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

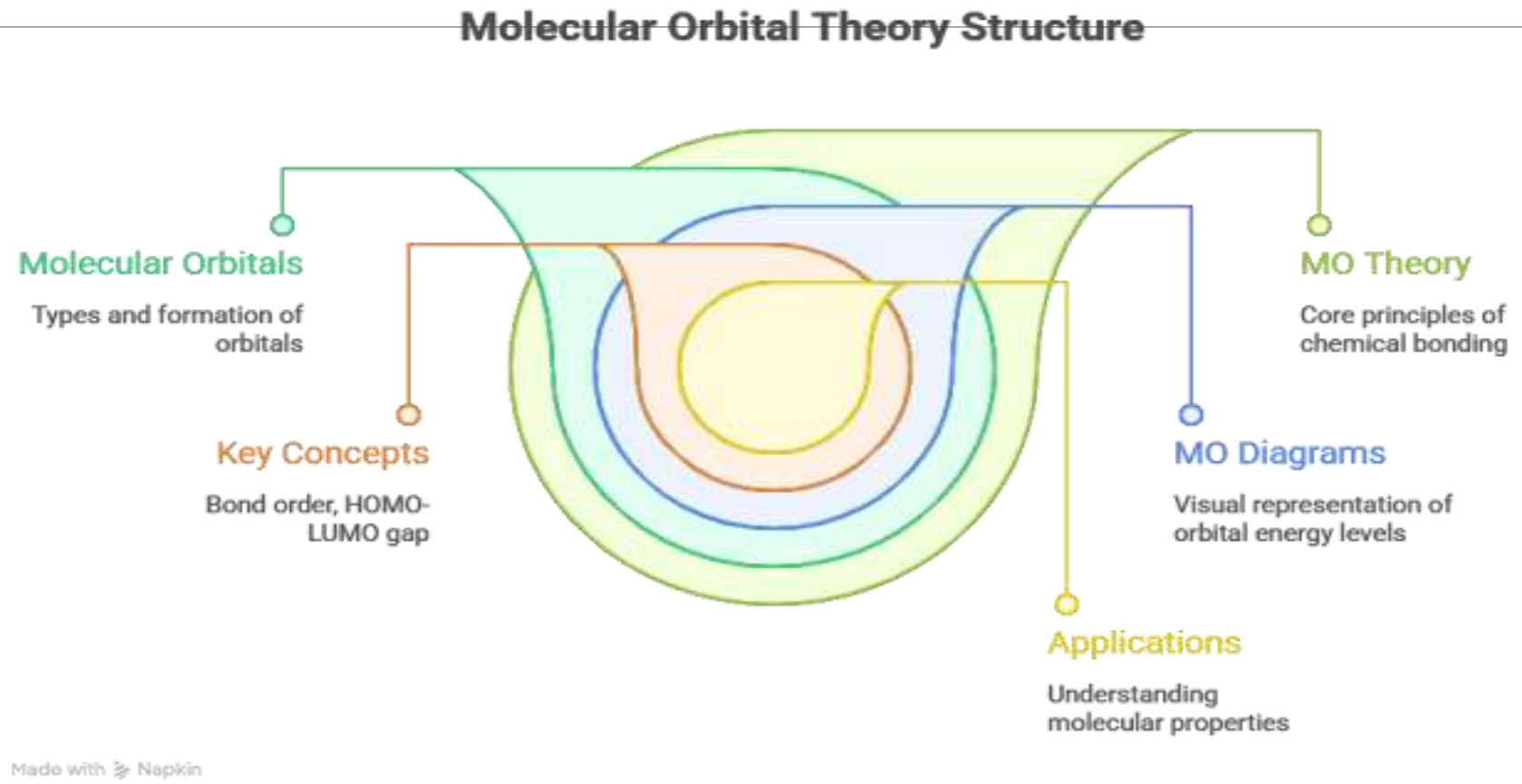
COURSE NAME : PHARMACEUTICAL ORGANIC CHEMISTRY-II

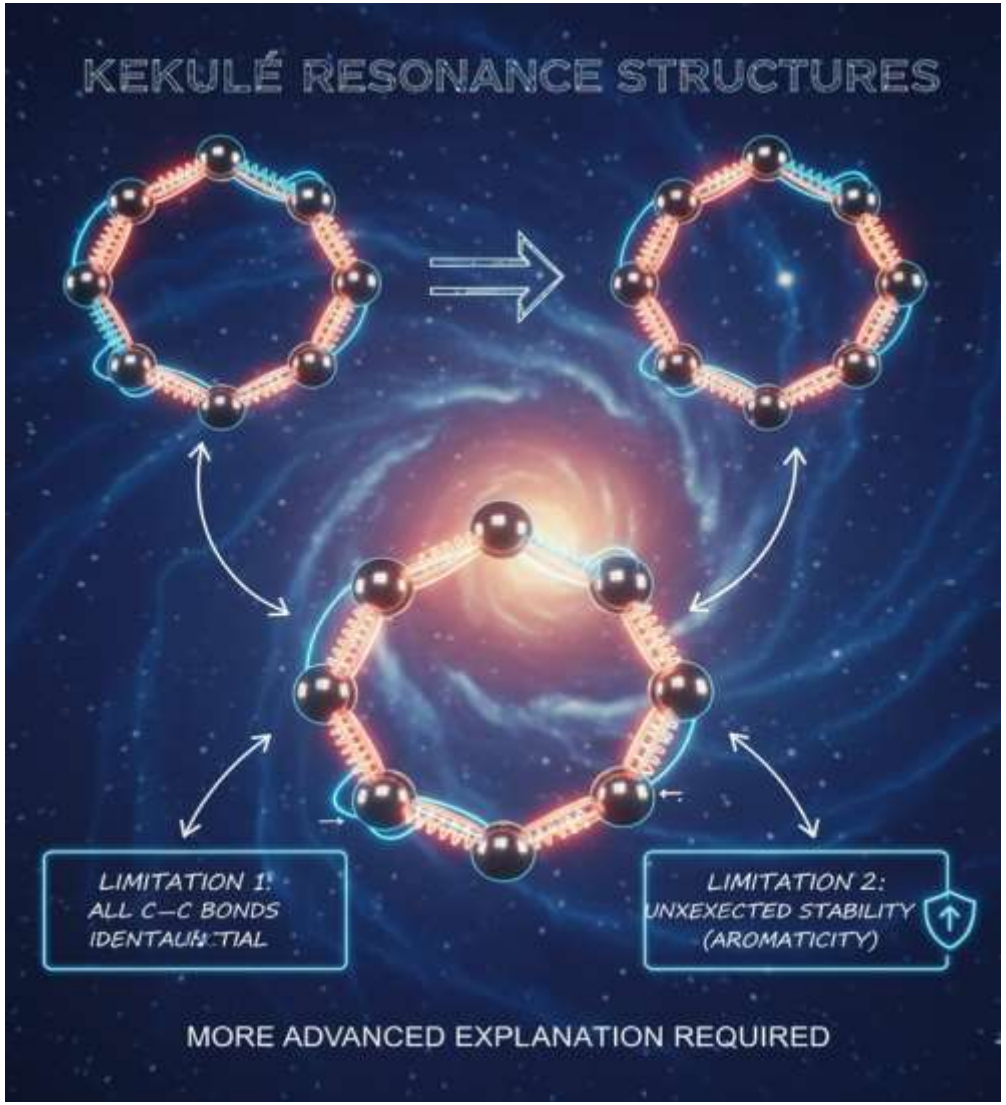
III SEM / II YEAR

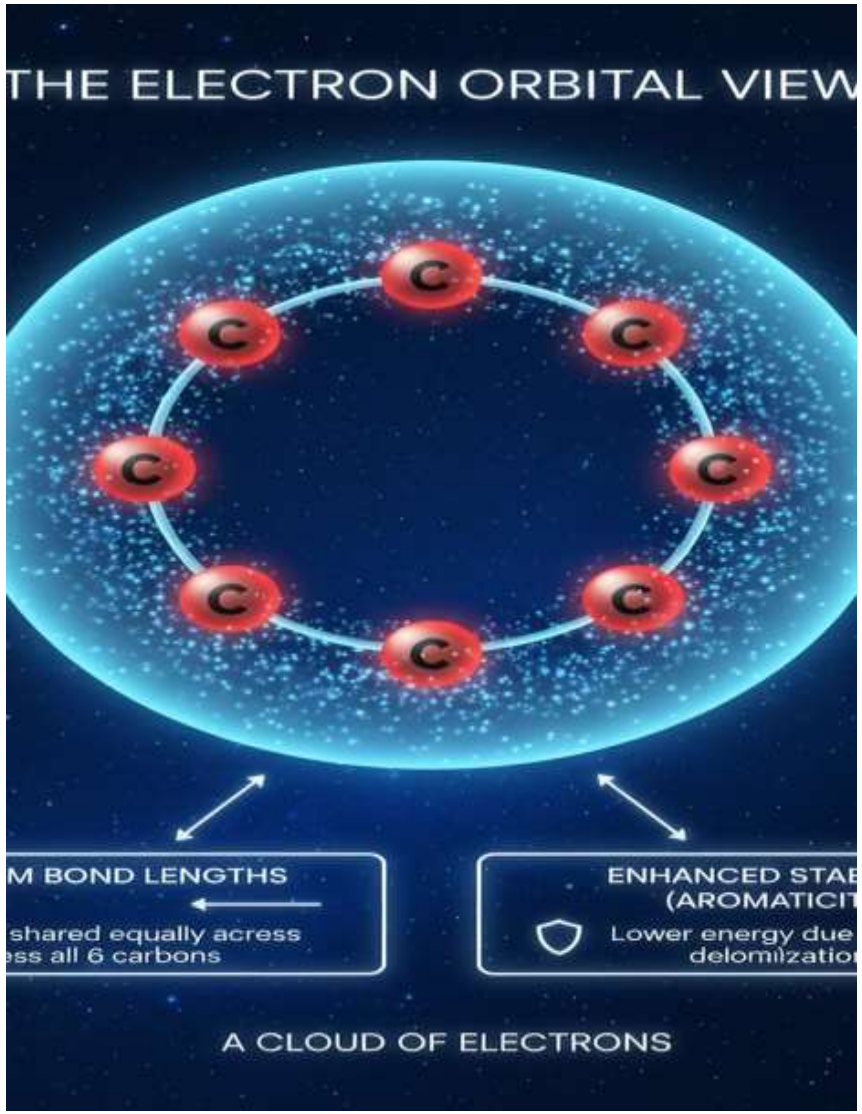
TOPIC 1 : MOLECULAR ORBITAL THEORY OF BENZENE


