Chapter 10: Chemical bonding II: Molecular shapes and bonding

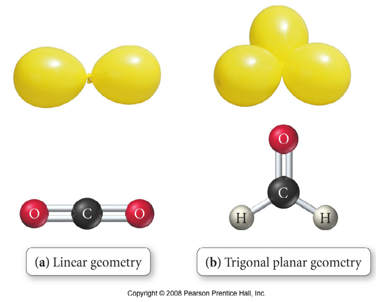
VSEPR Theory: Valence shell electron pair repulsion

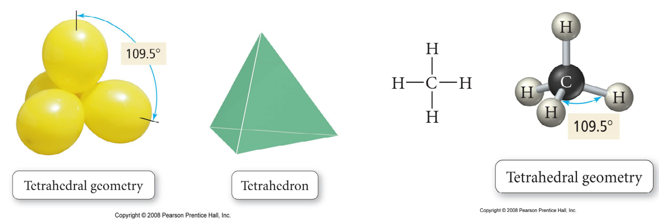
- Electron groups repel one another through coulombic forces
- They will spread as far apart as possible on a molecule's central atom
- 1 electron group:
  - 1 single bond
  - 1 double bond
  - 1 triple bond
  - 1 lone (unshared) pair of electrons

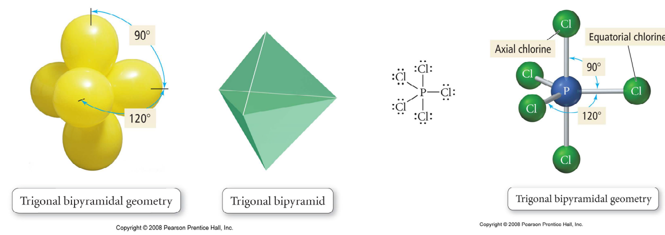
The five major electron group geometries:

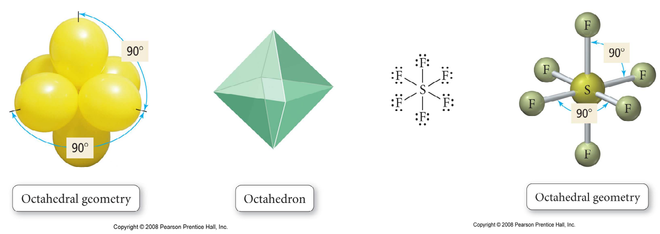
# e^- groups	Geometry	Structure	Ideal bond angle
2	Linear		
3	Trigonal planar		
4	Tetrahedral		
5	Trigonal bipyramidal		
6	Octahedral		

Electron group geometries









Lone pairs and molecular geometry

Electron group geometry is the arrangement of the electron groups

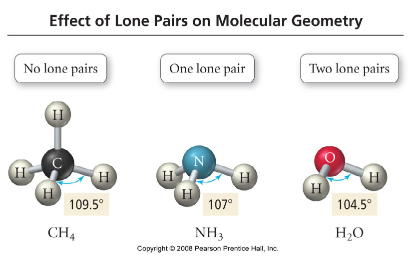
Molecular geometry is the arrangement of the atoms

These are the same if only **bonding** electron groups are attached to the central atom.

Nonbonding electrons (lone pairs) on the central atom will change the **molecular geometry**.

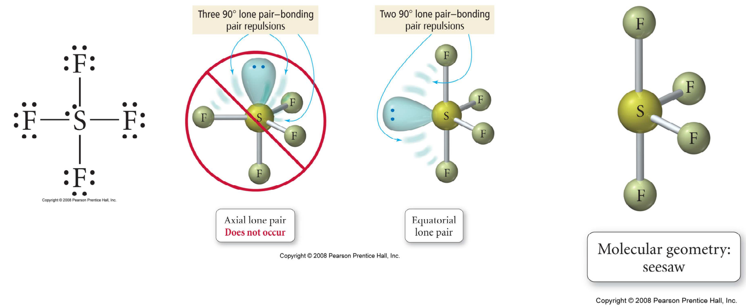
	# e^- groups	# lone pairs	e^- group geom.	molec. geom.	structure
CH_4					
NH_3					
H_2O					

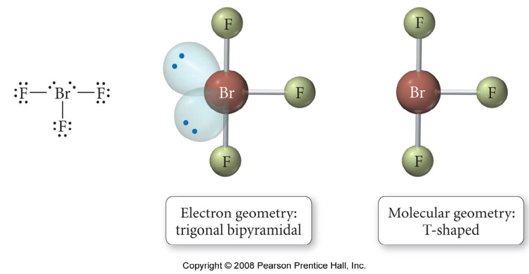
Lone pairs will actually repel the bonds a little more than a bond would, decreasing bond angles slightly.

