

WILEY

Chapter 9
Theories of Bonding and
Structure

Chemistry, 7th Edition
International Student Version
Brady/Jespersen/Hyslop

Chapter in Context

- Learn to draw the five basic molecular geometries
- Use the VSEPR model to predict the shape of molecules and ions
- Understand the influence of shape on the polarity (dipole moment) of molecules
- Explore how valence bond theory explains bonding
- Use hybridization to refine valence bond theory
- Use orbital diagrams and hybridization to describe the nature of multiple bonds
- Use orbital diagrams and hybridization to describe the nature of multiple bonds

Molecular Structures

- Molecules containing three or more atoms may have many different shapes
- Almost all are “3-dimensional”
- Shapes are made from **five basic geometrical structures**
- Shapes classified according to number of electron **domains** they contain around central atom

VSEPR Theory

Valence Shell Electron Pair Repulsion

- Simple model using the electron domain concept
- Two types of electron domains
 - **Bonding domains**
 - Electron pairs involved in bonds between two atoms
 - **Nonbonding domains**
 - Electron pairs associated with single atom
- All electrons in single, double, or triple bond considered to be in the **same** electron domain

VSEPR Theory

- Simple theory for predicting shapes of molecules

Fact

- Negative electrons repel each other very strongly

Result

- Electron pairs are arranged to be as far apart as possible
- Minimizes repulsions

Result

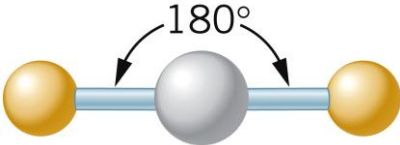
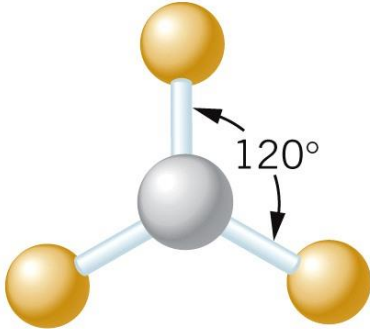
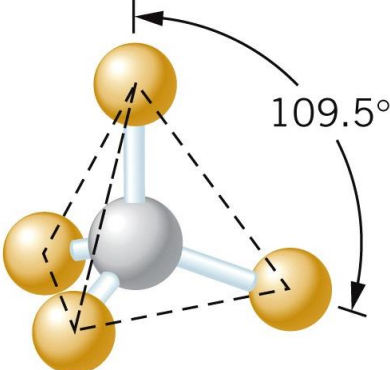
- Electron pairs are arranged to have lowest possible potential energy

VSEPR Theory

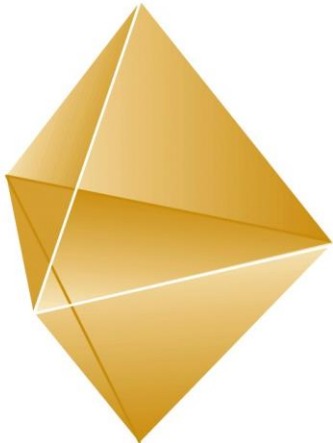
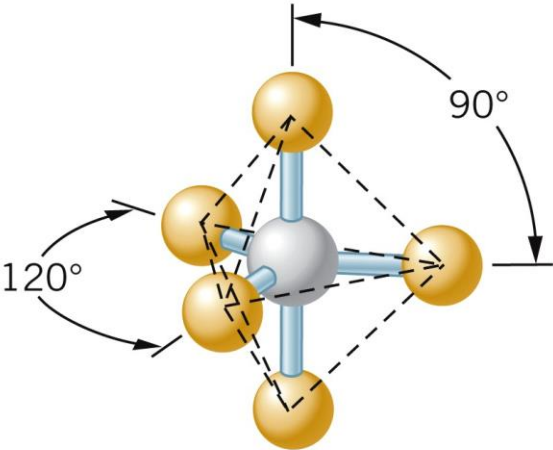
Assumes

- Bonds are shared pairs of electrons
 - Covalent bonds
- Central atom will have 2, 3, 4, 5, or 6 pairs of electrons in its valence shell
- Model includes central atoms with
 - Incomplete octet
 - Complete octet
 - Extended octet
- **Electron domains**
 - Lone electron pairs, single bonds, double bonds, and triple bonds all count as just one electron domain

Five Basic Electron Domains

Electron Domains	Shape	Electron Pair Geometry
2		linear
3		trigonal planar
4		tetrahedral

Five Basic Electron Domains (con't.)

Electron Domains	Shape	Electron Pair Geometry	
5	 <p data-bbox="397 1062 736 1100">A trigonal bipyramid</p>	 <p data-bbox="819 1062 1348 1100">A trigonal bipyramidal molecule</p>	<p data-bbox="1493 639 1870 782">trigonal bipyramidal</p> <p data-bbox="1470 815 1895 1033">has equatorial and axial positions.</p>

Five Basic Electron Domains (con't.)

**Electron
Domains**

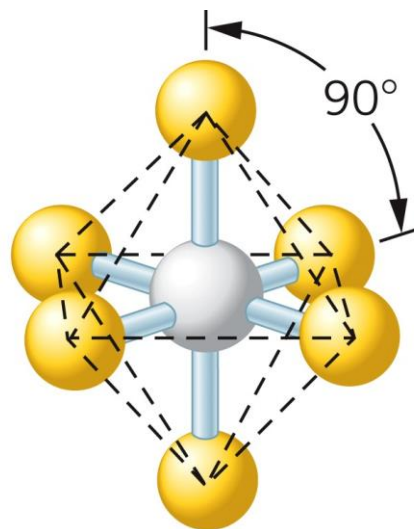
Shape

**Electron Pair
Geometry**

6



An octahedron



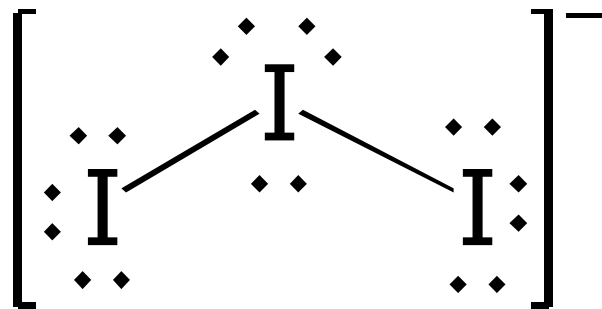
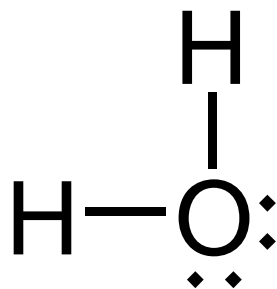
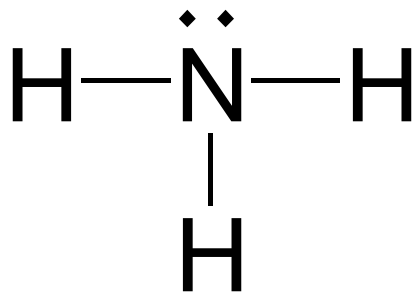
An octahedral molecule

octahedral
All positions
are equivalent

Learning Check

Identify, for each of the following:

1. Number of electron domains
2. Electron pair geometry



Your Turn!

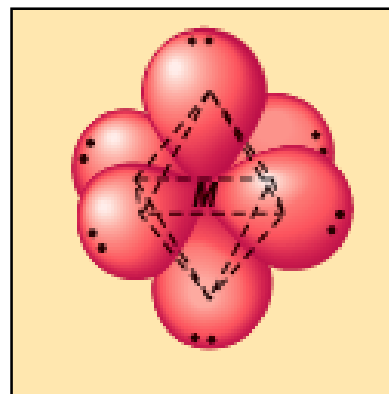
A central atom has two lone pair of electrons around it and two single bonds to other atoms. What is the electron pair geometry around the central atom?

- A. tetrahedron
- B. pentagon
- C. trigonal bipyramid
- D. square pyramid
- E. octahedron

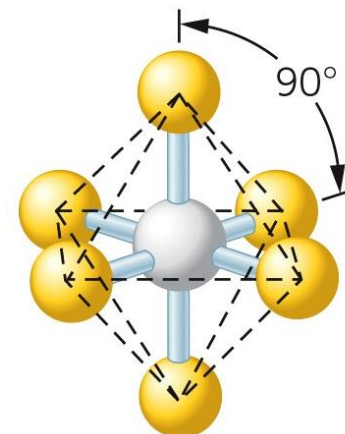
Your Turn!

- What is the electron pair geometry around an atom that has six electron domains?
- What are the angles between the electron pairs?
- Sketch it in a way that implies the three dimensionality of the structure.

- A. tetrahedron, 109.5°
- B. hexagon, 60° and 120°
- C. trigonal bipyramid, 120°
- D. square pyramid, 90°
- E. octahedron, 90°



or



Your Turn!

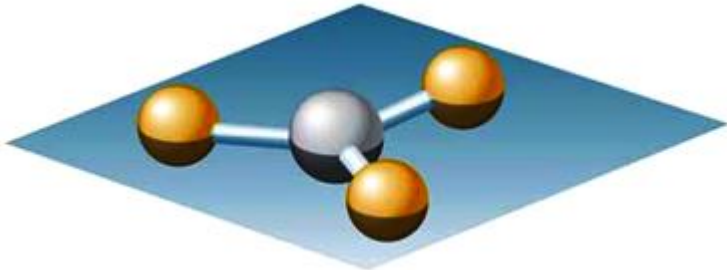
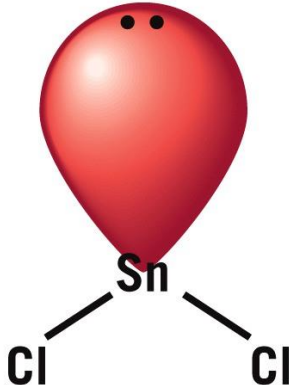
How many electron domains are there around the central atom in SF_4O ? What is the electron pair geometry for the compound?

