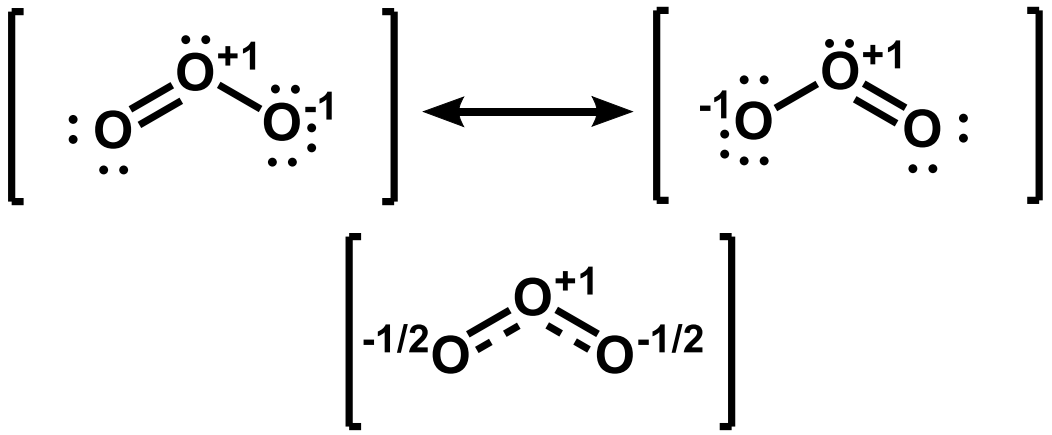
MO diagrams for molecules sometimes get complicated.

Ones we will cover: Molecules with delocalized electrons (resonance) using a combination of valence bond theory (hybridization) and MO theory

Example 1: O_3 molecule



<u>Resonance Structures:</u>

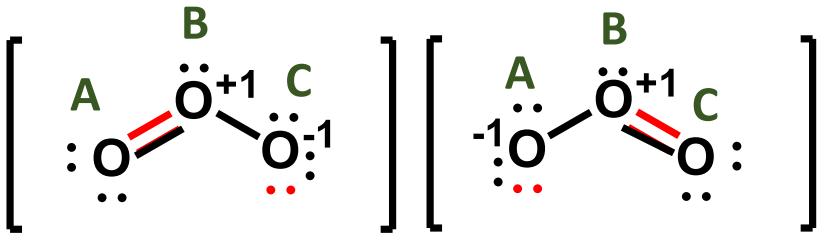
More than one possible Lewis structure

Both structures for Ozone are plausible Lewis structures

Only electrons move (movement of lone pairs or multiple bonds)

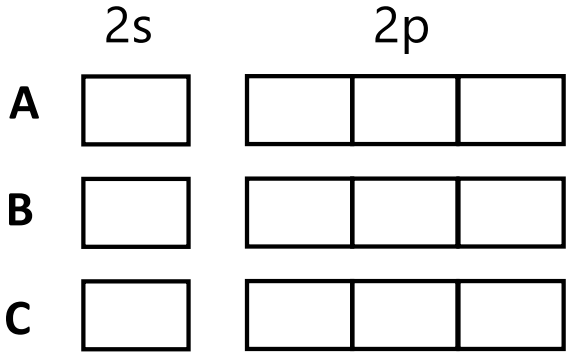
Atoms **<u>do not</u>** move

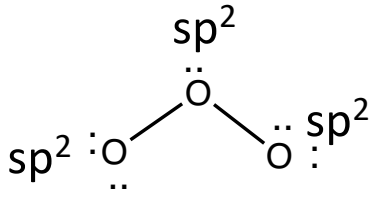
For ozone – a mix of valence bond theory and MO theory can help explain (and simplify) the bonding



Each oxygen has **4** valence orbitals

In O_3, total **12** valence orbitals





9 hybrid orbitals.

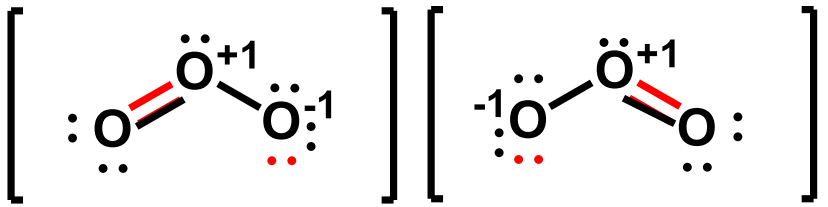
3 hybridized p orbitals.