BENZENE
DELOCILAIZED ELECTRONS
AROMATICITY

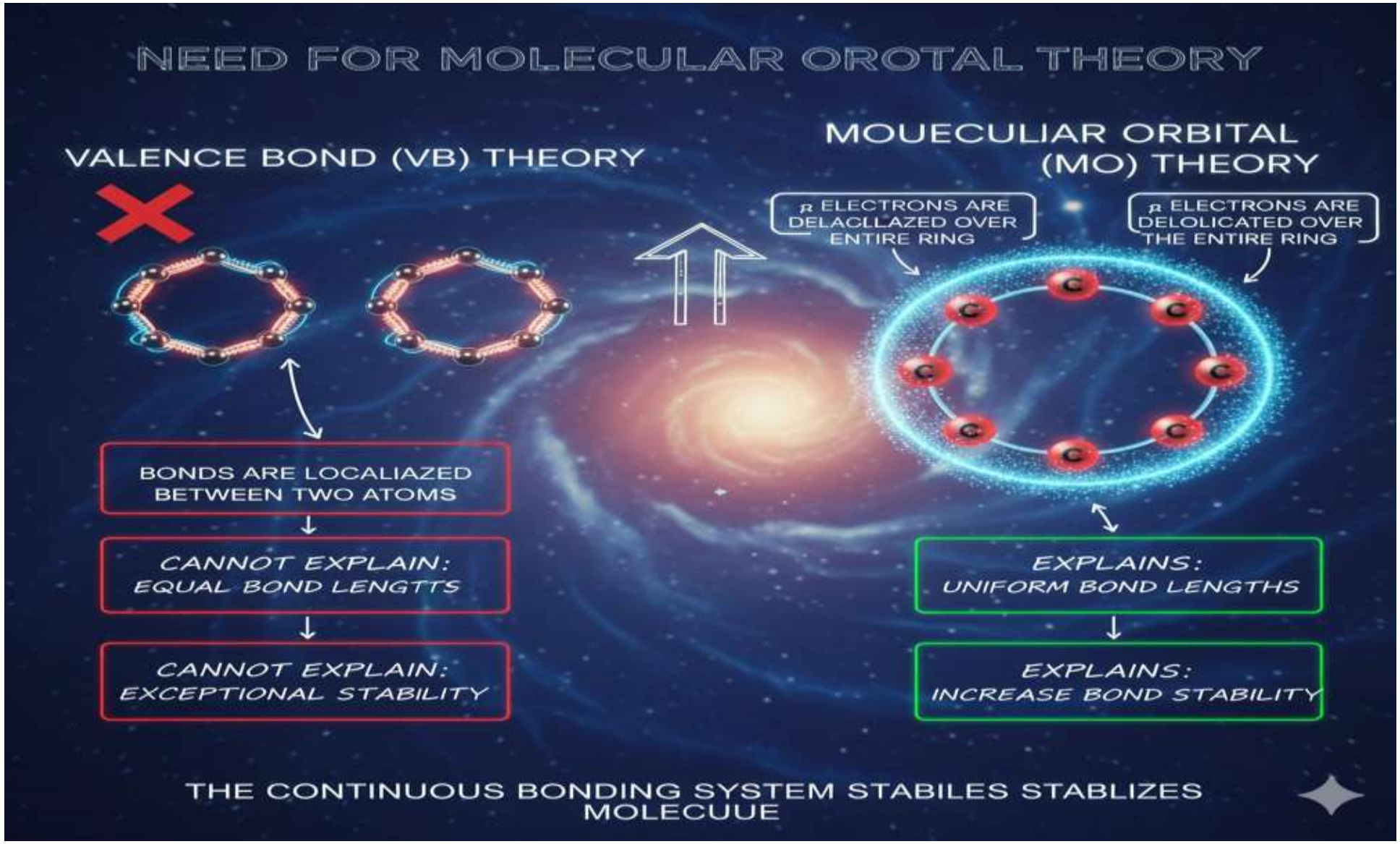
MOLECULAR ORBITAL THEORY-MINDMAP



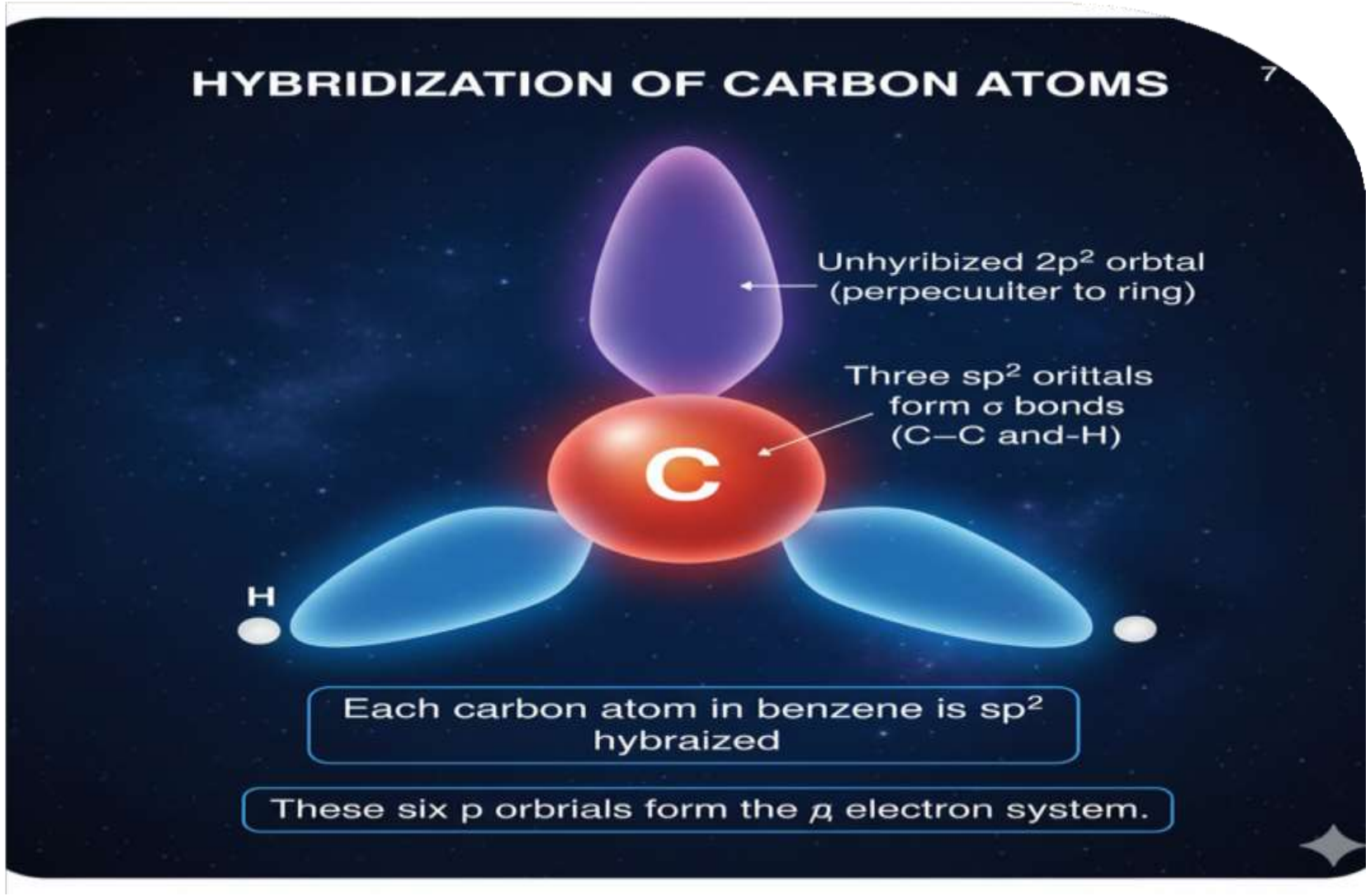

KEKULÉ RESONANCE STRUCTURES
LIMITATION 1:
ALL C–C BONDS
IDENTAUNCTIAL
LIMITATION 2:
UNXEXECTED STABILITY
(AROMATICITY)
MORE ADVANCED EXPLANATION REQUIRED