- A. 4, tetrahedron
- B. 5, pentagon
- C. 5, trigonal bipyramid
- D. 4, square pyramid
- E. 6, octahedron

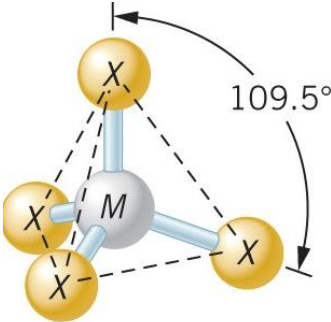
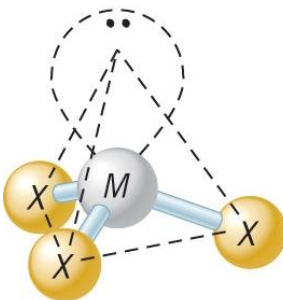
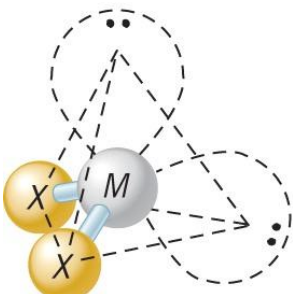
VSEPR (cont)

- **Shapes involving lone electron pairs**
 - **Lone pairs**
 - Take up more space around central atom
 - Effect overall geometry
 - Must be counted as electron domains
- **Shapes involving multiple bonds**
 - **Multiple bonds** (double and triple)
 - For purposes of molecular geometry
 - Treat as single electron domain
 - Same as single bonds

Structures Based on Three Electron Domains

Number of Bonding Domains	Number of Nonbonding Domains	Structure	Molecular Shape
3	0		<p>Planar Triangular (e.g., BCl_3) All bond angles 120°</p>
2	1		<p>Nonlinear Bent or V-shaped (e.g., SO_2) Bond $< 120^\circ$</p>

Four Electron Domains

Number of Bonding Domains	Number of Nonbonding Domains	Structure	Molecular Shape
4	0		Tetrahedron (e.g., CH ₄) All bond angles 109.5°
3	1		Trigonal pyramid (e.g., NH ₃) Bond angle less than 109.5°
2	2		Nonlinear, bent (e.g., H ₂ O) Bond angle less than 109.5°

Five Electron Domains

Number of
Bonding
Domains

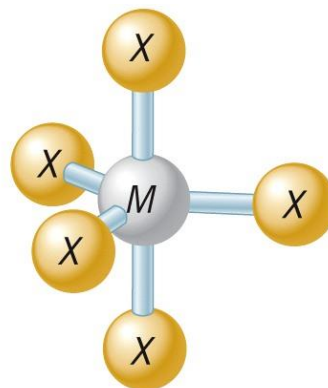
Number of
Nonbonding
Domains

Structure

Molecular Shape

5

0



Trigonal bipyramid

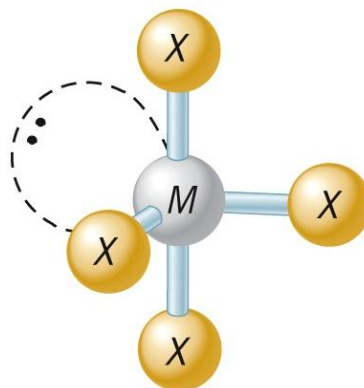
(**e.g.**, PF_5)

Ax-eq bond angles 90°

Eq-eq 120°

4

1



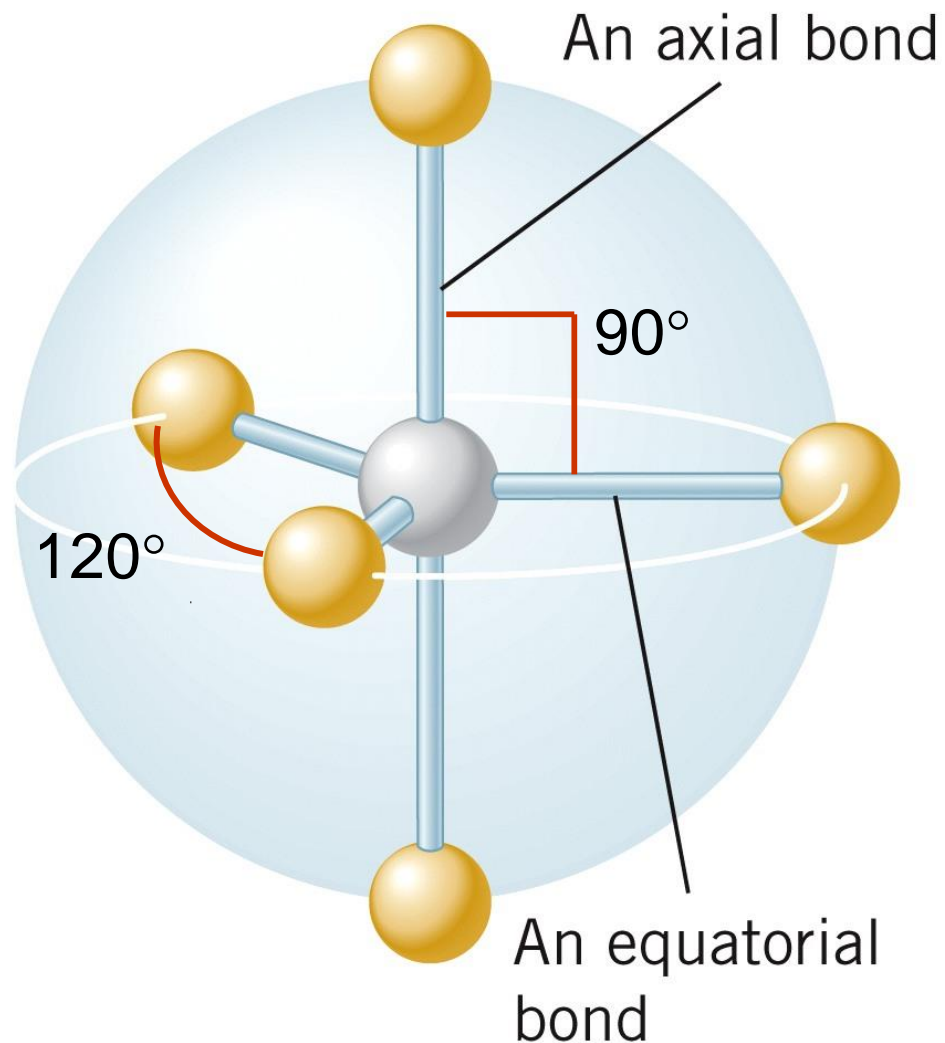
**Distorted
Tetrahedron, or
Seesaw**

(**e.g.**, SF_4)

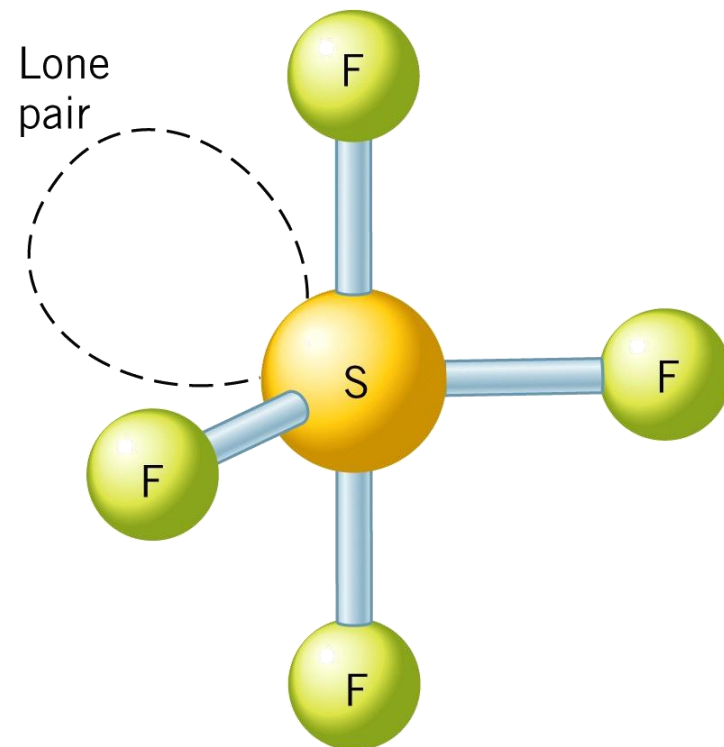
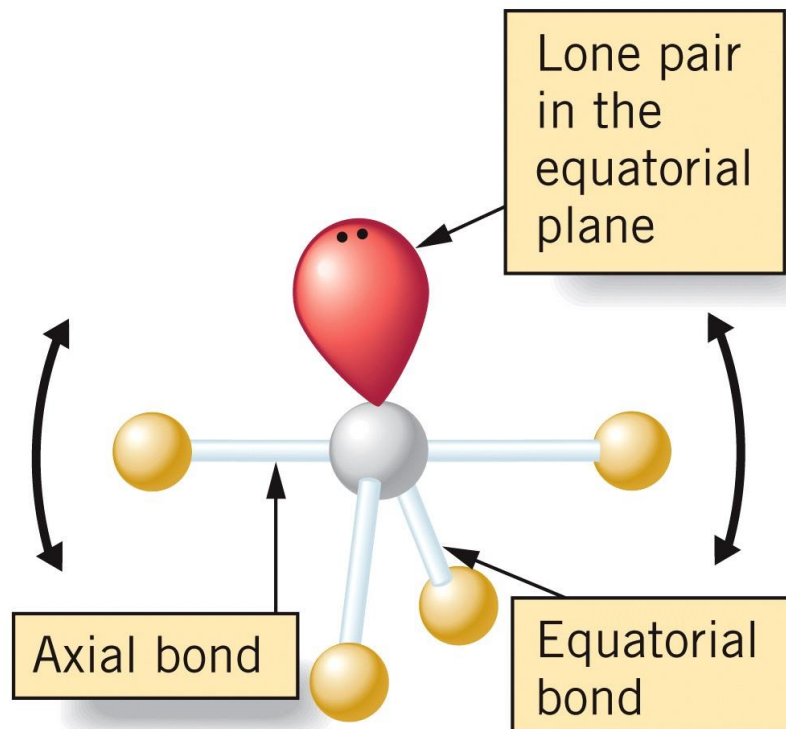
Ax-eq bond angles $< 90^\circ$

