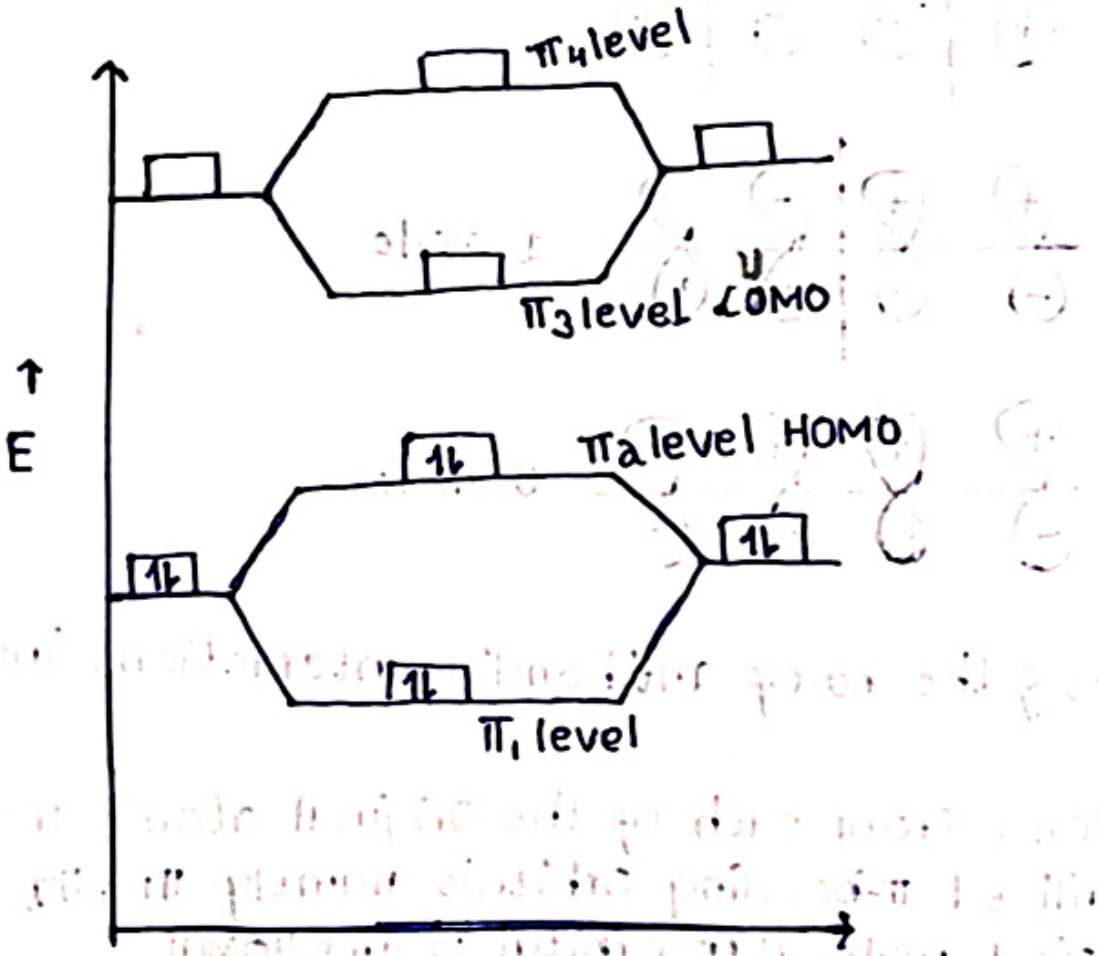
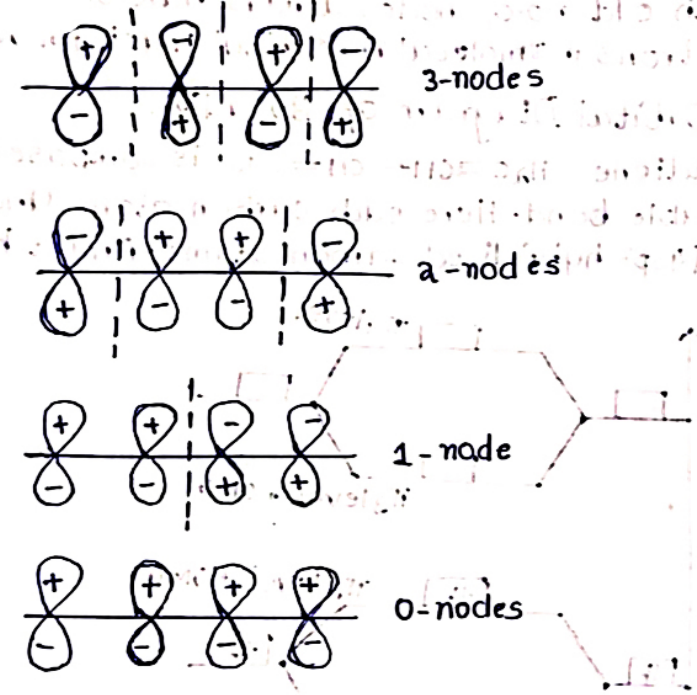
π- Molecular Orbital Diagram of Butadiene.

Ene → 1,3 butadiene $H_2C \equiv CH - CH = CH_2$ is composed of two conjugated double bond. Here each carbon atom Undergoes sp^2 hybridisation (4sp^2 hybridized carbon atoms). And it has





→ The no.of nodes & the no.of antibonding interactions increases from $\pi_1 - \pi_4$

→ When 4 π-electrons from each of the original atomic π orbital is Paired with sterilized π-bonding orbitals namely π_1 & π_2.

→ The highest occupied molecular orbital is π_2 (HOMO)

→ The Lowest Unoccupied molecular orbital is π_3 (LUMO)

(a) π_1 has bonding interactions b/w c_1-c_2 & c_2-c_3 & c_3-c_4 Thus resulting in 3 bonding interactions.

(b) π_2 has bonding interactions b/w c_1-c_2 & c_3-c_4, Antibonding interactions b/w c_2-c_3. Resulting in one bonding interaction.

(c) π_3 has bonding interactions b/w c_2-c_3, Antibonding interactions c_3-c_4 Resulting in one antibonding interaction.

(d) π_4 has antibonding interactions b/w c_1-c_2, c_2-c_3, c_3-c_4 resulting 3 antibonding interactions.

(e) Butadiene is composed of 4 carbons with 2-adjacent π bonds and this π bonds are also conjugated π bonds. all the 4 π-Orbitals are alinged with each other, so as to built into the largest pi system, The electron density is in resonance form.

[1) 2 Carbon π-Orbitals at the centre are flanked by one carbon Orbital on the sides.

2) If Butadiene act as electron donor (nuclophile), The electron will be lost from Homo

3) If Butadiene act as electron aceptor (Electrophile), The electrons will be donoted from LUMO.]