THE ELECTRON ORBITAL VIEW
C
C
C
C
C
C
M BOND LENGTHS
shared equally acress
ess all 6 carbons
ENHANCED STAE
(AROMATICIT
Lower energy due
delomlizatio
A CLOUD OF ELECTRONS

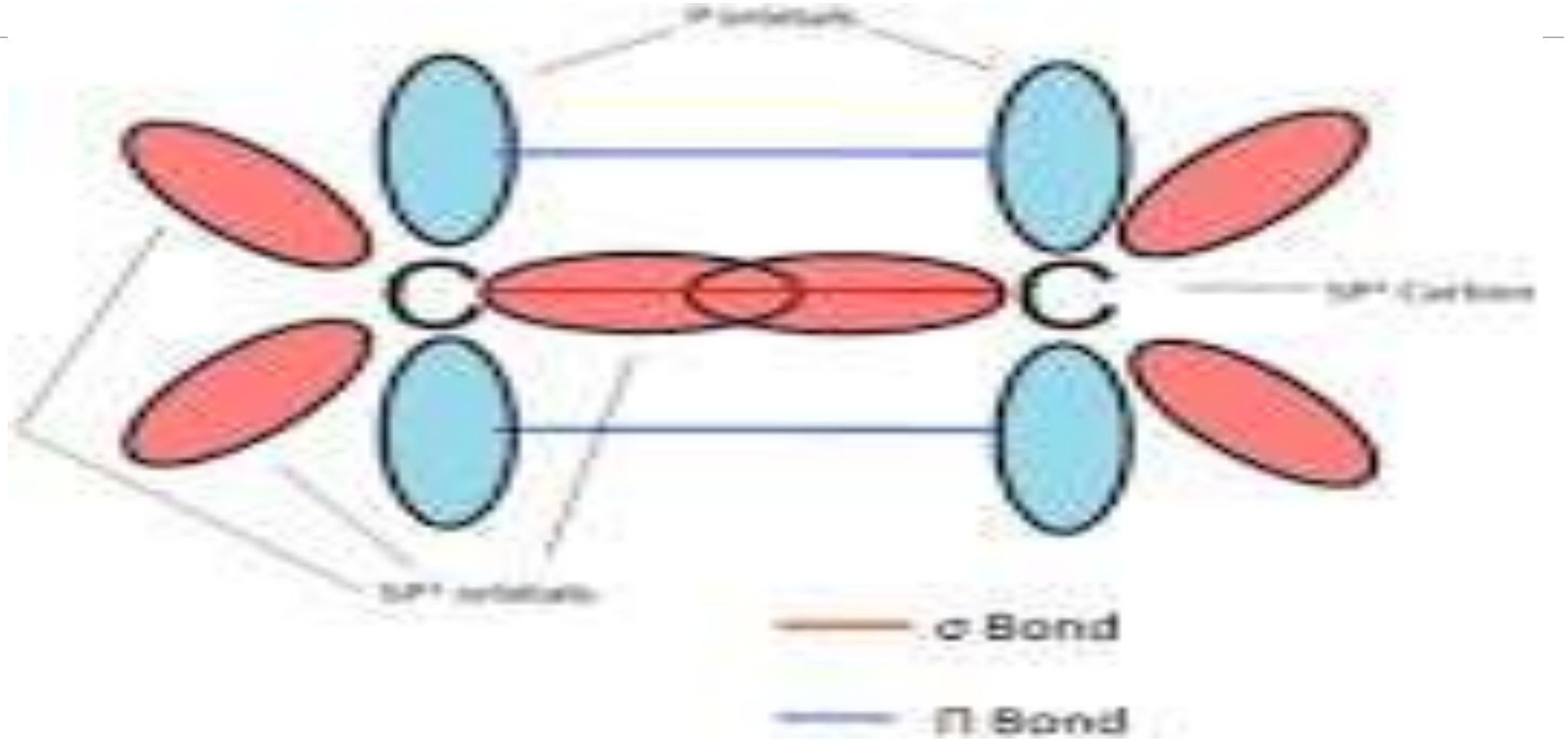
VALENCY ELECTRONS



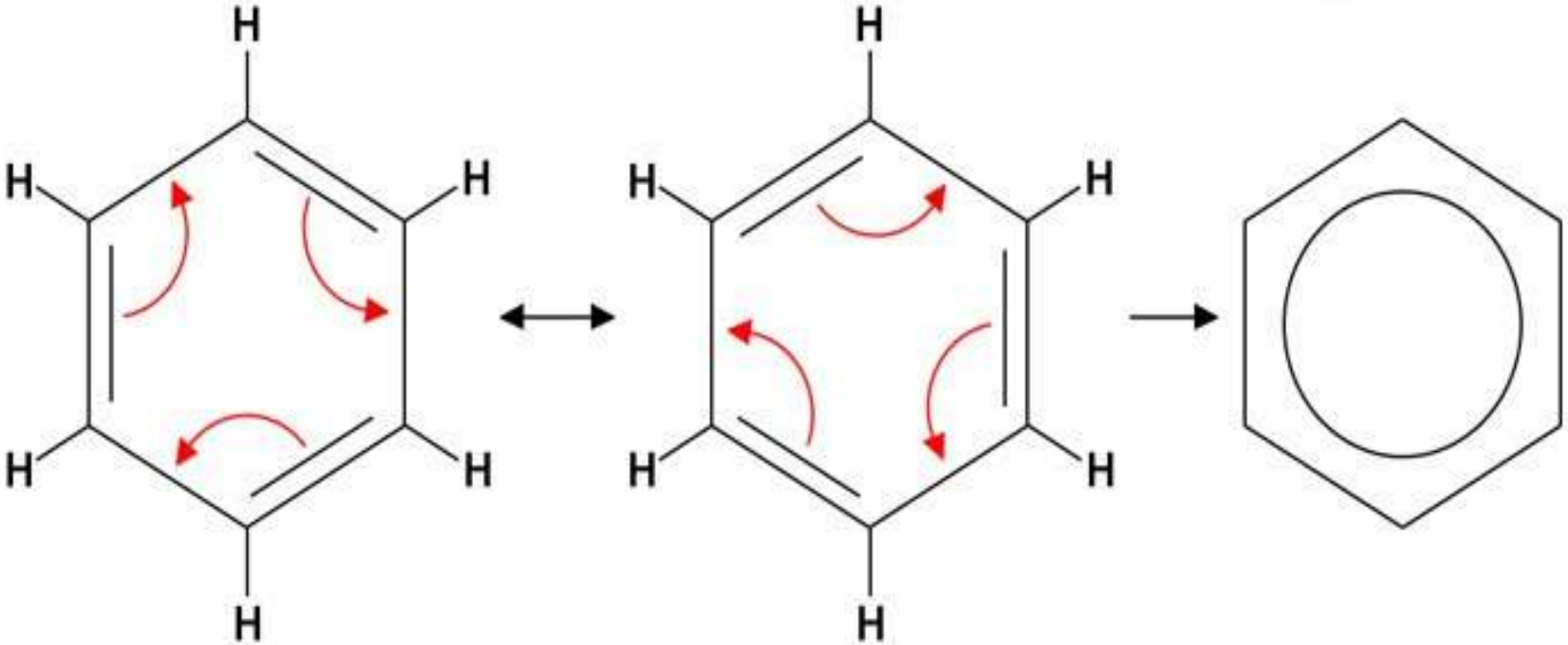
HYBRIDIZATION OF CARBON ATOMS