Trigonal Bipyramid

- Two atoms in axial position
 - 90° to atoms in equatorial plane
- Three atoms in equatorial position
 - 120° bond angle to atoms in axial position
 - More room here
 - Substitute here first



Where Do Lone Pairs Go?



The structure of SF₄

- Lone pair takes up more space
- Goes in equatorial plane
- Pushes bonding pairs out of way
- **Result:** distorted tetrahedron

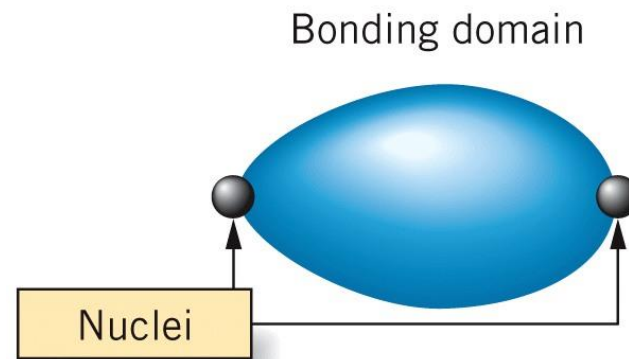
Five Electron Domains

Number of Bonding Domains	Number of Nonbonding Domains	Structure	Molecular Shape
3	2		<p>T-shape (e.g., ClF_3) Bond angles 90°</p>
2	3		<p>Linear (e.g., I_3^-) Bond angles 180°</p>

Relative Sizes of Electron Domains

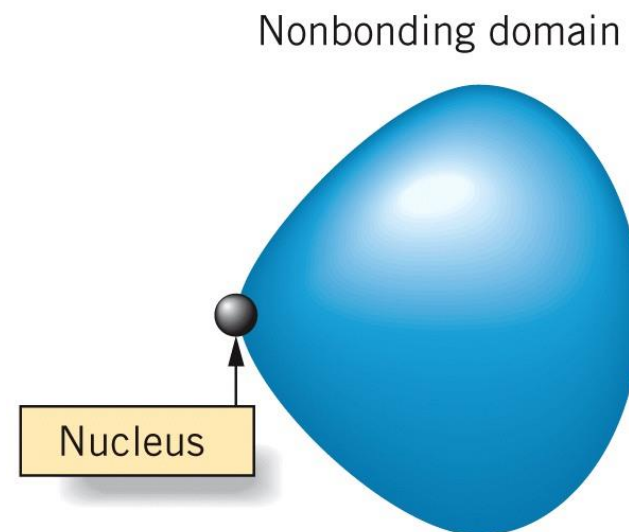
Bonding domains

- Oval in shape
- Electron density focused between two positive nuclei

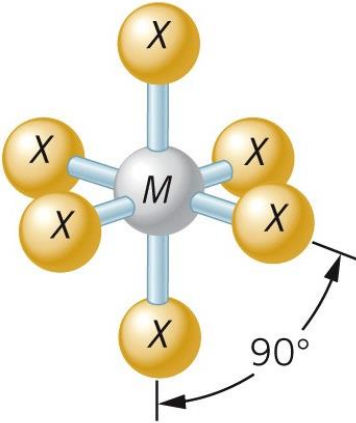
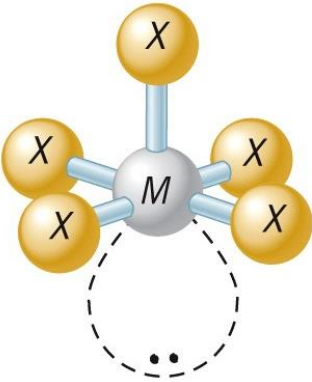


Nonbonding domains

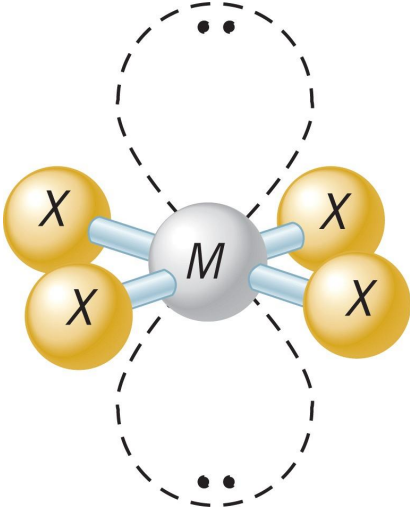
- More bell or balloon shaped
- Take up more space
- Electron density only has positive nuclei at one end



Six Electron Domains

Number of Bonding Domains	Number of Nonbonding Domains	Structure	Molecular Shape
6	0		Octahedral (e.g., SF ₆) Bond angles 180°, 90°
5	1		Square Pyramidal (e.g., BrF ₅) Bond angles 90°

Six Electron Domains cont'd

Number of Bonding Domains	Number of Nonbonding Domains	Structure	Molecular Shape
4	2		Square planar (e.g., XeF ₄) Bond angles 90°, 180°

Steps Used to Determine Three Dimensional Structures:

1. Draw Lewis Structure of Molecule

- Don't need to compute formal charge
- If several resonance structures exist, pick only one

2. Count electron pair domains

- Lone pairs and bond pairs around central atom
- Multiple bonds count as one set (or one effective pair)

Steps Used to Determine Three Dimensional Structures (Cont.)

3. Arrange electron pair domains to minimize repulsions

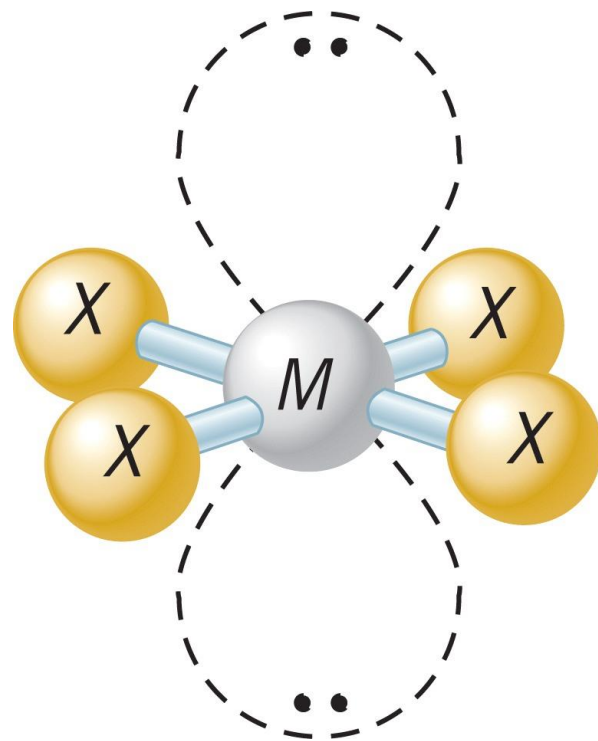
- Lone pairs
 - Require more space than bonding pairs
 - May slightly distort bond angles from those predicted
 - In trigonal bipyramid lone pairs are equatorial
 - In octahedron lone pairs are axial

4. Name **molecular geometry** by position of atoms considering *bonding electrons only*

Your Turn!

What is the molecular geometry of a molecule with four single bonds and two lone electron pairs attached to the center atom?

- A. trigonal bipyramid
- B. trigonal planar
- C. distorted tetrahedron
- D. square pyramid
- E. square planar



Your Turn!

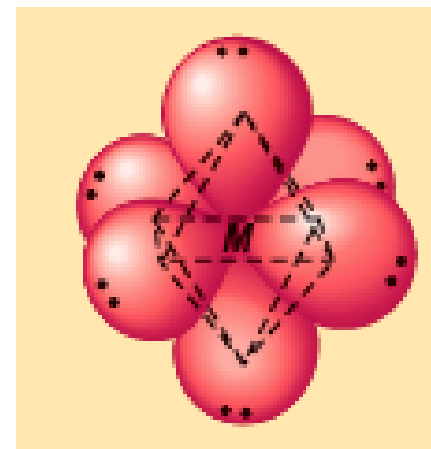
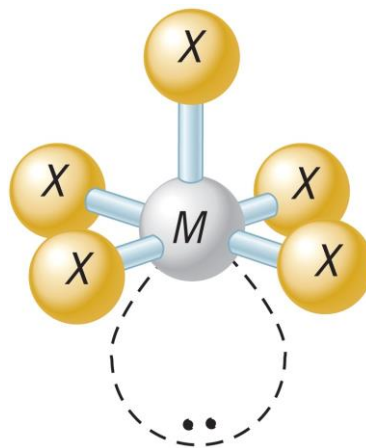
For the species, ICl_5 , how many bonding domains and how many nonbonding domains exist?

