own tail.

There were a number of problems with Kekulé's structure

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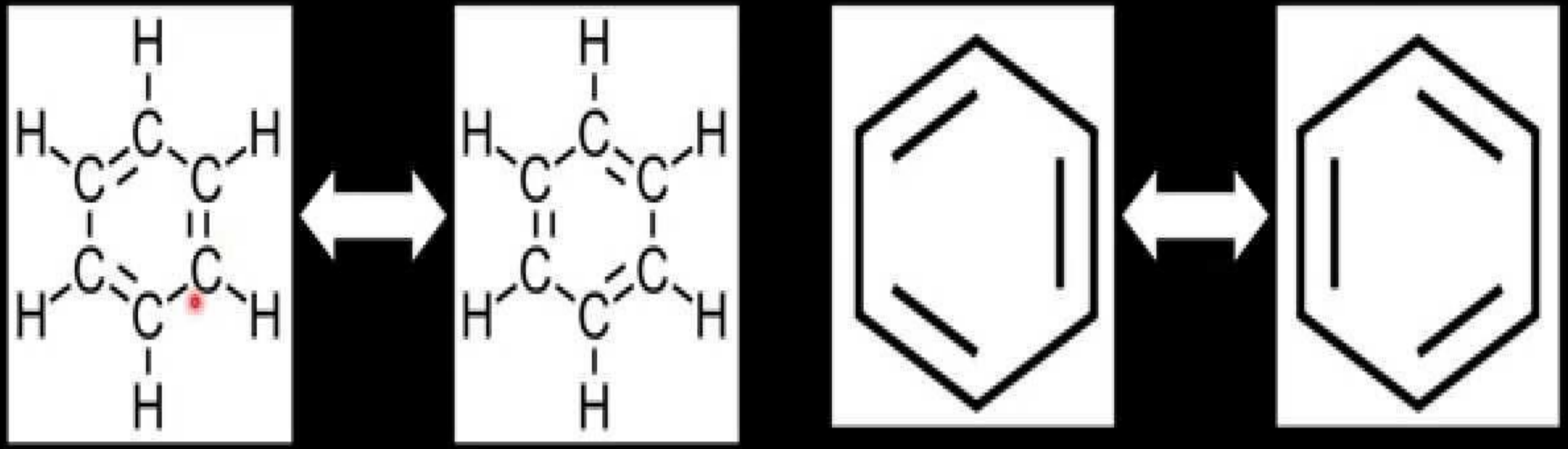
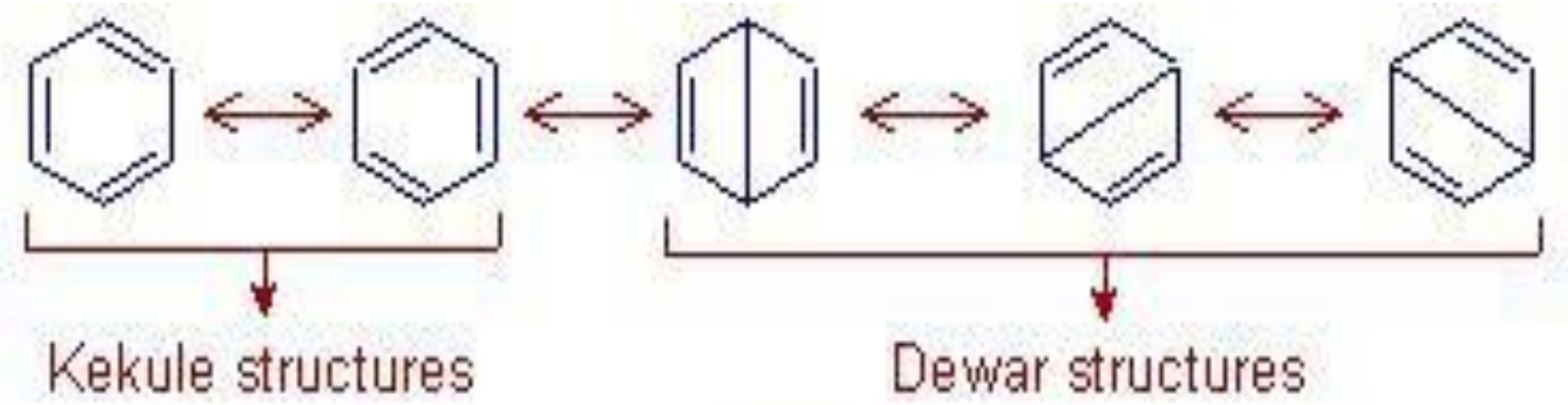
Structure of benzene

The Kekulé structure of benzene consists of alternating single and double bonds.