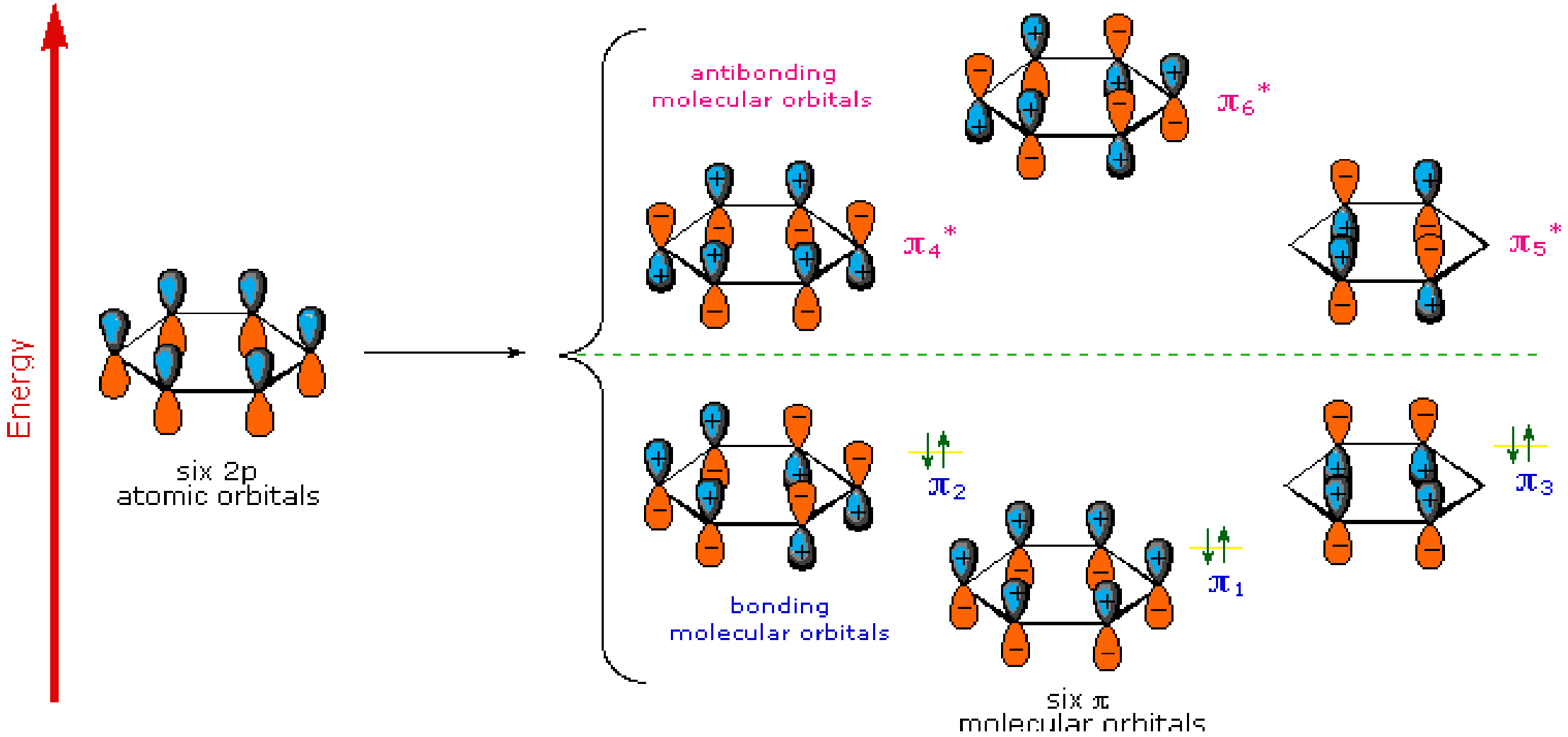
FORMATION OF THE Π SYSTEM

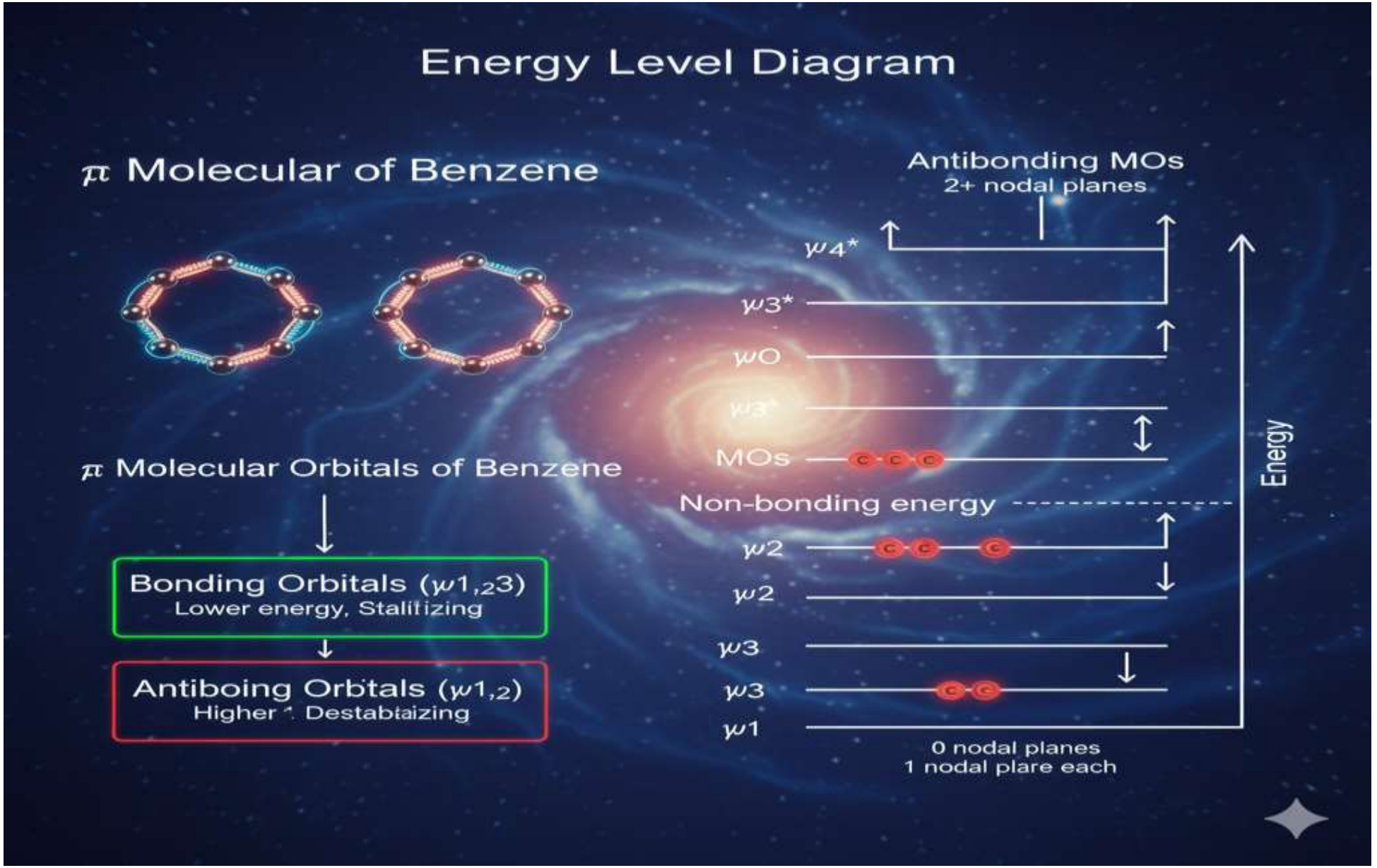


Delocalization of Pi Electrons in Benzene

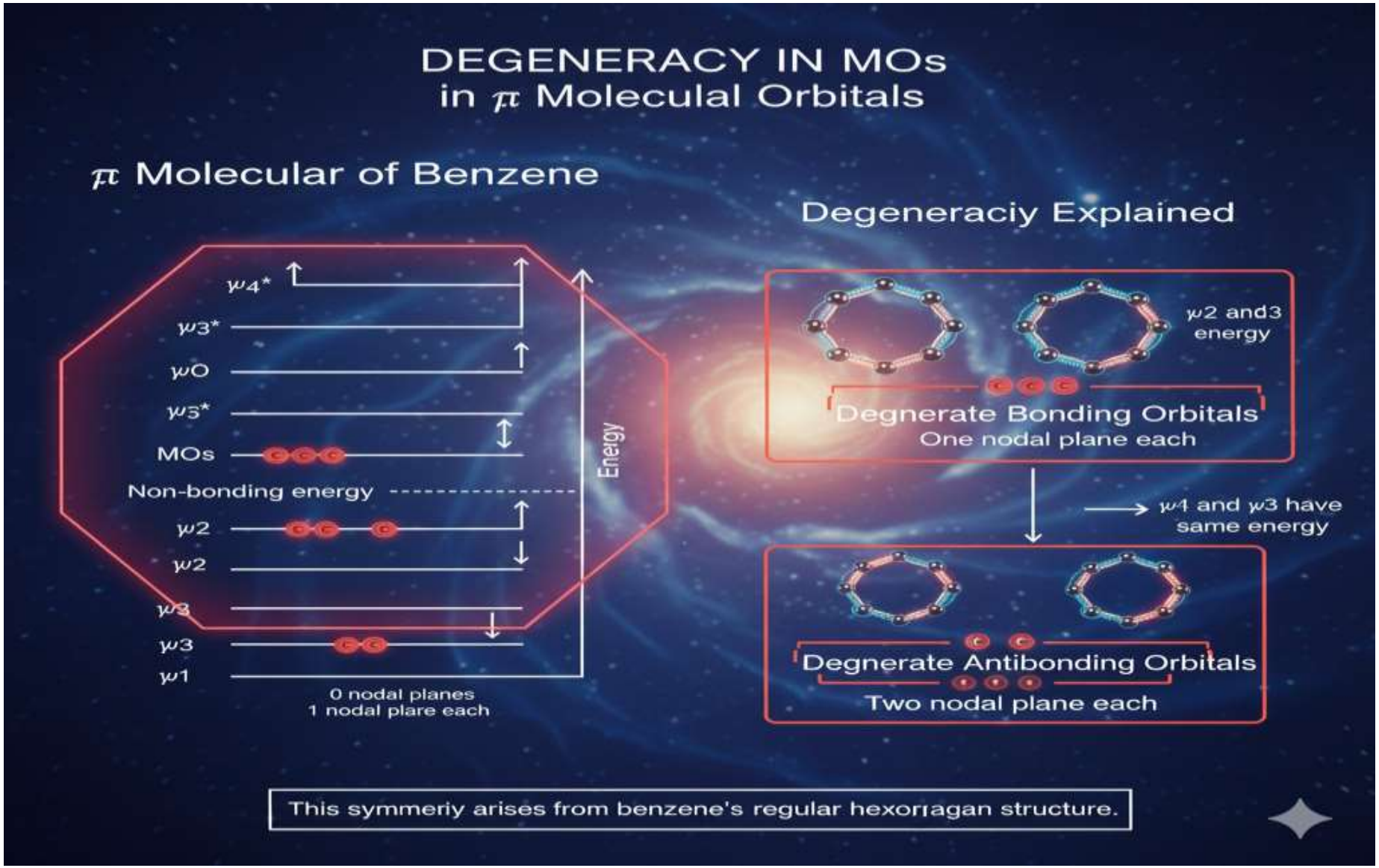


NUMBER OF MOLECULAR ORBITALS

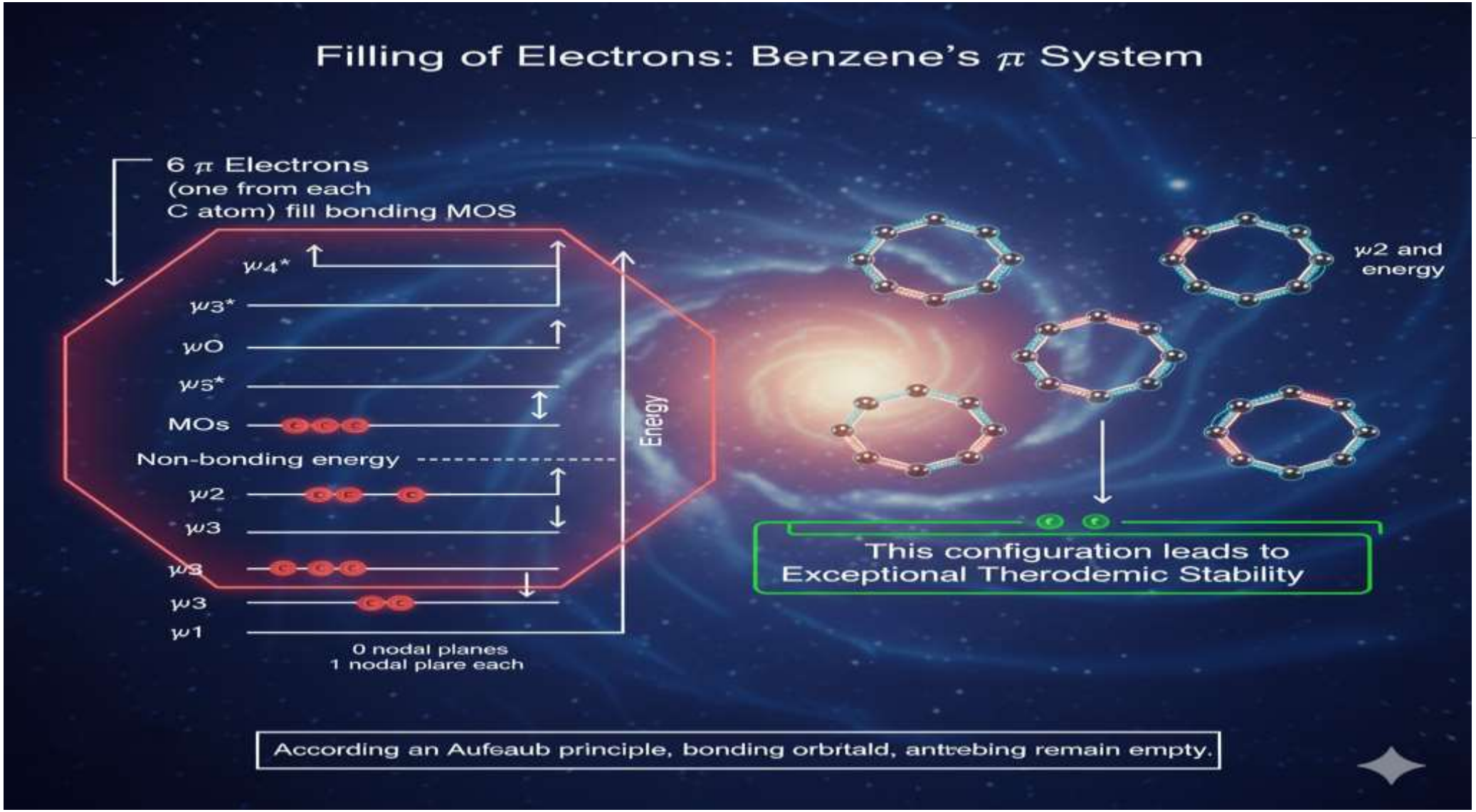


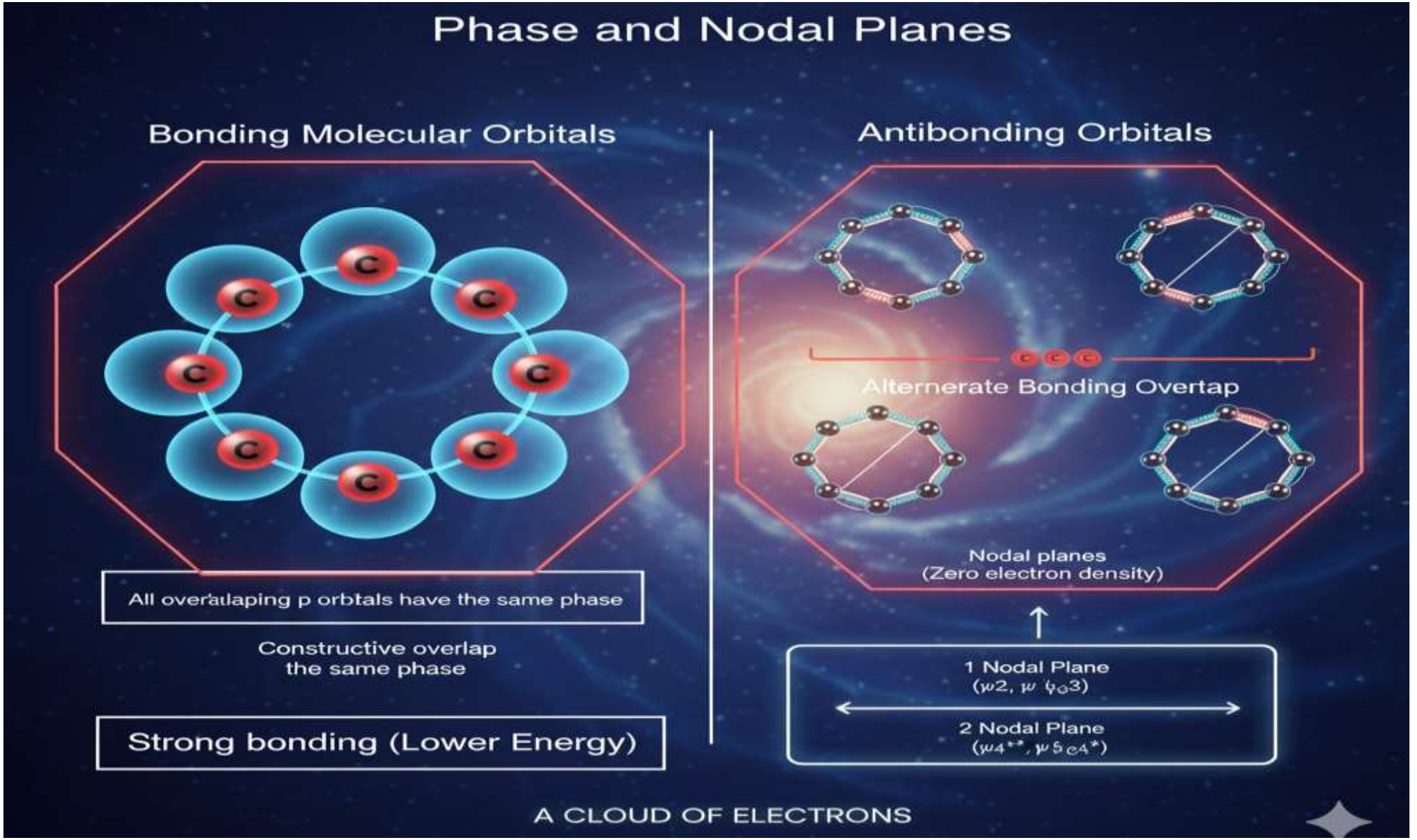

Energy Level Diagram
π Molecular of Benzene
π Molecular Orbitals of Benzene
Bonding Orbitals (ψ1,23)
Lower energy, Stalilizing
Antiboing Orbtals (ψ1,2)
Higher ¹ Destabtaizing
Antibonding MOs
2+ nodal planes
ψ4*
ψ3*
ψO
ψ3
MOs
Non-bonding energy
ψ2
ψ2
ψ3
ψ3
ψ1
Energy
0 nodal planes
1 nodal plare each