- A. 1, 5
- B. 4, 1
- C. 1, 4
- D. 5, 2
- E. 5, 1

Your Turn!

For the species that you just considered, ICl_5 , what is the *electron domain geometry*?

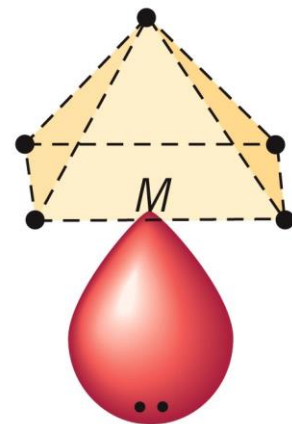
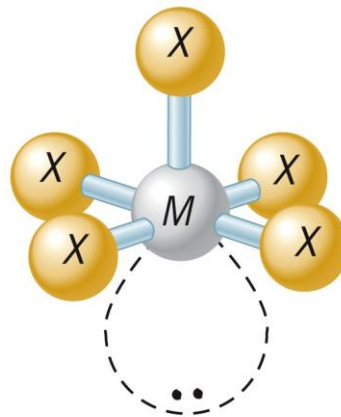
- A. trigonal planar
- B. tetrahedron
- C. trigonal bipyramid
- D. octahedron



Your Turn!

For the species that you just considered, ICl_5 , what is the *molecular geometry*?

- A. trigonal bipyramid
- B. trigonal planar
- C. distorted tetrahedron
- D. square pyramid

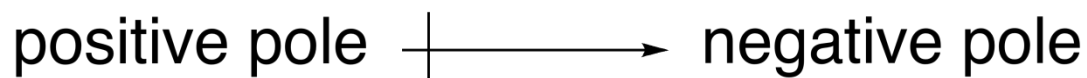


Polar Molecules

- Have net dipole moment
 - Negative end
 - Positive end
- Polar molecules attract each other
 - Positive end of polar molecule attracted to negative end of next molecule
 - Strength of this attraction depends on molecule's dipole moment
 - Dipole moment can be determined experimentally

Polar Molecules

- Polarity of molecule can be predicted by taking **vector** sum of bond dipoles
- Bond dipoles are usually shown as crossed arrows, where arrowhead indicates negative end

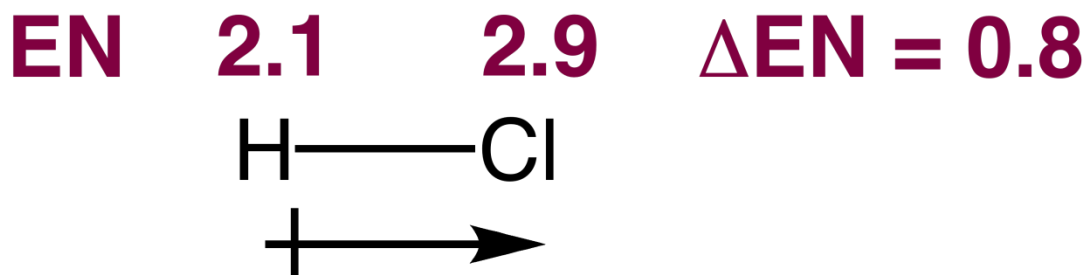


Molecular Shape and Molecular Polarity

- Many physical properties (melting and boiling points) affected by molecular polarity
- For molecule to be polar
 - Must have polar bonds
- Many molecules with polar bonds are nonpolar
 - Possible because certain arrangements of bond dipoles cancel

Why Nonpolar Molecules can Have Polar Bonds

- Reason depends on molecular shape
- Diatomics: just consider two atoms
- Calculate ΔEN



- For molecules with more than two atoms, must consider the ***combined effects*** of **all** polar bonds

Polar Molecules are Asymmetric

To determine polarity of molecule:

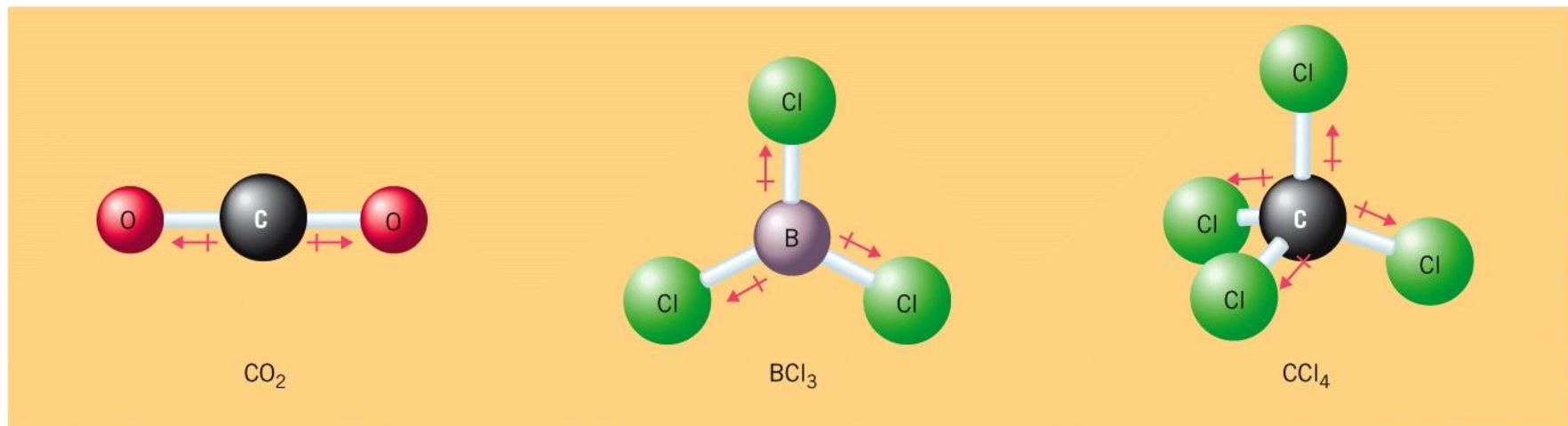
1. Draw structure using proper molecular geometry
 - there is no way to determine the polarity of most molecules without drawing the molecule
2. Draw bond dipoles
3. If they cancel, molecule is non-polar
4. If molecule has uneven dipole distribution, it is polar

Molecular Polarity

1. Molecule is **nonpolar** if

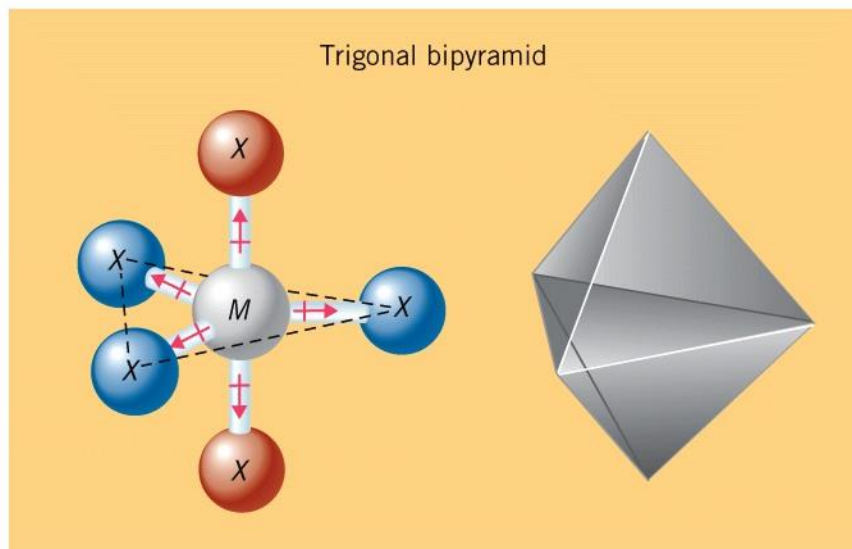
- All electron pairs around central atom are bonding pairs and
- All terminal groups (atoms) are same
- The individual bond dipoles cancel

Molecular Polarity

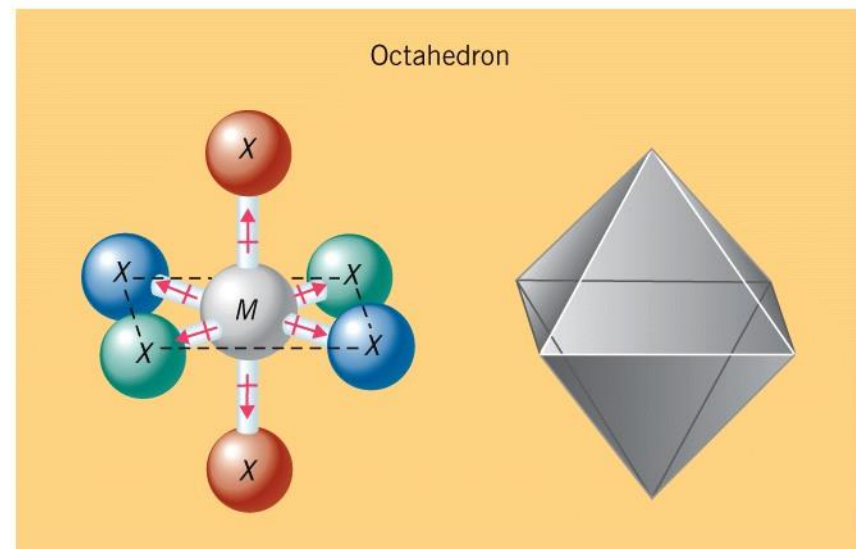


- **Symmetrical** molecules
 - Nonpolar because bond dipoles cancel
- All five shapes are symmetrical when all domains attached to them are composed of identical atoms

