Chem 111

Lecture 34

Announcement

- Exam 3: Dec. 6th in class

→Same deal as before

  - No Makeups
  - Pyramid
  - Bring pencils, calculator, ID card and a good erasers

- Practice Exam:

http://courses.umass.edu/chem111-bbotch/

Announcement Part 2

- SI sessions

- Sunday 4 – 6 PM, ISB 135, Prof. Vachet

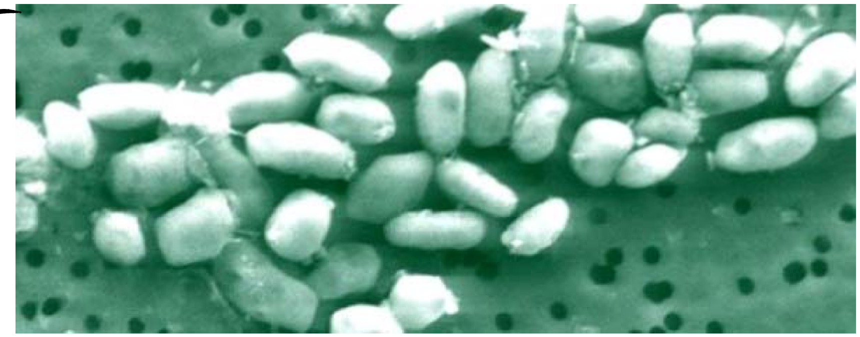
- Owl homework, unchecked homework should be correct for everything except chapter 8 & 9 work.

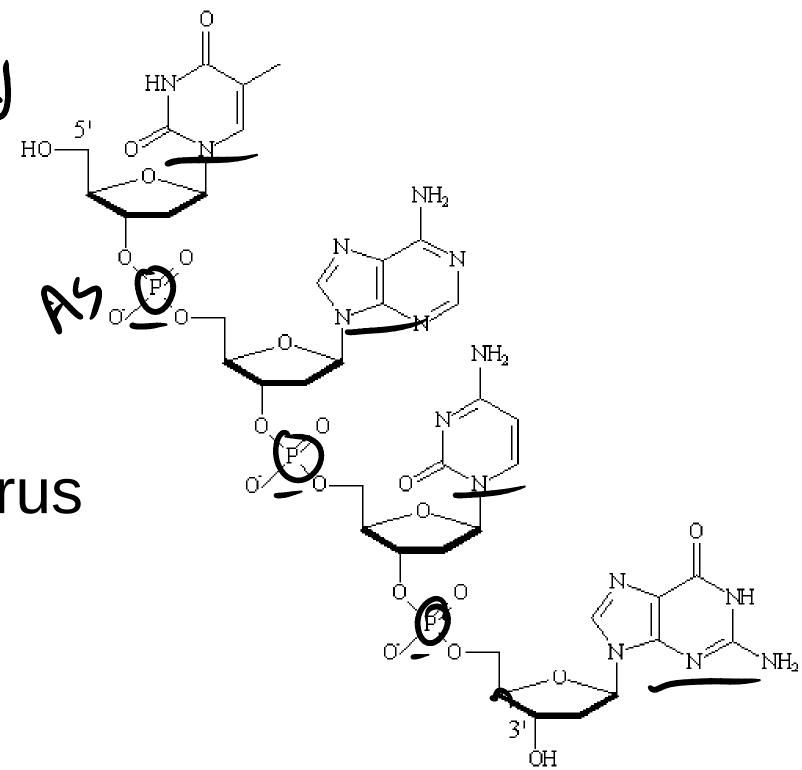
Homework

- ~~Start~~ Reading Chapter 9
  Continue
- Owl Homework

→ Some homework was added late and will be on the Exam (Due Sunday)