The actual structure of benzene is a resonance hybrid structure with delocalized electrons.

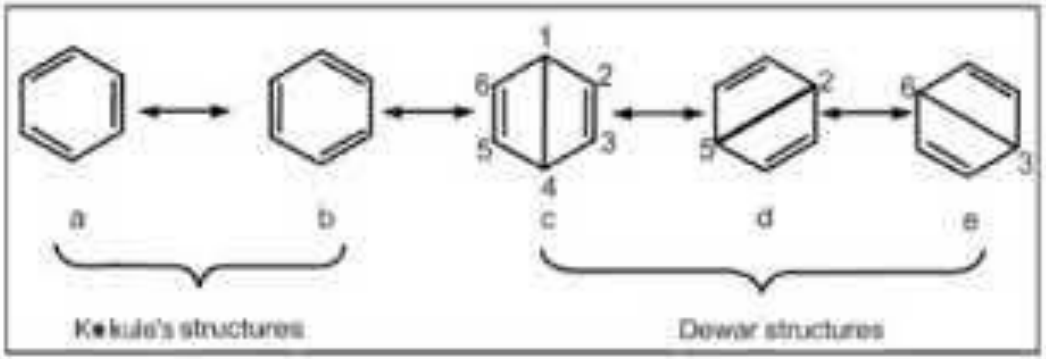


resonance hybrid of benzene

The Resonance Method:

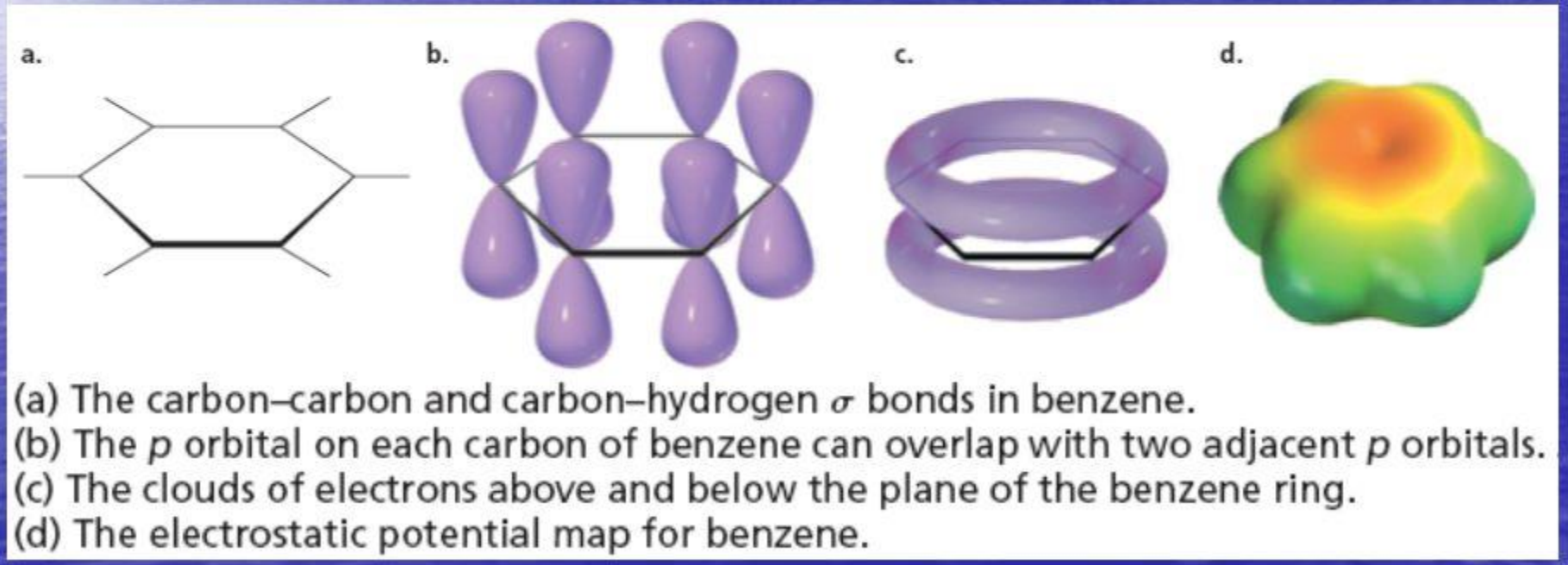
What is resonance Resonance ?

