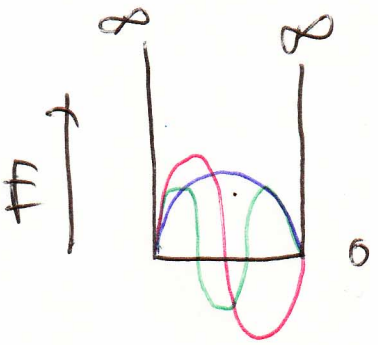
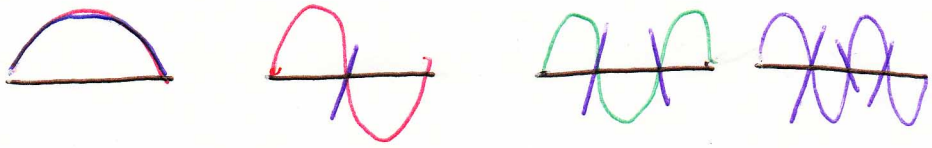
Particle in a box



$y = \sin \omega x$



n = 1 — 0 nodes

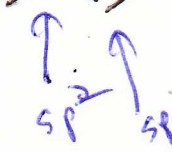
n = 2 — 1 node

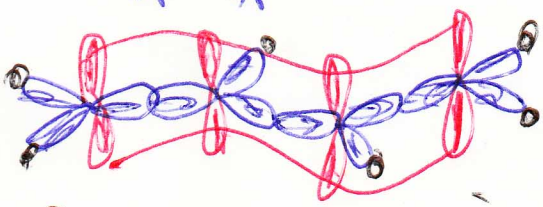
n = 3 — 2 nodes

n = 4 — 3 nodes

buta-1,3-diene

buta-1,2-diene

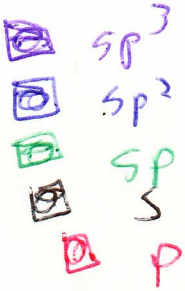


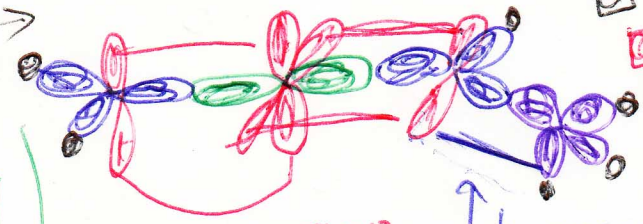


Due to conjugation, the single bond in buta-1,3-diene is shorter than an average C-C bond.

(carbon)

Cumulated diene





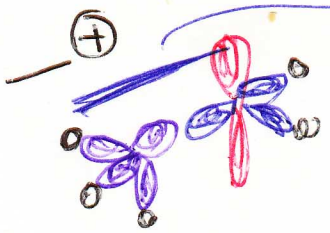
↑ hyperconj.

Since the two π bonds are ⊥ to each other, there is no conjugation.

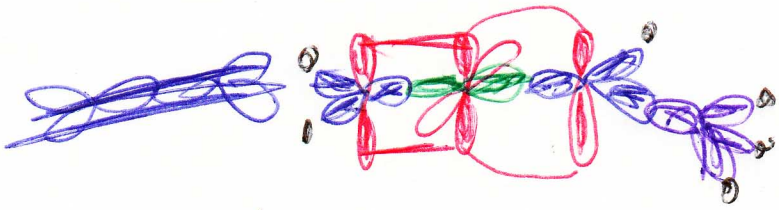
---

hyperconjugation – the partial donate of electron density to a neighboring orbital through an interaction that does not involve a bond.

Conjugation – the full delocalization of e⁻ density across multiple orbitals due to full ~~σ~~ bonding overlaps.

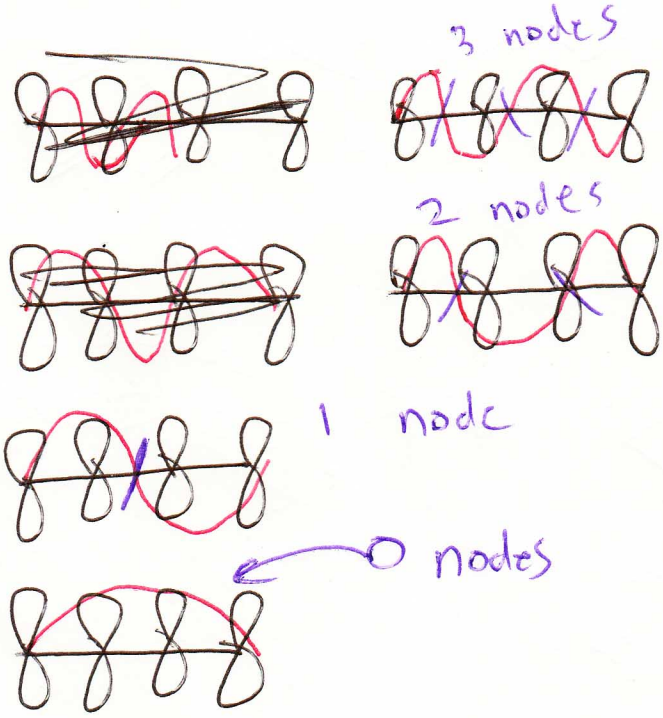


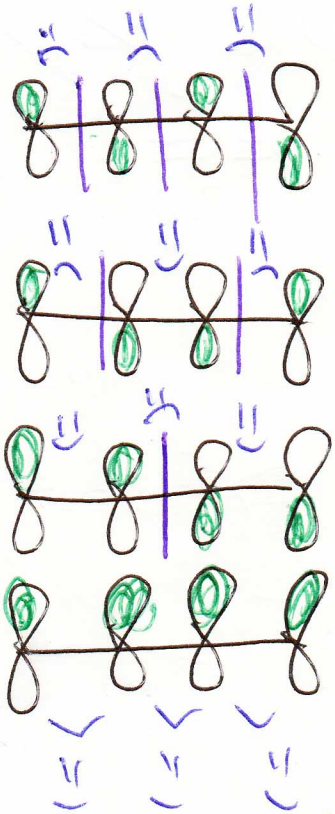
hyperconjugation

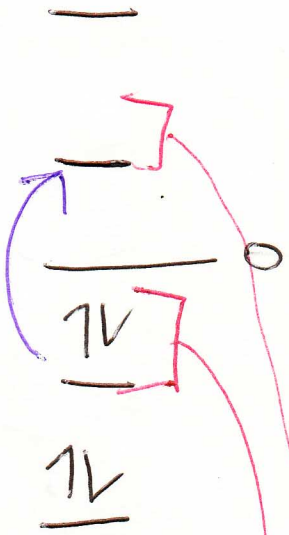


← 2 π bonds → 4 π e⁻

The # of MOs in a π system is always equal to the # of p orbitals in that system.







Bond order = $\frac{\#\text{ bonding } e^- - \#\text{ antibonding}}{2}$

HOMO-LUMO

High-Occupied Molecular Orbital

Lowest-Unoccupied Molecular Orbital