Chapter 9

Molecular Geometry & Bonding Theories

I) Molecular Geometry (Shapes)

Chemical reactivity of molecules depends on the nature of the bonds between the atoms as well on its 3D structure

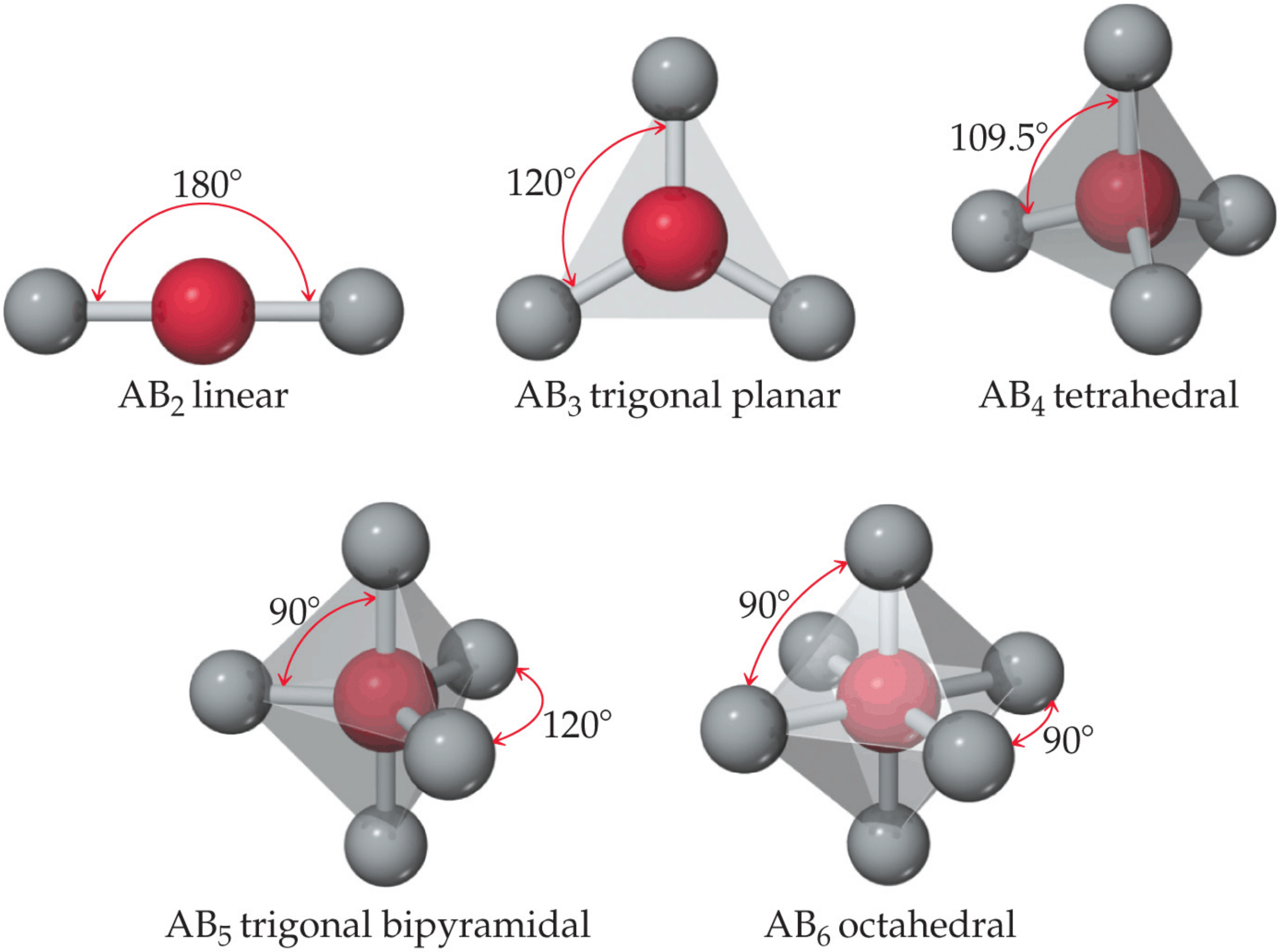
Molecular Geometry

Arrangement or positions of atoms relative to each other

Bond Angles

Angles made by lines joining the nuclei of atoms bonded

A) Basic AB$_n$ Arrangements



Various molecular shapes can arise from the 5 basic AB_n shapes.

$n = 2$: linear, bent

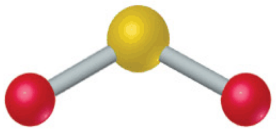
$n = 3$: trigonal planar, trigonal pyramidal, T-shaped

$n = 4$: tetrahedral, square planar, see-saw

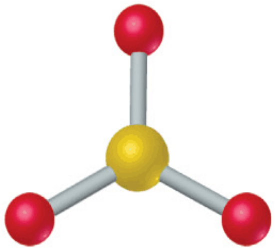
$n = 5$: trigonal bipyramidal, square pyramidal

$n = 6$: octahedral

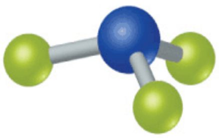
CO_2
AB_2 linear



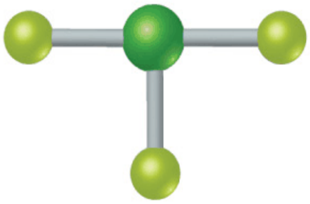
SO_2
AB_2 bent



SO_3
AB_3 trigonal planar



NF_3
AB_3 trigonal pyramidal



ClF_3
AB_3 T-shaped

II) VSEPR Theory

Valence-Shell Elecron-Pair Repulsion

e^- pair: lone pair e^- or bonding e^-
(single, double & triple
bonds treated same)

- really considering

regions of e^- density (domains)

VSEPR: e^- pairs arrange
themselves as far apart
as possible to minimize
repulsions between them

- controls geometry
around central atom

A) Types of Geometry

1) Electron-Domain Geom.

arrangement of bonding and nonbonding e^- pairs (domains) about the central atom

2) Molecular Geom. (Shapes)

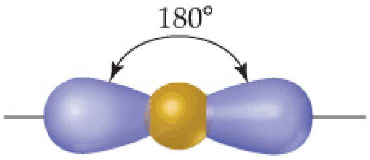
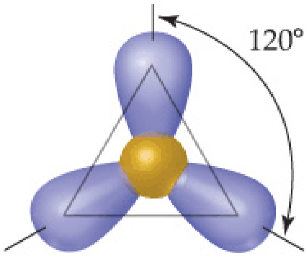
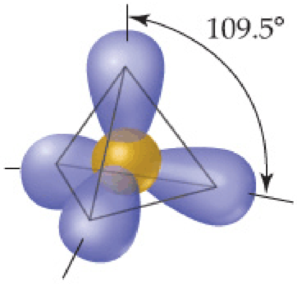
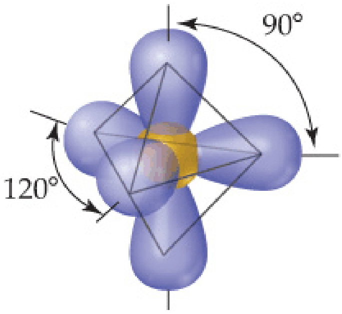
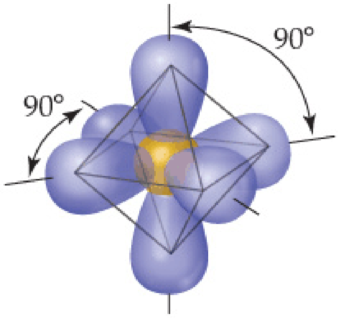
arrangement of bonded atoms about the central atom

described using ONLY the ATOMS

Distinction is very important!

Electron-Domain Geom

TABLE 9.1 • Electron-Domain Geometries as a Function of Number of Electron Domains

Number of Electron Domains	Arrangement of Electron Domains	Electron-Domain Geometry	Predicted Bond Angles
2		Linear	180°
3		Trigonal planar	120°
4		Tetrahedral	109.5°
5		Trigonal bipyramidal	120° 90°
6		Octahedral	90°

ED and MG for AB_2, AB_3 & AB_4 EDs

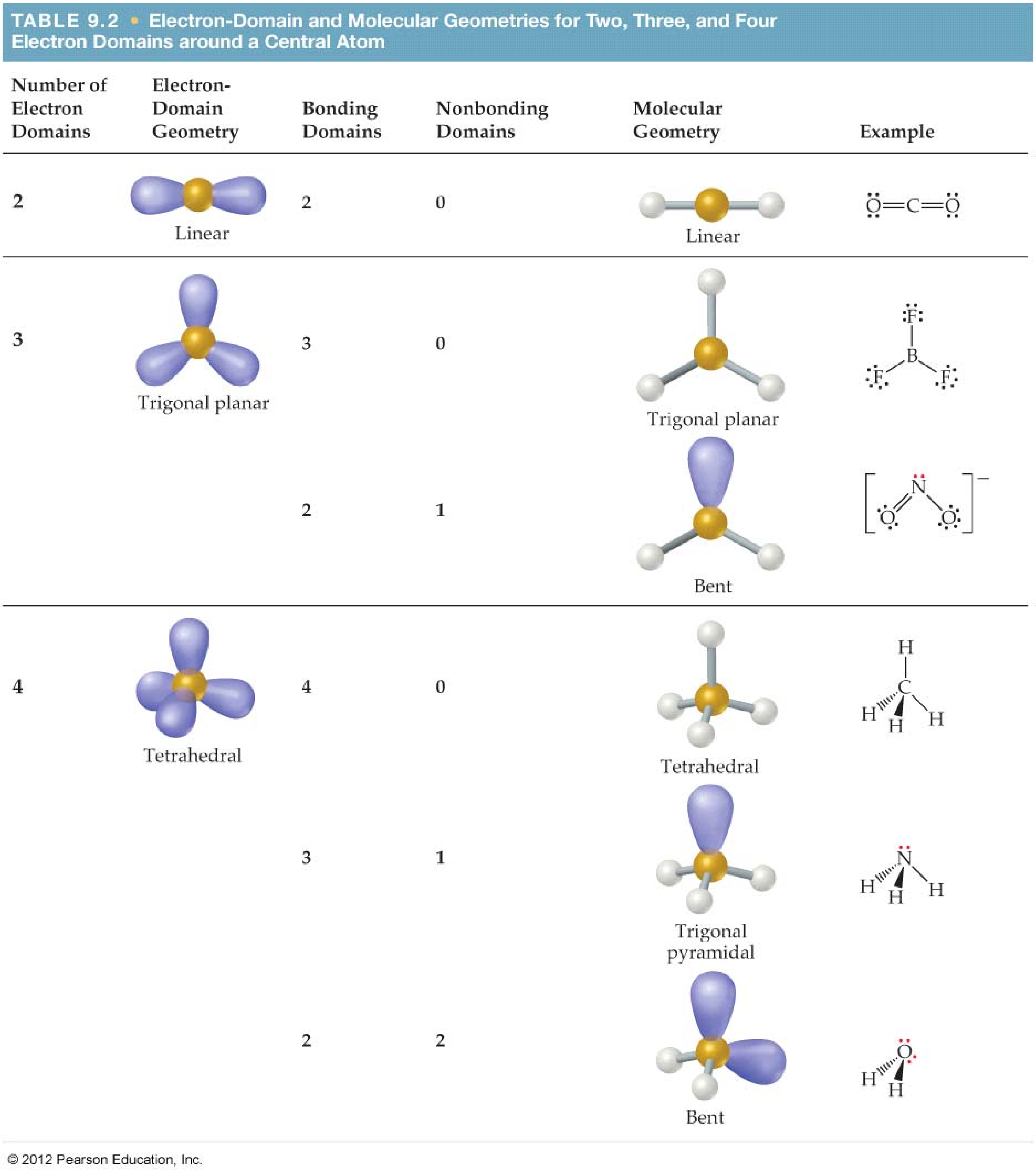
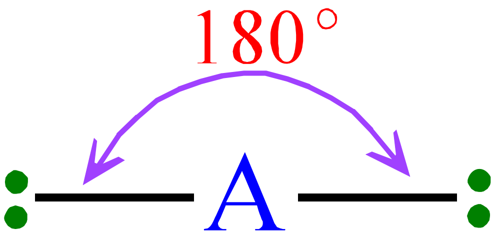


TABLE 9.2 • Electron-Domain and Molecular Geometries for Two, Three, and Four Electron Domains around a Central Atom

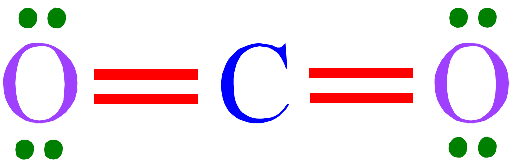
Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
2	Linear	2	0	Linear	$\ddot{O}=C=\ddot{O}$
3	Trigonal planar	3	0	Trigonal planar	F B F F
		2	1	Bent	$[O=N-O]^-$
4	Tetrahedral	4	0	Tetrahedral	H C H H H
		3	1	Trigonal pyramidal	N H H H
		2	2	Bent	O H H

B) 2 e^- Pairs

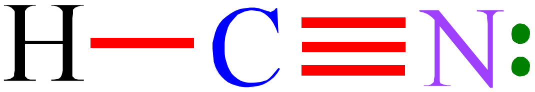


LINEAR

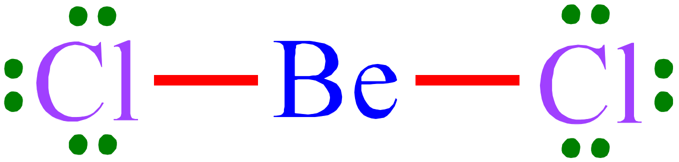
1) CO_2



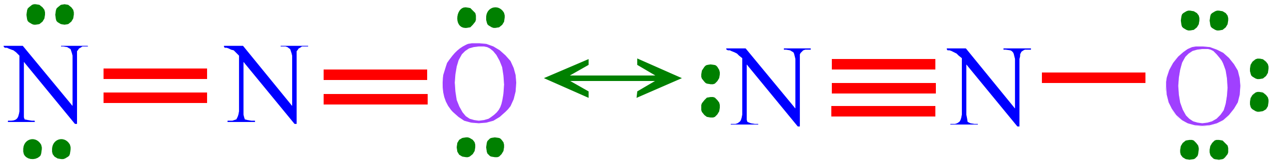
2) HCN



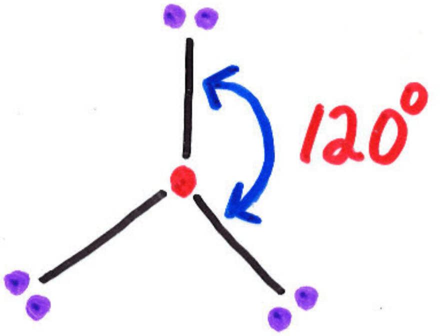
3) $BeCl_2$



4) N_2O



C) 3 e^- Pairs



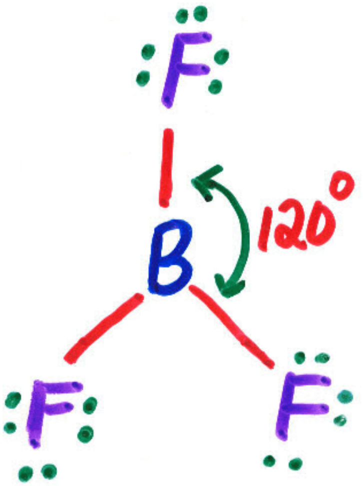
Trigonal Planar

Basic e^- pair geometry

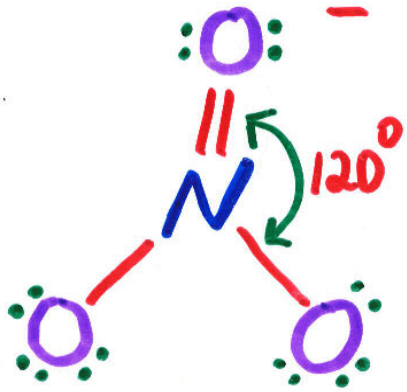
⇒ 2 possible molecular geom. or shapes

1) 3 bonding pairs

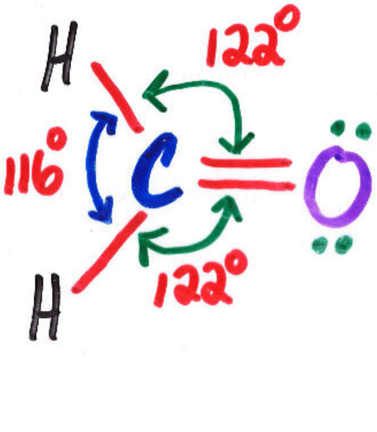
BF_3



NO_3^-



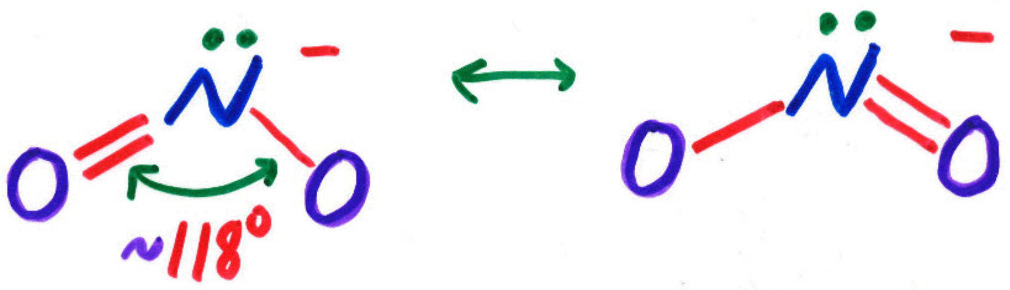
H_2CO



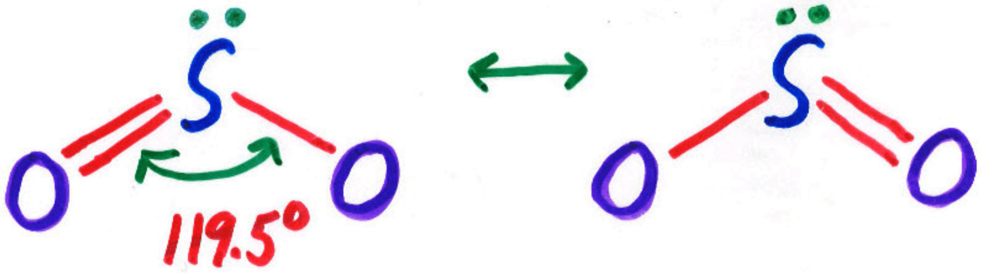
2) 2 bonding & 1 nonbonding

BENT (angular); Angle < 120°

NO_2^-



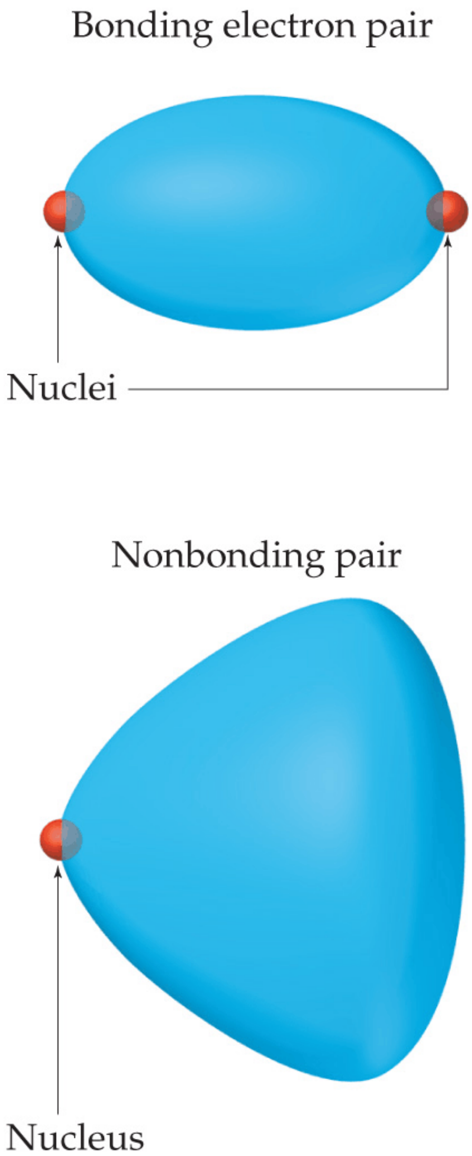
SO_2



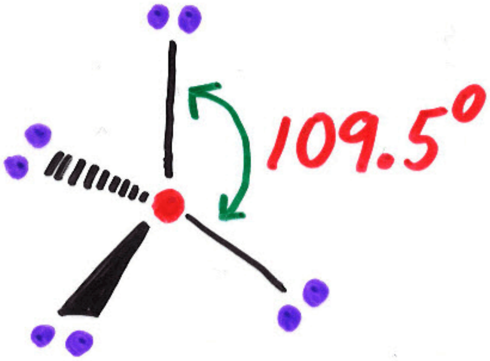
Molecular geom. is determined by arrangement of e^--pairs but is described by positions of the nuclei.