"The possibility of different pairing schemes of valence electrons of atoms is called resonance" and the different structures thus arranged are called "Resonance structures". The resonance is represented by a double headed arrow (↔) e.g. the following different pairing schemes of the fourth valence (the p-electrons) of carbon atoms are possible in benzene.

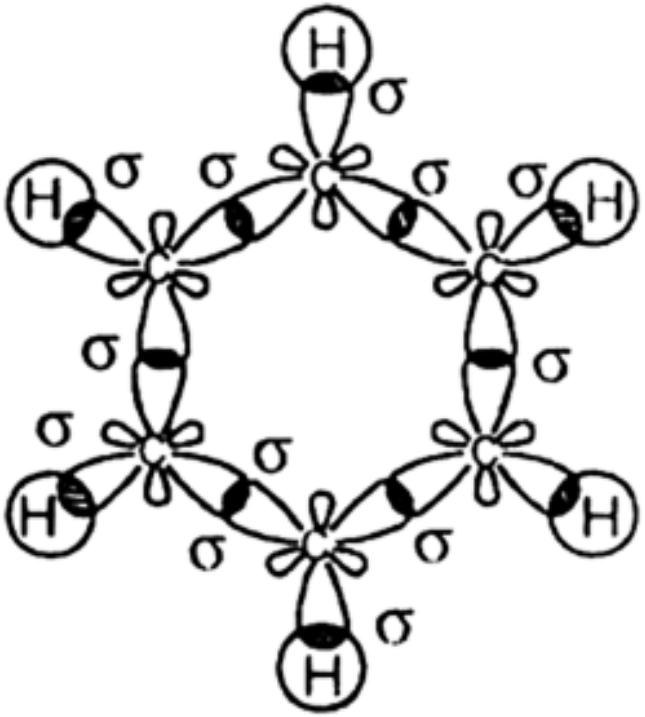


(a), (b) were proposed by Kekule and c, d, e, were proposed by Dewar. The stability of a molecule increases with increase in the number of its resonance structures. Thus molecule of benzene is chemically quite stable.

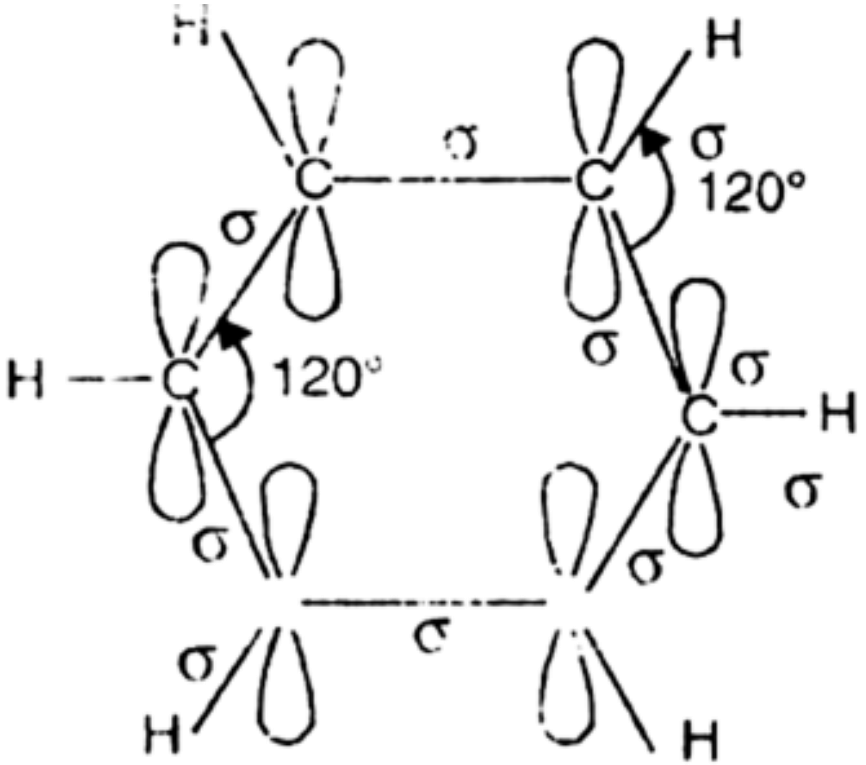
This type of representation makes it clear that there are no double bonds in benzene. The actual structure of benzene is a Kekulé structure with delocalized electrons.