Cancellation of Bond Dipoles In Symmetrical Trigonal Bipyramidal and Octahedral Molecules



(a)



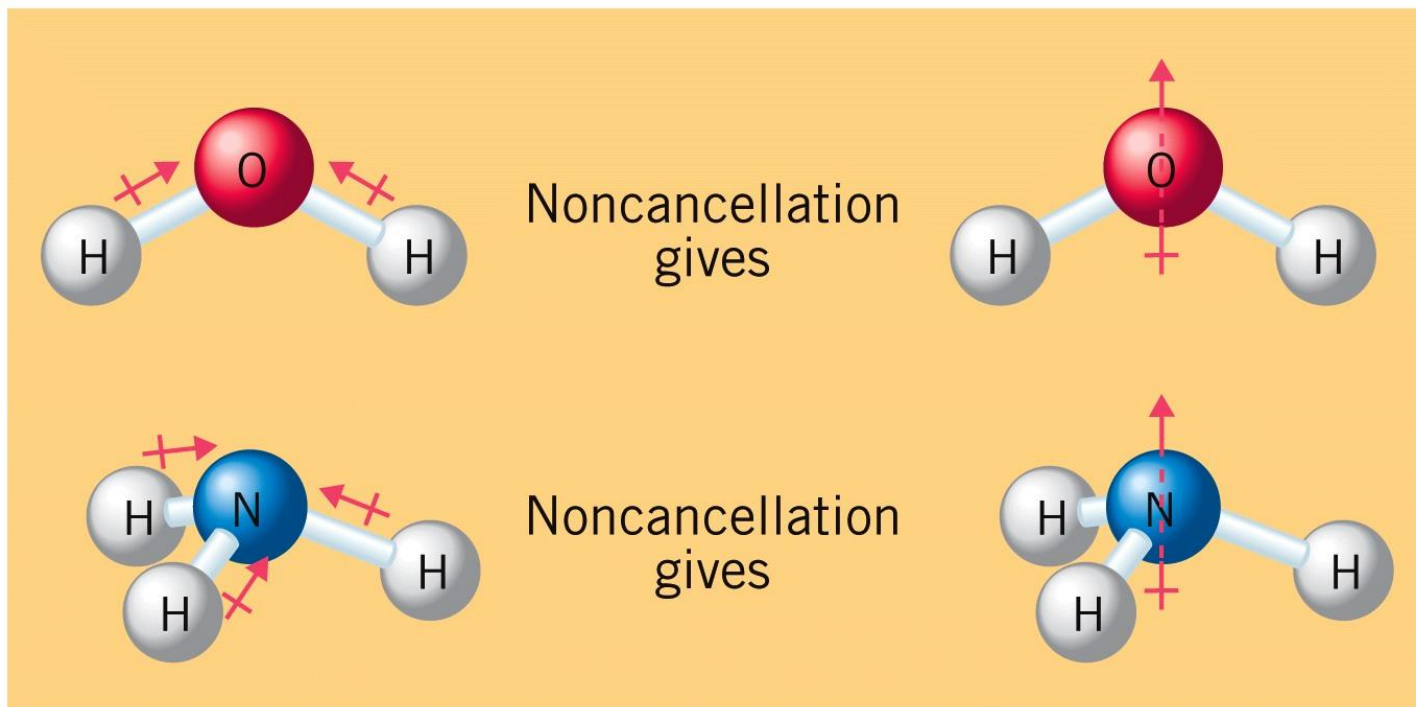
(b)

Molecular Polarity

2. Molecule is usually **polar** if

- All atoms attached to central atom are NOT same
- Or,
- There are one or more lone pairs on central atom

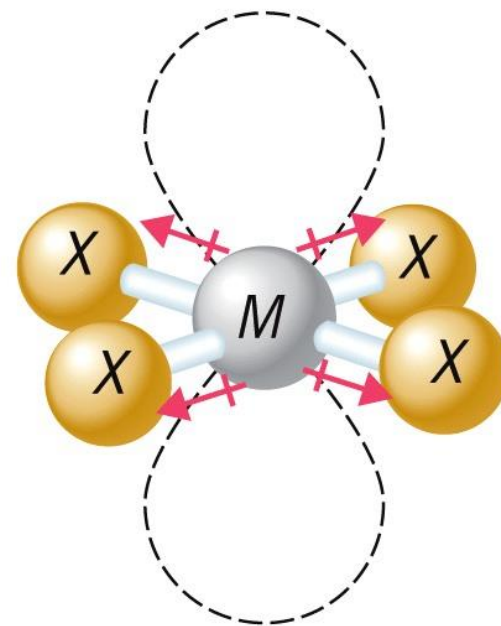
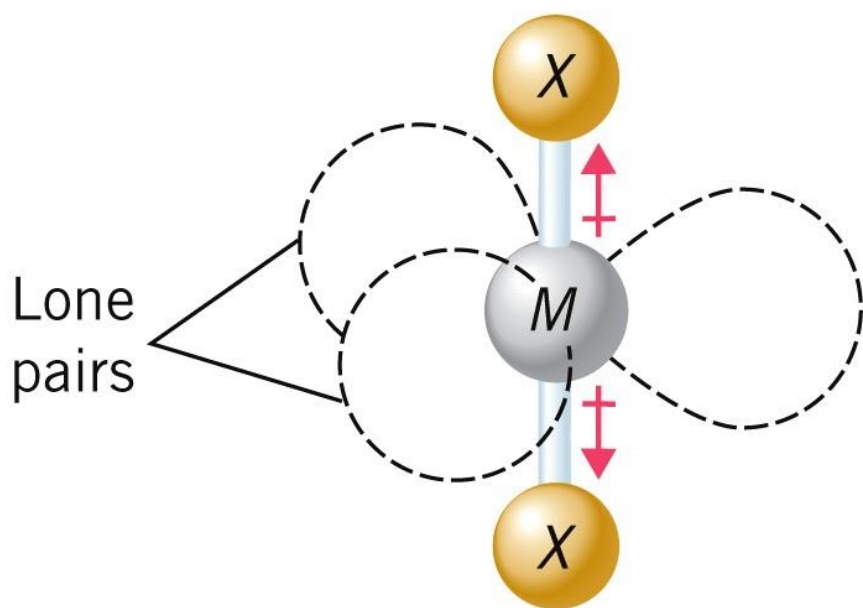
Molecular Polarity



- Water and ammonia both have non-bonding domains
- Bond dipoles do not cancel
- Molecules are polar

Molecular Polarity

- Following exceptions to rule 2 are **nonpolar**
- Nonbonding domains (lone pairs) are symmetrically placed around central atom

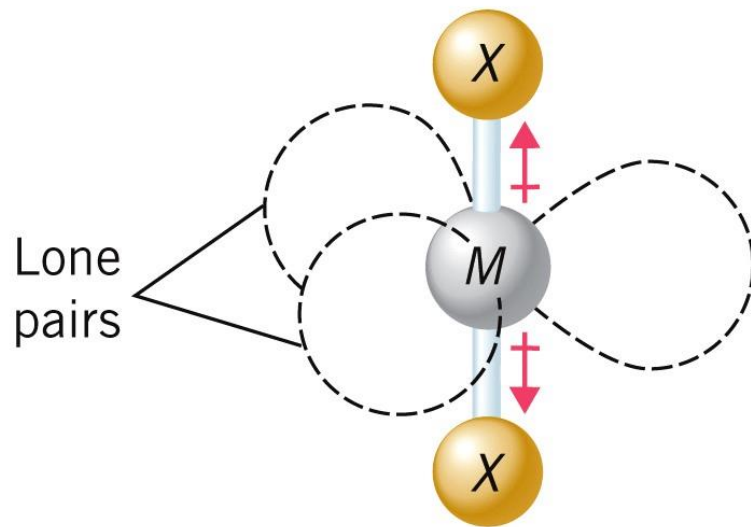


No net dipole

Your Turn!

Imagine a molecule, MX_2 , in which both X atoms are bonded to M and M also has 3 lone electron pairs on it. What is the *electron domain* geometry and is this molecule polar?

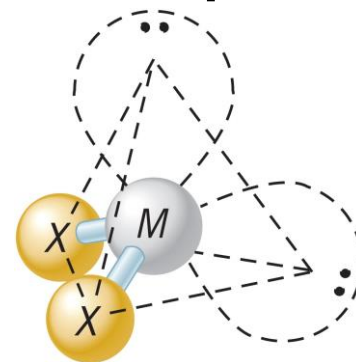
- A. square pyramidal, yes
- B. trigonal bipyramidal, no
- C. tetrahedral, yes
- D. tetrahedral, no
- E. linear, no



Your Turn!

Imagine a molecule, MX_2 , in which both X atoms are bonded to M and M also has 2 lone electron pairs on it. What is the *electron domain* geometry and is this molecule polar?