Why is the bond angle not exactly 120° ?

Lone-pair e^- (nbe) not trapped between two atoms and thus spread out and take up more space. Repulses bonding pairs and reduces the bond angles.



D) 4 e⁻ Pairs

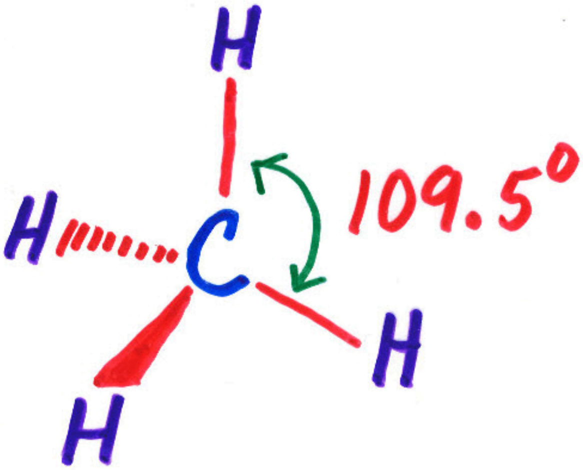


Tetrahedral

3 possible molecular geom. or shapes

1) 4 bonding pairs

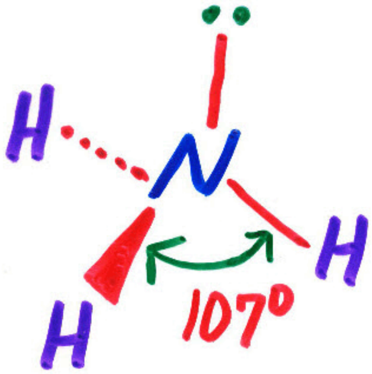
CH_4 PH_4^+ NH_4^+ SO_4^{2-}



Tetrahedral

2) 3 bonding & 1 nonbonding

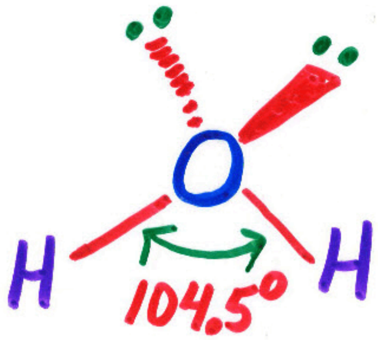
$:NH_3$ $H_3O:^+$ $:AsO_3^{3-}$



Trigonal pyramidal

3) 2 bonding & 2 nonbonding

$H_2\ddot{O}:$ $\ddot{\underset{..}{N}}H_2^-$



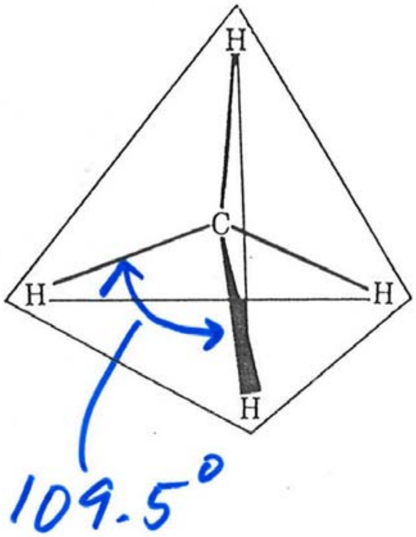
Bent

Note: bond angle dec. by ~ 2° for each lone pair of e⁻

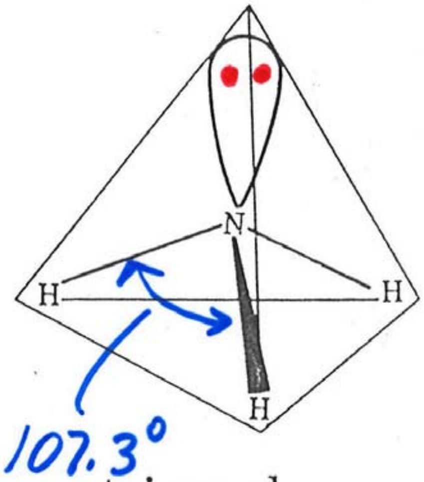
Arrangement of Electron Pairs and Geometry of Some Simple Molecules

Tetrahedral arrangement of electron pairs

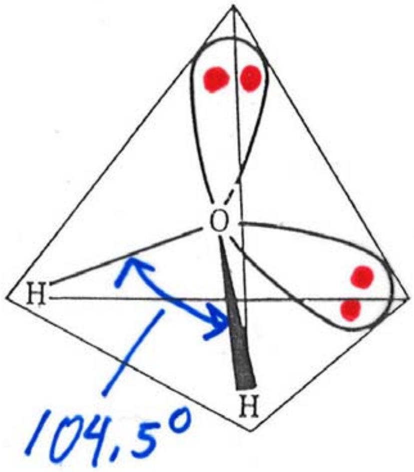
Molecular geometry:



tetrahedral



trigonal pyramidal



angular

ED and MG for AB_5 & AB_6 EDs

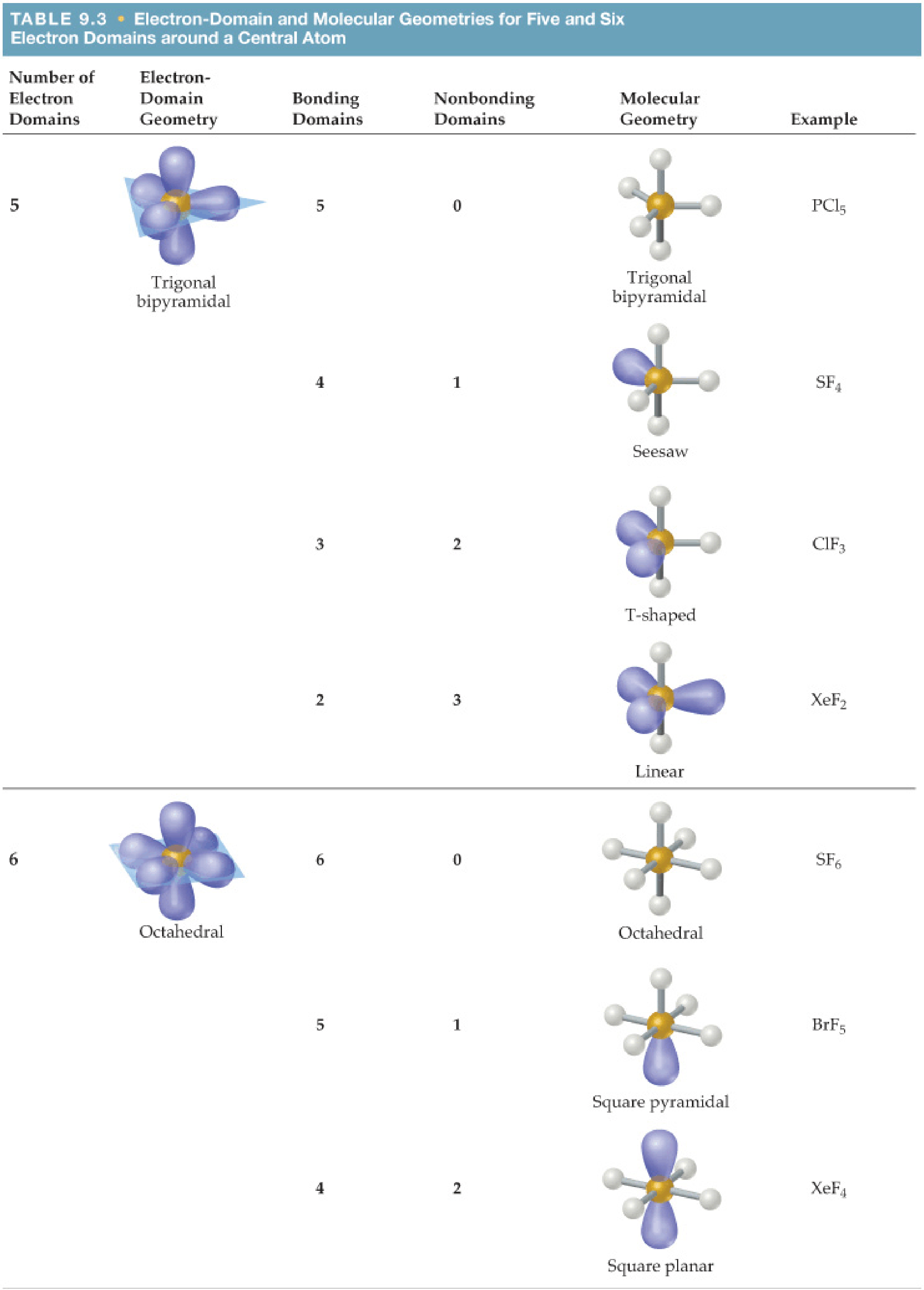
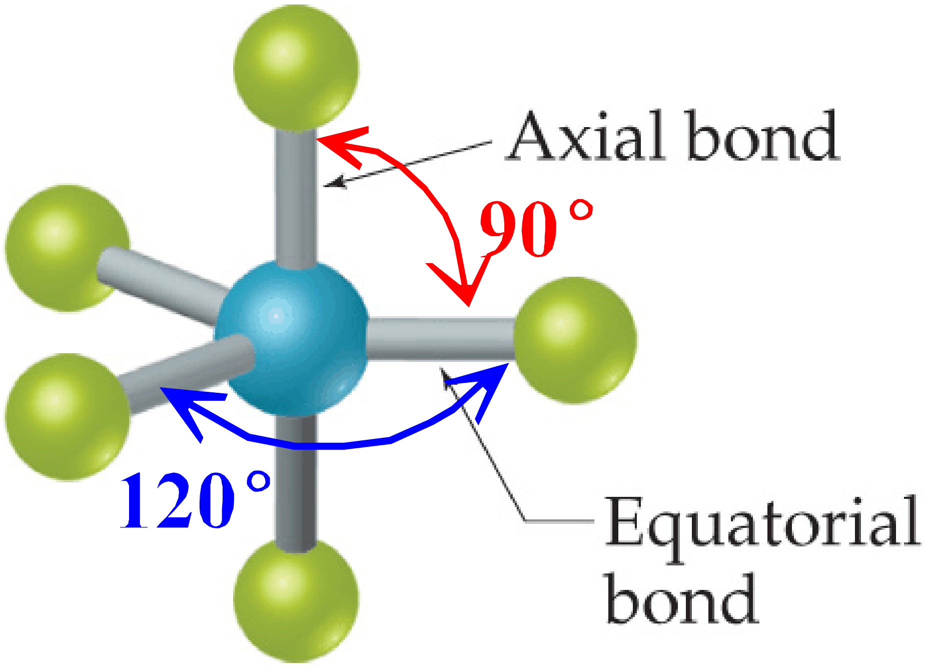


TABLE 9.3 • Electron-Domain and Molecular Geometries for Five and Six Electron Domains around a Central Atom

Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
5	Trigonal bipyramidal	5	0	Trigonal bipyramidal	PCl_5
		4	1	Seesaw	SF_4
		3	2	T-shaped	ClF_3
		2	3	Linear	XeF_2
6	Octahedral	6	0	Octahedral	SF_6
		5	1	Square pyramidal	BrF_5
		4	2	Square planar	XeF_4

E) 5 e$^-$ Pairs Domains



Two “different” bonds.

3 equatorial bonds forming
a trigonal planar arrangement
w. 120° angles

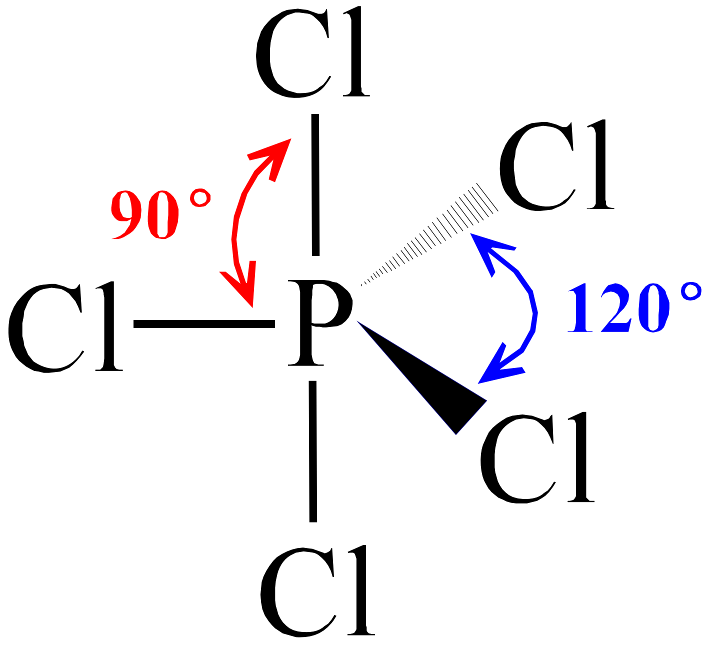
2 axial bonds which are perpendicular
to the trigonal planar equatorial
bonds (90° angles)

4 Molecular Geometries

1) trigonal bipyramidal

Angles: 120° & 90°

PCl_5



For seesaw, T-shaped, linear

Lone-pair e^- & Bonding Pairs

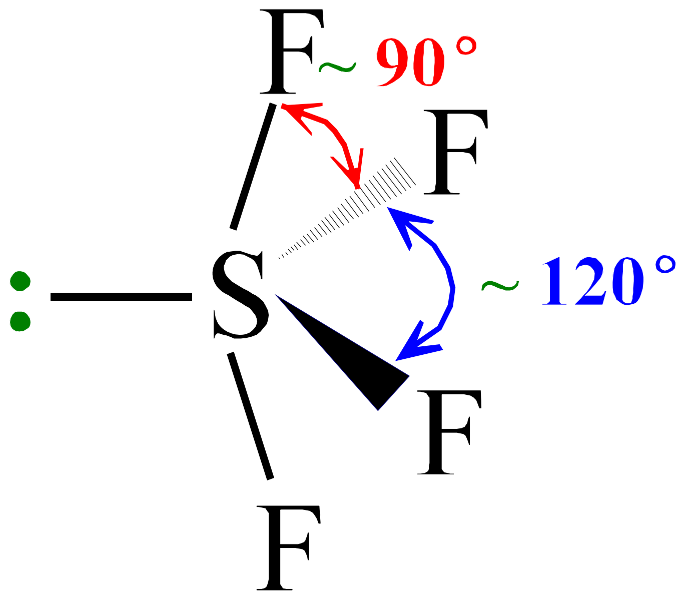
lpe$^-$ wind up in the equatorial positions to maximize separation and reduce repulsions.