DEGENERACY IN MOS

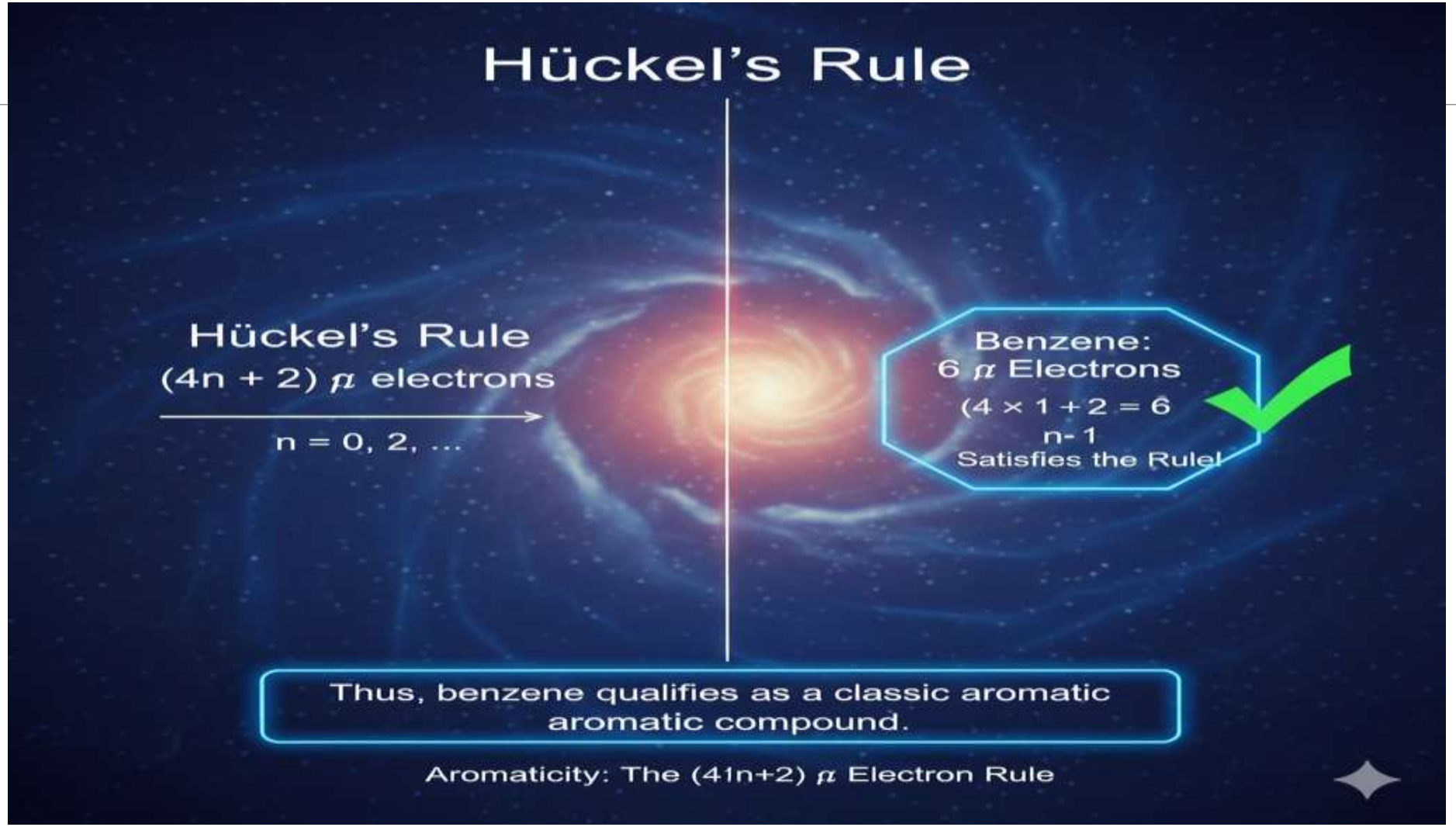


FILLING OF ELECTRONS IN BENZENE

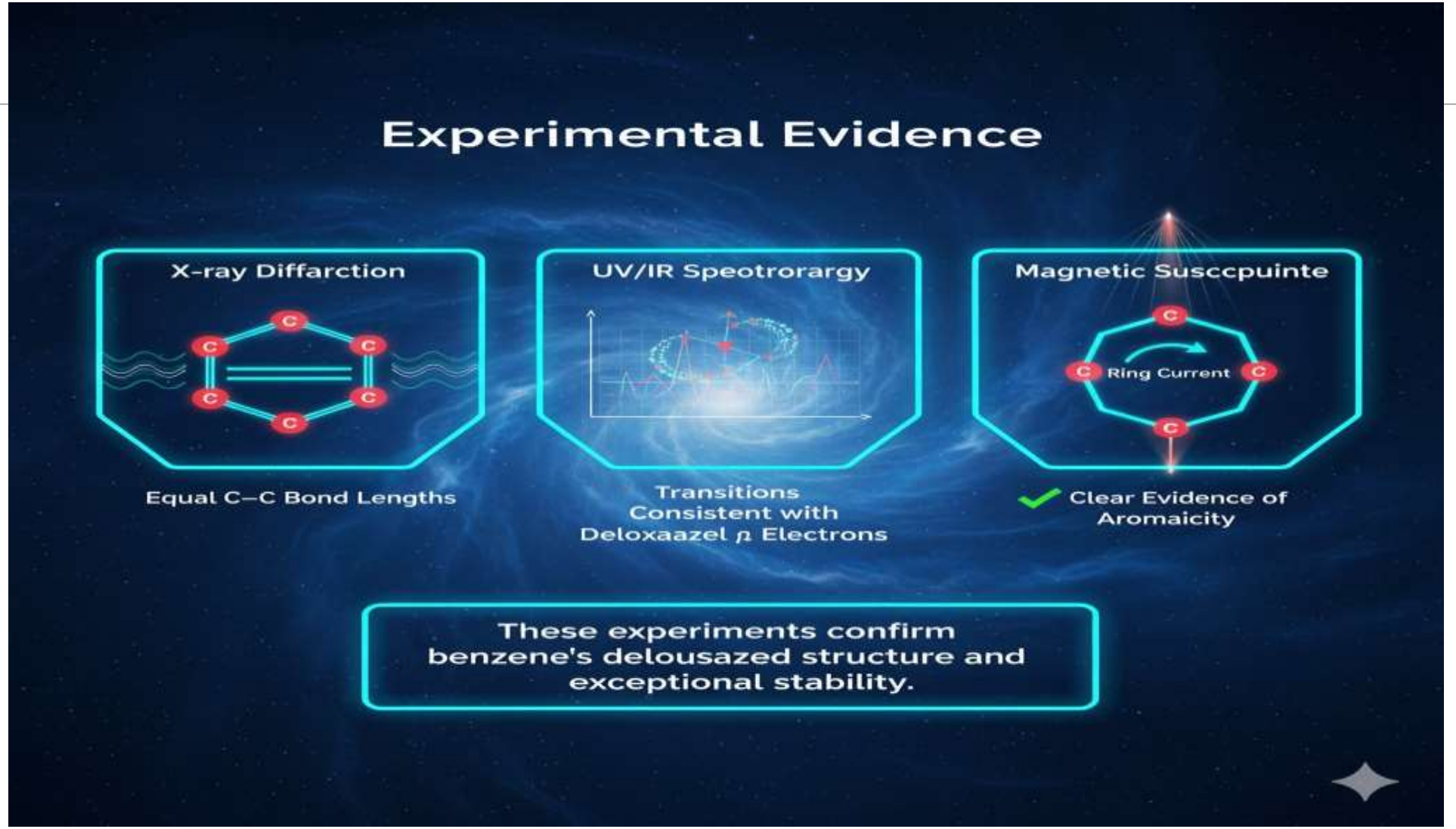



Phase and Nodal Planes
Bonding Molecular Orbitals
Antibonding Orbitals
C
Alternerate Bonding Overtap
All overalaping p orbtals have the same phase
Constructive overlap
the same phase
Strong bonding (Lower Energy)
Nodal planes
(Zero electron density)
1 Nodal Plane
2 Nodal Plane
A CLOUD OF ELECTRONS