- A. square pyramidal, yes
- B. trigonoal bipyramidal, no
- C. tetrahedral, yes
- D. tetrahedral, no
- E. linear, no



H_2O is an example:



Your Turn!

Which of the following molecules is polar?



Modern Atomic Theory of Bonding

- Based on wave mechanics
- Gives us
 - Electrons and shapes of orbitals
 - Four quantum numbers
 - Heisenberg uncertainty principle
 - **Electron** probabilities
 - Pauli Exclusion Principle

Valence Bond Theory

- Individual atoms, each have their own orbitals and orbitals overlap to form bonds
- Extent of overlap of atomic orbitals is related to bond strength

Molecular Orbital Theory

- Views molecule as collection of positively charged nuclei having a set of molecular orbitals that are filled with electrons (similar to filling atomic orbitals with electrons)
- Doesn't worry about how atoms come together to form molecules

Both Theories

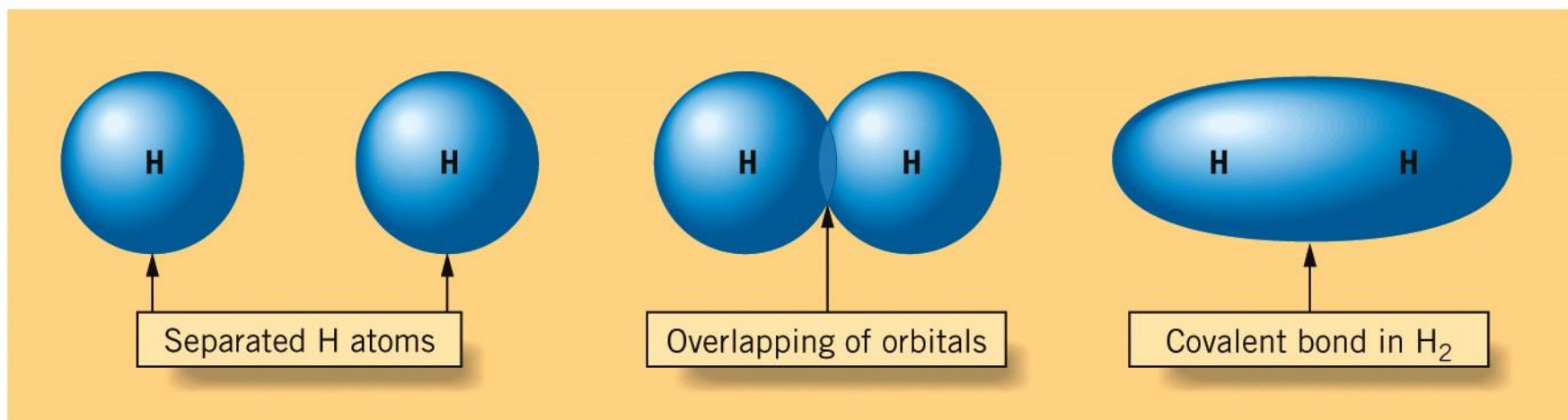
- Try to explain structure of molecules, strengths of chemical bonds, bond orders, etc.
- Can be extended and refined and often give same results

Valence Bond Theory

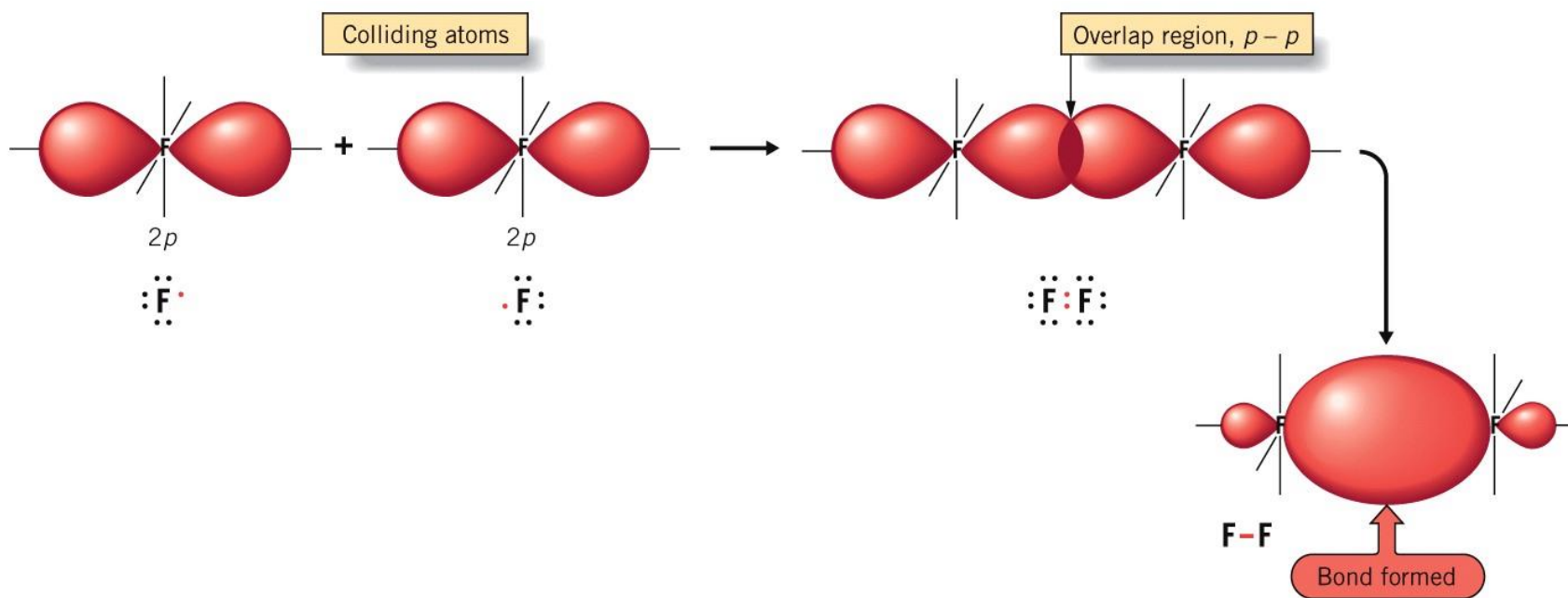
- Bond between two atoms formed when pair of electrons with paired (opposite) spins is shared by two overlapping atomic orbitals

Valence Bond Theory – H₂

- H₂ bonds form because **1s** atomic valence orbital from each H atom overlaps



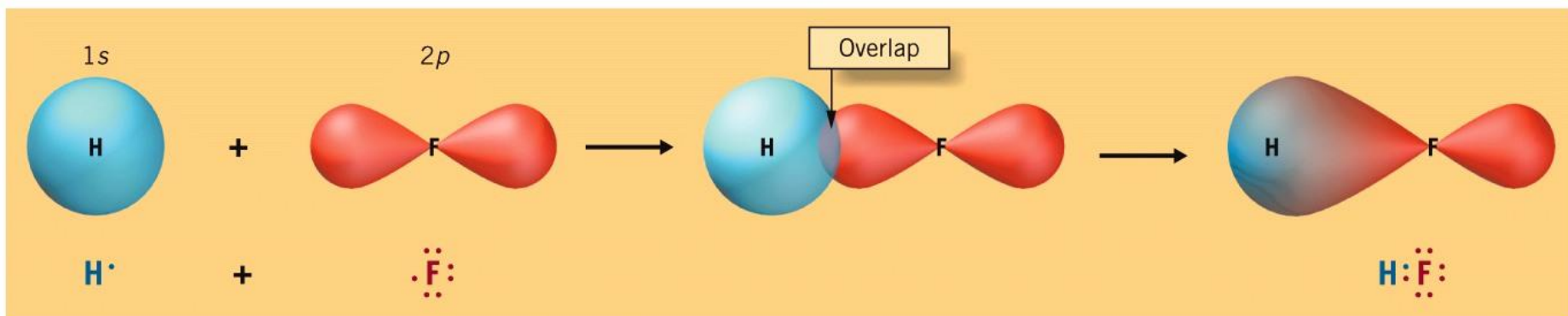
Valence Bond Theory – F₂



- F₂ bonds form because atomic valence orbitals overlap
- Here **2p** overlaps with **2p**
- Same for all halogens, but different **np** orbitals

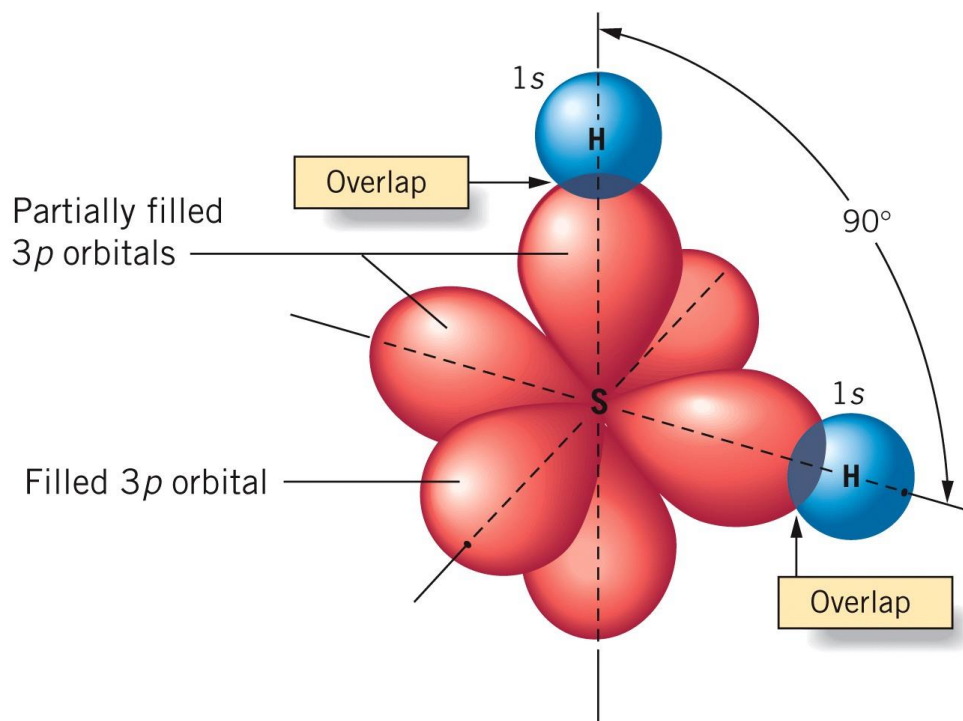
Valence Bond Theory – HF

- HF involves overlaps between **1s** orbital on H and **2p** orbital of F



Valence Bond Theory and H₂S

- Assume that unpaired electrons in S and H are free to form paired bond
- We may assume that H—S bond forms between **s** and **p** orbital