O $1s^2$ $2s^2$ $2p^4$

O $2s^2$ $2p^4$
(valence orbitals)

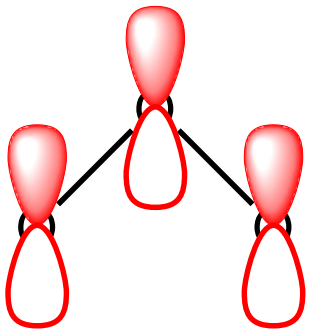
For all the sigma bonds use valence bond theory and hybridization
- the central oxygen is sp^2 hybridized (in either structure)
- One sigma bond each with the two terminal oxygen atoms
- Third sp^2 orbital contains the lone pair of electrons on the central atom

Ozone : delocalized p electrons



Still remaining:
3 of these orbitals are p orbitals
(one on each oxygen)

4 electrons delocalized



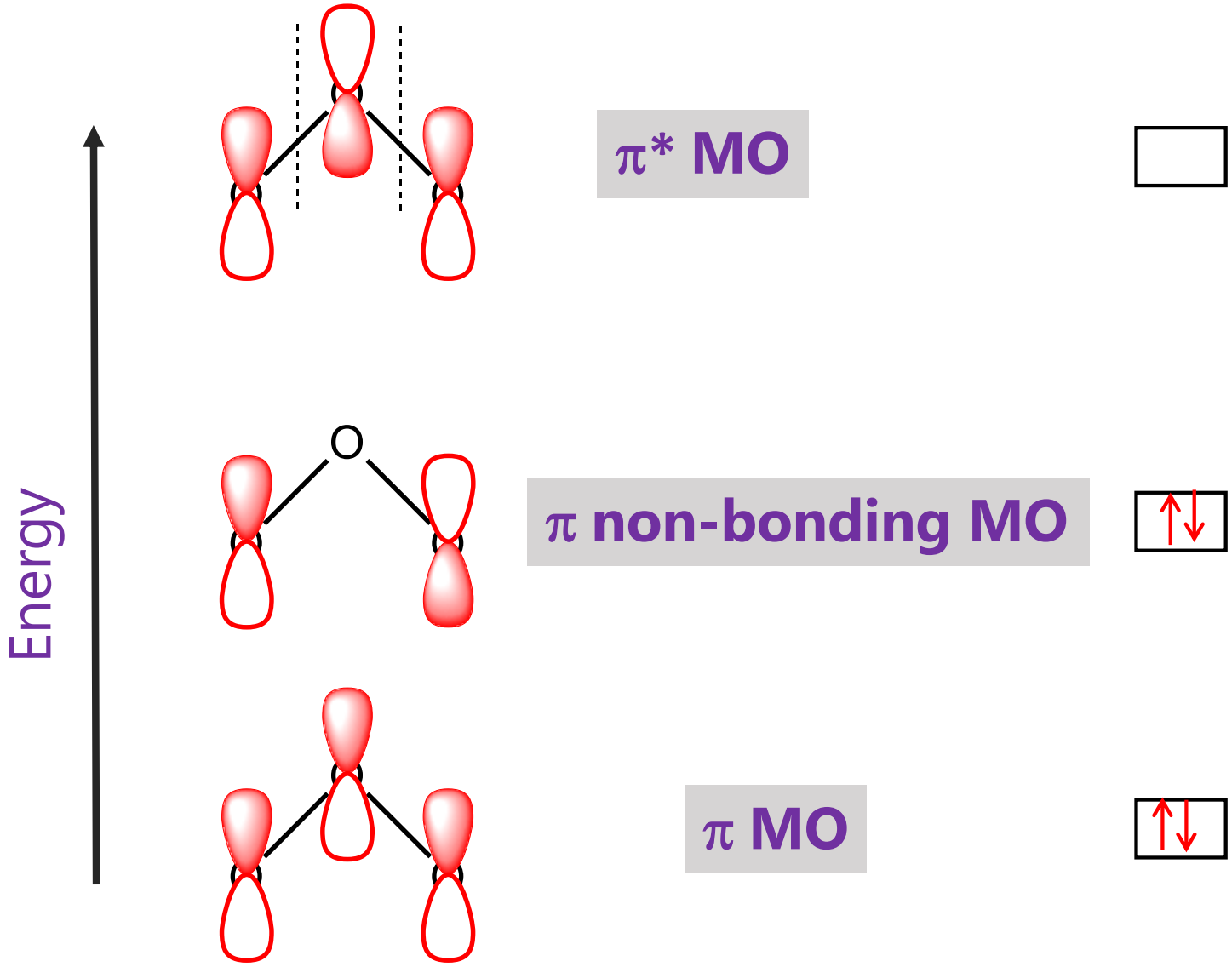
From LCAO of 3 p orbitals

- **π* MO**
- **π non-bonding MO**
- **π MO**

3 π MOs

McGill

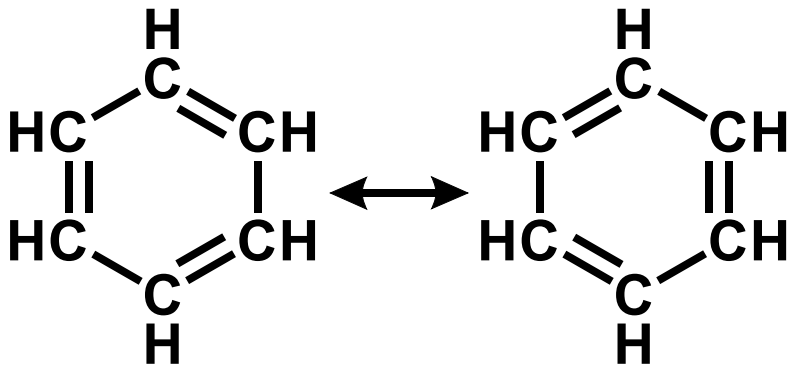
Ozone MO energy diagram (delocalized π system)

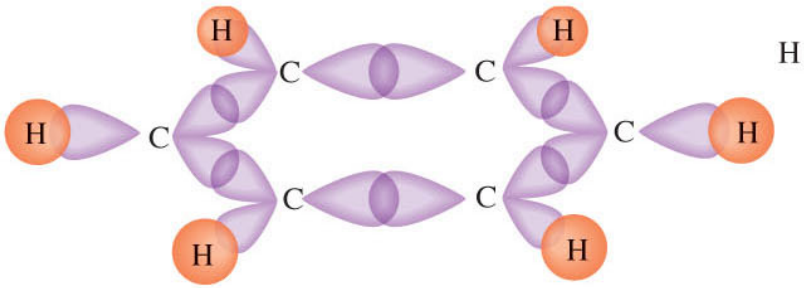


Example 2: Benzene Molecule (C_6H_6)

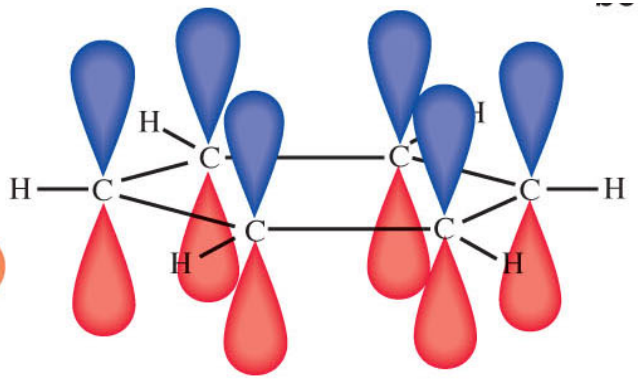
30 total valence orbitals
Each carbon has 4, and each hydrogen has 1

24 orbitals form 12 sigma bonds
There are 6 unhybridized p orbitals that form 6 π MOs