Chemistry Today





Bacteria called GFAJ-1
Uses Arsenic instead of Phosphorus

Mono lake

Recap

- Orbital Overlap
- Hybridization
- sp^2 and sp^3

OCN^-

B, Be, Al — central atom

n=3

n>3

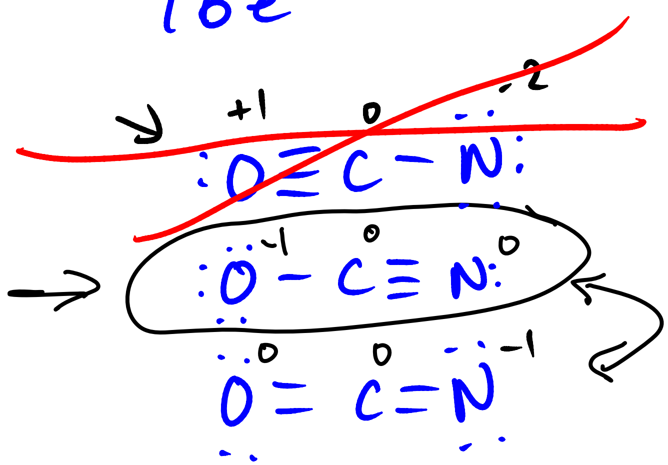
O : 6

C : 4

N : 5

e 1

16e$^-$



$FC = G\# - (lpe - \frac{1}{2} be)$

4

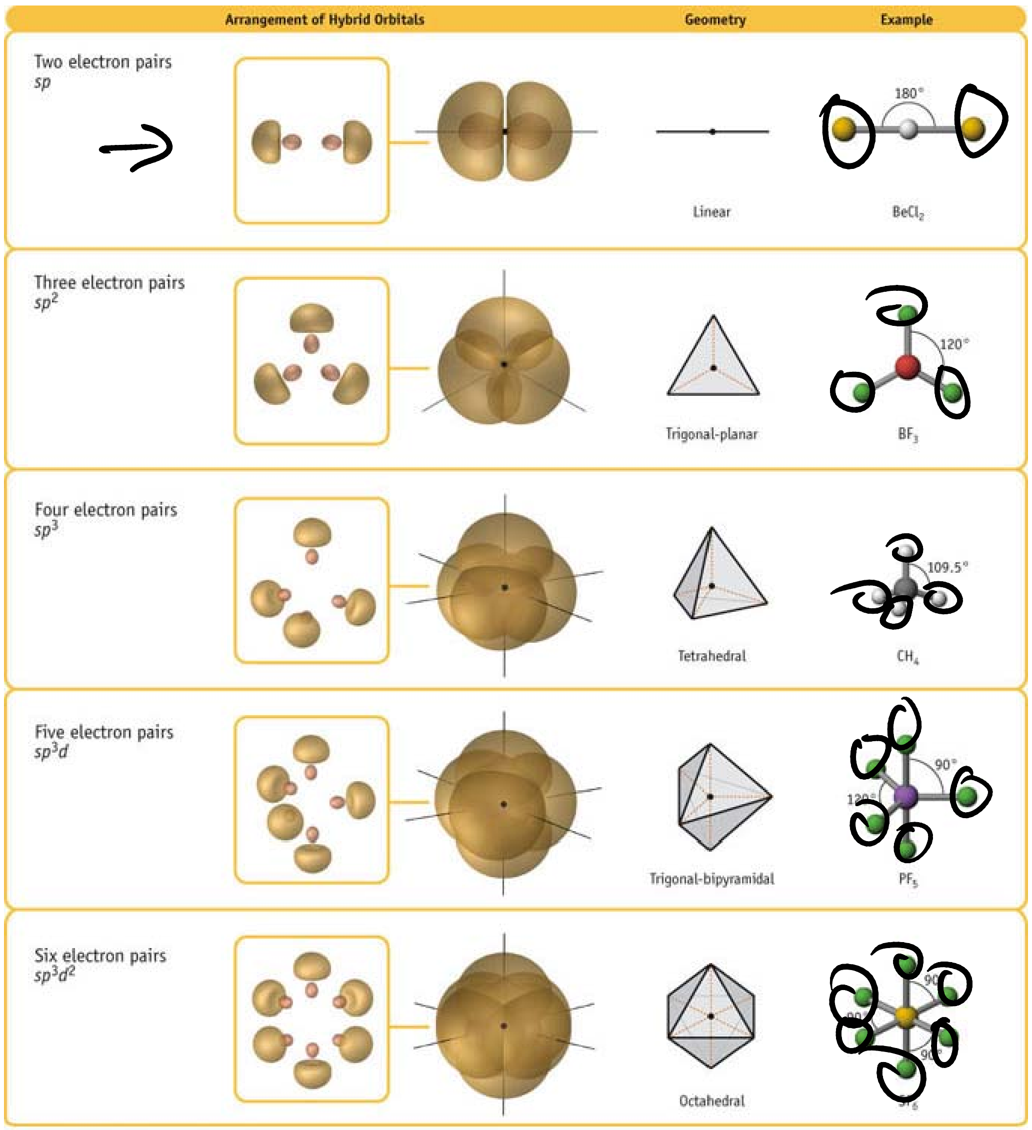
5-7 = -2

5-5 = 0

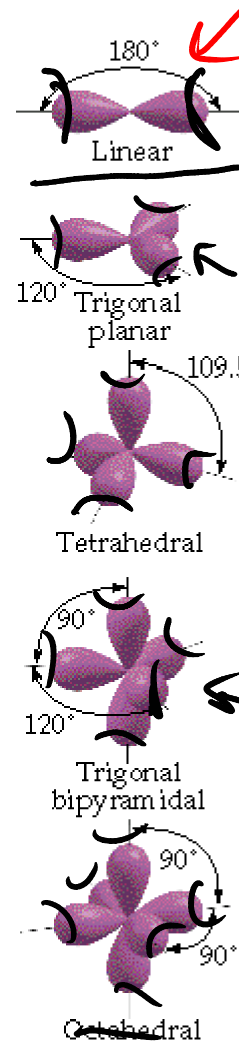
5-6 = -1

Hybridization

Memorize



Atomic Orbital Set	Hybrid Orbital Set	Geometry	Examples
s,p	Two sp	Linear	BeF_2, $HgCl_2$
s,p,p	Three sp^2	Trigonal planar	BF_3, SO_3
s,p,p,p	Four sp^3	Tetrahedral	CH_4, NH_3, H_2O
s,p,p,p,d	Five sp^3d	Trigonal bipyramidal	PF_5, SF_4, BrF_3
s,p,p,p,d,d	Six sp^3d^2	Octahedral	SF_6, ClF_5, XeF_4



Summary for Hybridization

1. Draw the Lewis structure for the molecule or ion
2. Determine the electron-pair geometry using VSEPR model.
3. Specify the hybrid orbitals needed to accommodate the electron pairs based on their geometrical arrangement.

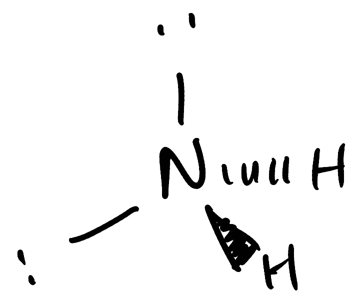
S → P → D

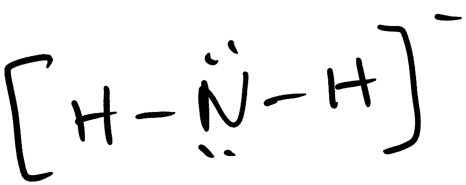
s p, p, p, d

Let's Practice

Indicate the hybridization of orbitals employed by the central atom in each of the following: NH_2^- and SF_6.