lpe$^-$ pushes bonding pairs closer together and reduces angles

2) seesaw

Angles: ~ 120° & ~ 90°

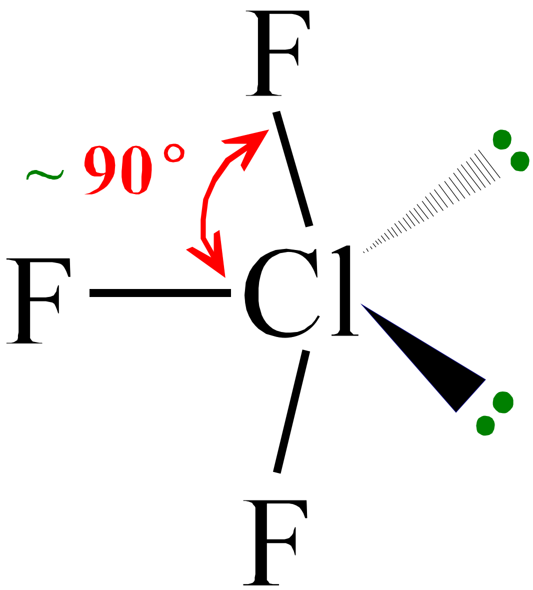
SF_4



3) T-shaped

Angles: ~ 90°

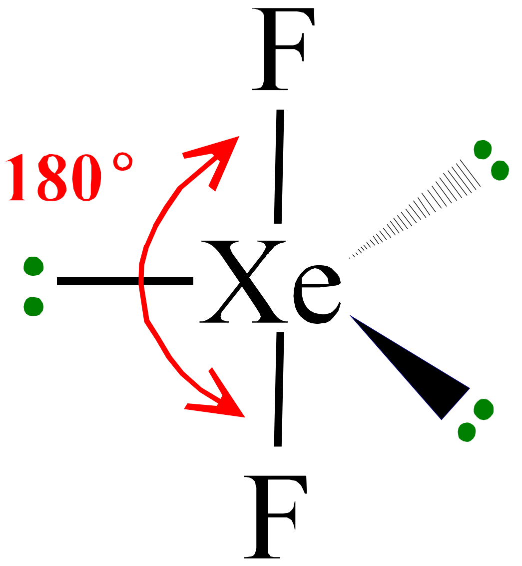
ClF_3



4) linear

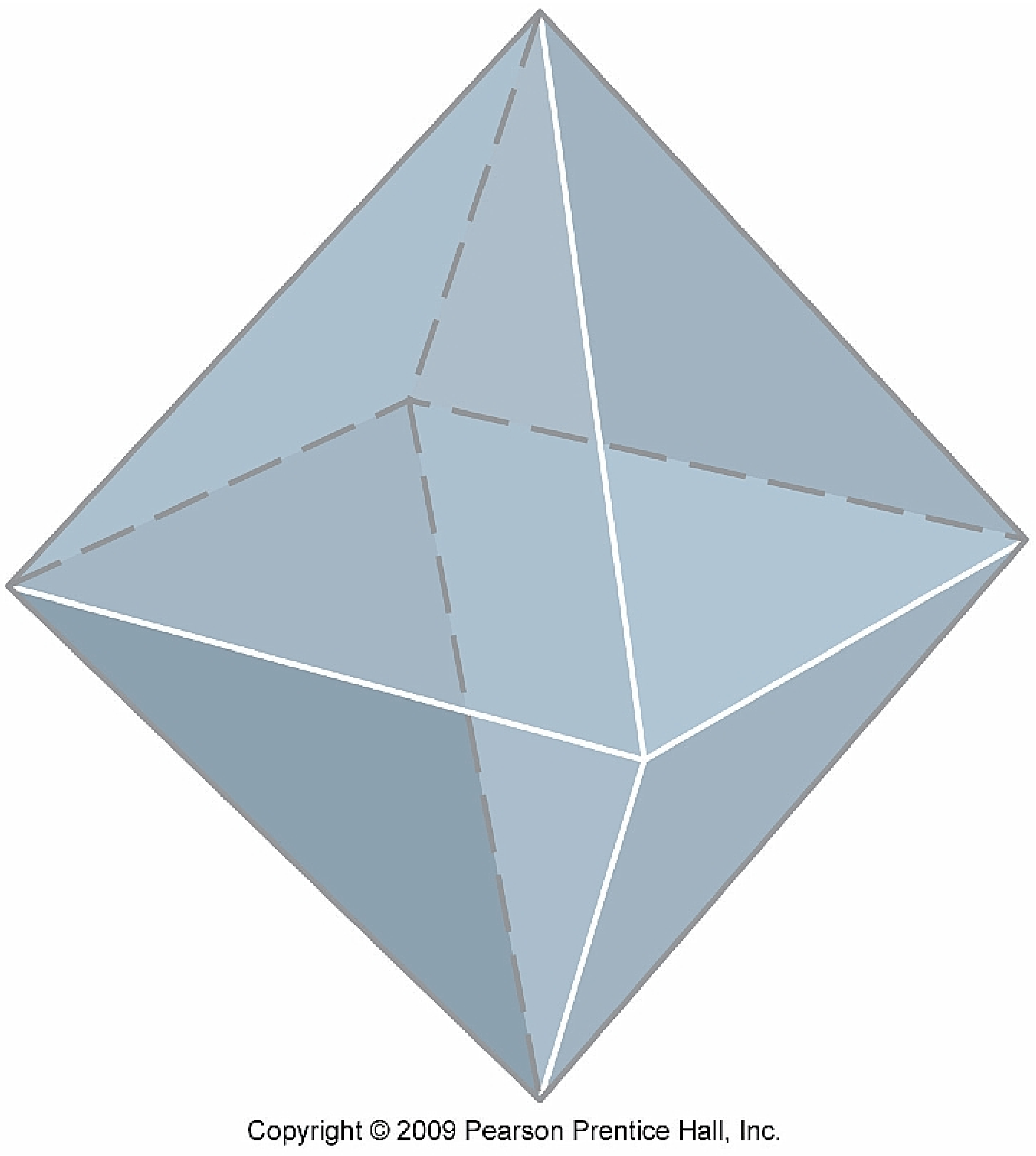
Angle: 180°

XeF_2



F) 6 e^- Pair Domains

Octahedral structure

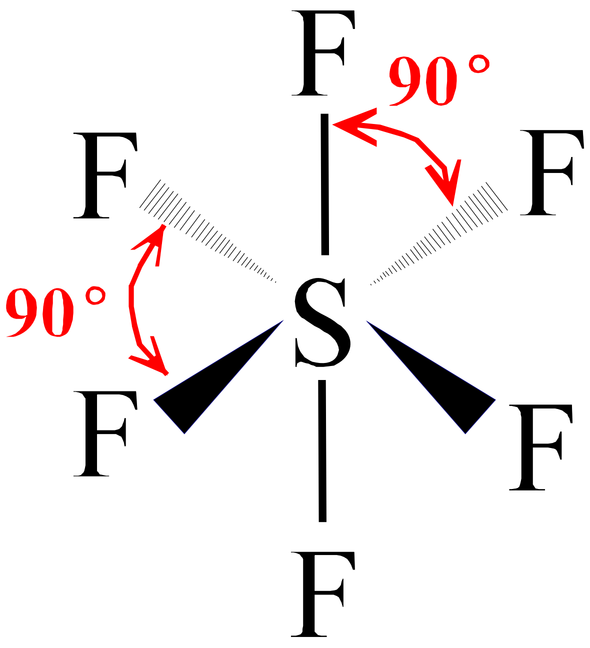


3 Molecular Geometries

1) octahedral

Angles: 90°

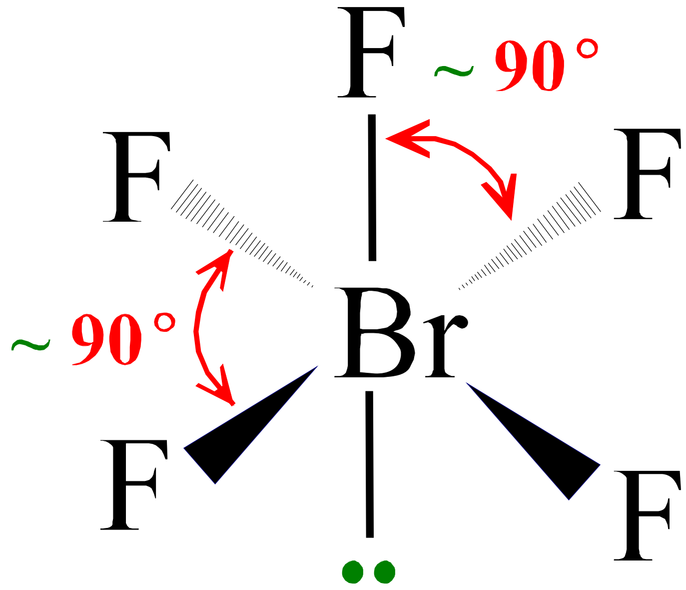
SF_6



2) square pyramidal

Angles: ~ 90°

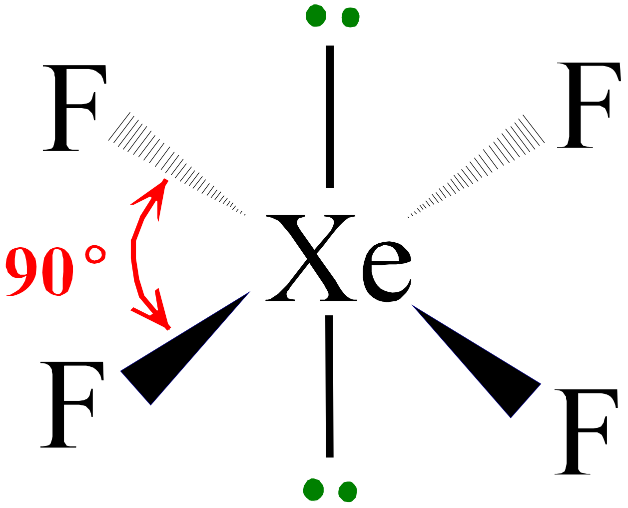
BrF_5



3) square planar

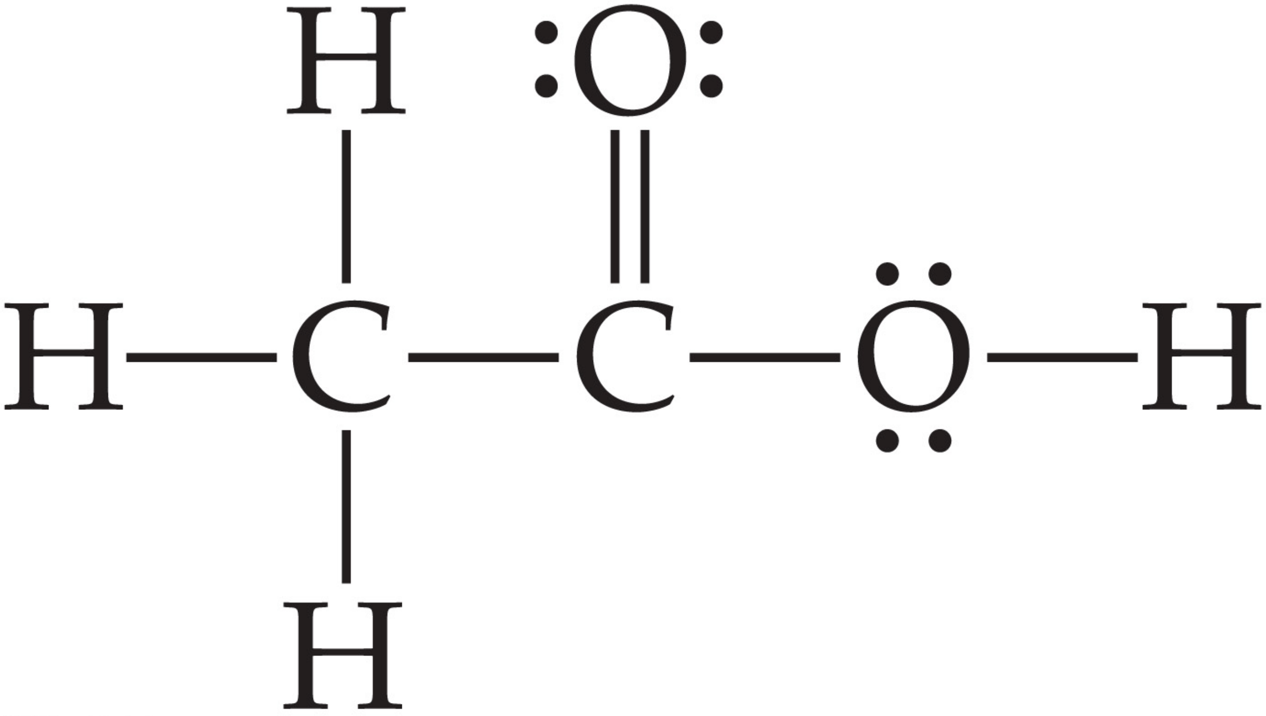
Angles: 90°

XeF_4



G) Shapes of Larger Molecules

Same rules apply to individual atoms in larger molecules.



H) Examples

1) $SnCl_3^-$

2) ICl_4^-

III) Molecular Shape and Polarity

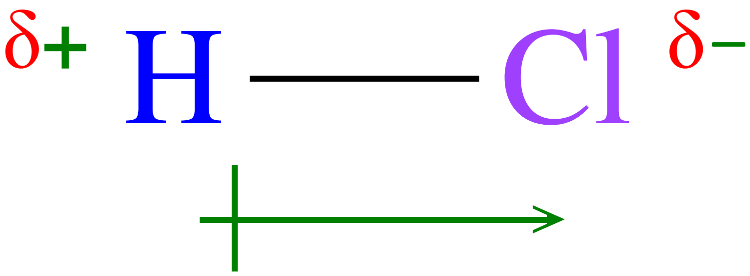
MUST have polar bonds

MUST consider shape

If the centers of + and – charges do not coincide, the molecule is polar.

A) Diatomic Molecules

A diatomic molecule w. a polar bond is polar



B) Polyatomic Molecules

For polyatomic molecules geometry is very important in predicting if the centers of + and – charges coincide.

The dipole moment is for the entire molecule

vector sum of ALL of the individual bond dipole moments.

1) $BeCl_2$ $Cl-Be-Cl$

2) CO_2 $O=C=O$

3) HCN $H-C\equiv N$

4) H_2O

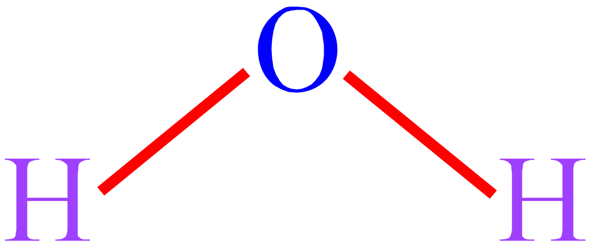
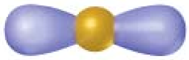
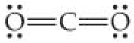
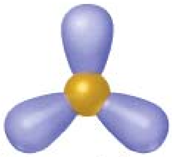
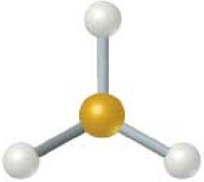
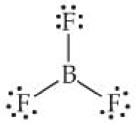
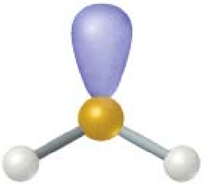
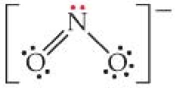
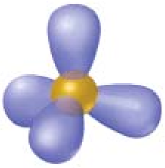
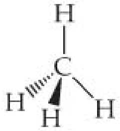
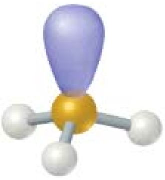
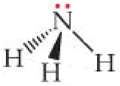
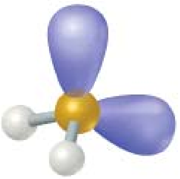
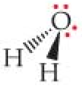


TABLE 9.2 • Electron-Domain and Molecular Geometries for Two, Three, and Four Electron Domains around a Central Atom

Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
2	 Linear	2	0	 Linear	 $O=C=O$
3	 Trigonal planar	3	0	 Trigonal planar	
		2	1	 Bent	
4	 Tetrahedral	4	0	 Tetrahedral	
		3	1	 Trigonal pyramidal	
		2	2	 Bent	

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5) Trigonal Bipyramidal & Octahedral EDs

PCl_5

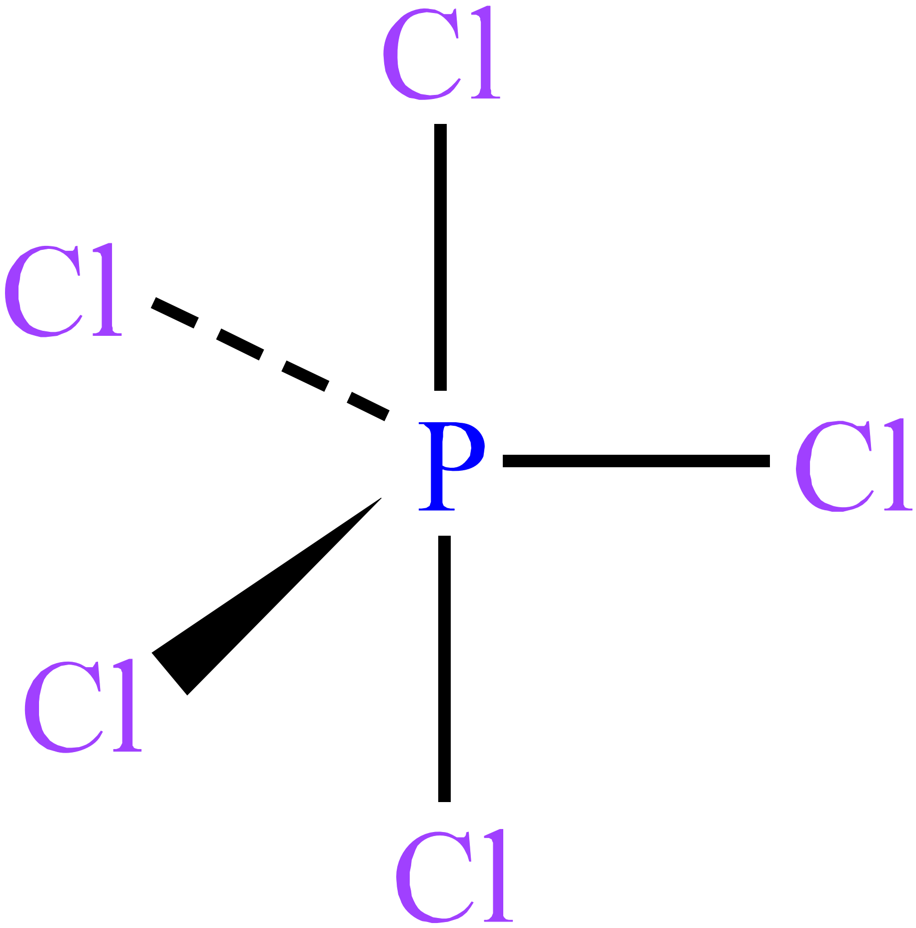
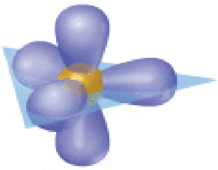
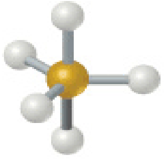
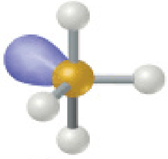
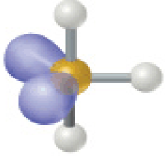
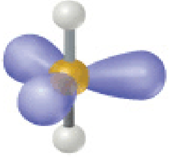
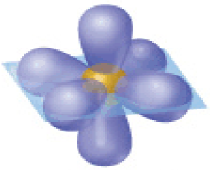
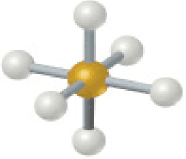
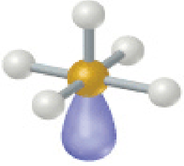
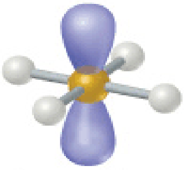


TABLE 9.3 • Electron-Domain and Molecular Geometries for Five and Six Electron Domains around a Central Atom

Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
5	 Trigonal bipyramidal	5	0	 Trigonal bipyramidal	PCl_5
		4	1	 Seesaw	SF_4
		3	2	 T-shaped	ClF_3
		2	3	 Linear	XeF_2
6	 Octahedral	6	0	 Octahedral	SF_6
		5	1	 Square pyramidal	BrF_5
		4	2	 Square planar	XeF_4

BLANK

Note:

1) All the basic shapes are non-polar if all bonding positions are the same

2) If lpe$^-$ on central atom it's usually polar around the central atom

   - exceptions

     linear (trig. bipyr. ED, XeF_2)

     sq. planar (octahed. ED, XeF_4)

3) lpe$^-$ play a role in polarity

BLANK

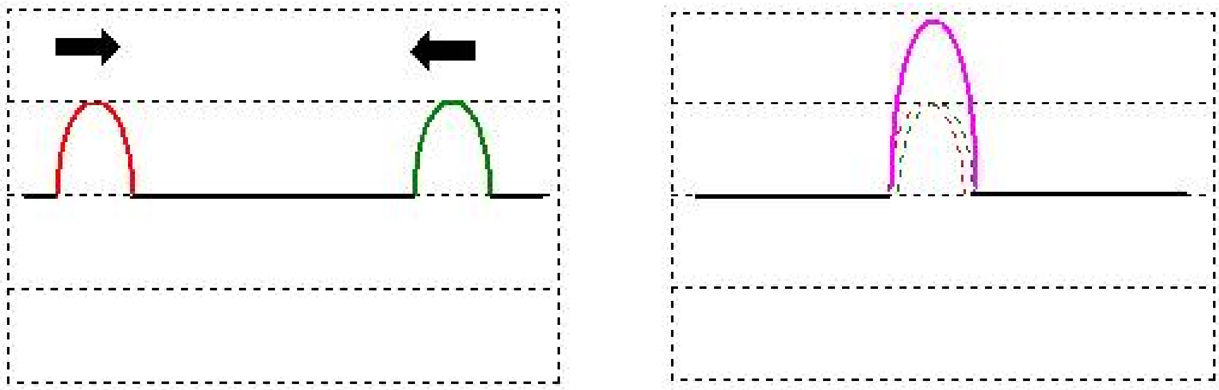
IV) Covalent Bonding and Orbital Overlap

A) Wave Interference:

e^- behave like any other wave & when 2 waves meet they can interact constructively or destructively.

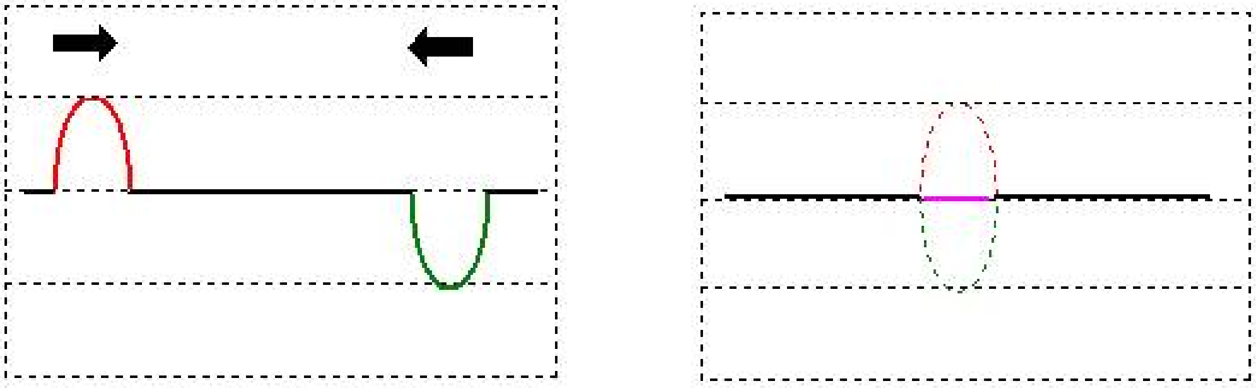
1) Constructive interference:

waves add together and
get a bonding orbital



2) Destructive interference:

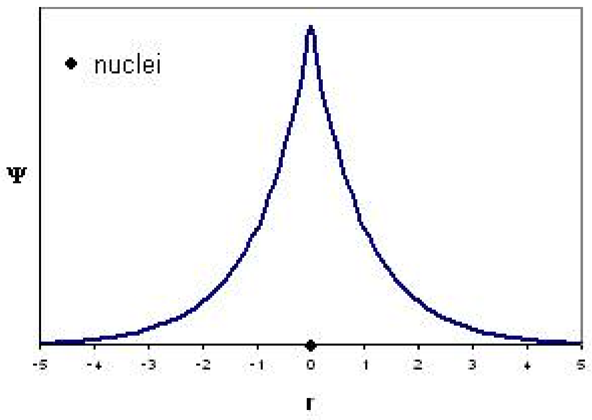
waves subtract from each other and get an anti-bonding orbital

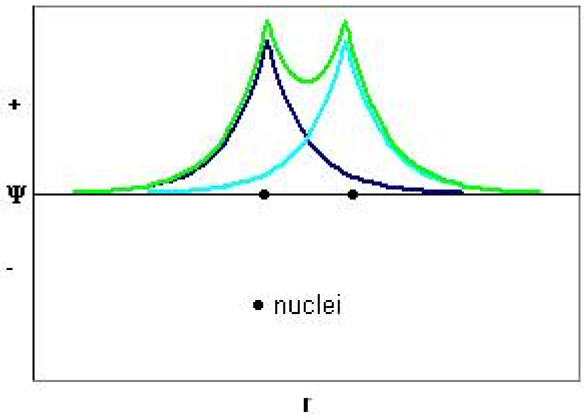


B) Effect in Chemistry

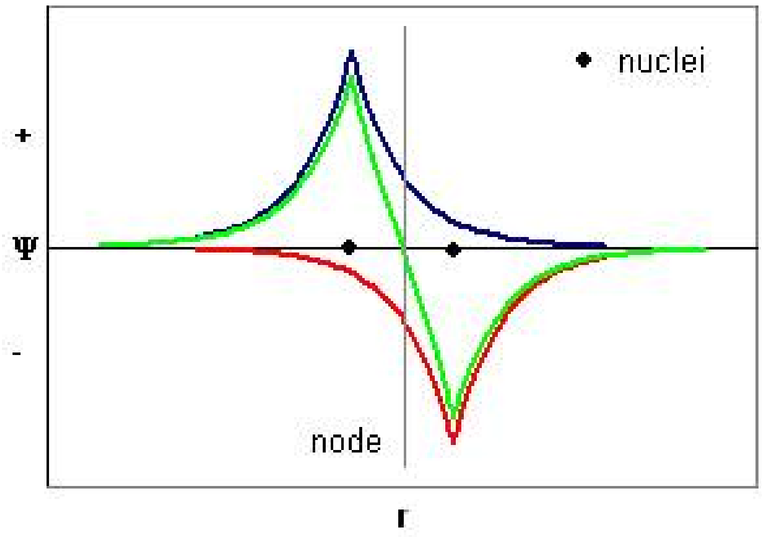
The wavefunction (ψ) which describes the electrons works the same way