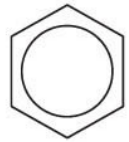




(a) σ bond framework



(b) Carbon 2p orbitals to be used in π bonding



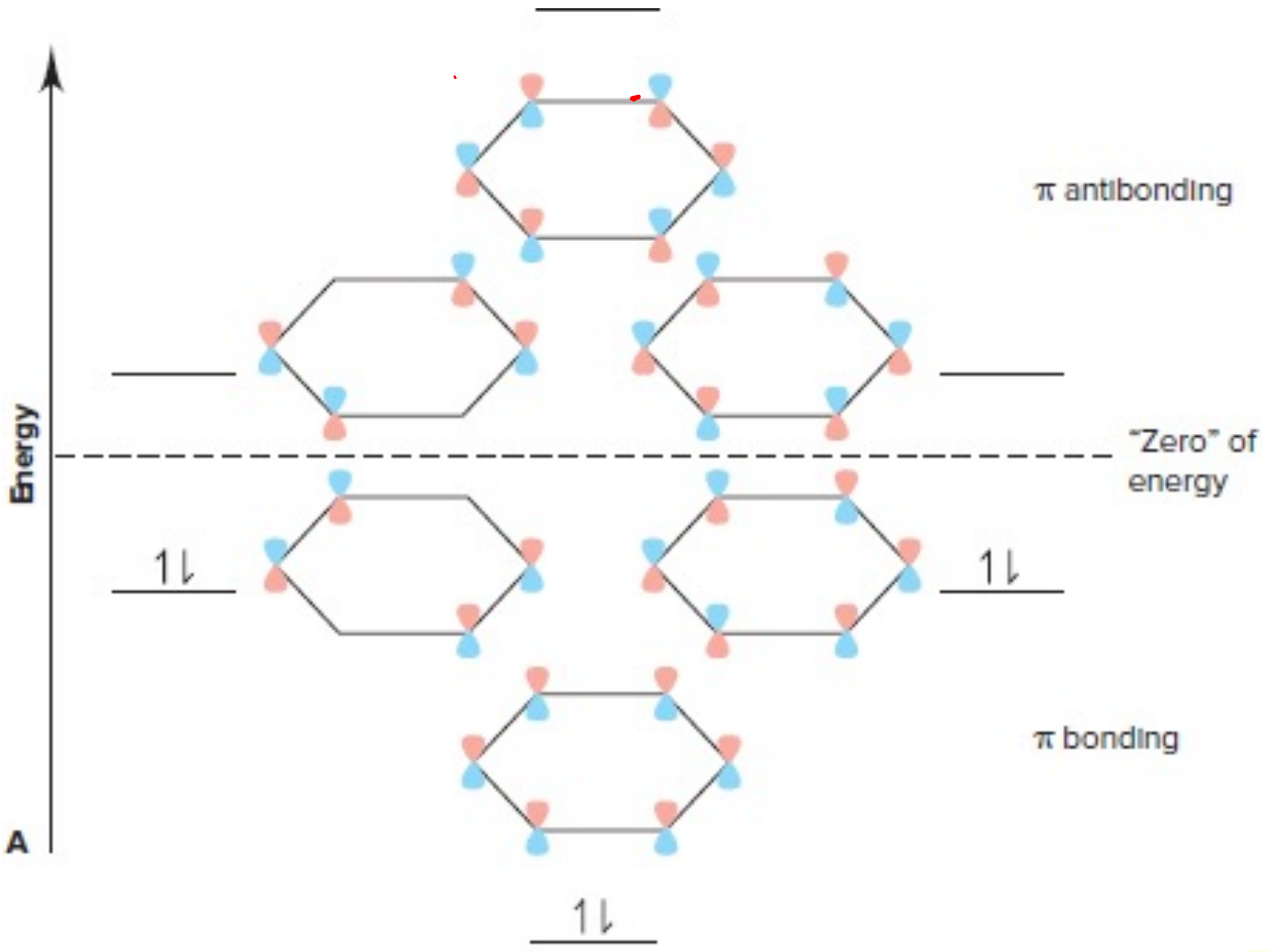
(c) Symbolic representation

Each carbon is sp2 hybridized