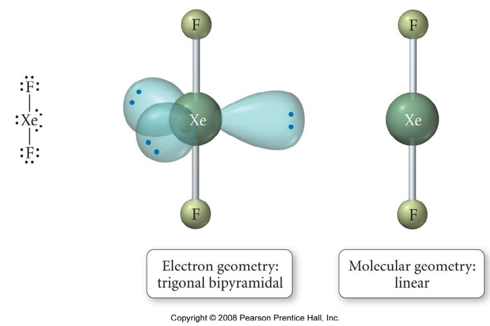


5 electron groups with lone pairs

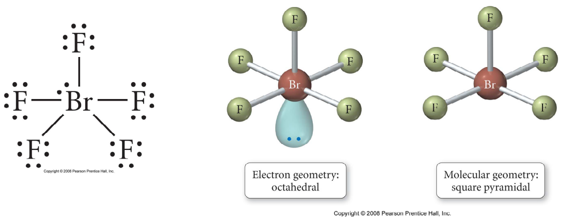
Lone pairs will **only** be placed in equatorial positions in the trigonal bipyramidal electron group geometry.



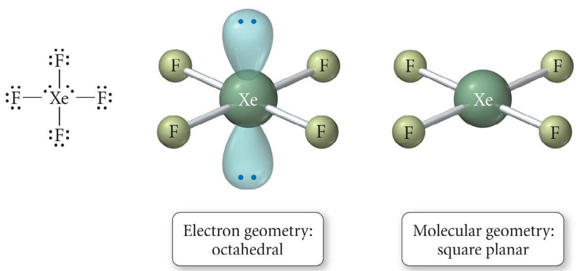




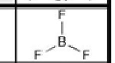
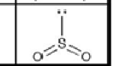
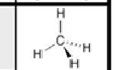
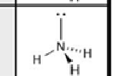
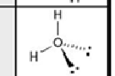
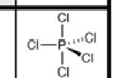
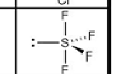
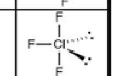
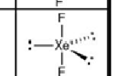
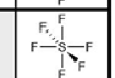
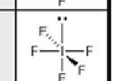
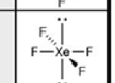
6 electron groups with lone pairs



Two lone pairs in an octahedral electron group geometry will add across from each other to minimize lone pair-lone par repulsions.



Geometries summary

Electron groups	Bonding groups	Nonbonding groups	Molecule shape	Example	Drawing
2	2	0	Linear	BeF_2	
3	3	0	Trigonal planar	BF_3	
	2	1	Bent	SO_2	
4	4	0	Tetrahedral	CH_4	
	3	1	Trigonal pyramid	NH_3	
	2	2	Bent	H_2O	
5	5	0	Trigonal bipyramid	PCl_5	
	4	1	Seesaw	SF_4	
	3	2	T-shaped	ClF_3	
	2	3	Linear	XeF_2	
6	6	0	Octahedral	SF_6	
	5	1	Square pyramid	IF_5	
	4	2	Square planar	XeF4	

Geometry practice

What is the electron group and molecular geometry of IBr_5? Draw its flat Lewis structure and its 3-dimensional structure.

What is the electron group and molecular geometry of ICl_2^-? Draw its flat Lewis structure and its 3-dimensional structure.

Molecular shape and polarity

The dipoles of polar bonds will add together geometrically to form a **net dipole moment** for the molecule. Molecules with a net dipole moment are **polar**.