1) **Constructive interference** between two orbitals ("**in-phase**" combination) will produce a "**bonding orbital**" (a large area spanning both atoms in which the two electrons are free to move, *i.e.* the atoms share the electrons!!!). This orbital is lower in E than the two AOs (atomic orbitals)





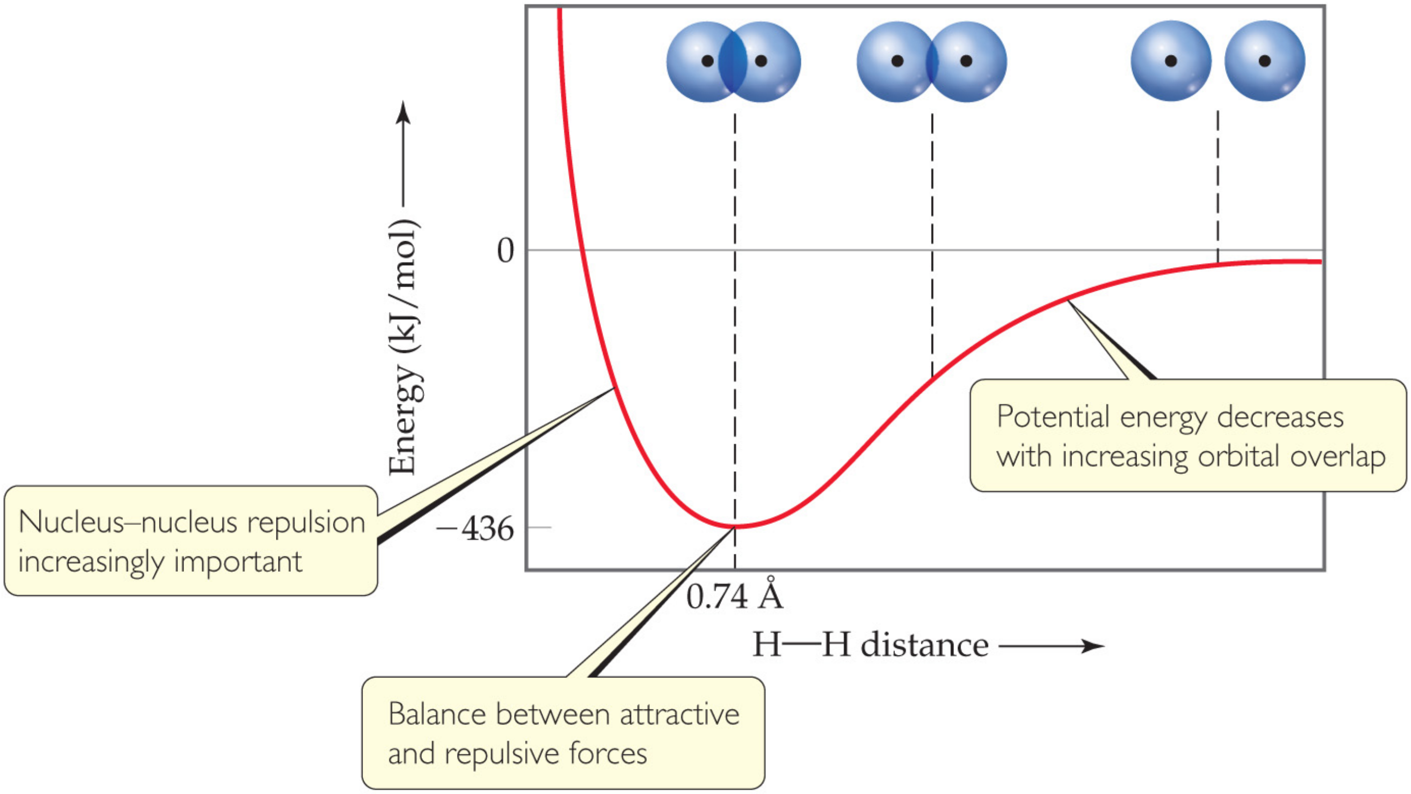
2) **Destructive interference** (the "**out-of-phase**" combination) will produce an "anti-bonding **orbital**", where there will be a node (point where the wavefunction has a value of 0) between the two atoms. This orbital is higher in E than the two AOs or the bonding orbital.



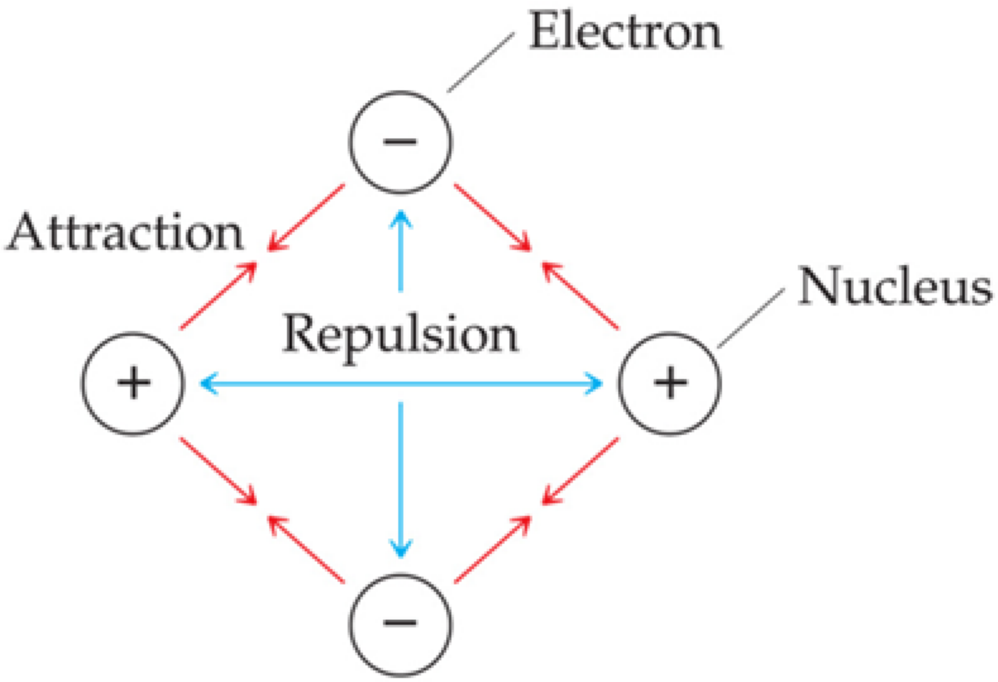
A) Sigma (σ) Bonds

High e^- density concentrated between nuclei along the internuclear axis

Morse Potential Energy curve



Bond is attraction of e^- - nuclei & repulsion of nuclei.



Bond strength depends on:

1) The degree of orbital overlap

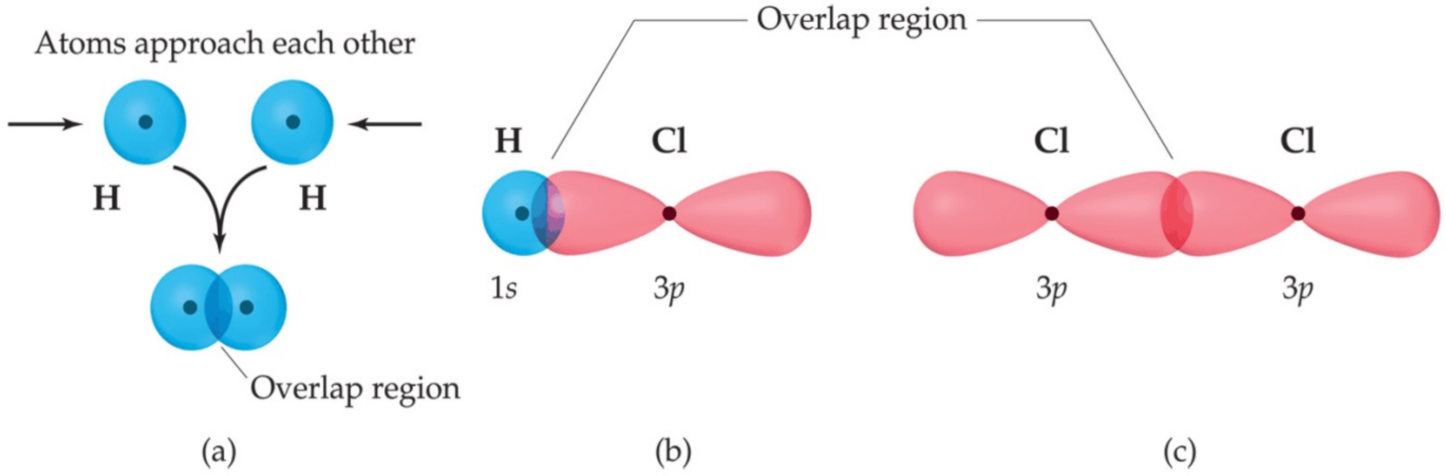
2) The relative energies of the AOs which form the bond

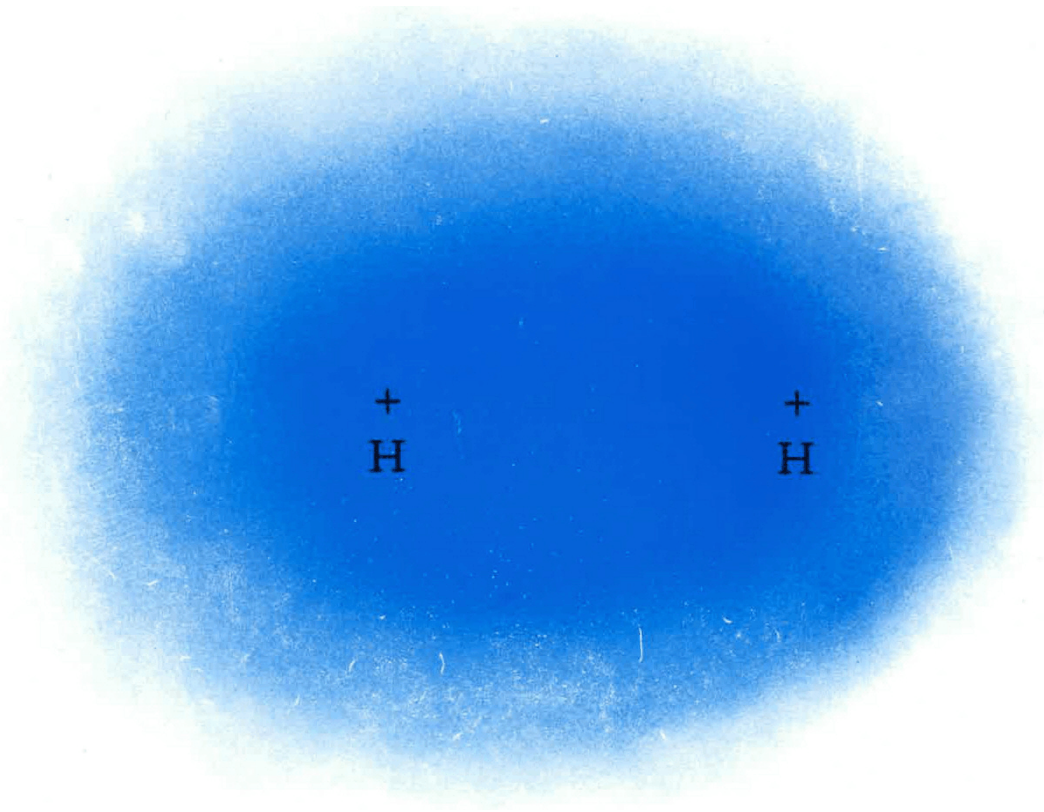
Result from overlap of 2 "*s*" orb., "*s*" & "*p*" (end on), 2 "*p*" (end on), "*s*" & hybrid orb., 2 hybrid orb (end on)

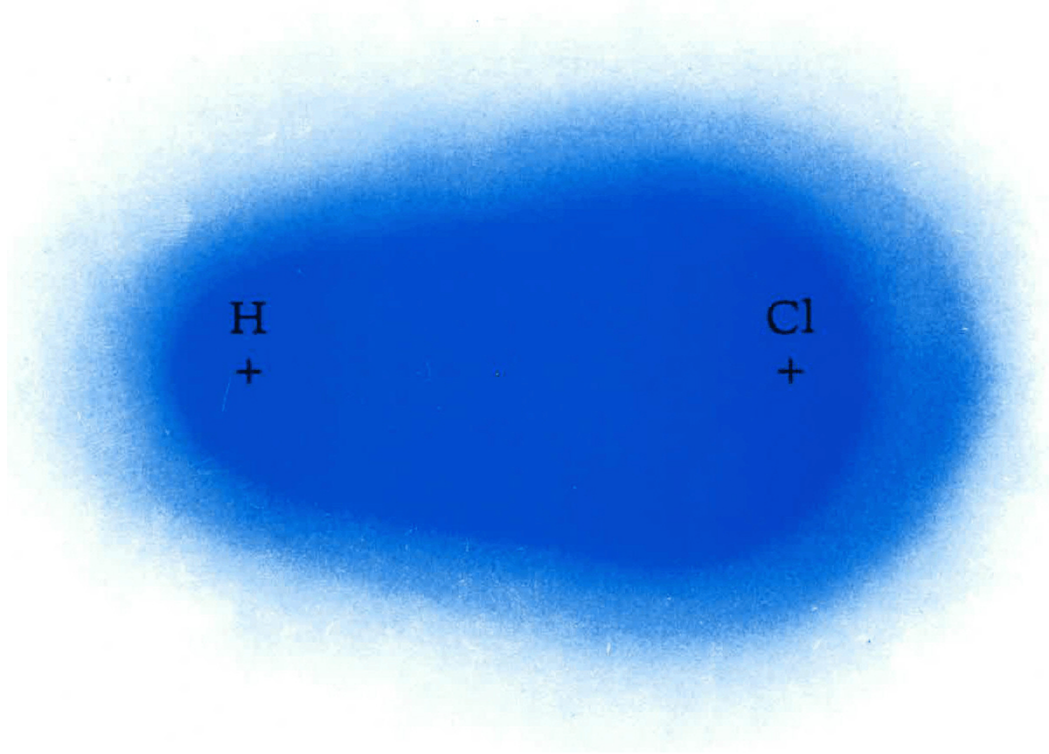
$s + s \Rightarrow \sigma$

$s + p \Rightarrow \sigma$

$p + p \Rightarrow \sigma$



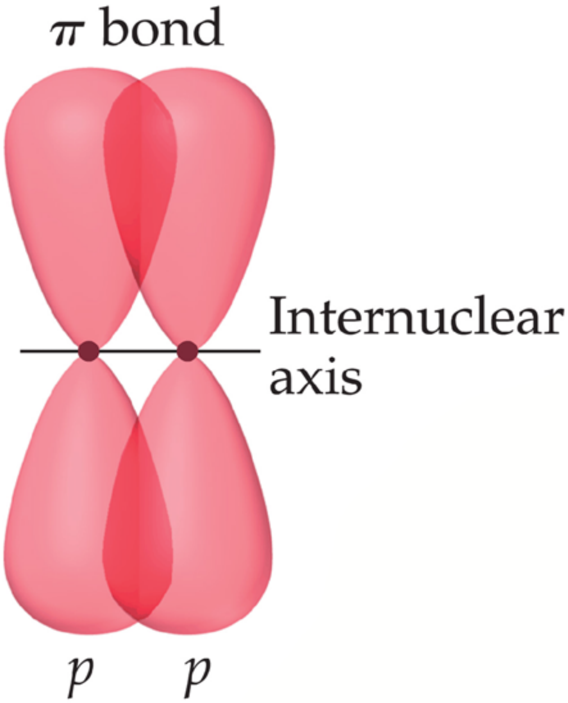

+
H
+
H

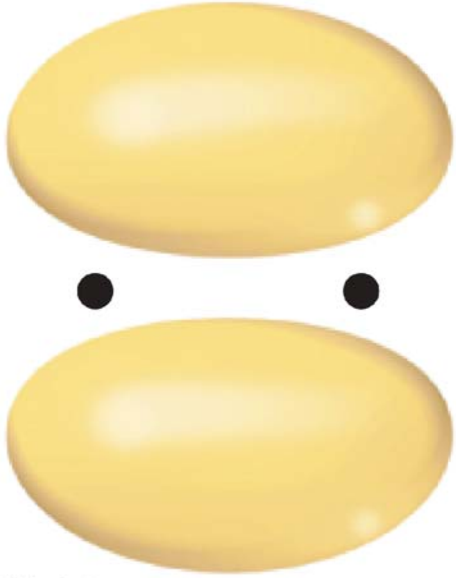

H
+
Cl
+

B) Pi (π) Bonds

e^- density above and below internuclear axis

Results from sideways overlap of parallel ***p*** orbitals





The side-side overlap in **π** bonds is less efficient than for **σ** bonds

- **π** bonds weaker than **σ** bonds

C) Bonding Theories

Any theory of bonding needs to explain why & how bonds form and the resulting observed molecular geometries.

There are two basic theories:

1) Valence Bond theory

2) Molecular Orbital (MO) theory

Both use the idea of orbital overlap to create bonds. The main difference is when orbitals are allowed to merge.

V) Hybrid Orbitals - Valence Bond Theory

Bonds are created by orbital overlap to produce **σ** or **π** bonds

To explain many observed molecular geometries, pure "s" and "p" atomic orbitals are combined to produce a set of "hybrid" orbitals on atoms.

These hybrid orbitals then form bonds between atoms producing the correct geometry.

A) *sp* Hybrid Orbitals

BeF_2 linear with 2 single bonds

Be atom:

[He] $\underline{\uparrow\downarrow}\qquad\qquad \underline{\quad\ }\quad \underline{\quad\ }\quad \underline{\quad\ }$

2s 2p

Should not form bonds

- no singly occupied orbitals

As it forms bonds it can absorb enough energy to "promote" one 2*s* e^- to a 2*p* orbital.

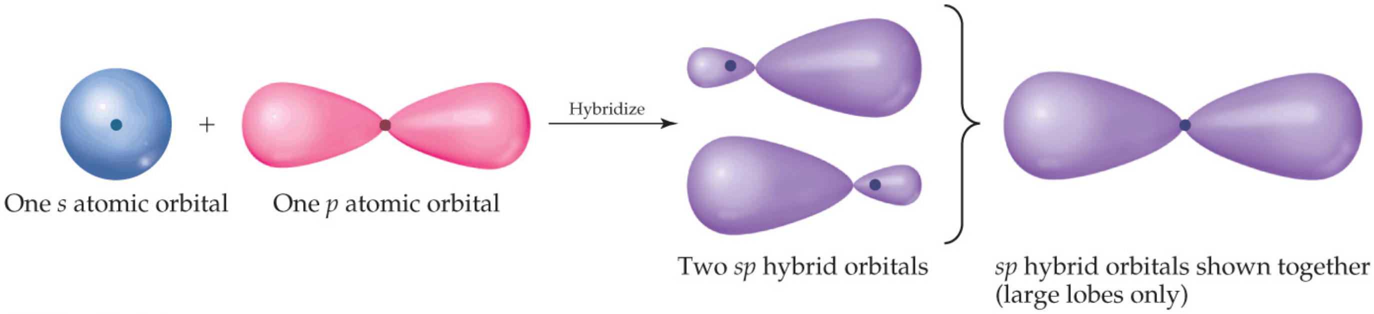
[He] $\underline{\uparrow\ \ }\qquad\qquad \underline{\uparrow\ \ }\quad \underline{\quad\ }\quad \underline{\quad\ }$

2s 2p

The *s* and *p* orbitals then mix or "hybridize" to form two degenerate ***sp*** *hybrid* orbitals.

These ***sp*** *hybrid* orbitals have two lobes similar to a p orbital.

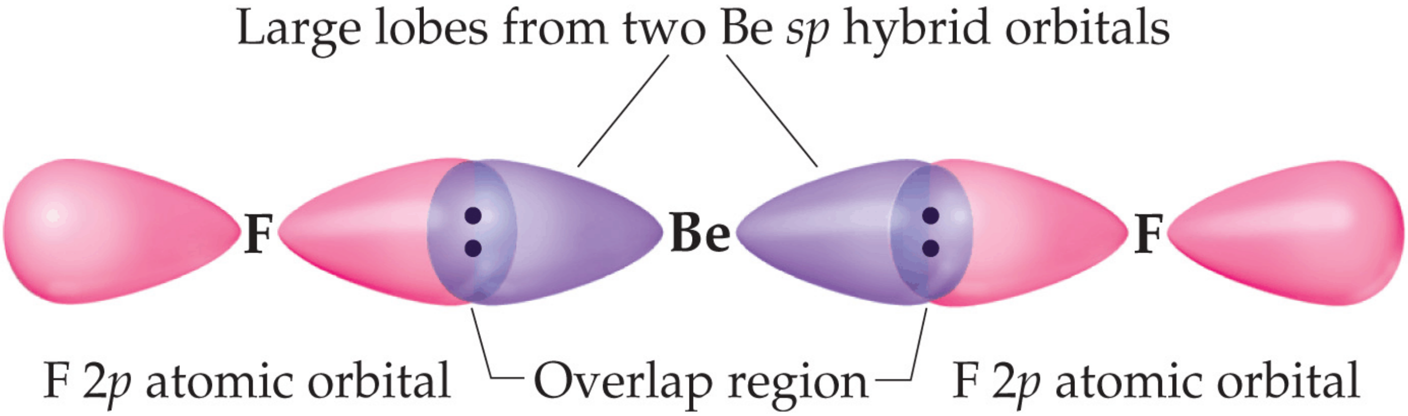
One of the lobes is larger and more rounded as is the *s* orbital.