(a) The carbon–carbon and carbon–hydrogen σ bonds in benzene.
(b) The *p* orbital on each carbon of benzene can overlap with two adjacent *p* orbitals.
(c) The clouds of electrons above and below the plane of the benzene ring.
(d) The electrostatic potential map for benzene.



Formation of C–C and C–H sigma bonds

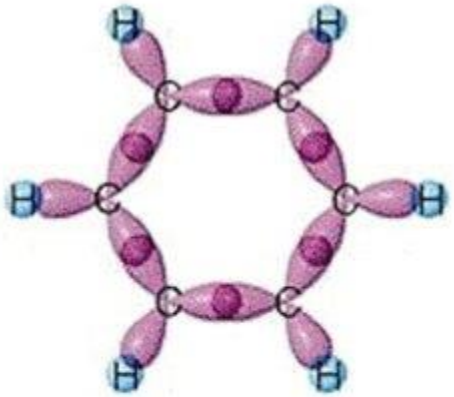


Sigma skeleton of benzene molecule

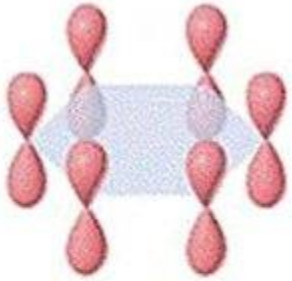
Delocalized π Bonding

In the case of benzene (C_6H_6) there are

- **6 C-C σ bonds, all equal;**
- **6 C-H σ bonds, all equal.**
- **Each C atom is sp^2 hybridized.**
- **There are 6 *p* orbitals on each C atom.**