H_2O:

CO_2:

BF_3:

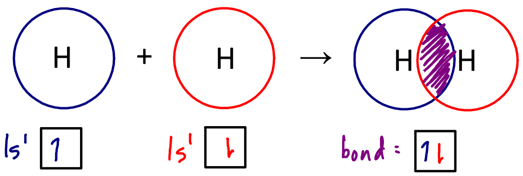
CH_2F_2:

CO_3^{2-}:

Valence bond theory

In valence bond theory, bonds are formed by the orbitals of two atoms overlapping.

$$H\cdot + \cdot H \rightarrow H{-}H$$



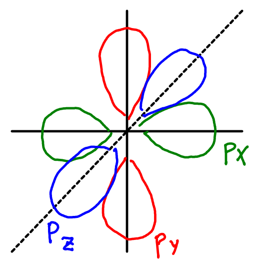
But, many times the orbitals cannot combine as-is.

$$4\,H\cdot + \cdot\dot{\underset{\cdot}{C}}\cdot \rightarrow CH_4$$

C: ☐ ☐☐☐

2s 2p

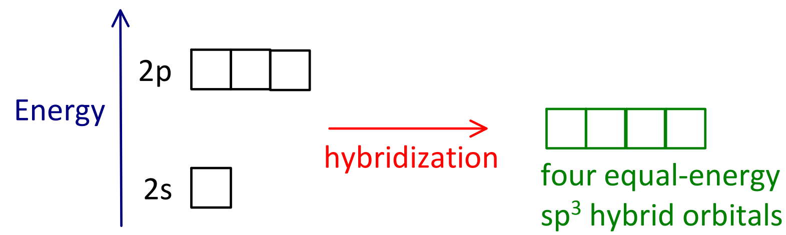
Remember, p orbitals are oriented on the *x*, *y*, and *z* axes:



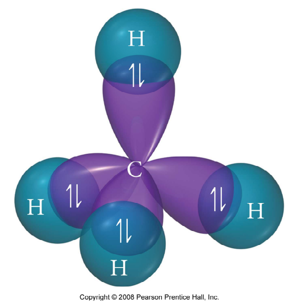
Using VSPER, what is the shape of the CH_4 molecule?

sp^3 hybrid orbitals

The one s and three p orbitals in carbon's valence shell combine together into 4 equivalent **hybrid orbitals** so carbon can make 4 bonds.



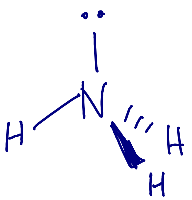
According to VSEPR, four equivalent hybrid orbitals (each containing one electron group) will best fit around a central atom with a _______________ geometry.



Any time there's a ________________ electron group geometry, the hybridization of the central atom is _____.

sp^3 hybrid orbitals

NH_3: electron group geometry:
molecular geometry:
electron groups on central atom:



(The number of electron groups on the central atom is the number of hybrid orbitals that need to be formed!)

Energy

2p

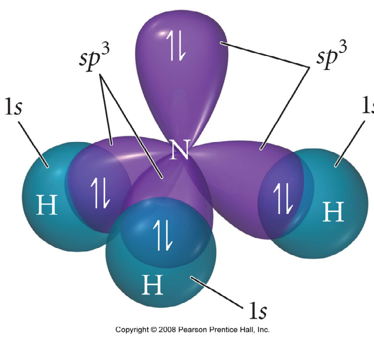
2s

N

hybridization

sp^3 hybrid orbitals

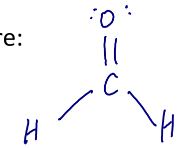
(three unpaired electrons to form bonds, and one lone pair!)



sp^2 hybrid orbitals

CH_2O: # electron groups on central atom:
hybrid orbitals to be formed:

CH_2O Lewis structure:



Energy

2p

2s

C
(central atom)

