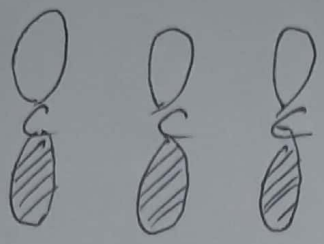
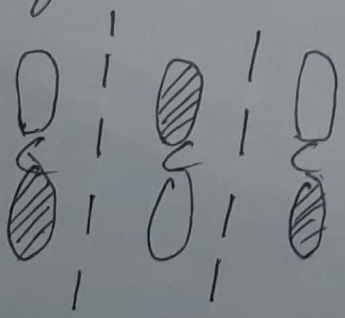
Pi Molecular Orbital of Butadiene:

- No. of MO (n) for a pi-system is equal to no. of contributing P orbital. For allyl system n=3 and we had three contributing p orbitals and thus three pi molecular orbitals.
- The lowest energy orbitals has zero nodes b/w the p orbitals that is in the lowest energy orbitals, all phases of the contributing p-orbitals are aligned the same way.



π_1 0 nodes b/w orbitals

- The no. of nodes ↑ed by one for each successive energy level such that the highest energy orbital has (n-1) nodes (all phases of contributing p-orbitals alternate).

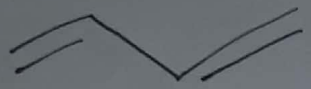


(2 nodes b/w orbitals)

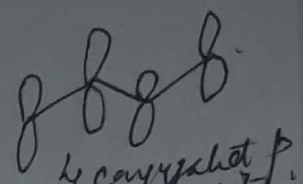
- The lowest and highest energy orbitals are always the easiest pi molecular orbitals to draw It's helpful to draw them first.
- Nodes are positioned in such a way that they are symmetrical relative to the centre. A system with 1 node has the node smack in the centre A system with 2 node will have nodes at equal distance relative to centre.