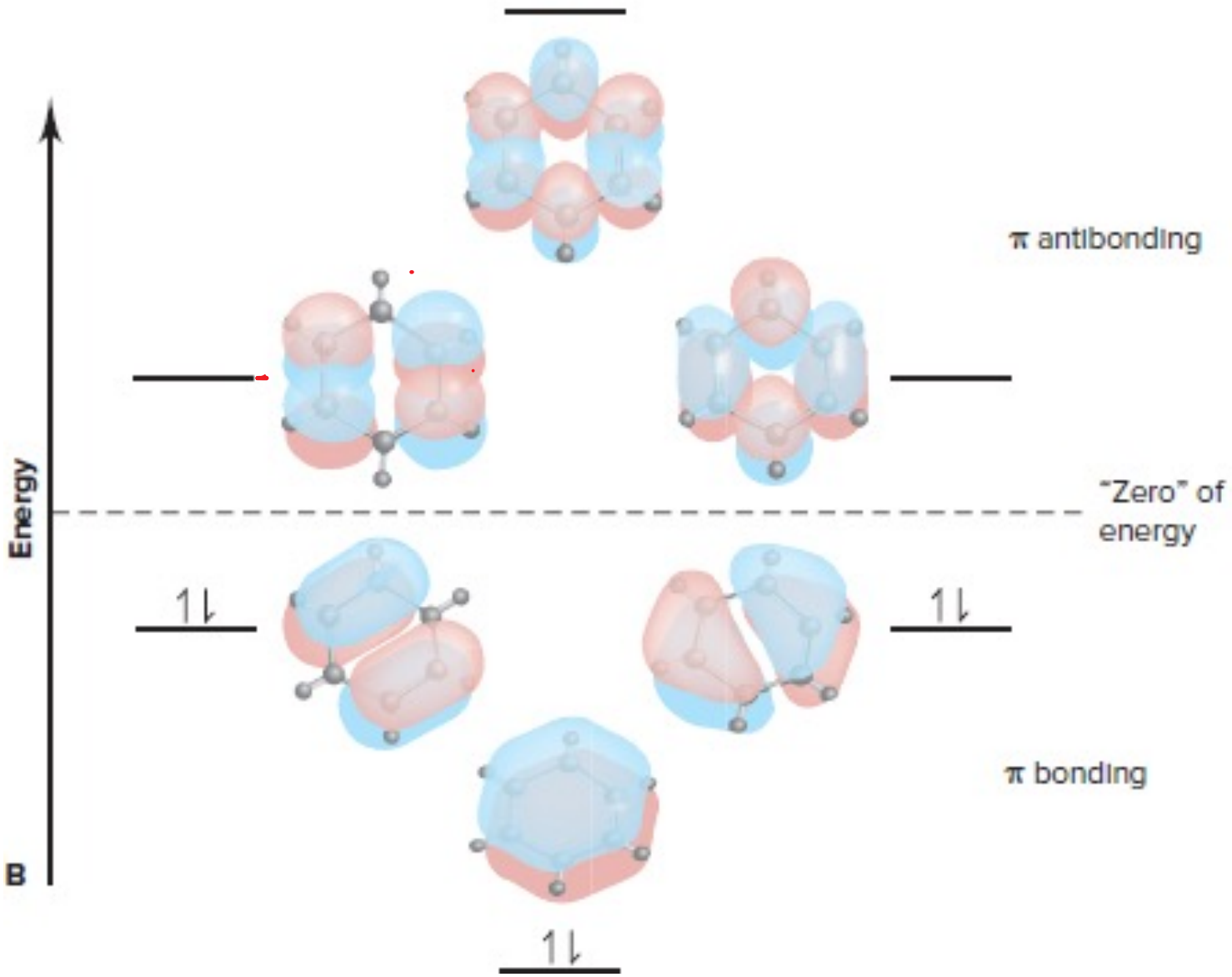
Bond angle = 120

Trigonal planar

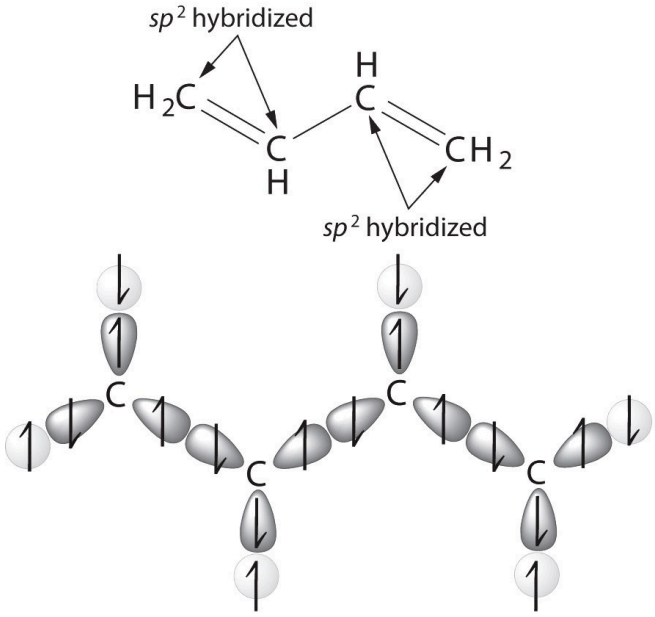
Benzene : delocalized π electrons (For your interest only – not assessed on exams)