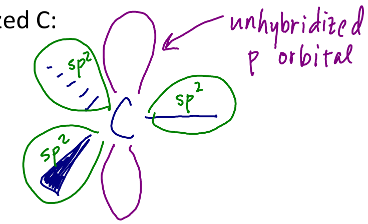
hybridization

one unhybridized p orbital

three equal-energy sp^2 hybrid orbitals

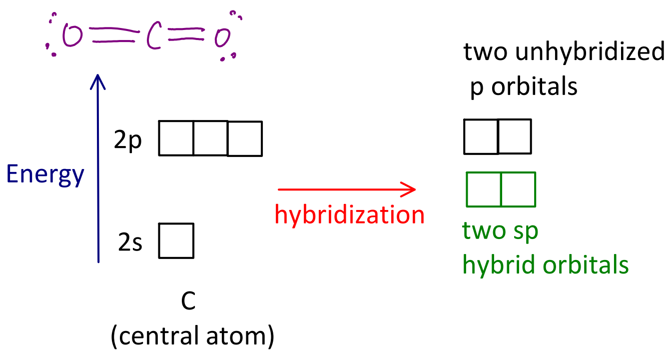
The three sp^2 hybrid orbitals will be ________________ in shape. The unhybridized p orbital is perpendicular.

sp^2 hybridized C:



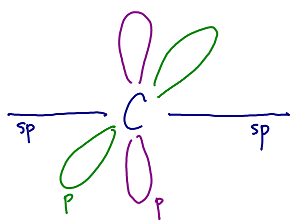
sp hybridization

CO_2: 2 electron groups around C, so 2 hybrid orbitals



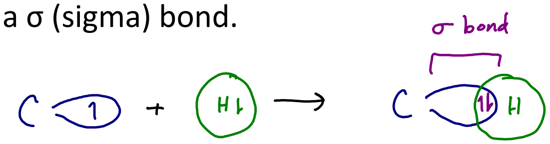
An sp hybridized central atom will be _________ in shape.

sp hybridized C:

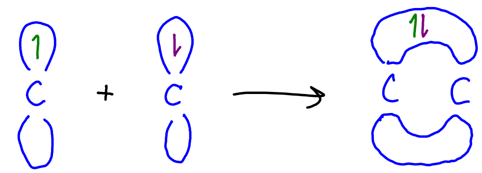


σ and π bonds

The bonds in valence bond theory are classified by their positions relative to the two bonding atoms. If two half-filled orbitals combine straight between the two atoms, it's called a σ (sigma) bond.

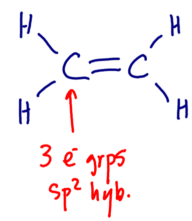


When two half-filled p orbitals combine side-by-side, it's called a π (pi) bond.



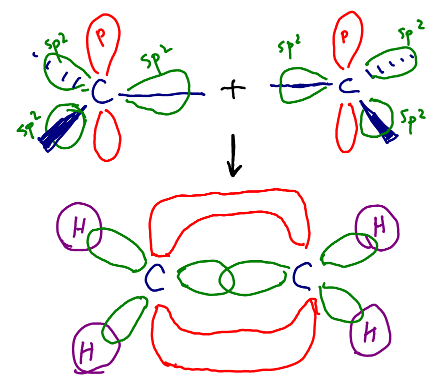
A **single bond** from Lewis theory like the C–H bonds in CH_4 is made of a single σ (sigma) bond.

A **double bond** from Lewis theory like the C=C bond in C_2H_4 is formed by one σ bond and one π bond.



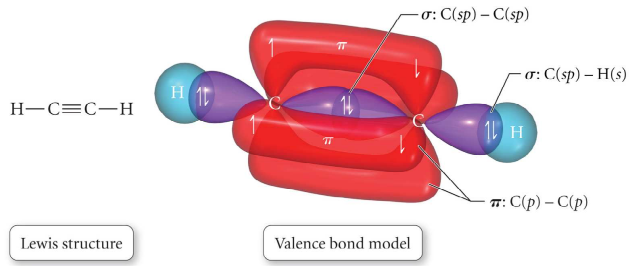
how many σ ?

how many π ?



σ and π bonds

If an atom is sp hybridized, it has 2 hybrid orbitals and 2 unhybridized p orbitals.



Summary of σ and π bonding:

Bond type:	Lewis:	Valence bond theory:
Single	—	___ σ, ___ π
Double	$=$	___ σ, ___ π
Triple	$\equiv$	___ σ, ___ π

Summary of hybrid orbitals

# of electron groups on central atom	hybridization	unhybridized p orbitals
4		
3		
2		