These two degenerate orbitals align themselves 180° from each other:

linear

Consistent with the observed geometry of Be compounds.



B) ***sp***^{2} Hybrid Orbitals

BF_3: trigonal planar, 120°

[He] ↿⇂ ↿ __ __

2s 2p

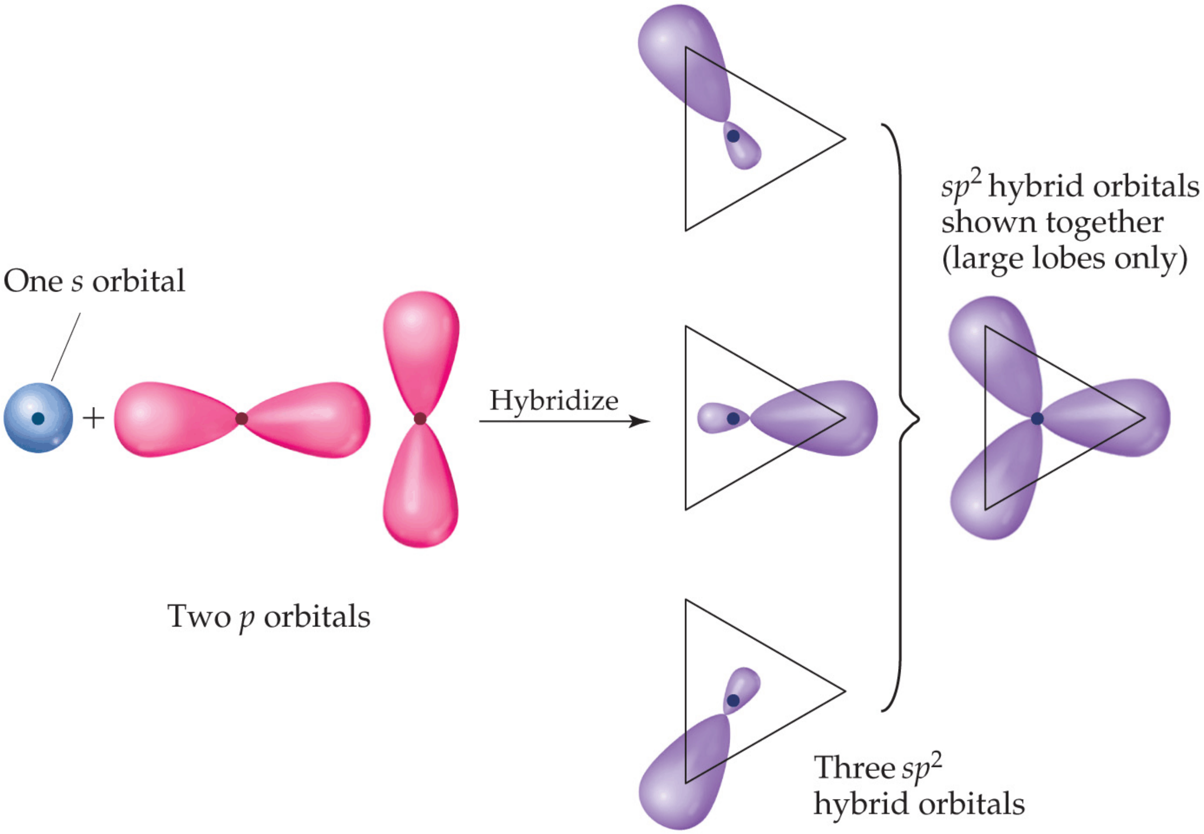
As it forms bonds it can absorb enough energy to "promote" one 2*s* e$^-$ to a 2*p* orbital.

[He] ↿ ↿ ↿ __

2s 2p

The *s* and *p* orbitals then mix or "hybridize" to form three degenerate ***sp*^{2}** *hybrid* orbitals.

These ***sp*^{2}** *hybrid* orbitals have three lobes with more p orbital character than for ***sp*** *hybrid* orb.



C) sp^3 Hybrid Orbitals

CH_4: tetrahedral, 109.5°

[He] ↿⇂ ↿ ↿ __

2s 2p

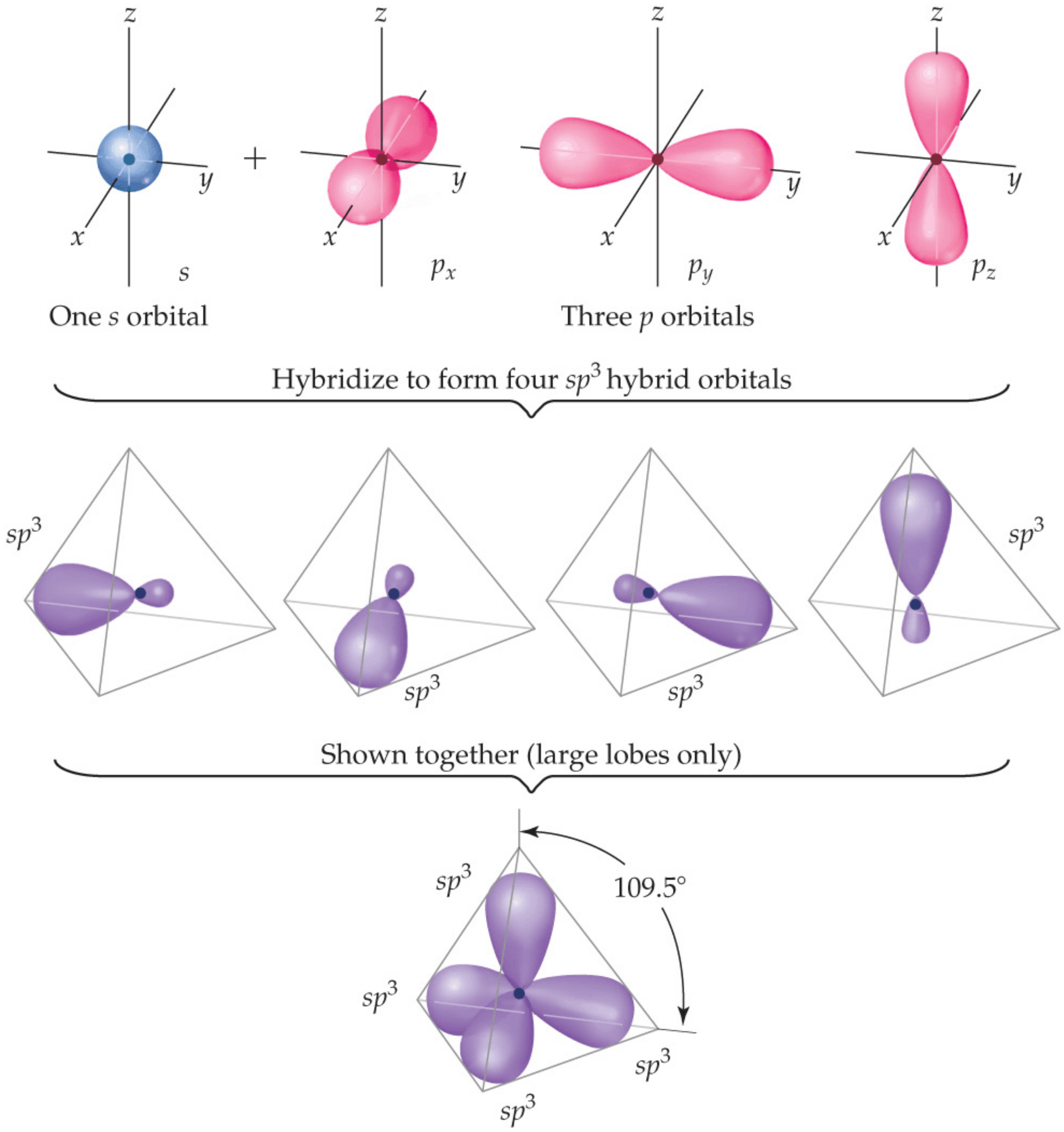
As it forms bonds it can absorb enough energy to “promote” one 2*s* e^- to a 2*p* orbital.

[He] ↿ ↿ ↿ ↿

2s 2p

The *s* and *p* orbitals then mix or “hybridize” to form four degenerate ***sp***^{3} *hybrid* orbitals.

These ***sp*^{3}** *hybrid* orbitals have four lobes with more p orbital character than for ***sp*^{2}** *hybrid* orb.



D) Hybrid Orbitals - Summary

Hybrid orbitals are responsible for the ED geometries.

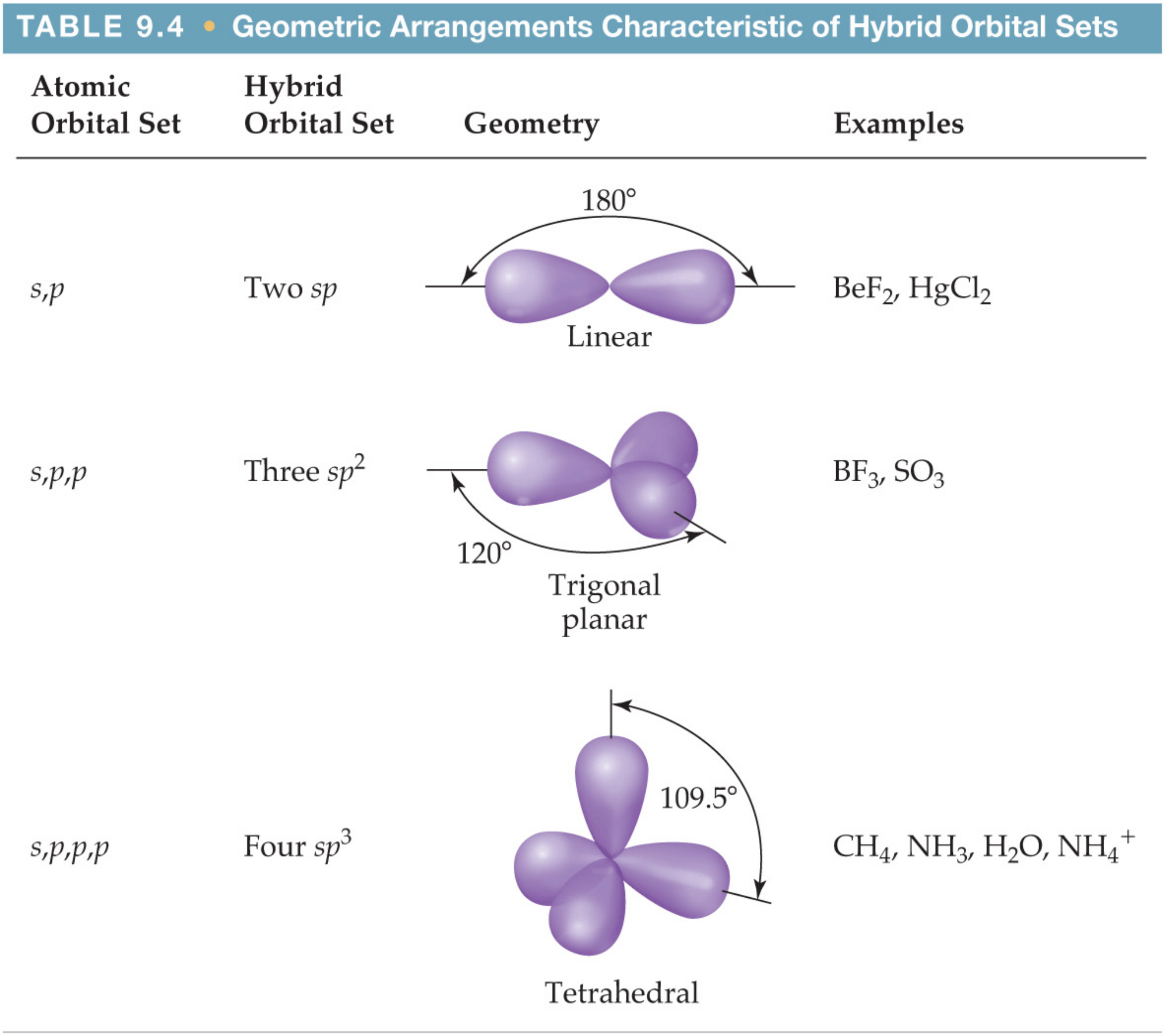


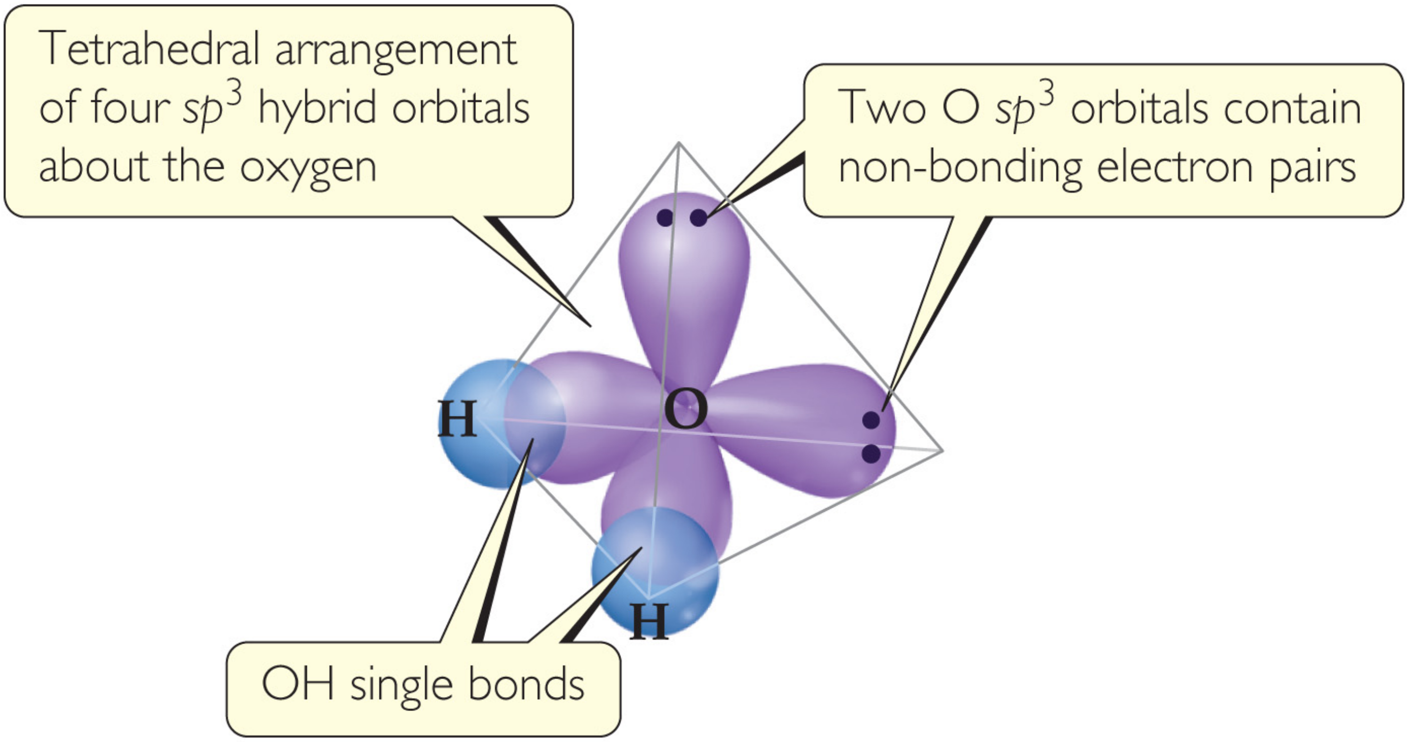
TABLE 9.4 • Geometric Arrangements Characteristic of Hybrid Orbital Sets

Atomic Orbital Set	Hybrid Orbital Set	Geometry	Examples
s,p	Two *sp*	180° Linear	BeF_2, $HgCl_2$
s,p,p	Three sp^2	120° Trigonal planar	BF_3, SO_3
s,p,p,p	Four sp^3	109.5° Tetrahedral	CH_4, NH_3, H_2O, NH_4^+

1) Ex: H_2O

ED geom. tetrahedral

Molecular geom. bent



E) Hypervalent Cmpds - Hybrid Orbitals?

Are hybrid orbitals necessary for ED geometries of trigonal bipyramidal and octahedral?

- some say yes some say no

In VB theory you need to hybridize the n***d*** orbitals with the n***s*** & n***p*** (e.g. 3s, 3p and 3d).

sp^3d	5 hybrids	trig. bipyr.
sp^3d^2	6 hybrids	octahedral

VI) Multiple Bonds

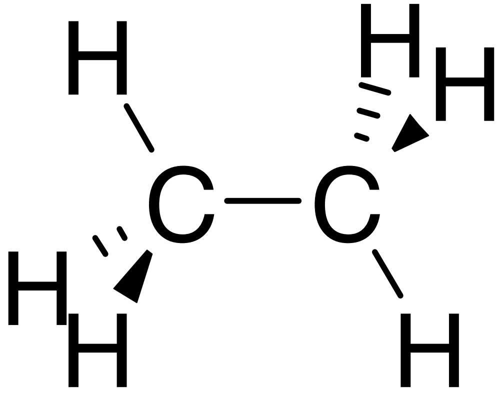
Overlap of hybrid orbitals with *s* or *p* or other hybrid orbitals (end-to-end):

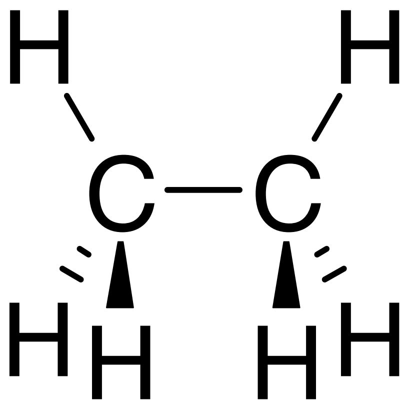
σ bonds.

e⁻ density is symmetric about the internuclear axis of **σ** bond, groups can rotate about the bond without breaking it.