N: 5
H: 1 x 2 = 2
e^-: 1
$8e^-$





4e/8

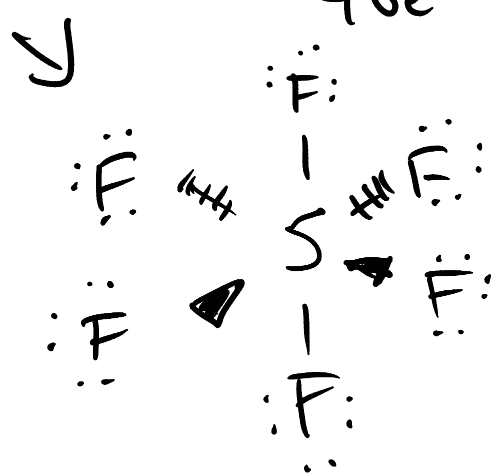
s p p p

sp^3

~~sp~~

S – $6e^-$
F – 7 x 6 = 42e
$48e^-$

$48e^-/48e^-$

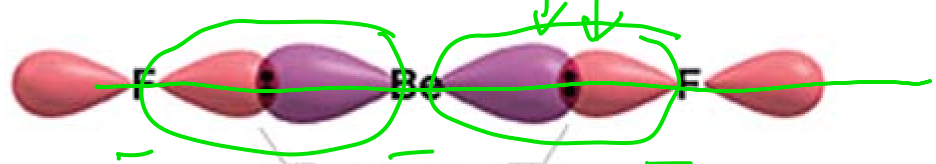


s p p p d d ⇒ sp^3d^2

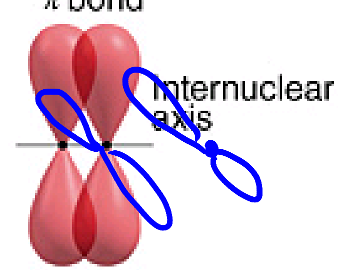
Multiple Bonds

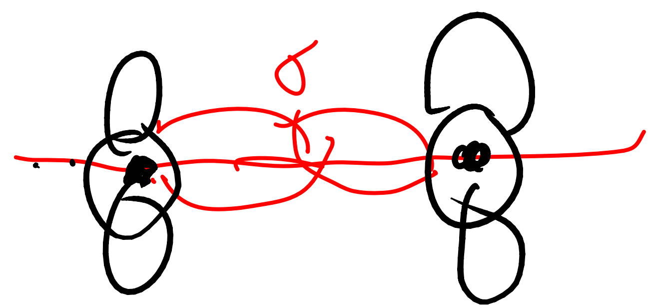
Internuclear Axis - Line connecting the nuclei of two bonded atoms

Sigma (σ) bond – is a covalent bond in which the overlap region lies along the internuclear axis.

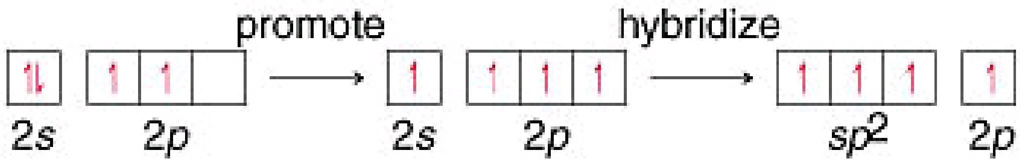


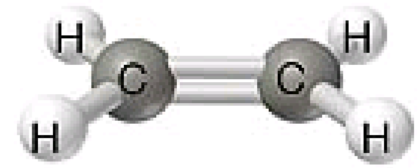
Pi (π) bonds – is a covalent bond in which the overlap regions lie above and below the internuclear axis.