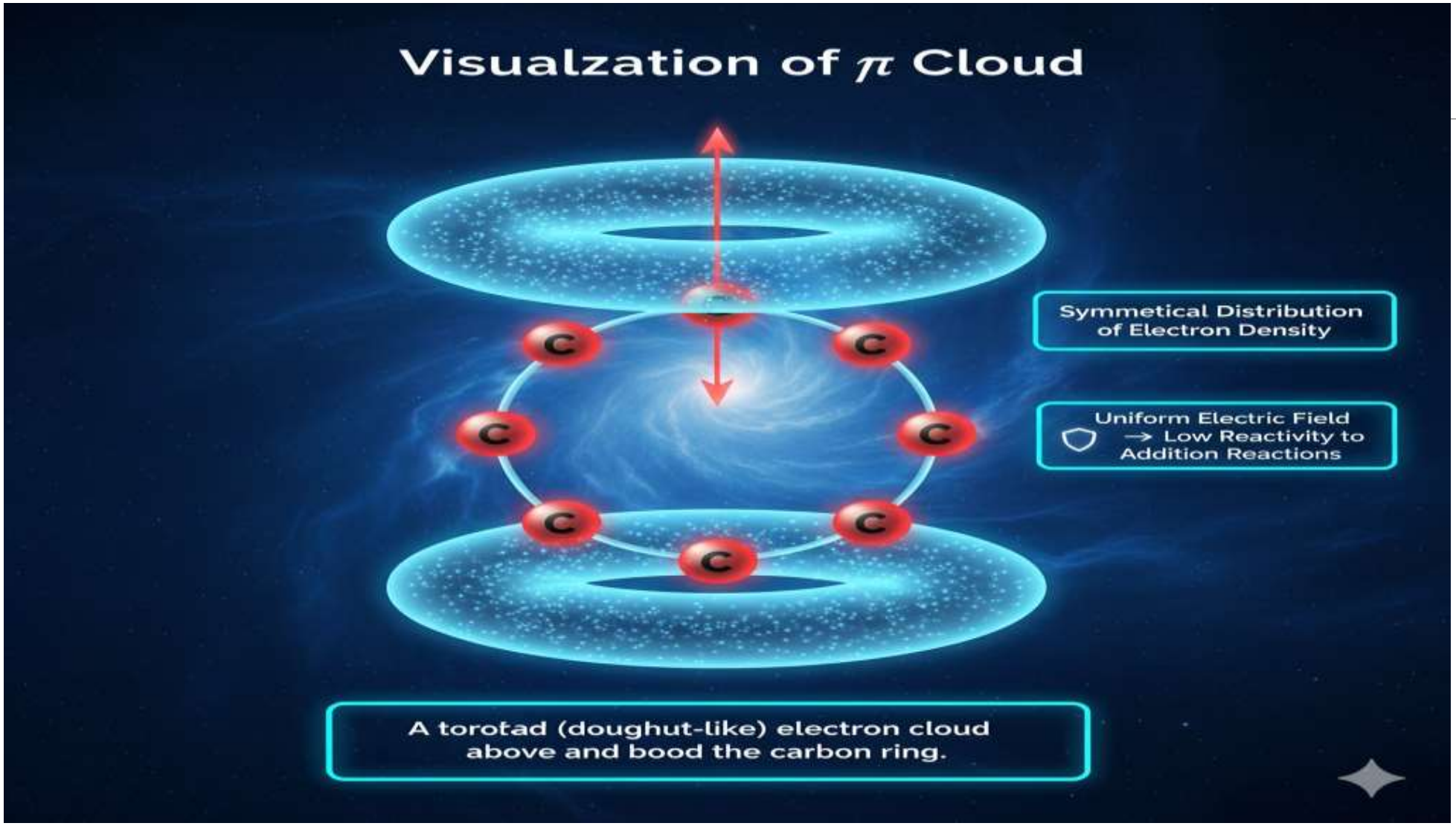
HÜCKEL'S RULE



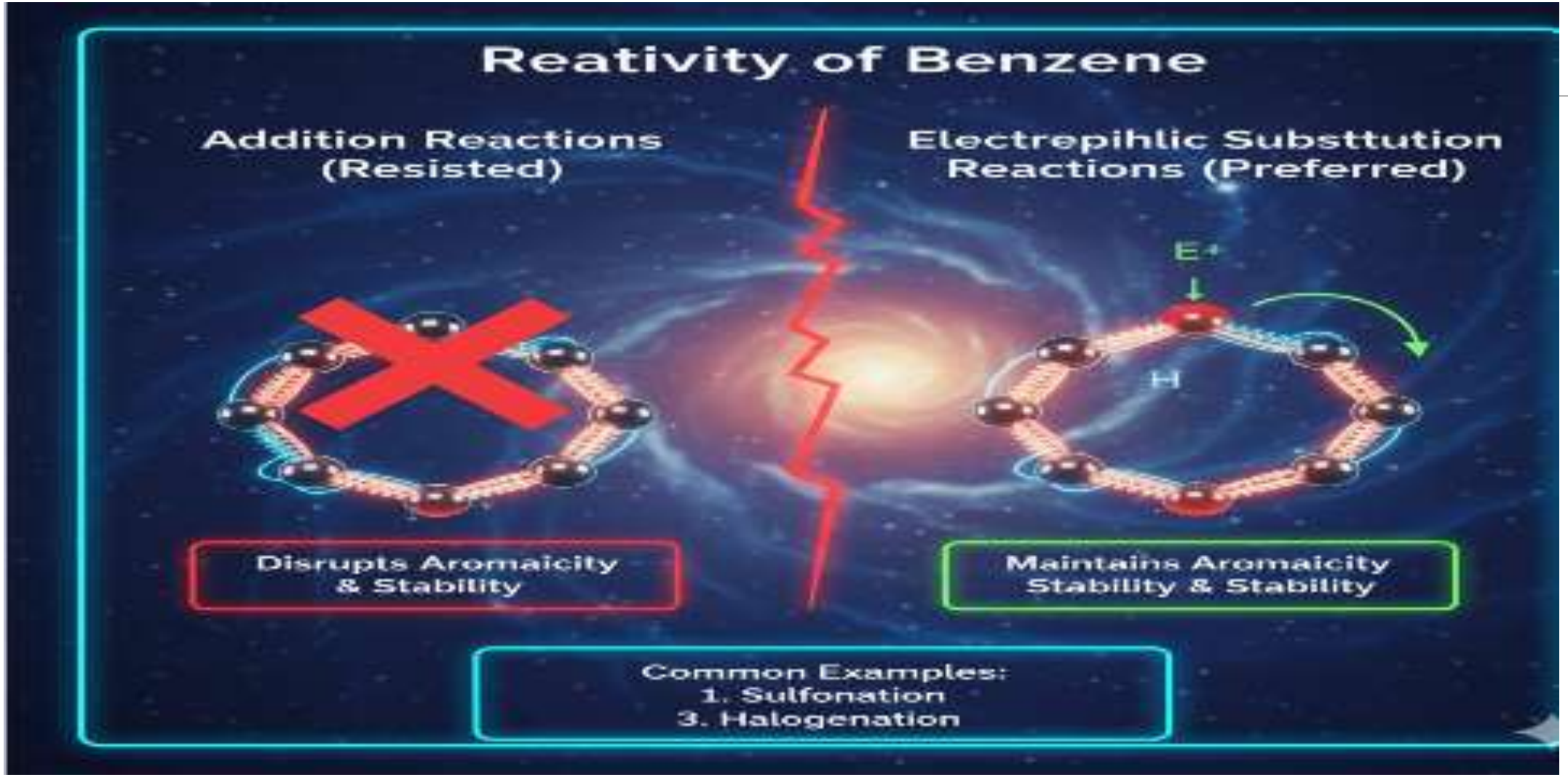
EXPERIMENTAL EVIDENCES



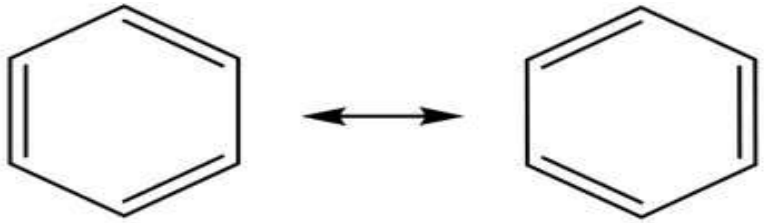
VISUALISATION OF PI ELECTRONIC CLOUD



REACTIVITY OF BENZENE

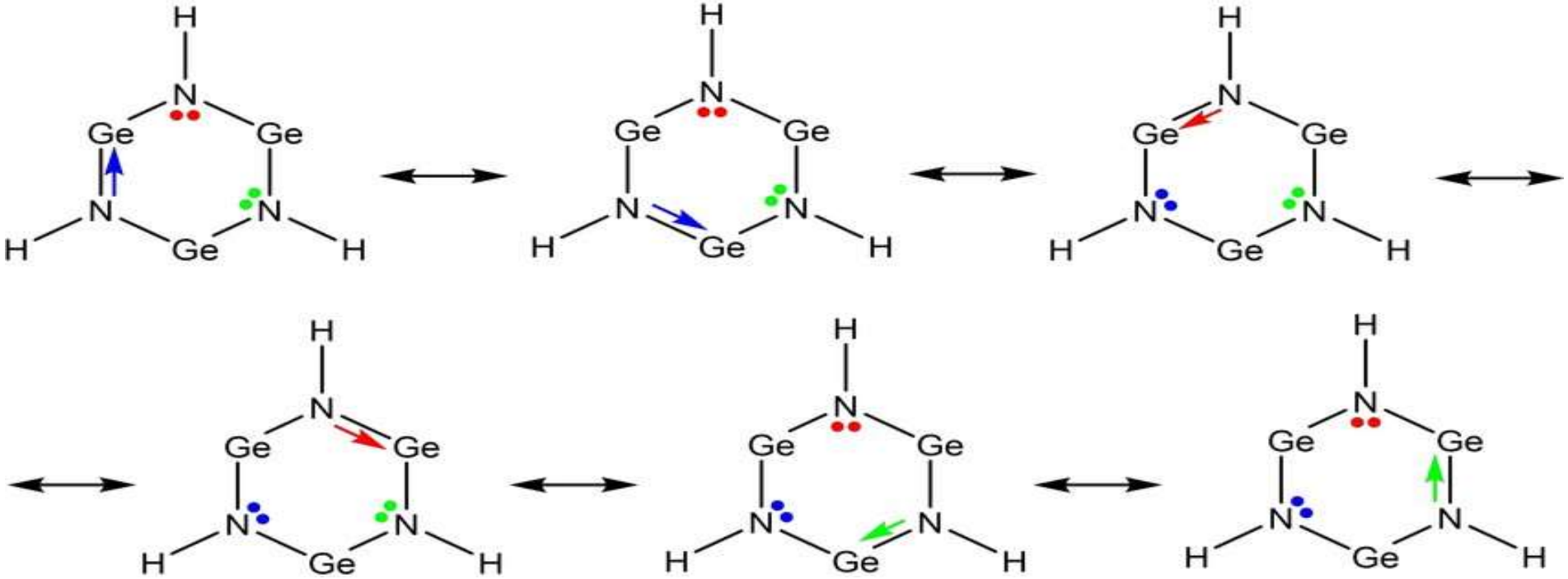


DELOCALISATION IN SUBSTITUTED BENZENE



Benzene

vs.



Molecular Orbital Theory Concepts

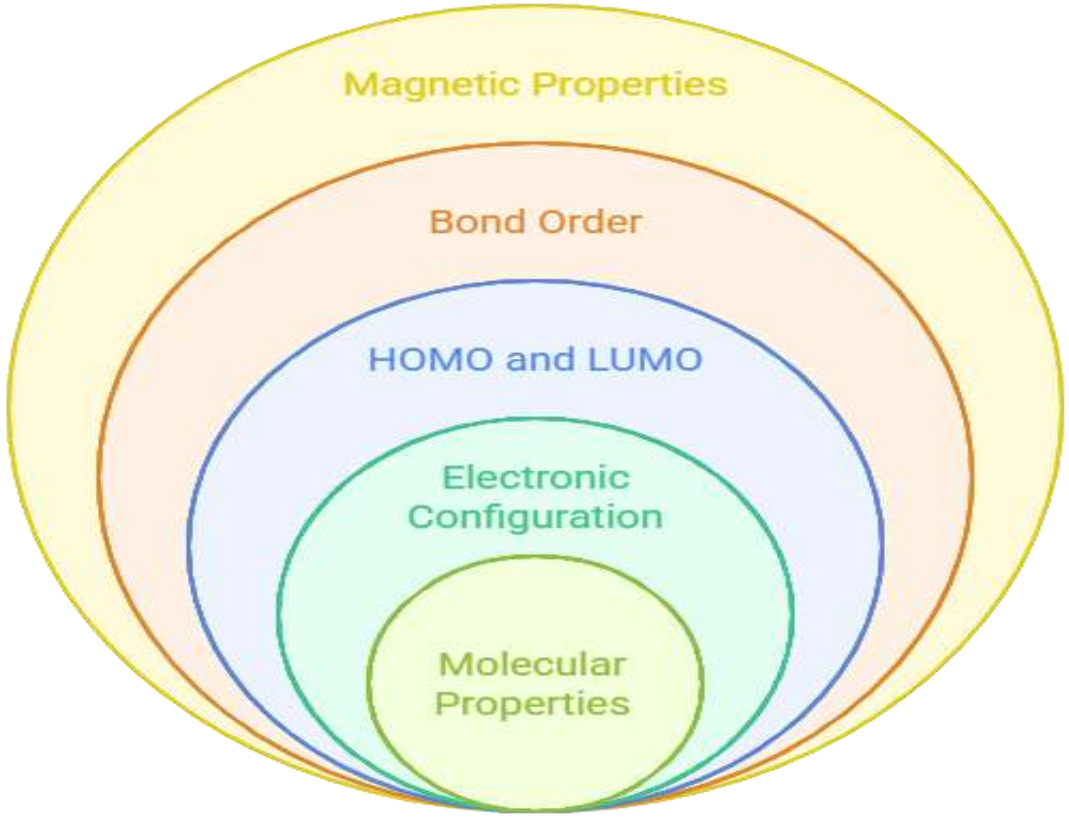
Behavior in magnetic fields

Strength and length of bonds

Orbitals for reactivity and transitions