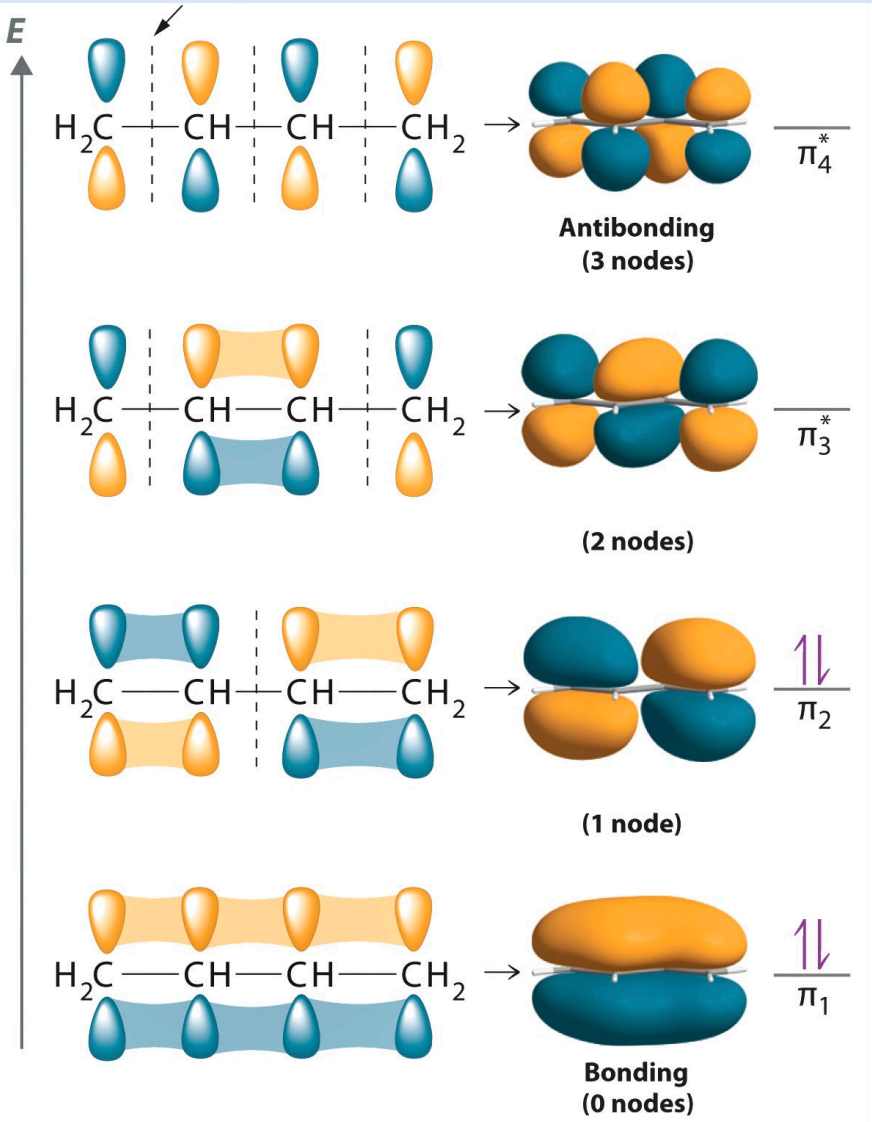
Benzene : delocalized π electrons (For your interest only – not assessed on exams)



Using VBT + MO Theory to explain delocalized systems



(a) 1,3-Butadiene σ-bonded framework



(b) 1,3-Butadiene π bonding