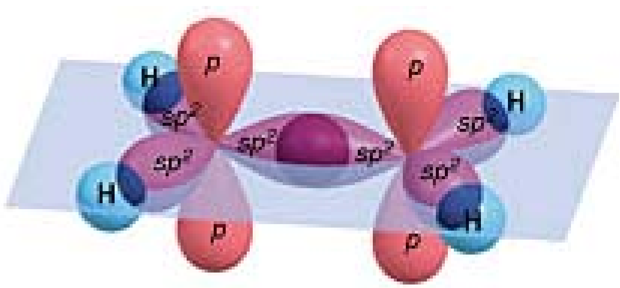


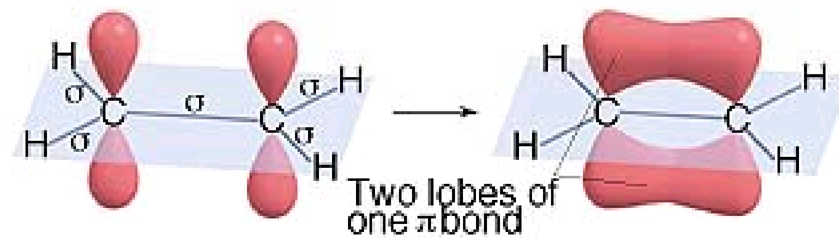


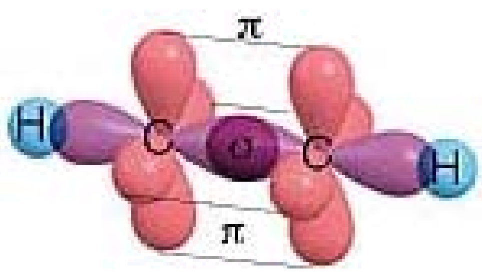
Multiple Bonds





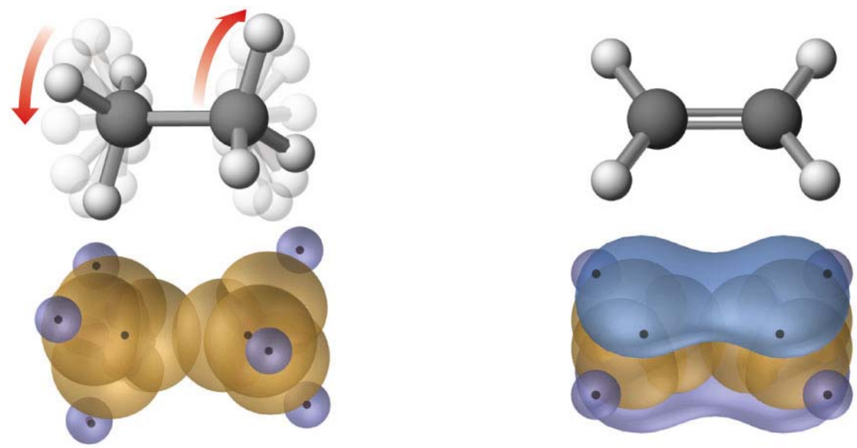




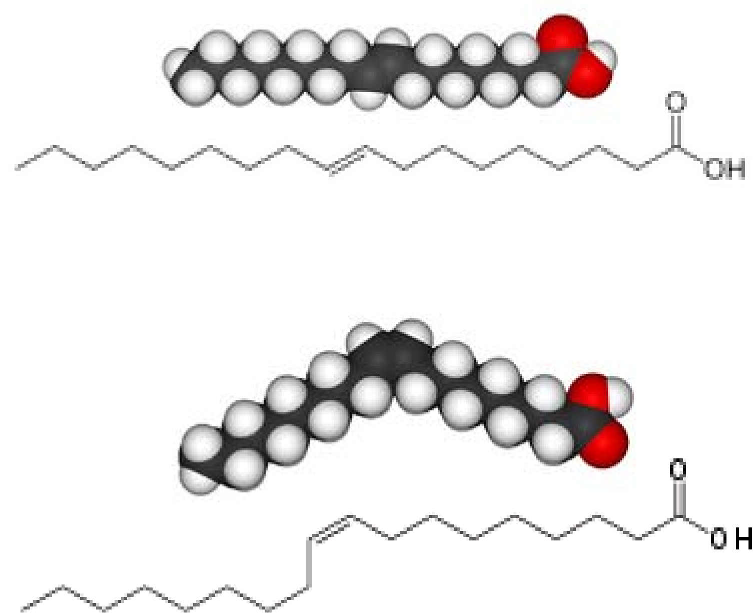


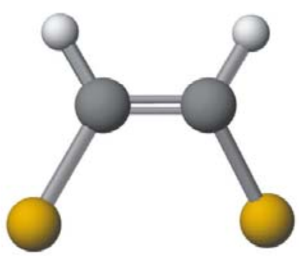
Double bond = 1 σ bond and 1 π bond
Triple bond = 1 σ bond and 2 π bond
πbond usually happen with unhybridized p orbitals, therefore sp and sp^2 hybridization.
πUsually C, O, N, and S

Cis-Trans Isomers

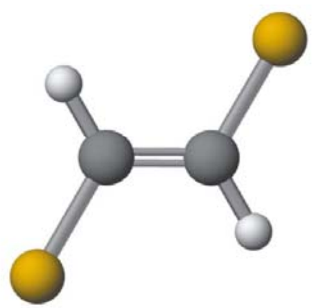


Isomers – are compounds that have the same formula but different structures.