For Butadiene

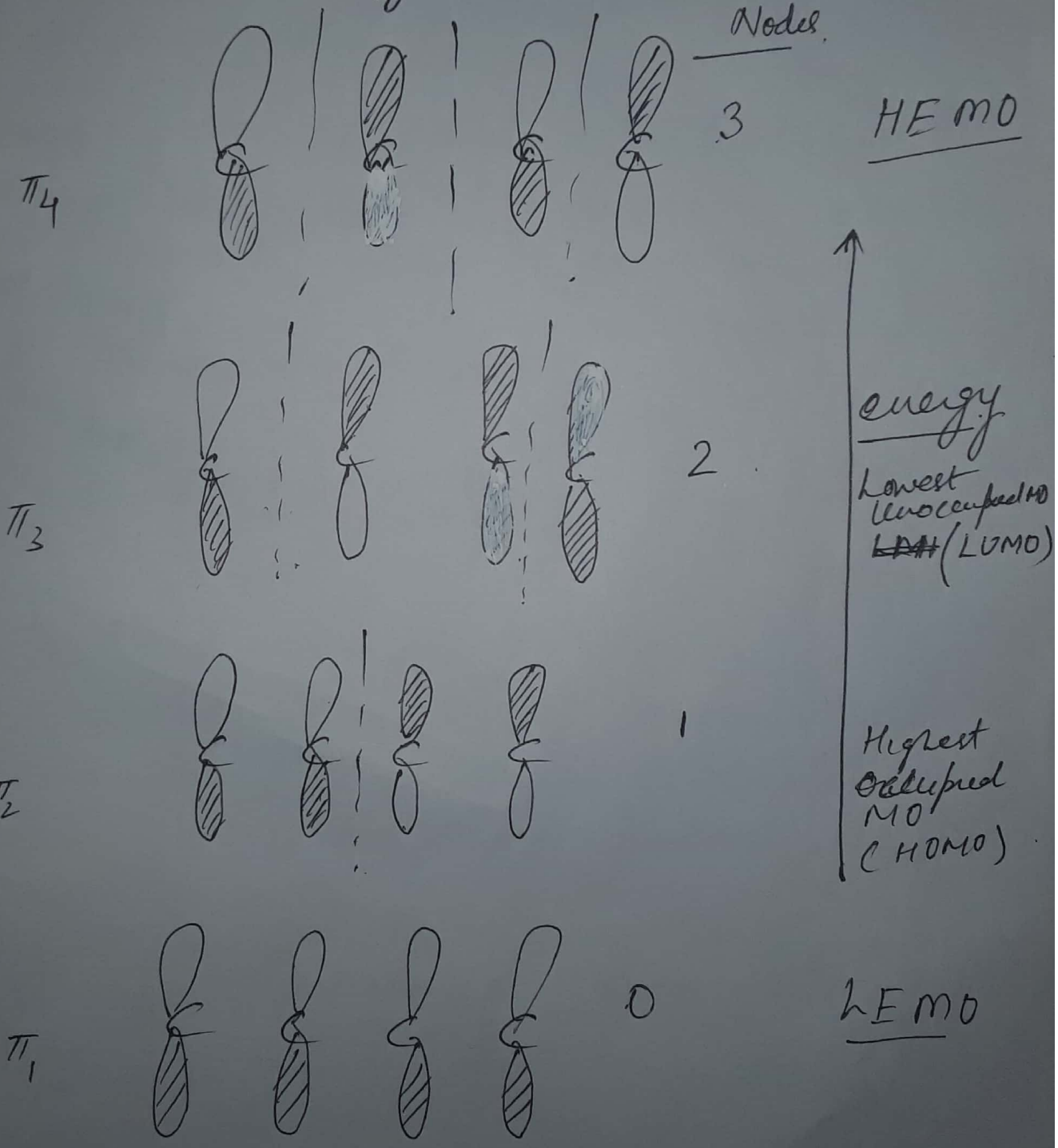
C=C−C=C



4π electrons.



Butadiene has 2 double bonds & 4 π e' We fill up the lowest energy Molecular Orbital LEMO



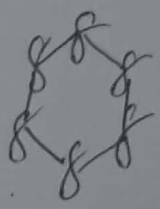
We have considered HOMO and LUMO ie π_2 and π_3 respectively. HOMO is like the Valance electrons of the pi system. they are most readily lost. If butadiene participates in the rxn where it is e⁻ donor that is (Nucleophile), it's electrons are going to come from that Orbital.

LUMO is π_3. if butadiene participates in the rxn where it is a e⁻ acceptor ie electrophile the e⁻ will be donated to that Orbital.

Now for Benzene

6 p orbitals ∴
So 6 ~~MO~~ Pi(MO) Molecular Orbitals.

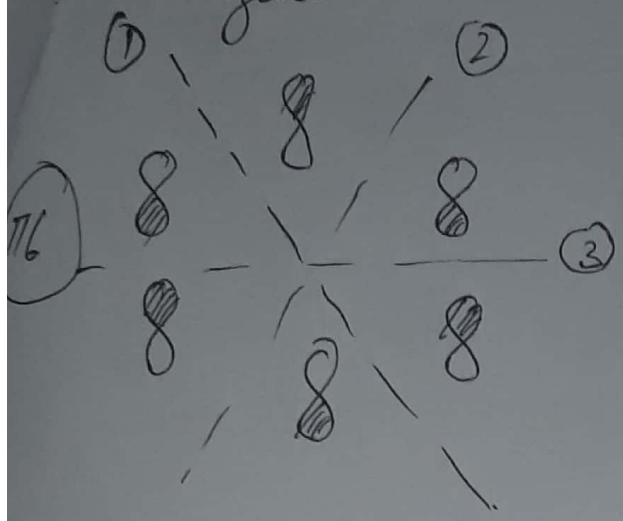
C_6H_6



n = 6

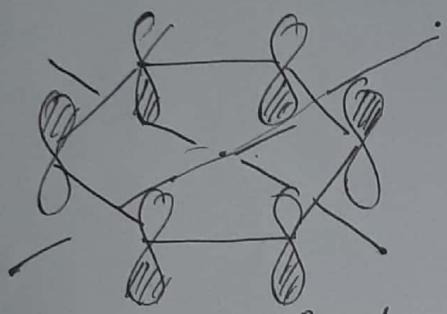
Now the no. of nodes Pes with each successive energy level :- A node is where there is change in phase b/w adjacent P-Orbitals. (where they can't constructively overlap). At lowest energy level (0 node). It provides the greatest possible delocalization of the electron the highest level has (n-1) nodes. (alternate all phases)
Nodes are always placed symmetrically wrt centre of the orbital.
- A single node must cut through the centre of MO.
- 2 nodes must be placed at equal distance from centre.
- Each successive energy level adds an extra node.
an orbital c an odd no. of nodes will have a node in centre.
- Then fill MO c electron using Aufbau rule