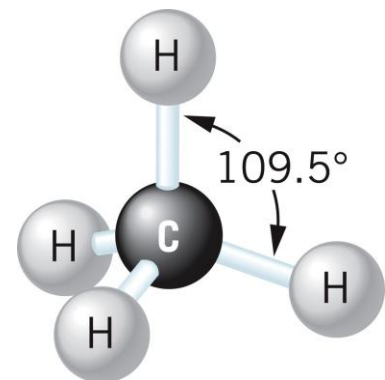


- Predicted 90° bond angle is very close to experimental value of 92°

Difficulties With Valence Bond Theory

Example: CH_4 C $1s^2 2s^2 2p^2$ and H $1s^1$

- In methane, CH_4
 - All four bonds are the same
 - Experimental bond angles are all 109.5°
- Carbon atoms have
 - All paired electrons except two unpaired **$2p$**
 - **p** orbitals are 90° apart
 - Atomic orbitals *predict* CH_2 with 90° angles



Hybridization

- Mixing of atomic orbitals to allow formation of bonds that have realistic bond angles.
 - Realistic description of bonds often requires combining or blending two or more atomic orbitals
- Hybridization just rearranging of electron probabilities

Why do it?

- To get maximum possible overlap
- Best (strongest) bond formed

Hybrid Orbitals

- Blended orbitals result from hybridization process
- Hybrid orbitals have
 - New shapes
 - New directional properties
 - Each hybrid orbital combines properties of parent atomic orbitals

New Names for These New Orbitals?

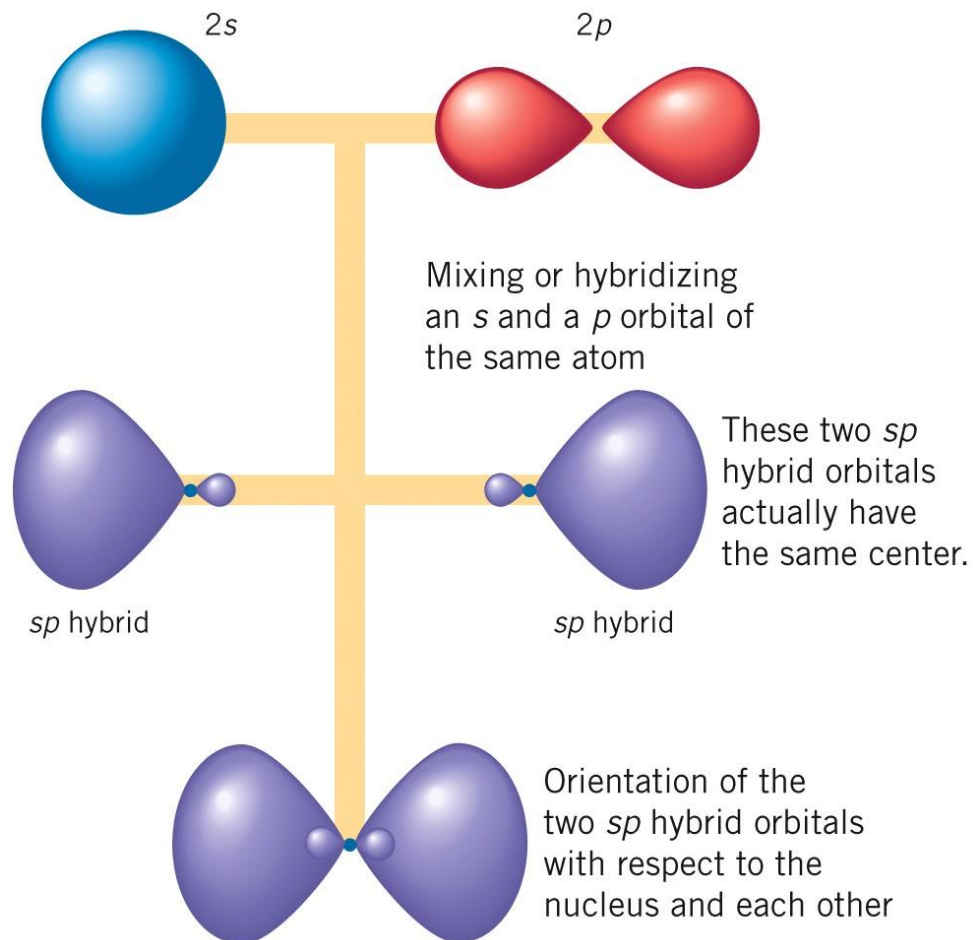
- Symbols for hybrid orbitals combine the symbols of the orbitals used to form them
 - Use $s + p$ form two sp hybrid orbitals
 - Use $s + p + p$ form three sp^2 hybrid orbitals
- One atomic orbital is used for each hybrid orbital formed
- Sum of exponents in hybrid orbital notation must add up to number of atomic orbitals used

Your Turn!

On the previous slide we saw that hybridizing $s + p + p$ forms three hybrid orbitals designated as sp^2 orbitals. Predict the number and designation of orbitals formed by hybridizing $s + p + p + p + d$ (i.e., hybridize one s, three p, and one d orbital).

- A. three, spd
- B. three, sp^3d
- C. five, spd
- D. five, sp^3d
- E. five, s^3pd

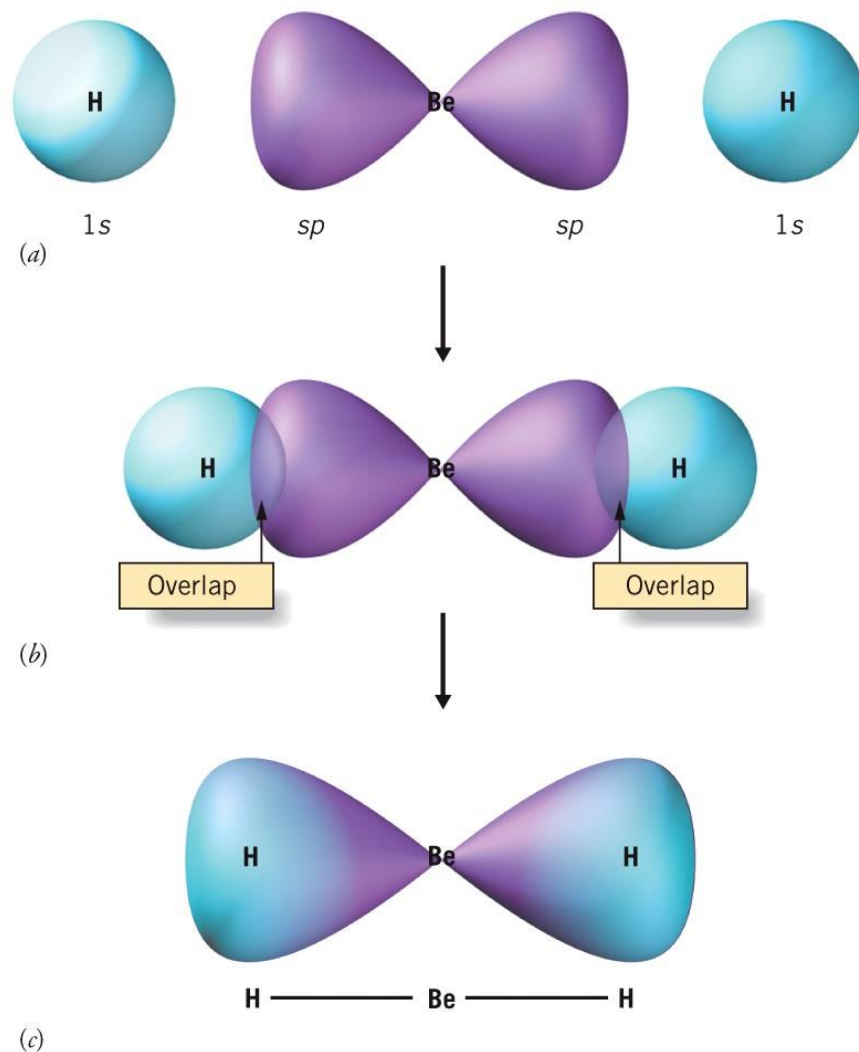
Let's See How Hybridization Works



- Mixing or hybridizing s and p orbital of same atom results in two sp hybrid orbitals
- Two sp hybrid orbitals point in opposite directions

Using *sp* Hybrid Orbitals to Form Bonds

- Now have two *sp* hybrid orbitals
- Oriented in correct direction for bonding
- 180° bond angles
 - As VSEPR predicts and
 - Experiment verifies
- Bonding =
 - Overlap of H *1s* atomic orbitals with *sp* hybrid orbitals on Be



What Do We Know?