cis-1,2-dichloroethylene

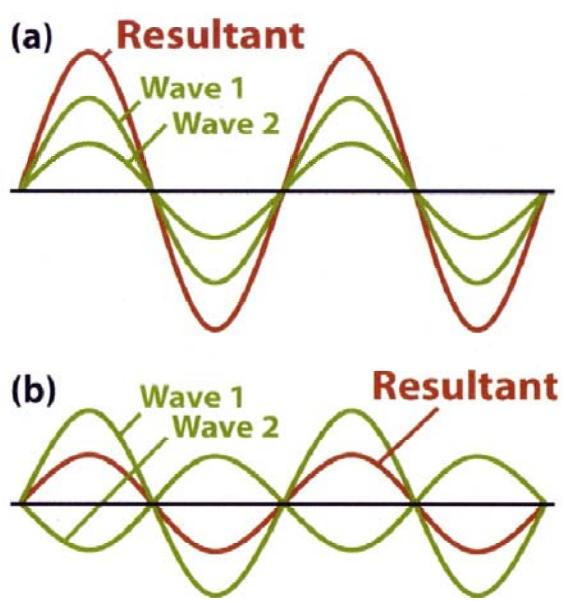


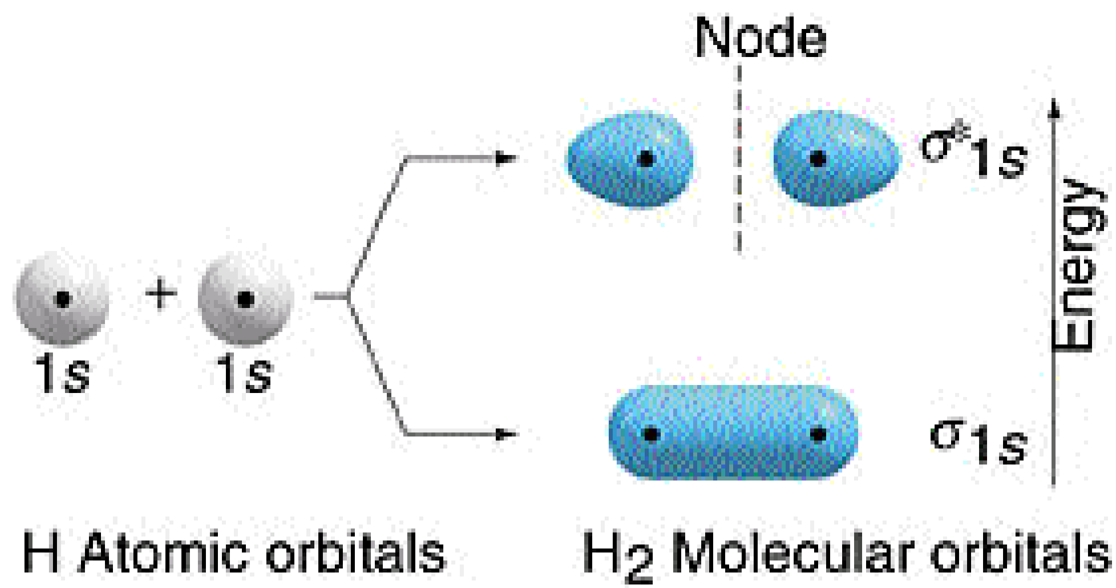
trans-1,2-dichloroethylene

Molecular Orbital Theory

Molecular orbitals have many characteristics similar to atomic orbitals: hold two electrons, have discreet energies.

Consider H_2





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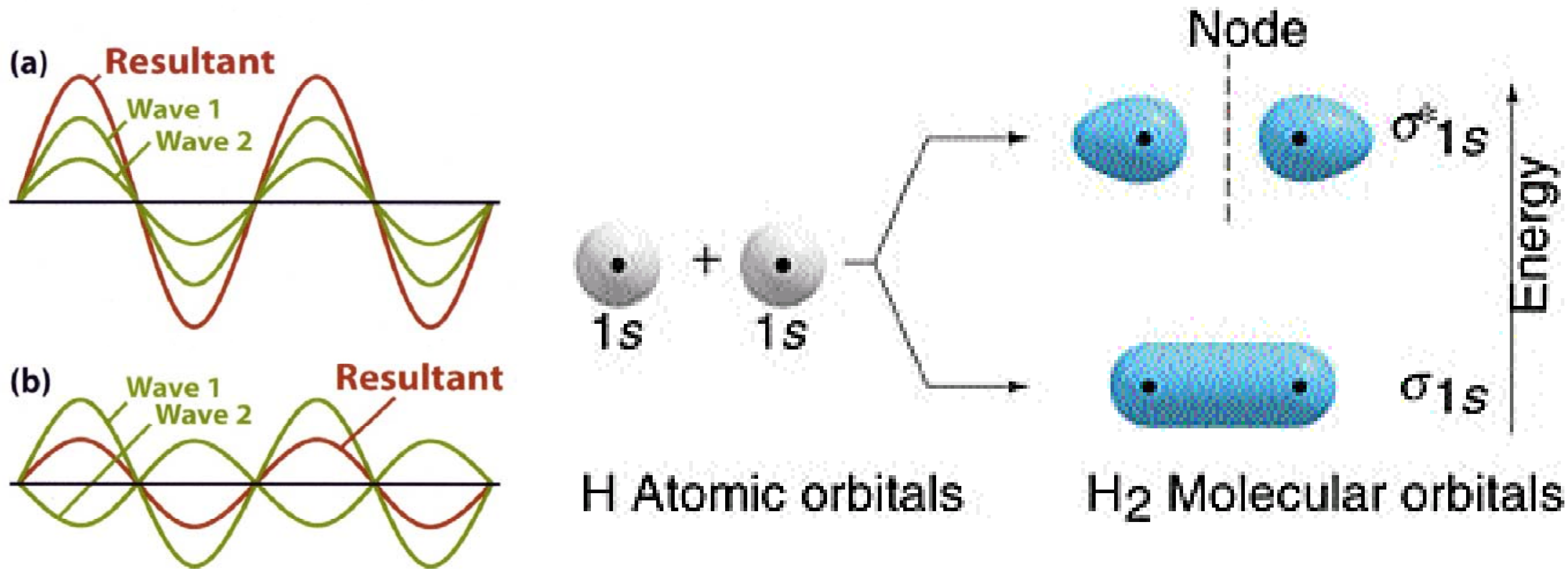
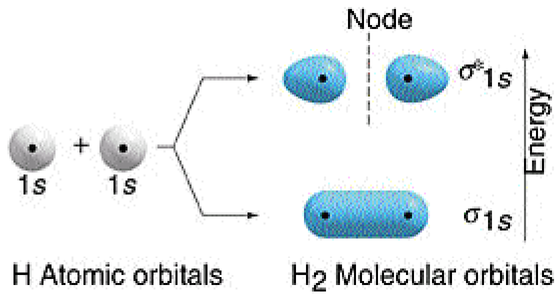


Molecular Orbital Theory

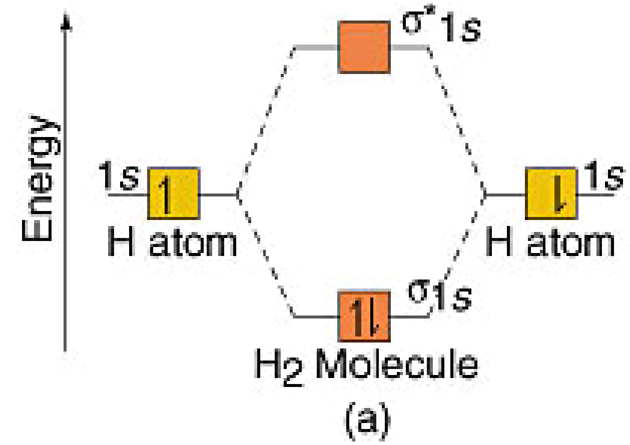


The total number of molecular orbitals created equal the total number of atomic orbitals used.