- free rotation about **σ** bonds

Single bonds are **σ** bonds





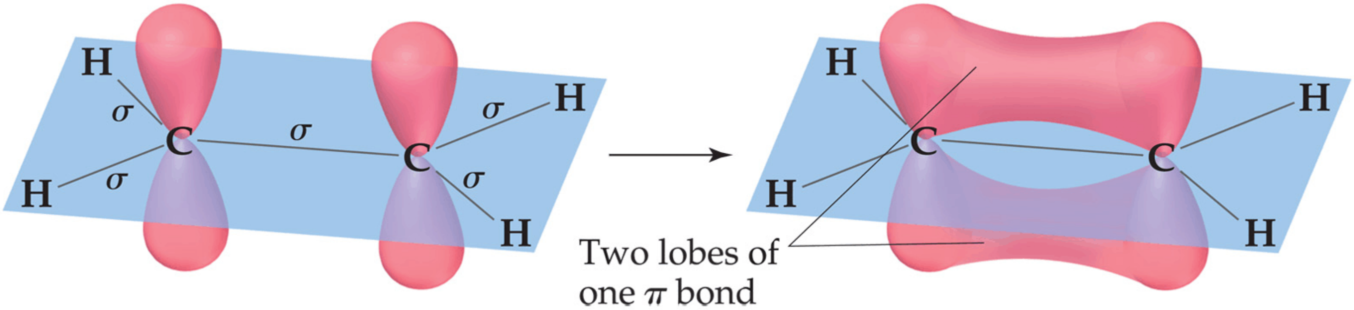
Multiple bonding requires π bonds

A) Double Bonds

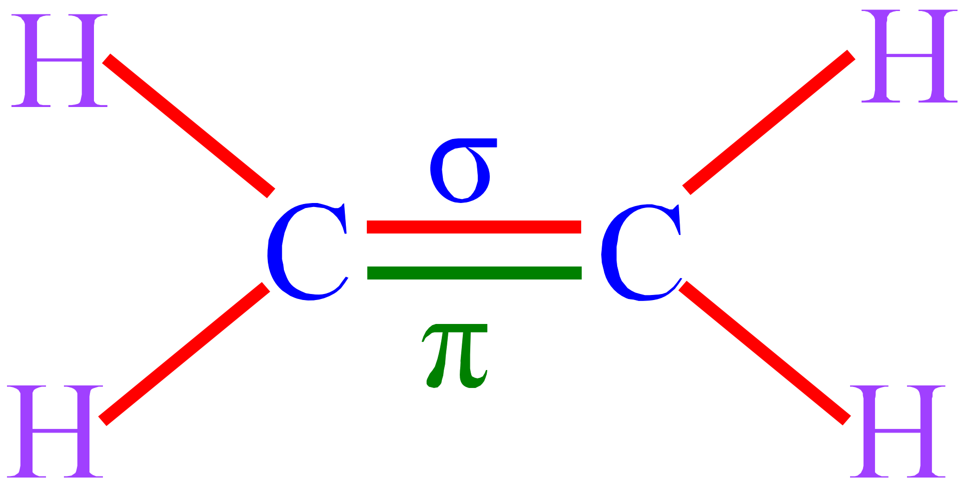
Look at ethylene: C_2H_4

σ bonds between C and H and both C atoms using sp^2 hybrid orbitals

leaves "*p*" orbitals on each C which can overlap sideways to form π bonds



Two lobes of one π bond



Trigonal planar around each C atom
- whole molecule is planar

π bond is perpendicular to plane

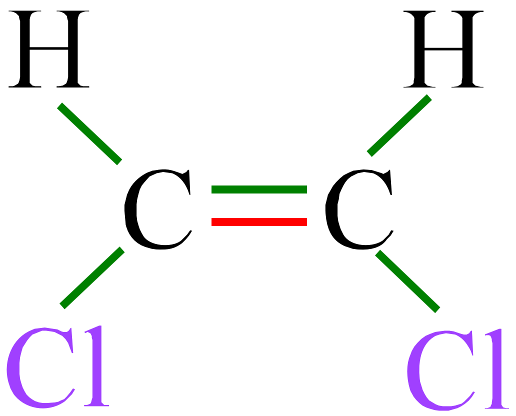
No free rotation between C atoms

Double bond ≡ 1 **σ** **+** 1 **π**

1) Cis-Trans Isomers

Isomers

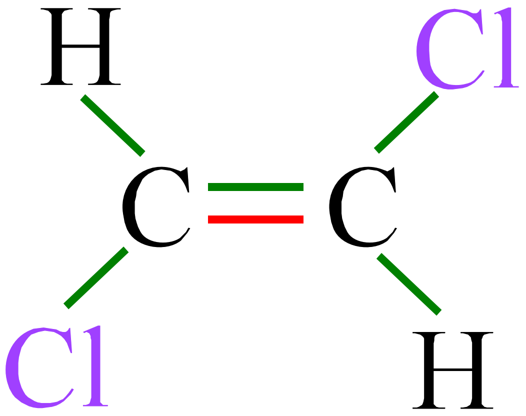
Cmpds. w. same molecular form. but diff. arrangements of atoms



cis-1,2-dichloroethene

b.p. = 60°C

DM = 1.85 D



trans-1,2-dichloroethene

b.p. = 48°C

DM = 0 D

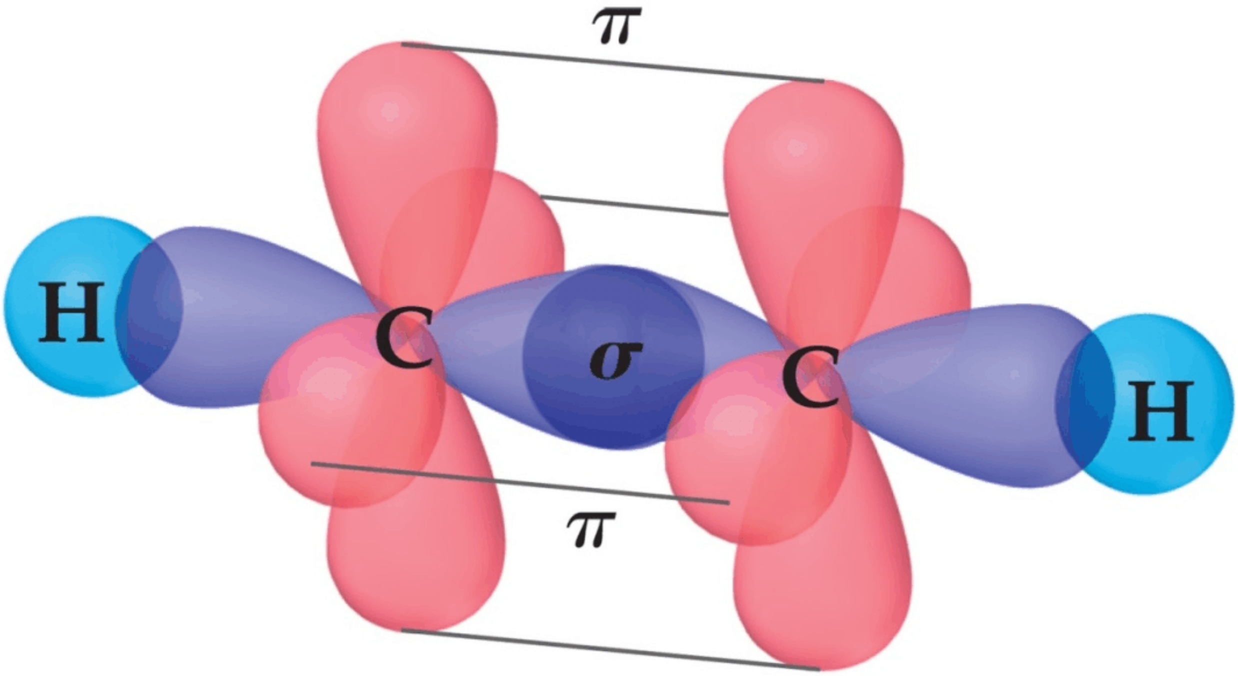
NO "free" rotation about double bond

B) Triple Bonds

Look at acetylene: C_2H_2

σ bonds between C and H and both C atoms using ***sp*** hybrid orbitals

leaves 2 sets of ”***p***” orbitals on each C which can overlap sideways to form 2 sets of **π** bonds



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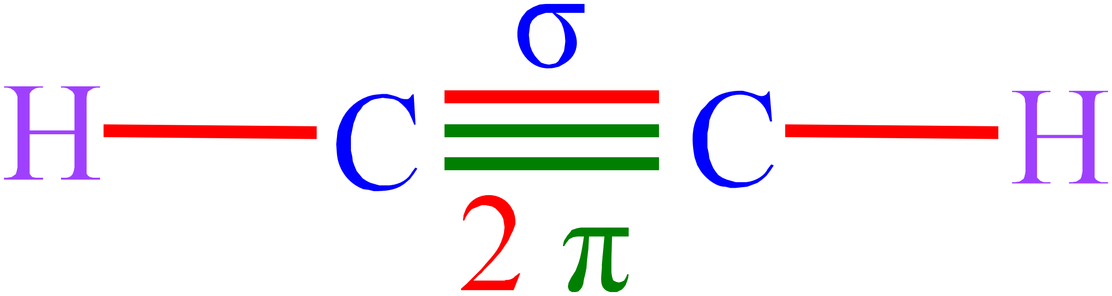


$H-C\equiv C-H$

Linear around each C atom

Triple bond $\equiv$ 1 **σ** **+** 2 **π**

C) VB Theory - Summary

For a given atom, all hybrid orbitals have the same energy.

total number hybrid orbitals

=

total number of AOs used

Unhybridized "***p***" orbitals can be used to form **π** bonds (or remain empty).

When atoms share more than
one pair of e^- one pair is used
to form a **σ** bond.
- Additional pairs form **π** bonds.

1) Good Points

a) Hybrid orbitals created by mixing ***s***, ***p*** (& ***d***) orbitals then form localized **σ** & **π** bonds

– simple model.

b) Geometries match VESPR very well

2) Problems

a) Does not explain O_2 paramagnetism (unpaired e^-)

b) Does not explain excited states

- impt for spectroscopy

c) Explains localized bonding - but resonance concepts have to be "added" for some molecules (i.e. doesn't explain delocalized bonding well).

D) Resonance & Delocalized Bonding

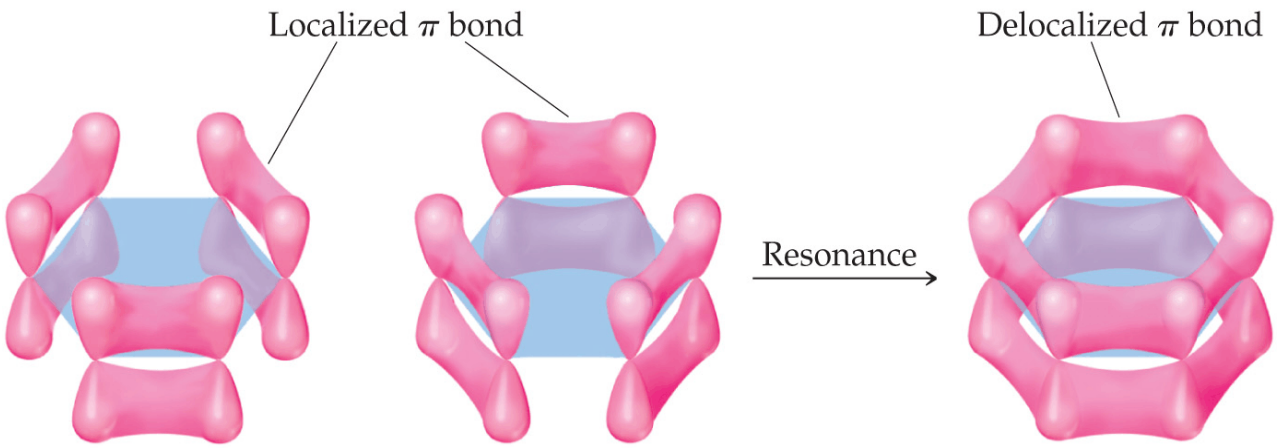
Localized σ and π bonds
can't explain resonance.

Instead can think of atoms
forming delocalized π bonding.

Benzene:

Each C atom is *sp*^{2} hybridized and
has 1 atomic *p* orbital left over

- form a delocalized π bond



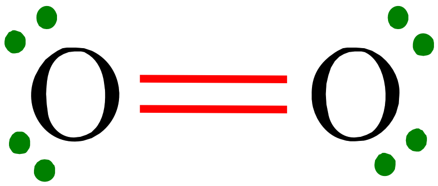
VII) Molecular Orbital Theory

Some things not explained by VB theory

Does NOT explain magnetic
or spectral prop.

Diamagnetic - NOT attracted to magnet
Paramagnetic - attracted to magnet

Simple VB theory predicts any molecule
w. an even # e^- should be diamagnetic



O_2 is paramagnetic

- must have unpaired e^-

In MO theory orbitals are constructed as combinations of AOs from **ALL** atoms in the molecule.

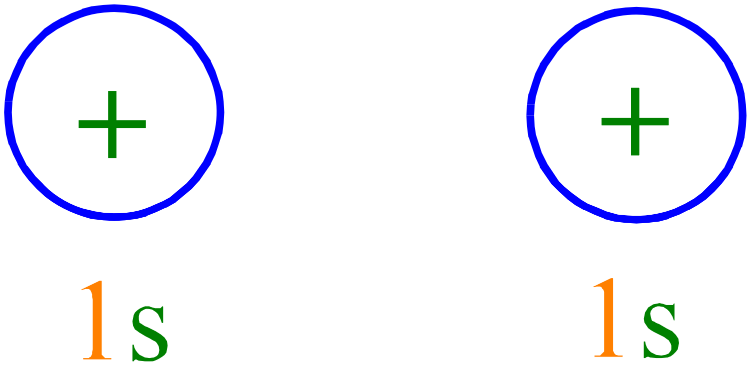
The MO can span more than 2 atoms.

Each MO can still only contain 2 e^-

In VB theory orbitals are mixed on individual atoms 1st then bonded together as needed

In MO theory the orbitals of all atoms mix and are then used to form the lowest energy molecular orbitals.

A) Bonding and Anti-bonding σ-Orbitals



Can either add or subtract the AOs (e^- density of the atoms)

1) Bonding MO

Add AOs - e^- density concentrated in region between nuclei

σ_{1s}

→ **MO has cylindrical shape about axis**

→ **MO obtained from 1s AO**

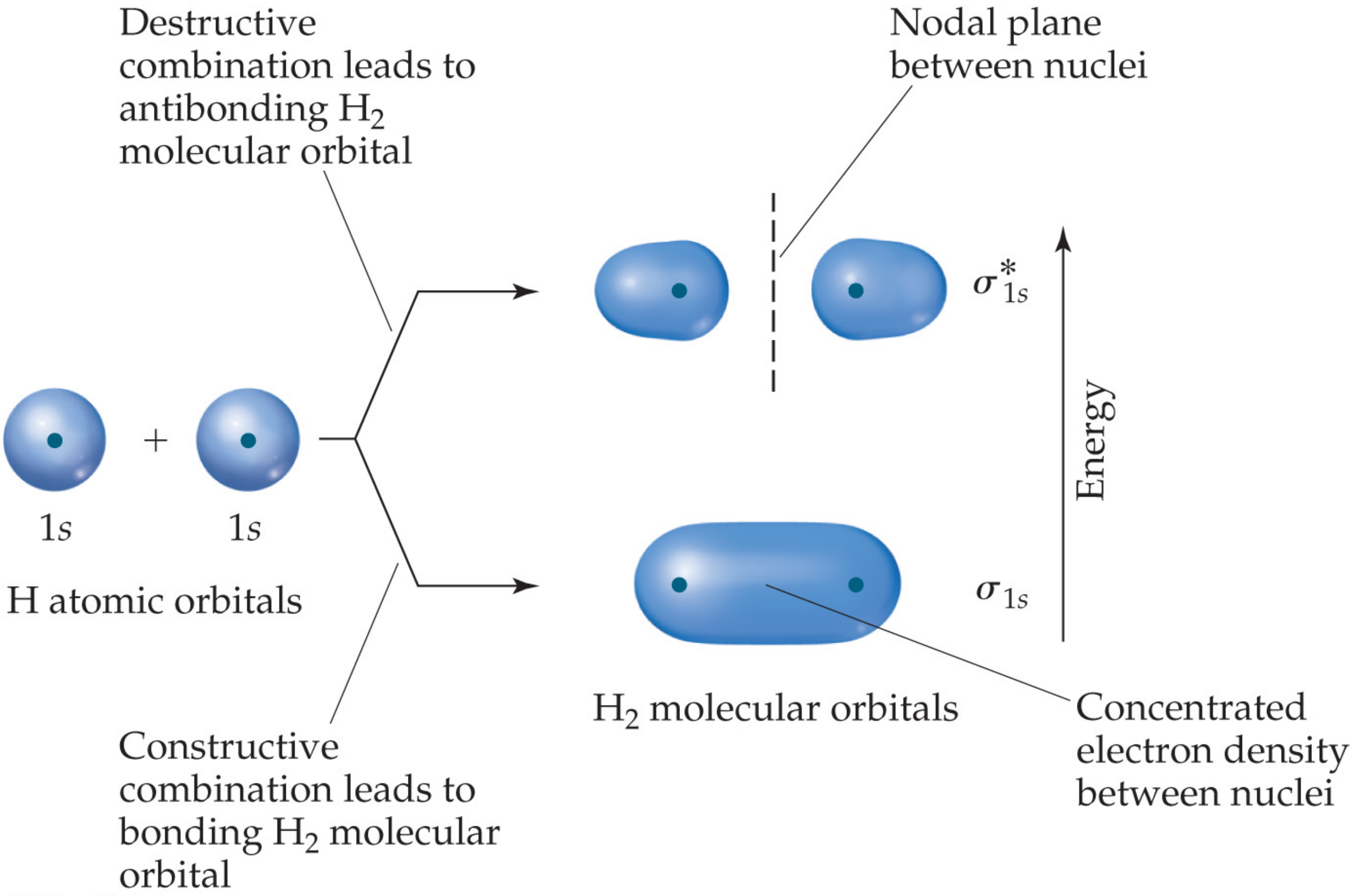
2) Antibonding MO

Subtract AOs - cancel each other in region between nuclei

Node between nuclei

- e^- density is zero

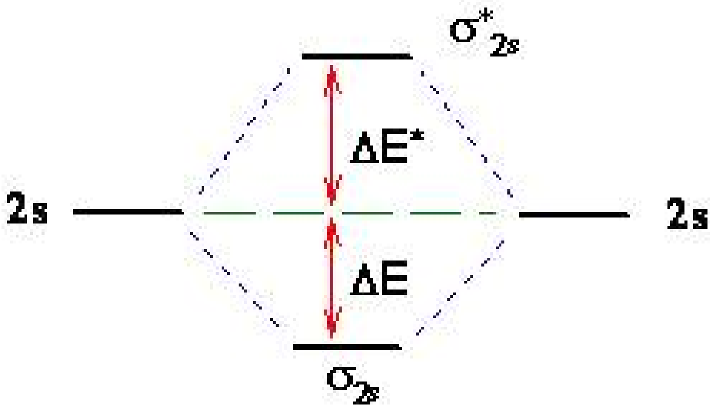
σ^*_{1s} → **signifies an anti-bonding MO**

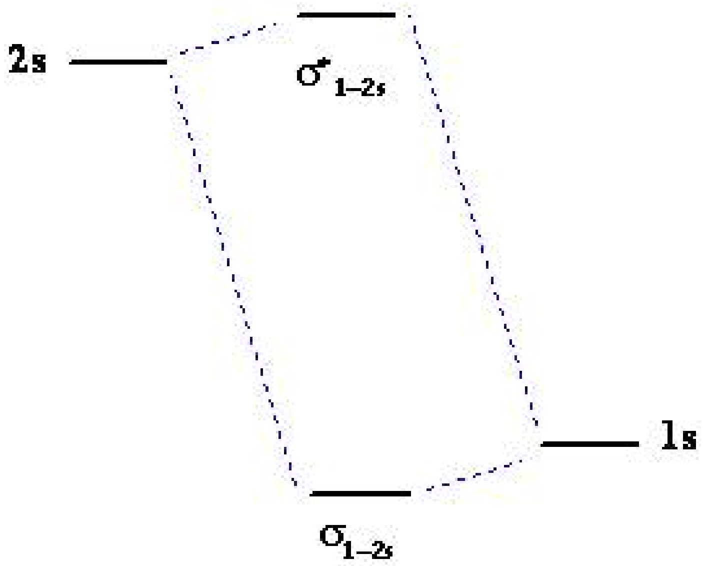

Destructive combination leads to antibonding H_2 molecular orbital
Nodal plane between nuclei
σ^*_{1s}
$1s$
+
$1s$
H atomic orbitals
Energy
σ_{1s}
H_2 molecular orbitals
Concentrated electron density between nuclei
Constructive combination leads to bonding H_2 molecular orbital

3) Effectiveness of Overlap & Mixing

a) How well two AOs overlap & mix depends on type of orb. (s vs. p or σ vs. π) & their relative energy

- closer in energy, better overlap

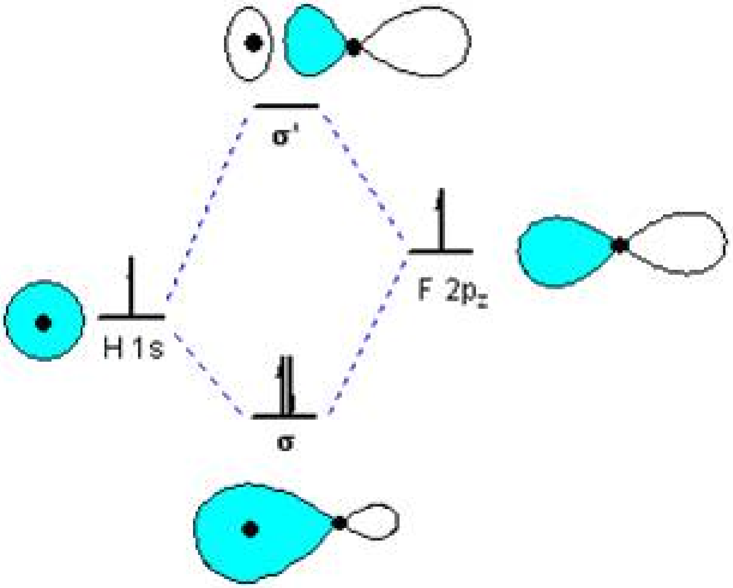




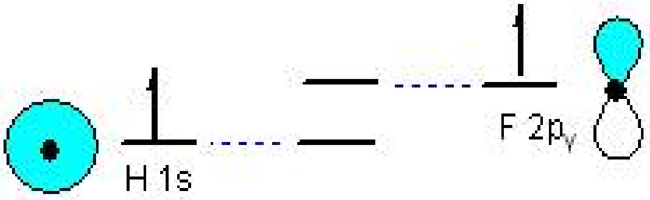
Note: $\Delta E^* > \Delta E$

b) The orbitals must have correct phases to overlap

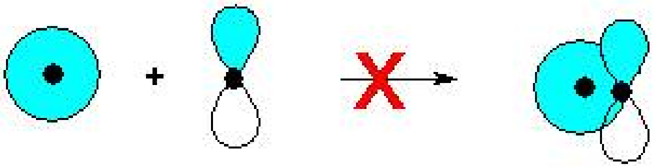
This is bonding combination, the H & F atoms on the z-axis, the $2p_z$ AO on F overlaps w. the H 1s to form the bonding & anti-bonding MOs



These orbitals do not have correct symmetry/phase to overlap so these AOs will not interact to form the MOs



Why not $2p_y$?