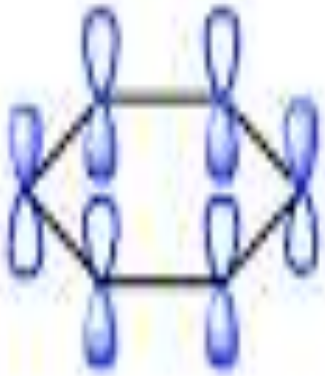
Electron distribution in MOs

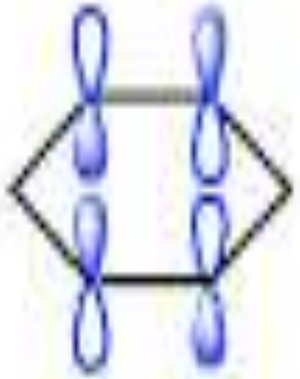
Determine molecule's characteristics

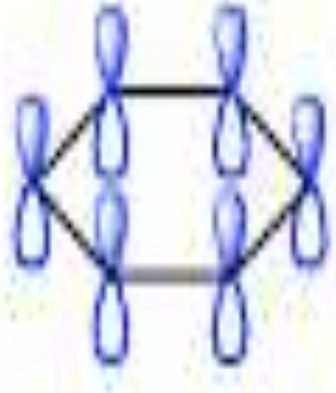


ASSESMENTS

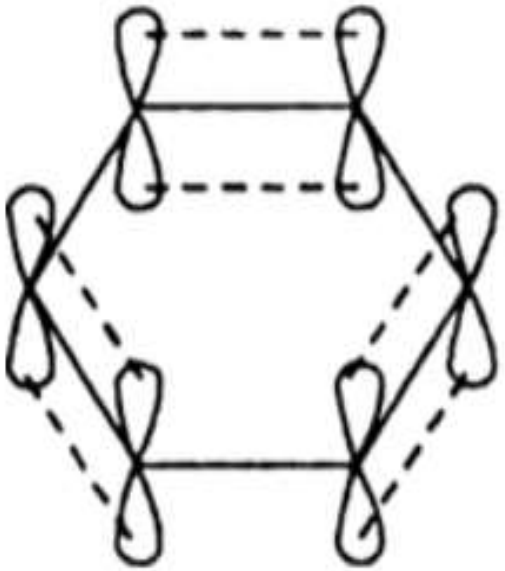
How many **nodal planes** are present in each of the following orbitals?
(not counting the plane of the ring cutting through each p-orbital)

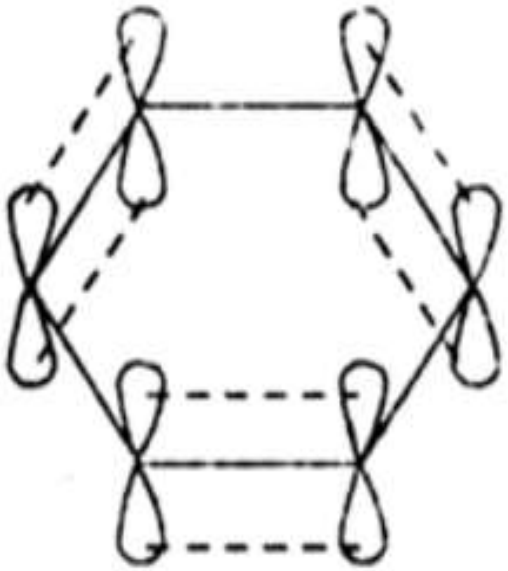


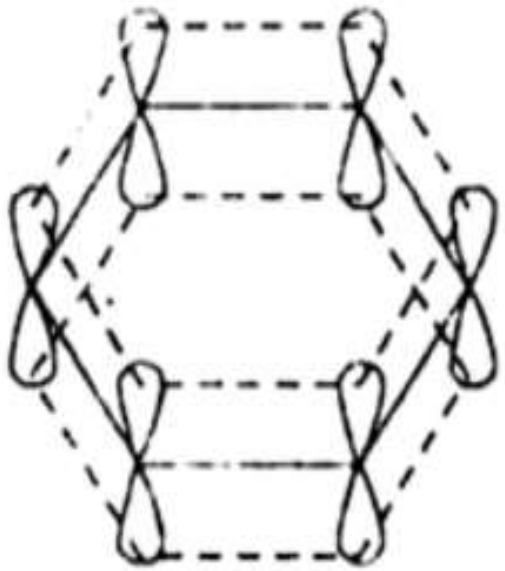




Explain the molecular orbital picture of Benzene








Thank You