Bonding orbital – lower energy orbital (than atomic orbitals) that concentrate electron density between the atoms.

Antibonding orbital – higher energy orbital (than atomic orbitals) that have little electron density between the atoms.

MOT Energy Level Diagram



sigma (σ) orbital – bonding molecular orbital centered around internuclear distance.

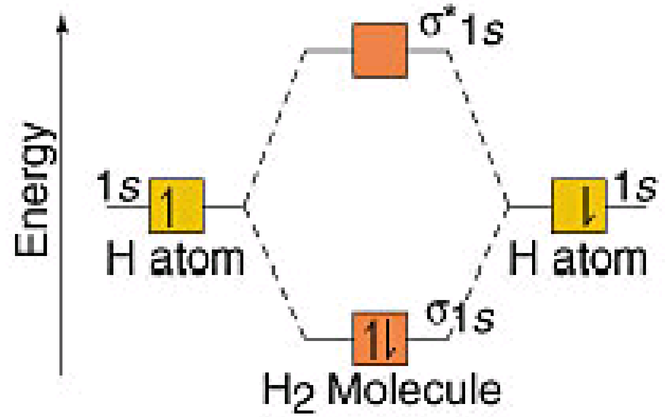
sigma-star (σ∗) bond – anitbonding molecular orbital centered around internuclear distance.

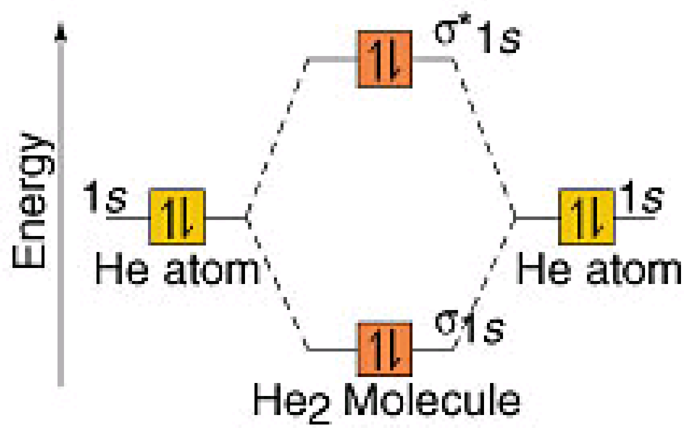
1s – denotes the character of the atomic orbitals that make up the molecular orbitals.

Electron fill like atomic orbitals, low energy first & spin paired.

Bond Order (Using MOT)

Bond order = ½ (# of bonding electrons - # of nonbonding electrons)



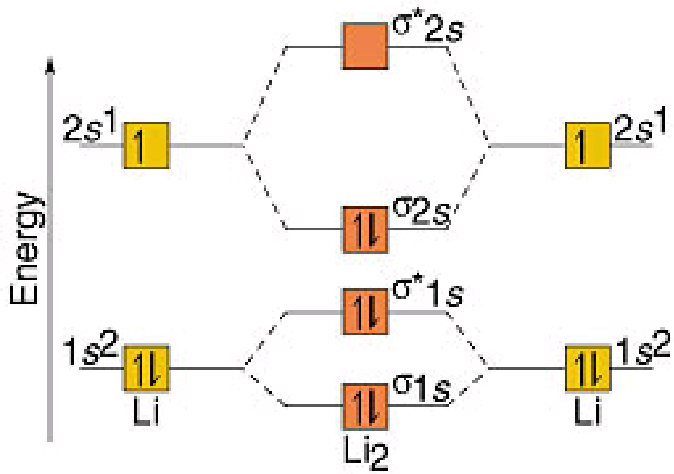


Let's Practice

Draw the molecular energy level diagram of He_2^+? What is the bond order?

MO of Li_2

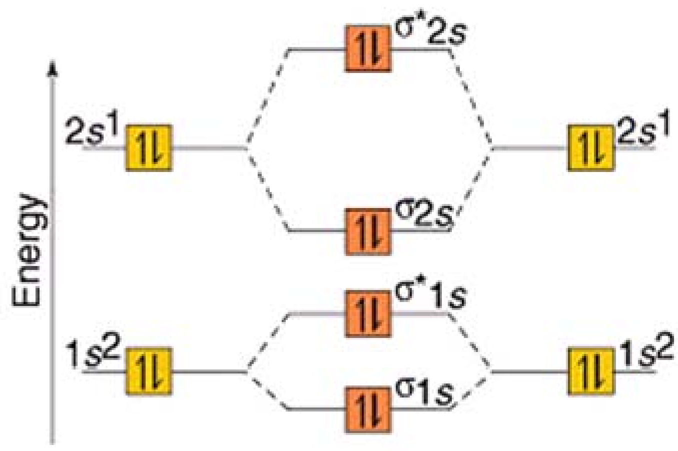
Atomic orbitals must be of similar energy to form molecular orbitals.



Core electrons usually don't do not contribute significantly to bonding in the molecule formation.