B) MOs formed from p AOs

1) σ MOs

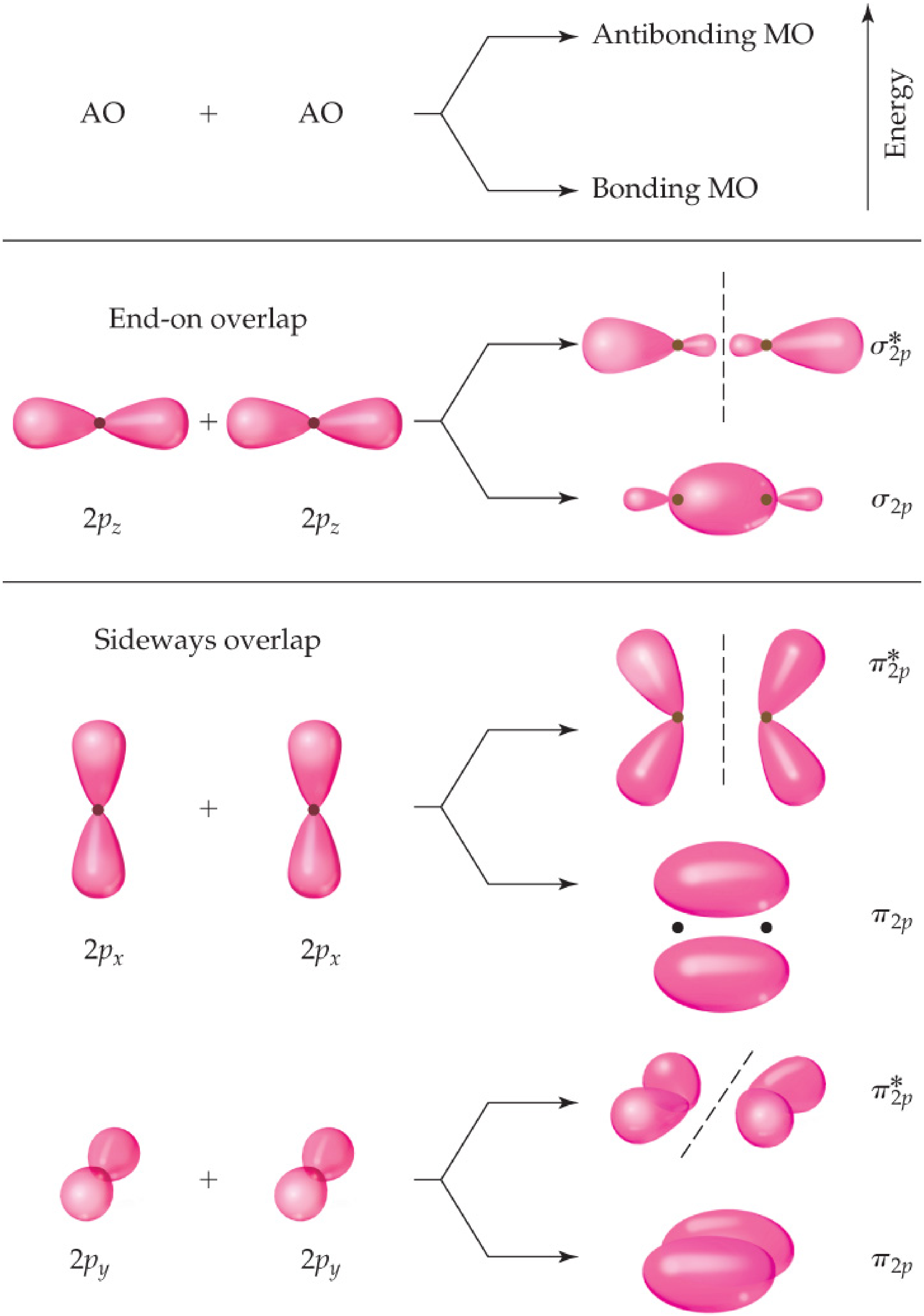
1 set of 2p AOs ($2p_z$) overlap end-to-end (head on)

$\boldsymbol{\sigma}_{2p}$ & $\boldsymbol{\sigma}_{2p}{}^{*}$

2) π MOs

Other 2 sets ($2p_x$ & $2p_y$) of parallel 2p AOs overlap sideways

2 $\boldsymbol{\pi}_{2p}$ & 2 $\boldsymbol{\pi}_{2p}{}^{*}$


AO + AO
Antibonding MO
Bonding MO
Energy
End-on overlap
$2p_z$ + $2p_z$
σ^*_{2p}
σ_{2p}
Sideways overlap
$2p_x$ + $2p_x$
π^*_{2p}
π_{2p}
$2p_y$ + $2p_y$
π^*_{2p}
π_{2p}

C) MO Energy-Level Diagrams, Electron Config. & Orbital Diagrams

1) Rules for Determining MO Diag.

a) # MOs formed = # AOs combined

b) AOs combine by both "in-phase" (addition) & "out-of-phase" (subtraction) interactions

c) AOs of similar energy combine most effectively

d) The more effectively AOs overlap the larger the energy diff. between the MOs

e) AOs may not form MOs if there is no other orbital for it to interact with (these are nbe$^-$ or lpe$^-$)

f) Only occupied MOs affect the E of the molecule

g) Pauli Exclusion Principle & Hund's Rule are obeyed

2) Period 1: Homonuclear Diatomics

a) electron configuration

$$(\sigma_{1s})^{nb}\ (\sigma_{1s}{}^{*})^{na}$$

nb = # bonding e^-
na = # anti-bonding e^-

b) Bond Order

bonds which exist between atoms

$$\text{B.O.} = \tfrac{1}{2}\,(nb - na)$$

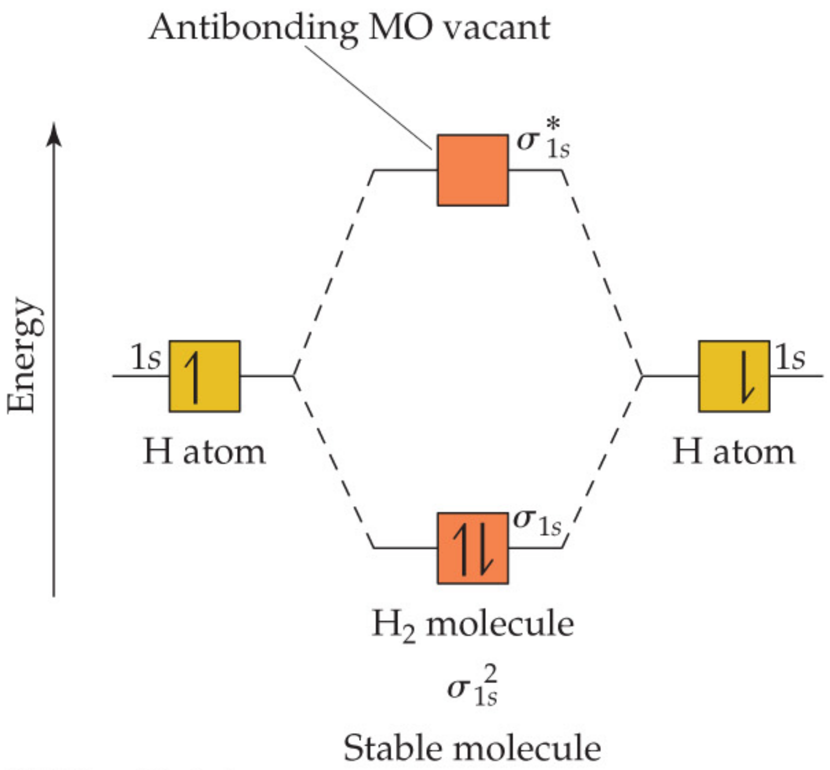
c) Bond Energy

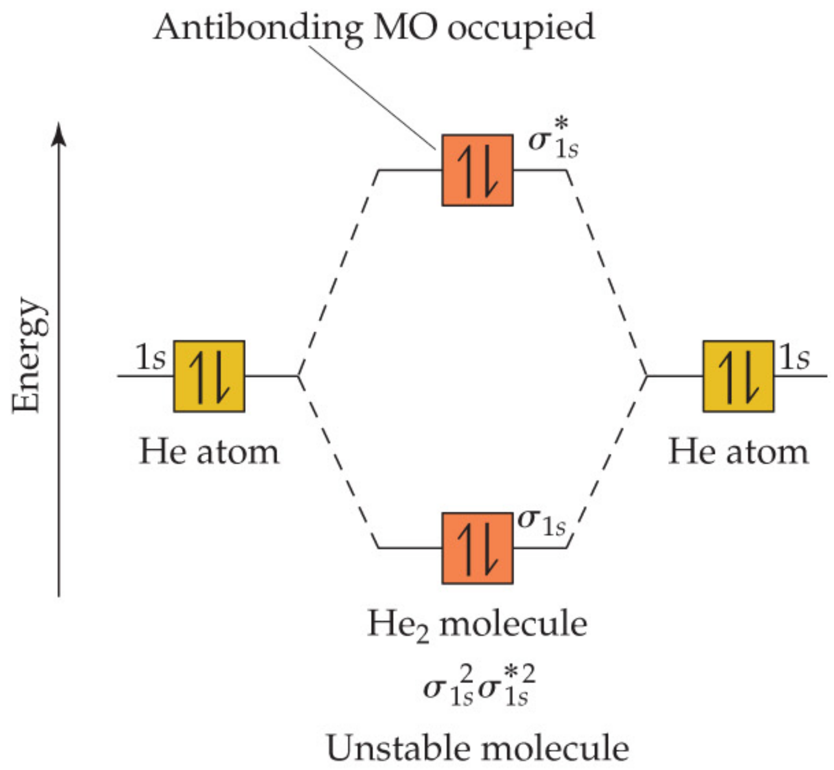
Energy necessary to break
1 mole of bonds

measure of bond strength
& stability

B.O.	type of bond	bond length	bond energy
0	unstable	—	—
1	single	Dec.	Inc.
2	double	↓	↓
3	triple	↓	↓

d) H_2 and He_2





(   )

(   ) (   )

B.O. =

B.O. =

e) He_2^+

3) Period 2 : Homonuclear Diatomics

a) “core” MOs

1s AOs ⟶ σ_{1s} & σ_{1s}^*

- do NOT overlap effectively
- remain mostly like the 1s AOs on atoms
- contribute almost nothing to bonding

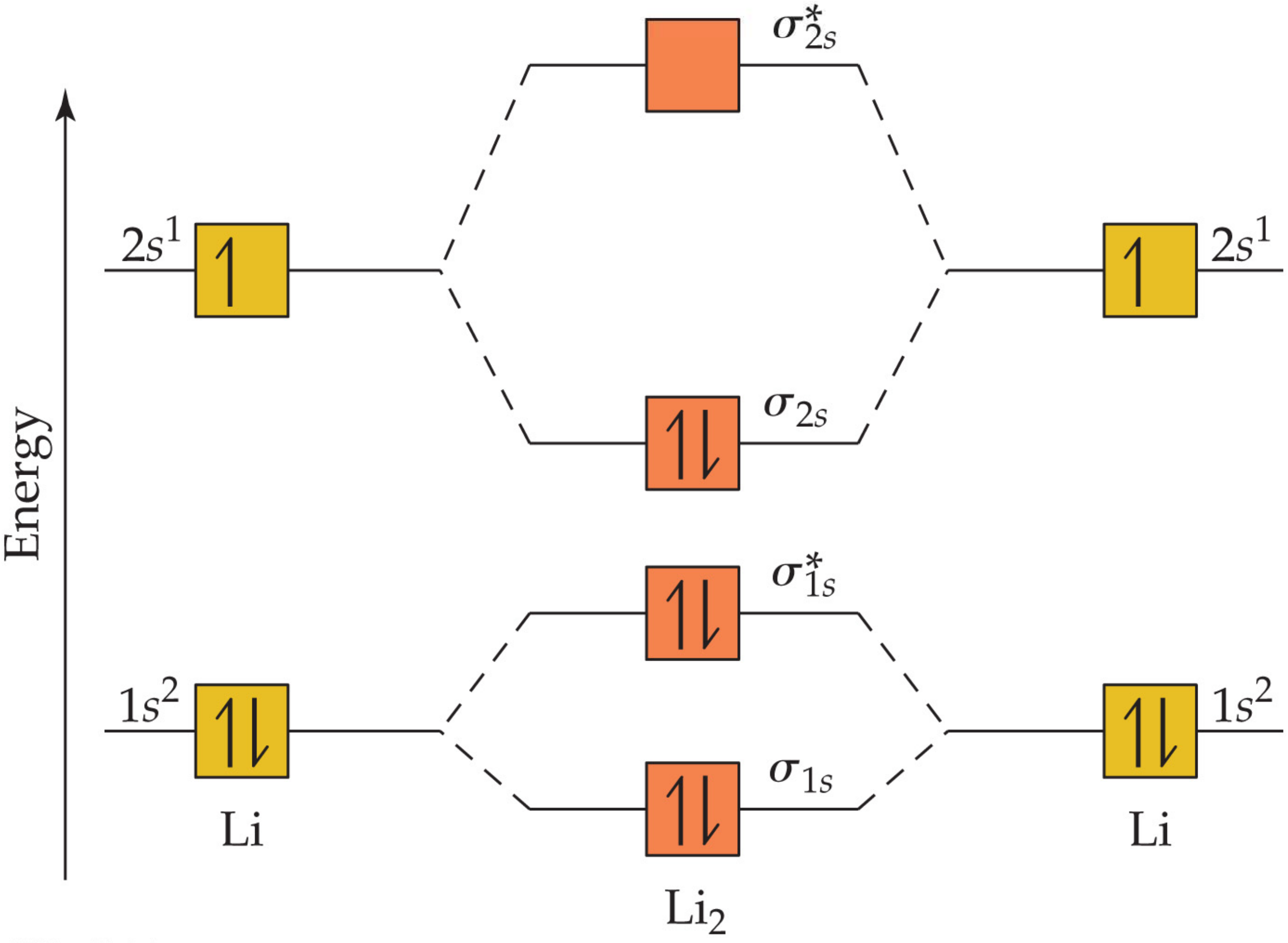
b) “Valence” MOs

2s AOs ⟶ σ_{2s} & σ_{2s}^*

overlap effectively

valence AOs combine to give “valence” MOs

c) Li_2 : 6 e^- total



full e^- config. :

shorthand :

B.O. =

d) Be_2 : 8 e^- total

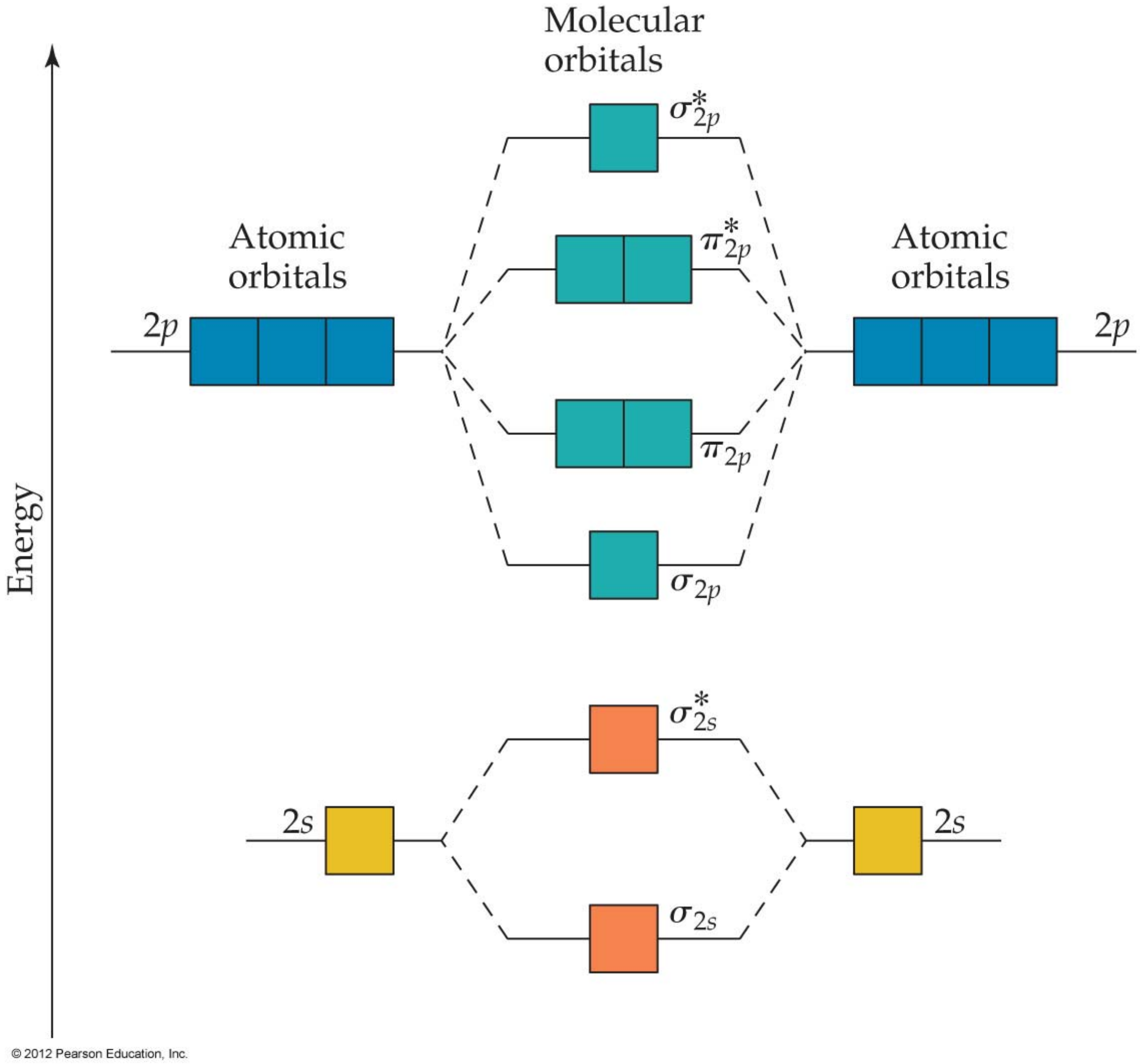
full e^- config. :

shorthand :

B.O. =

4) Period 2 : O_2 - Ne_2

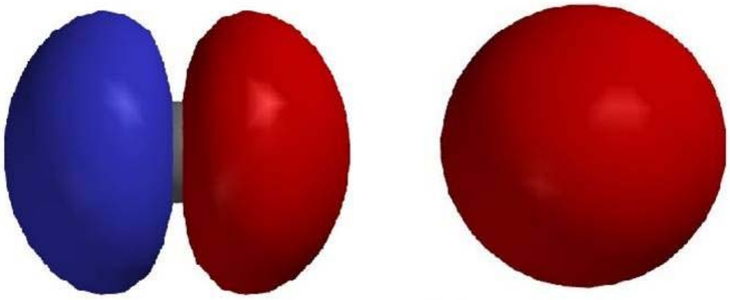
The following is expected based on σ bonds being stronger than π bonds and applies to O_2 - Ne_2 with no mixing (interaction) of 2s orbital on one atom w. 2p on other atom.