σ-bonds

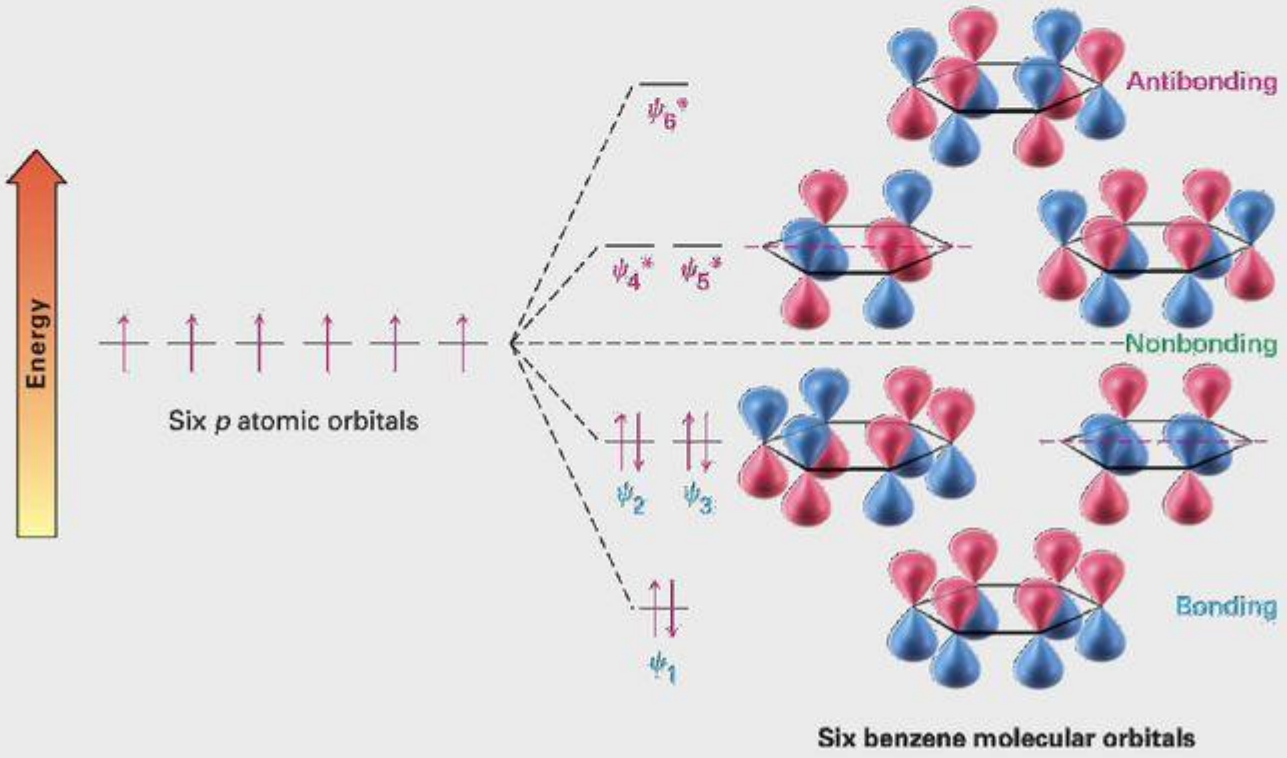


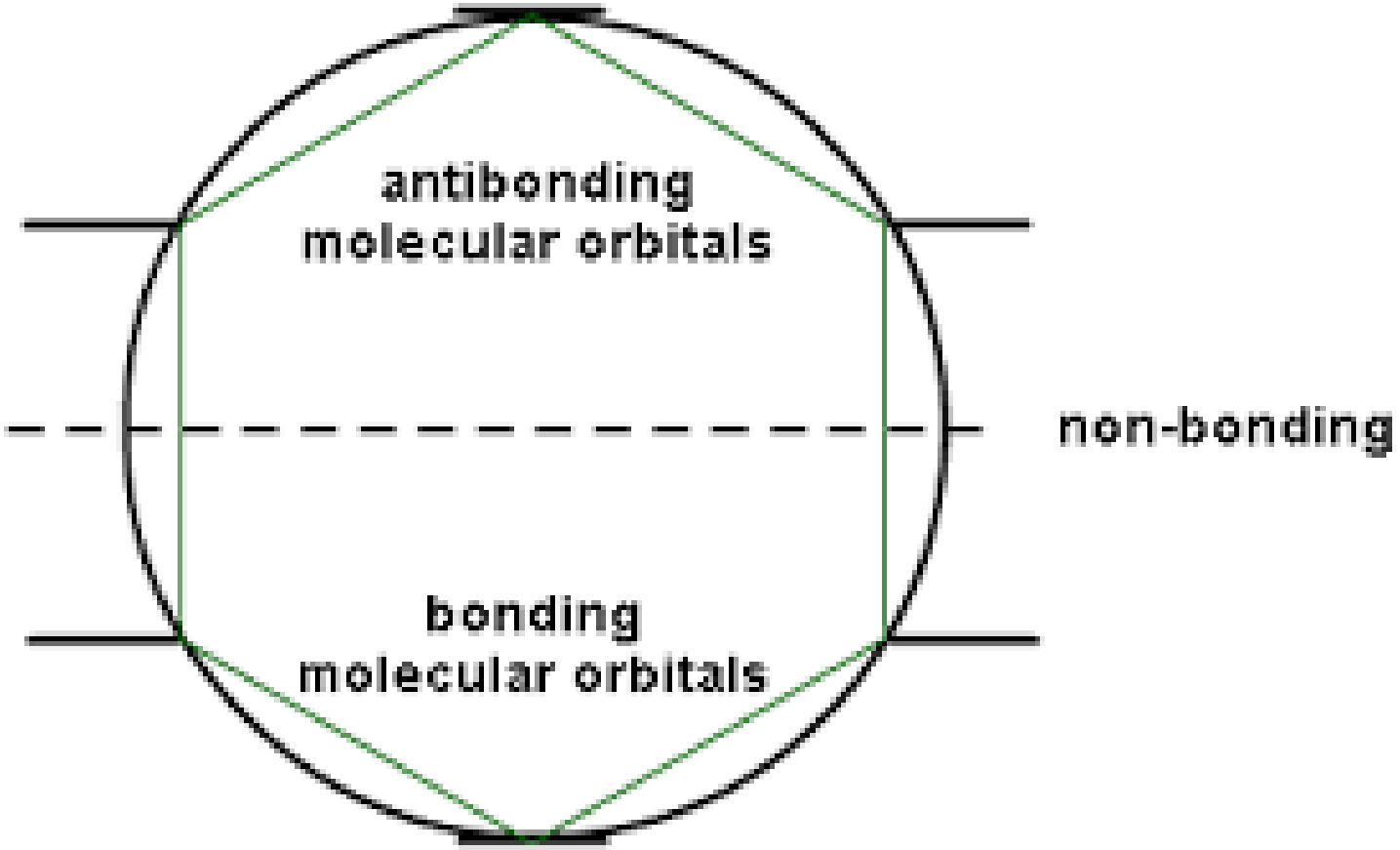
p orbitals

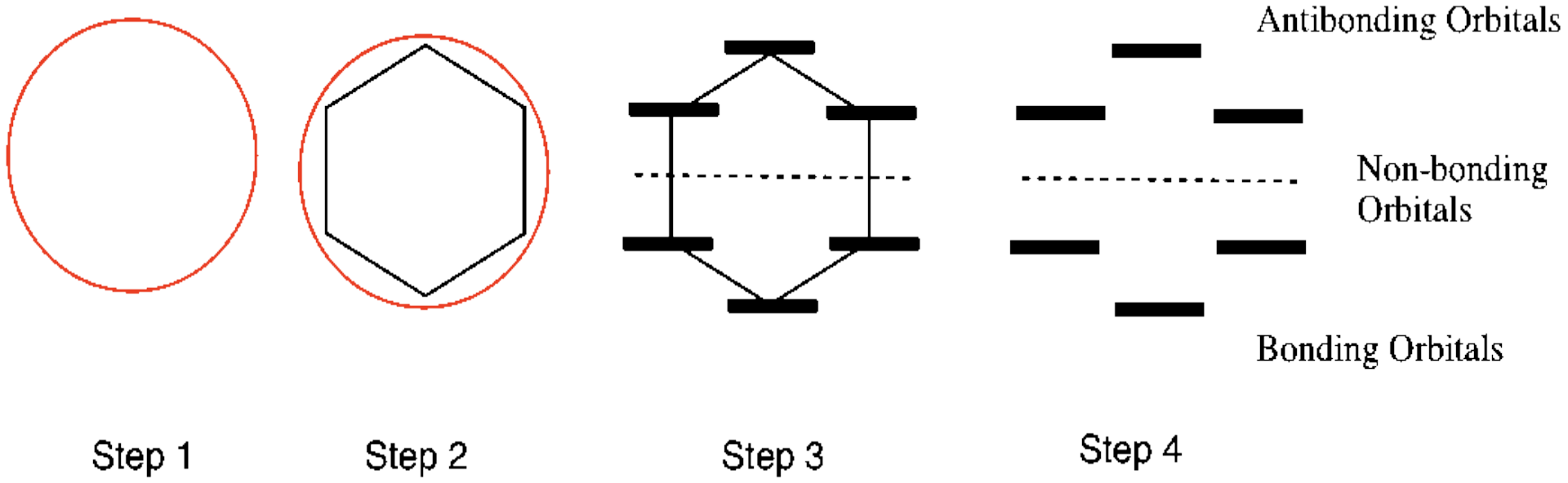
molecular orbital

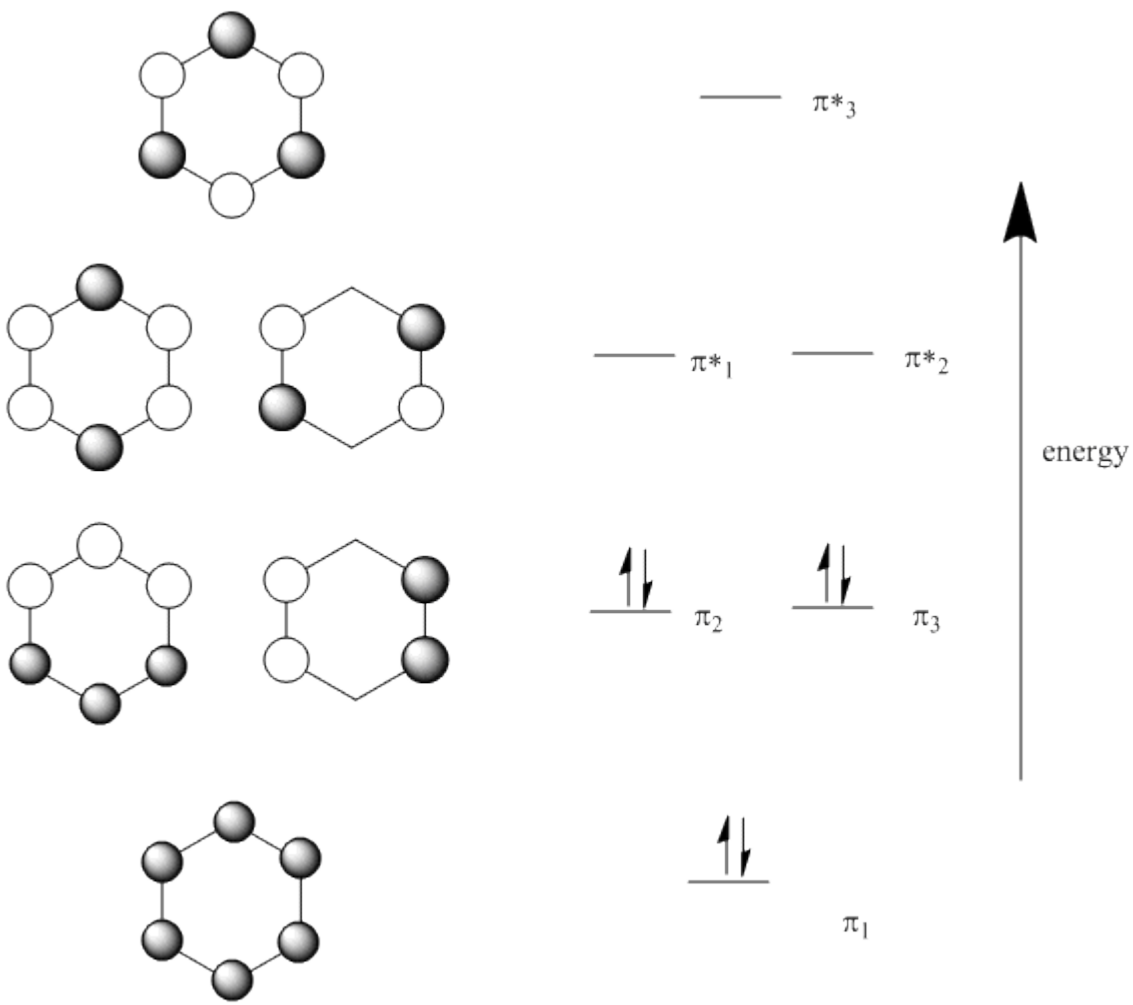
Benzene

- The 6 *p*-orbitals combine to give
  - Three bonding orbitals with 6 π electrons,