Benzene

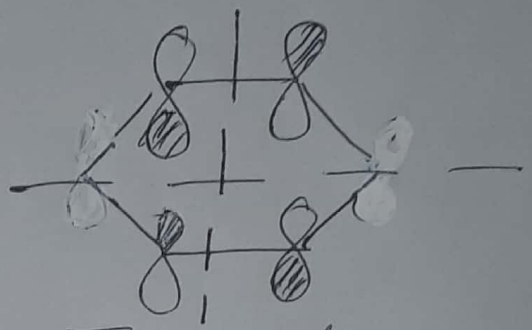


(4)

Lowest possible delocalisation of electron due to lack of overlap ∴ they are in highest energy.
6 nodes (3 nodal planes)

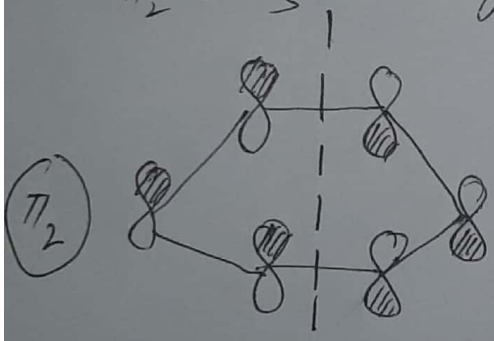


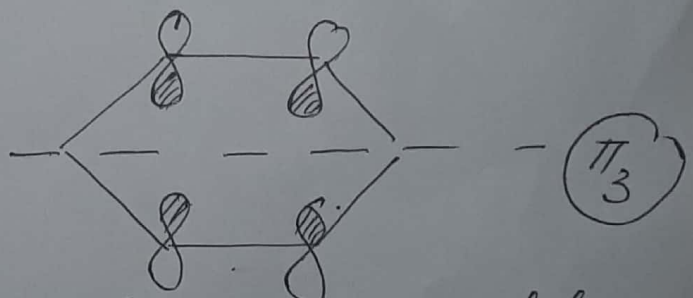
Through Bond



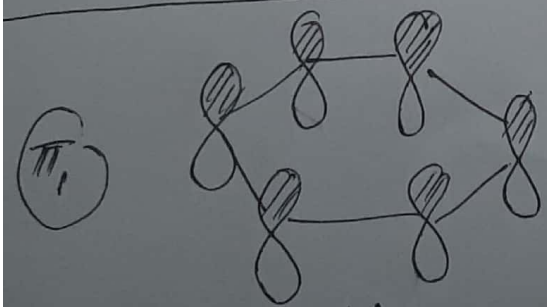
Through alon.

π_2 & π_3 are degenerate MO. π_2 and π_3 (same flow)





Benzene ē are nodal plane through-alon.

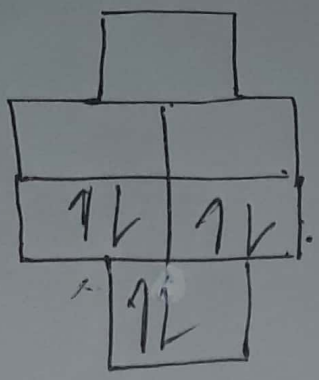


0

All p orbitals are aligned ē phases pointing in same direction. ē are delocalised over the length of the molecule resulting in greatest lowering of Energy.

In cyclic system (n-1) rule fails.

So filling of e⁻



A cyclic system allows 2 ways to place a single nodal plane this means 2, 3rd floors each having two units with same energy - they are degenerate. So Benzene is stable