Orbital Diagram 1 (OD1)

5) Period 2 : B_2 - N_2

s - p mixing: can occur between the 2s and 2p_z as they have the correct symmetry

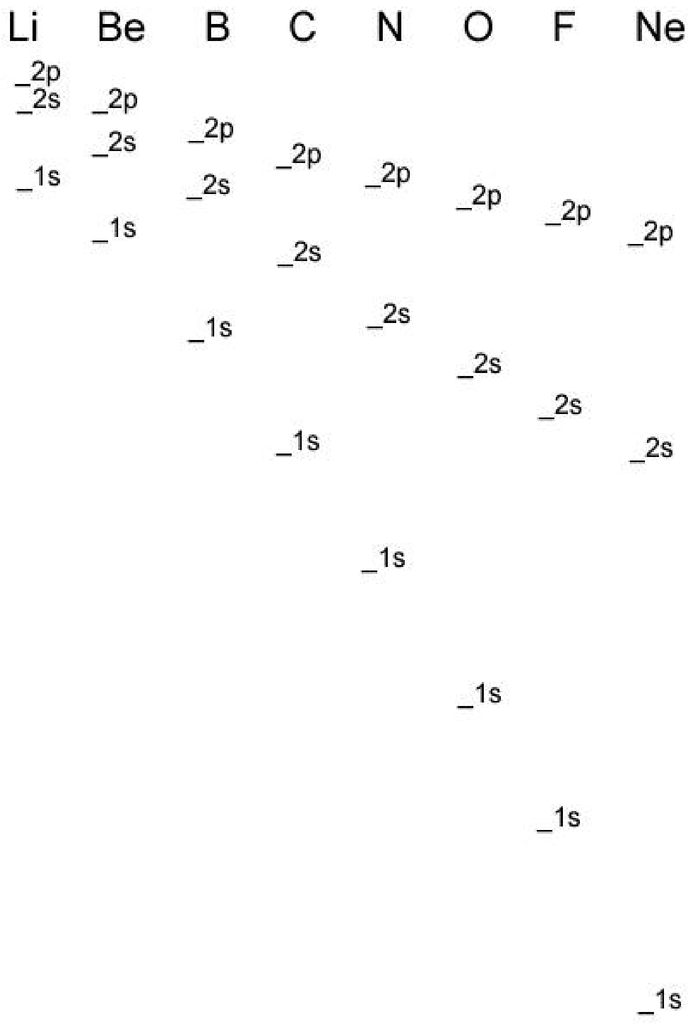


This depends on energy gap between the 2s & 2p_z AOs

Energy of AOs for 2nd row elements

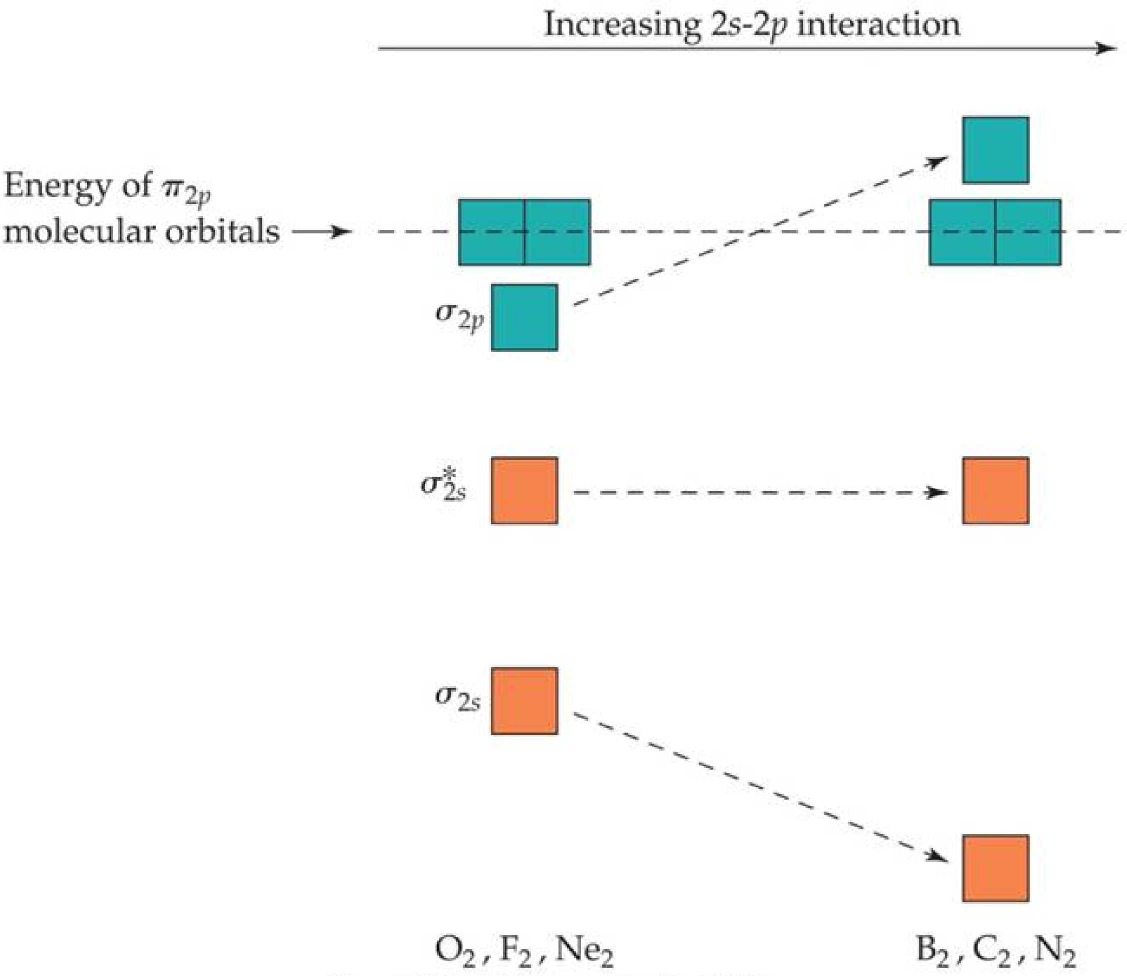
Element	E 2_s	E 2_p	E 2_p – E 2_s
Li	-521		
Be	-897		
B	-1350	-801	549
C	-1871	-1022	849
N	-2470	-1274	1196
O	-3116	-1524	1592
F	-3879	-1795	2084
Ne	-4680	-2084	2596

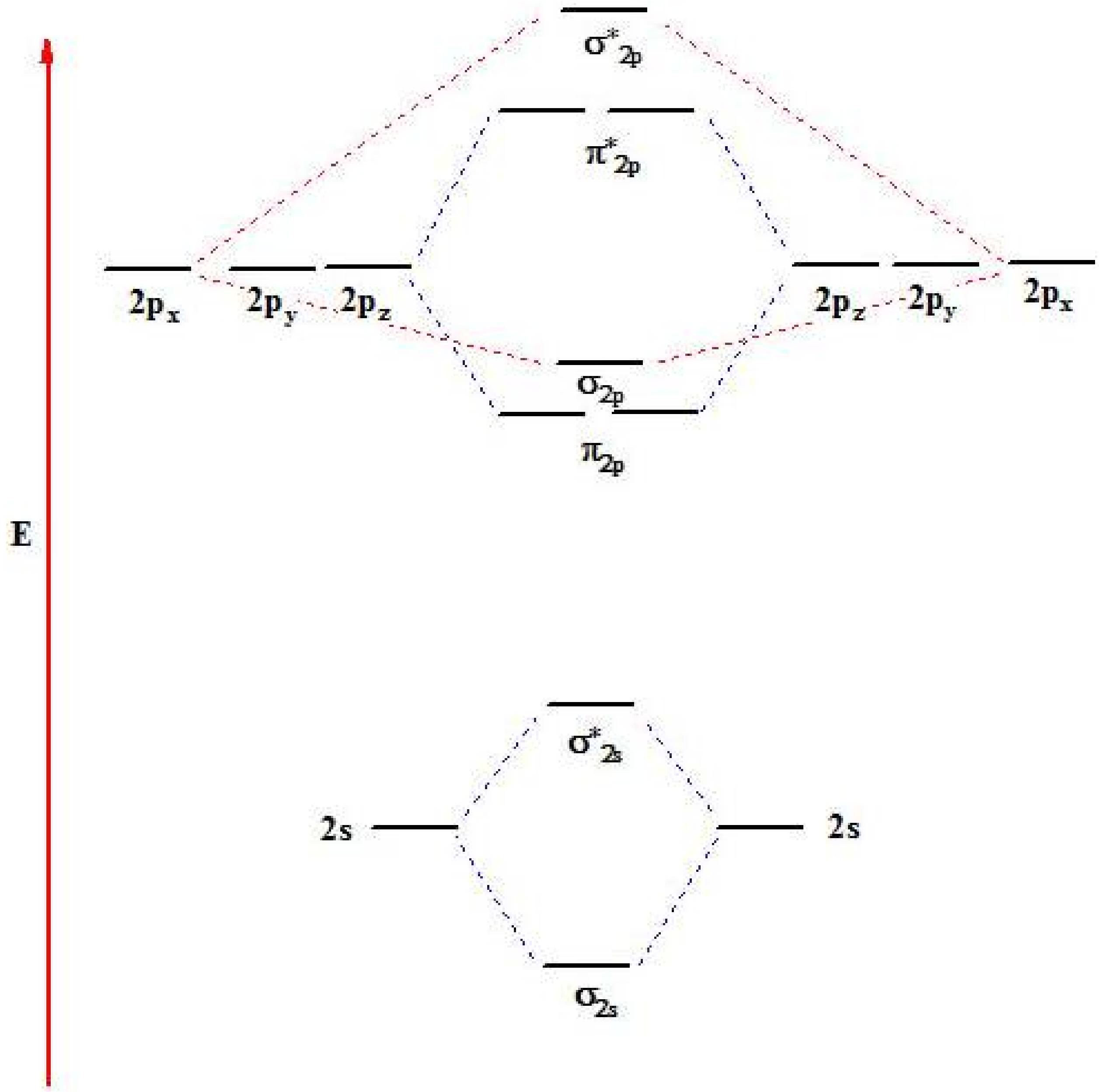
As can be seen in the figure below, the energies of the orb. change for each element. The gap between the 2s & 2p inc. as you go across the period. This means the energy gap is too large for s – p mixing to occur for O, F & Ne, but the gap is small enough for mixing to occur for B, C & N. This will affect the relative energy of MOs formed.



The MO diagram for B_2 - N_2 is diff. s - p mixing allows the σ_{2s} and σ_{2p} to interact, lowering the energy of the σ_{2s} & raising the energy of the σ_{2p}.

Note: has no effect on energies of the π and π^* MOs.



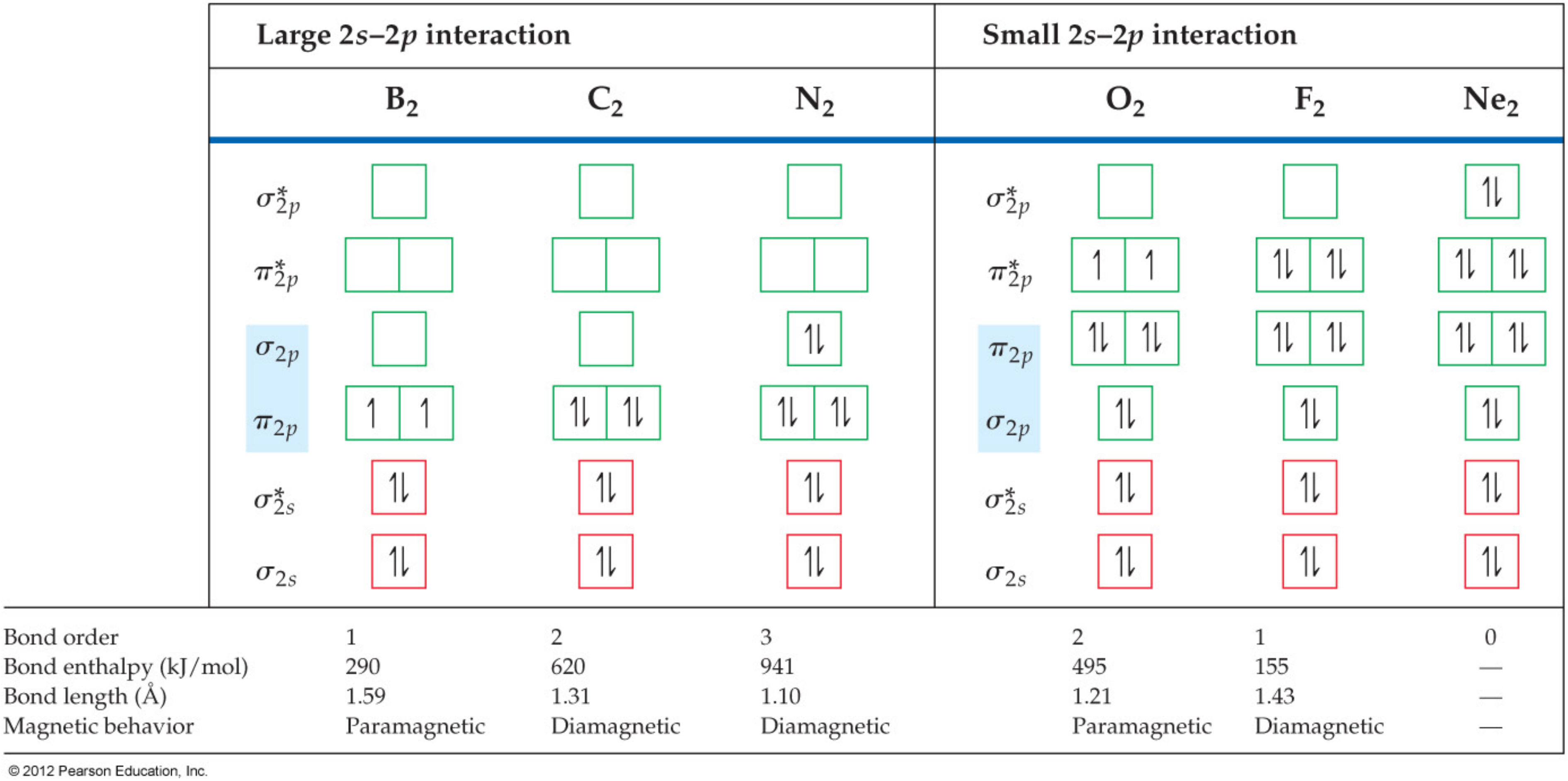


Orbital Diagram 2 (OD2)

The σ_{2p} and π_{2p} have switched order due to σ_{2s} and σ_{2p} interaction

2nd Row Diatomic Elements

MO Diagrams



Large 2*s*–2*p* interaction	B_2	C_2	N_2
σ^*_{2p}			
π^*_{2p}			
σ_{2p}			↿⇂
π_{2p}	↿ ↿	↿⇂ ↿⇂	↿⇂ ↿⇂
σ^*_{2s}	↿⇂	↿⇂	↿⇂
σ_{2s}	↿⇂	↿⇂	↿⇂

Small 2*s*–2*p* interaction	O_2	F_2	Ne_2
σ^*_{2p}			↿⇂
π^*_{2p}	↿ ↿	↿⇂ ↿⇂	↿⇂ ↿⇂
π_{2p}	↿⇂ ↿⇂	↿⇂ ↿⇂	↿⇂ ↿⇂
σ_{2p}	↿⇂	↿⇂	↿⇂
σ^*_{2s}	↿⇂	↿⇂	↿⇂
σ_{2s}	↿⇂	↿⇂	↿⇂

	B_2	C_2	N_2	O_2	F_2	Ne_2
Bond order	1	2	3	2	1	0
Bond enthalpy (kJ/mol)	290	620	941	495	155	—
Bond length (Å)	1.59	1.31	1.10	1.21	1.43	—
Magnetic behavior	Paramagnetic	Diamagnetic	Diamagnetic	Paramagnetic	Diamagnetic	—

a) Electron Config.

1) H_2 - N_2

$$(\sigma_{1s})^2(\sigma_{1s})^2(\sigma_{2s})^2(\sigma_{2s}*)^2(\pi_{2p})^4(\sigma_{2p})^2(\pi_{2p}*)^4(\sigma_{2p}*)^2$$

Shorthand Notation for 2nd Period

- use valence e^- only

$$KK\ (\sigma_{2s})^2(\sigma_{2s}*)^2(\pi_{2p})^4(\sigma_{2p})^2(\pi_{2p}*)^4(\sigma_{2p}*)^2$$

2) O_2 - Ne_2

$$KK\ (\sigma_{2s})^2(\sigma_{2s}*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}*)^4(\sigma_{2p}*)^2$$

3) Ex: O_2

12 valence e^-

6) Period 2 : Heteronuclear Diatomics

AOs of more electronegative element are lower in energy

Bonding MOs tend to be more like AOs of more EN element

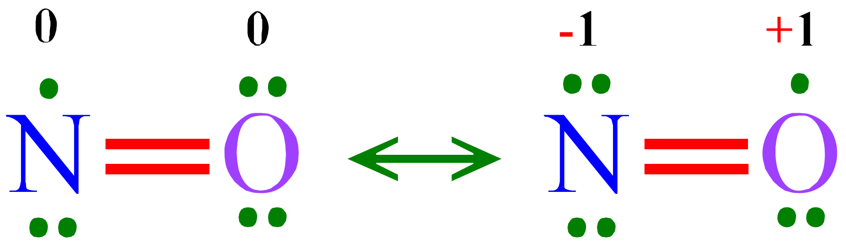
MO will have a greater contribution from the AO closest in energy

smaller ΔE ⇨ more orb. overlap ⇨ greater covalent character

greater ΔE ⇨ more polar bond ⇨ greater ionic character

A) nitric oxide, NO

Two possible Lewis Struct.

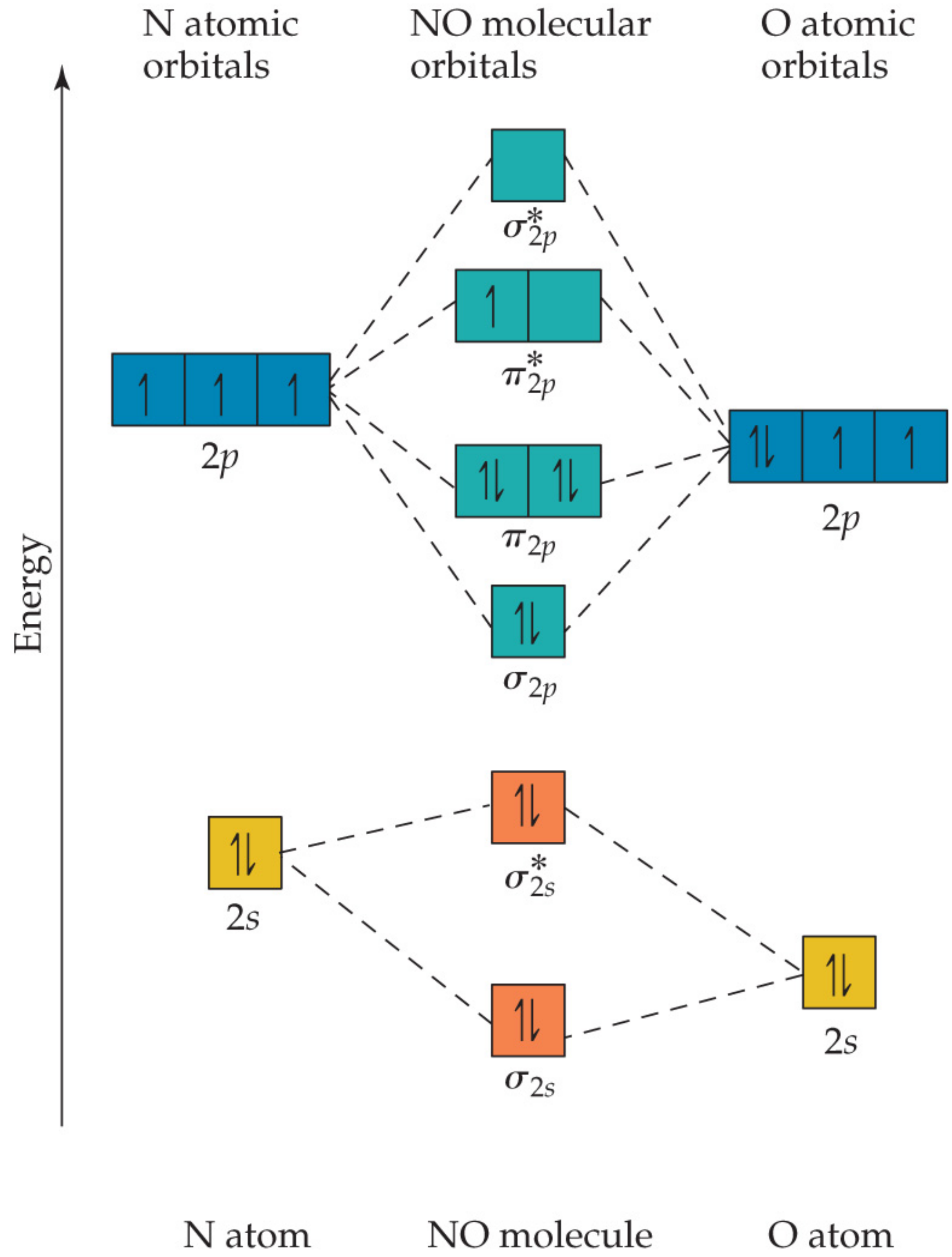


LS on left is the better struct.

Both show double bond

Bond length of 1.15 Å

- close to that in N_2
- implies bond between double and triple bond


N atomic orbitals
NO molecular orbitals
O atomic orbitals
Energy
σ^*_{2p}
π^*_{2p}
π_{2p}
σ_{2p}
σ^*_{2s}
σ_{2s}
2p
2s
2p
2s
N atom
NO molecule
O atom

B.O. =

7) MO Theory Summary

MOs are linear combinations of AOs

MOs can span multiple atoms

Best theory:

- delocalization not a problem
- excited states not a problem
- describes things like O_2 correctly