  - Three antibonding with no electrons
- Orbitals with the same energy are degenerate




antibonding
molecular orbitals
non-bonding
bonding
molecular orbitals

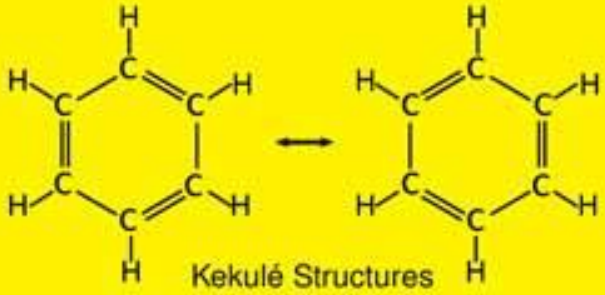

Antibonding Orbitals
Non-bonding Orbitals
Bonding Orbitals
Step 1
Step 2
Step 3
Step 4


π*3
π*1
π*2
energy
π2
π3
π1

Benzene Ring Structure

C_6H_6

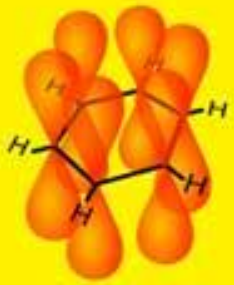
Benzene
Molecular formula



Kekulé Structures
(Resonance Forms)

Planar Hexagon
Bond Length 140 pm

Sigma Bonds
sp^2 Hybridized orbitals



6 p_z orbitals

delocalized pi
system

Benzene ring
Simplified depiction