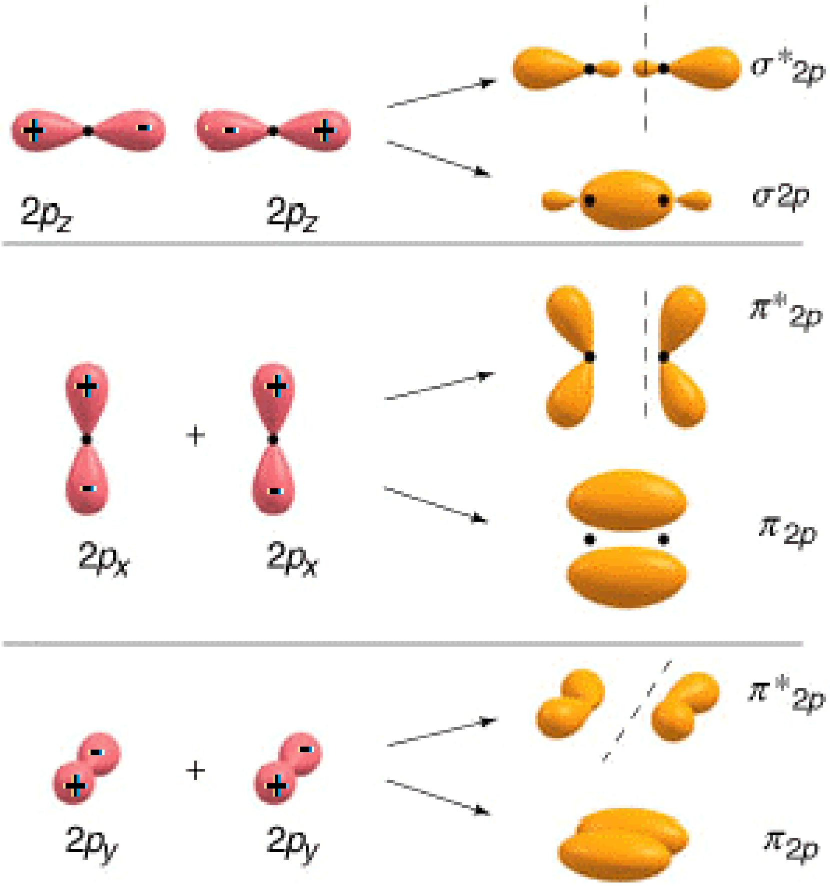
Li_2 MO Configuration = $(\sigma_{1s})^2(\sigma^*_{1s})^2(\sigma_{2s})^2$

MO of Be_2



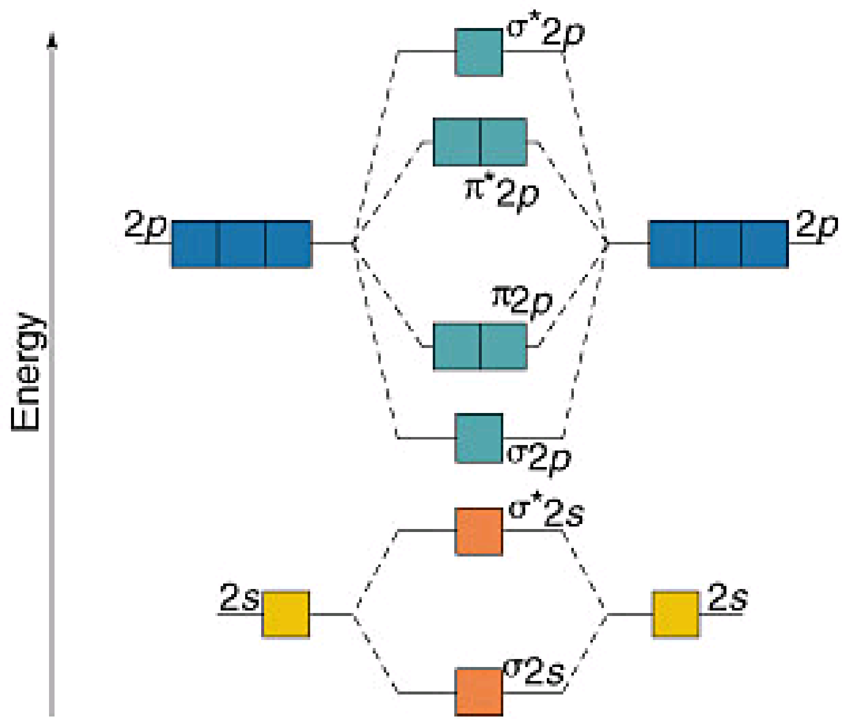
Be_2 MO Configuration = $(\sigma_{1s})^2(\sigma^*_{1s})^2(\sigma_{2s})^2(\sigma^*_{2s})^2$

Molecular orbitals from P orbitals

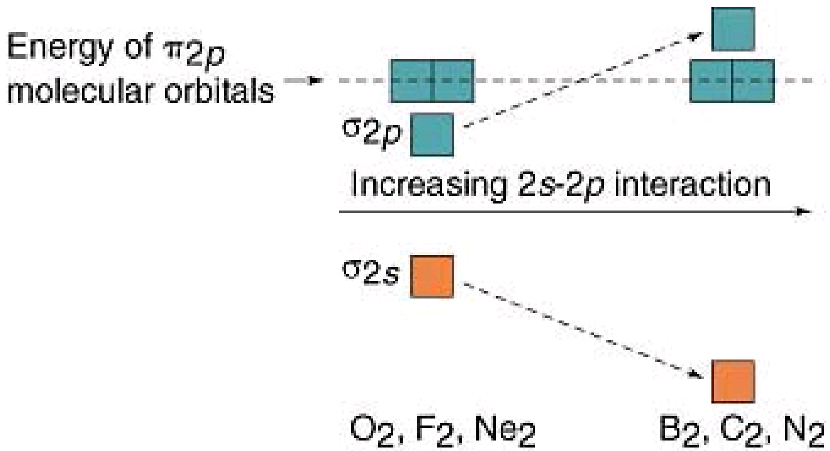


Note the amount they can mix and their relation to internuclear axis

MO Diagram



Energy
σ*2p
π*2p
2p
2p
π2p
σ2p
σ*2s
2s
2s
σ2s



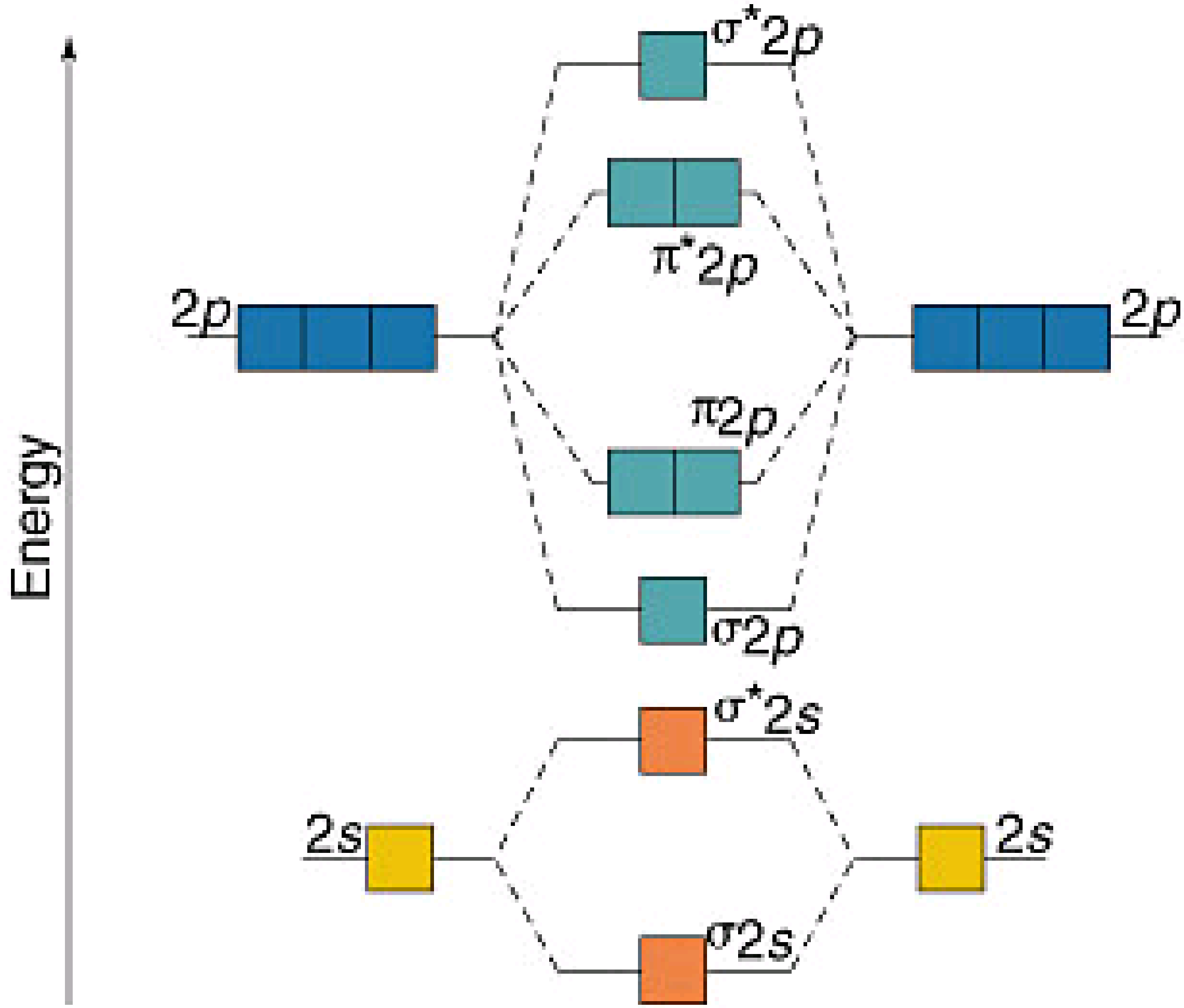
Energy of π2p molecular orbitals
σ2p
Increasing 2s-2p interaction
σ2s
O2, F2, Ne2
B2, C2, N2

MOT P block

Large 2*s*-2*p* interaction				Small 2*s*-2*p* interaction			
	B_2	C_2	N_2		O_2	F_2	Ne_2
σ^*2p				σ^*2p			↑↓
π^*2p				π^*2p	↑ ↑	↑↓ ↑↓	↑↓ ↑↓
$\sigma 2p$			↑↓	$\pi 2p$	↑↓ ↑↓	↑↓ ↑↓	↑↓ ↑↓
$\pi 2p$	↑ ↑	↑↓ ↑↓	↑↓ ↑↓	$\sigma 2p$	↑↓	↑↓	↑↓
σ^*2s	↑↓	↑↓	↑↓	σ^*2s	↑↓	↑↓	↑↓
$\sigma 2s$	↑↓	↑↓	↑↓	$\sigma 2s$	↑↓	↑↓	↑↓

Let's practice

What is the Bond Order O_2, O_2^-, O_2^{2-}, O_2^+



MOT-Heteronuclear Diatomics

- Differences from Homonuclear case:
  - Electrons will be drawn to the more electronegative element . Thus bonding orbitals will have more of that element character and antibonding orbitals will have more character from the less electronegative element.
  - As a result of having more A character, the molecular orbital will be closer in energy to that elements atomic orbital.