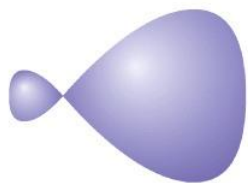
- Experiment and VSEPR show that
 - $\text{BeH}_2(g)$ is linear
 - 180° bond angle
- For Be to form these bonds it must have
 - Two hybrid orbitals on Be must point in opposite directions
 - Give correct bond angle
- Each Be orbital must contain one electron
 - Each resulting bond with H contains only two electrons
 - Each H supplies one electron

Hybrid Orbitals

Hybrid	Atomic Orbitals Used	Electron Geometry
<i>sp</i>	<i>s + p</i>	Linear Bond angles 180°
<i>sp²</i>	<i>s + p + p</i>	Trigonal planar Bond angles 120°
<i>sp³</i>	<i>s + p + p + p</i>	Tetrahedral Bond angles 109.5°
<i>sp³d</i>	<i>s + p + p + p + d</i>	Trigonal Bipyramidal Bond angles 90° and 120°
<i>sp³d²</i>	<i>s + p + p + p + d + d</i>	Octahedral Bond angles 90°

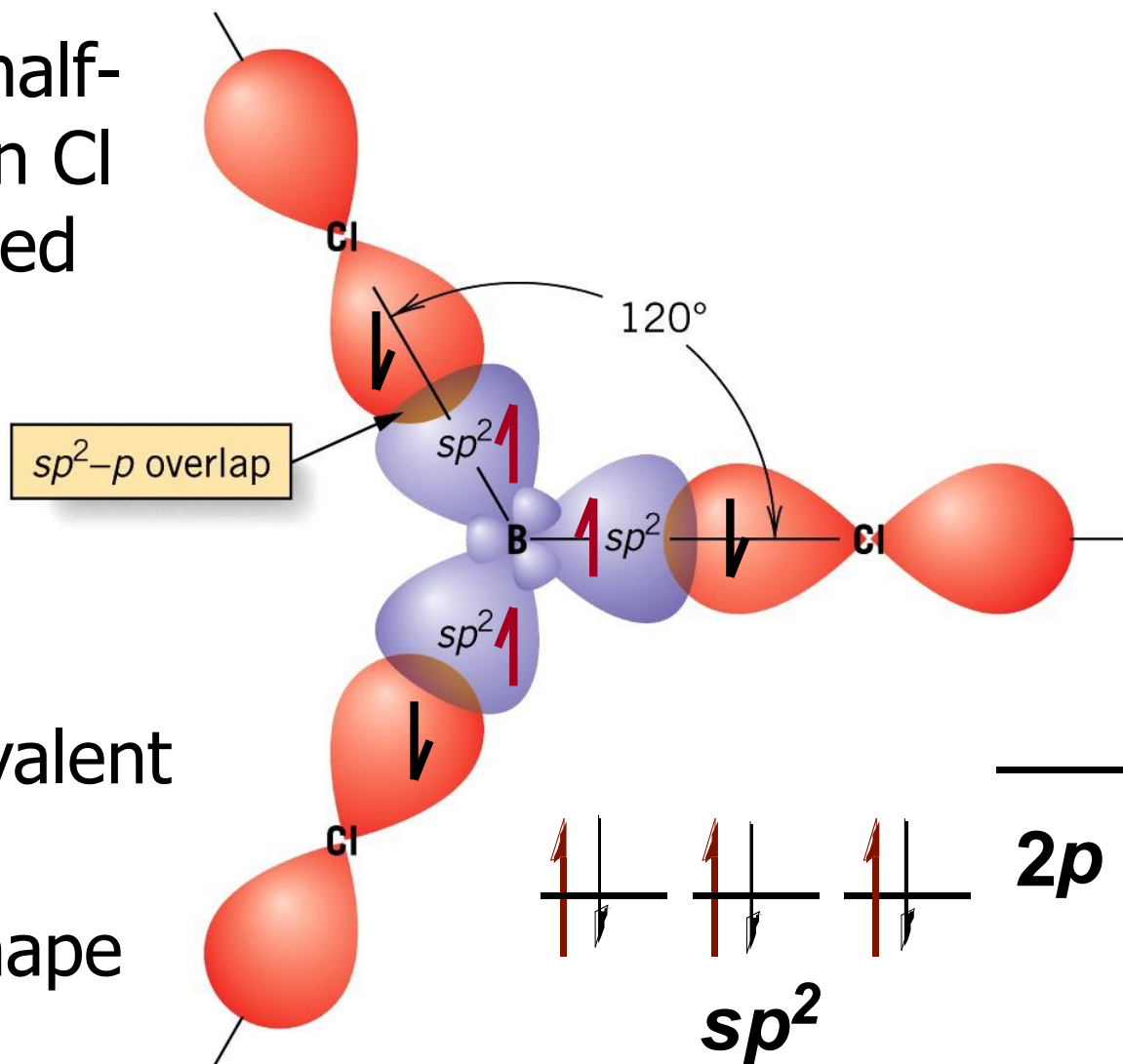
Bonding in BCl_3

- Overlap of each half-filled $3p$ orbital on Cl with each half-filled sp^2 hybrid on B



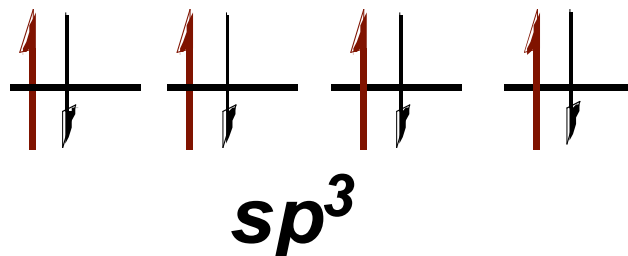
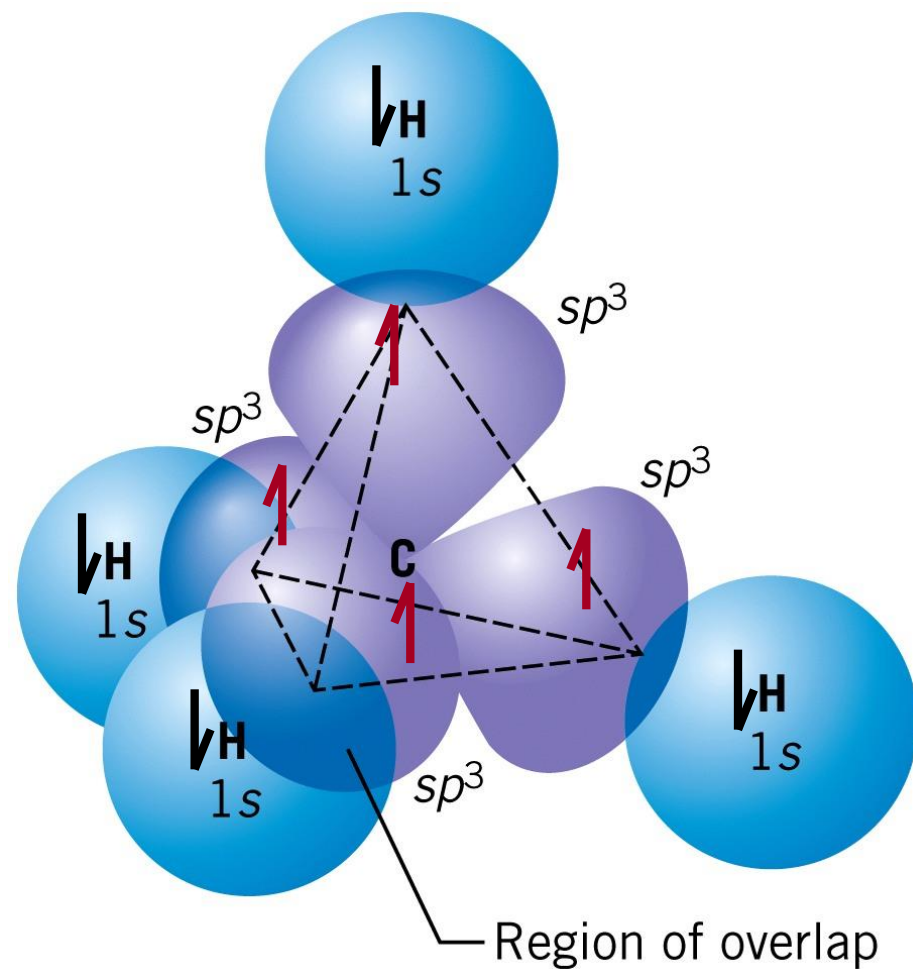
sp^2 hybrid orbital

- Forms three equivalent bonds
- Trigonal planar shape
- 120° bond angle



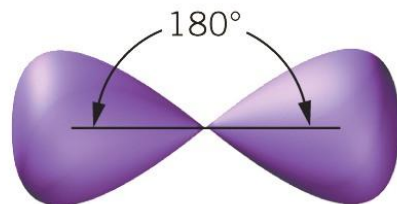
Bonding in CH₄

- Overlap of each half-filled 1s orbital on H with each half-filled sp^3 hybrid on carbon
- Forms four equivalent bonds
- Tetrahedral geometry
- 109.5° bond angle



Hybrid Orbitals

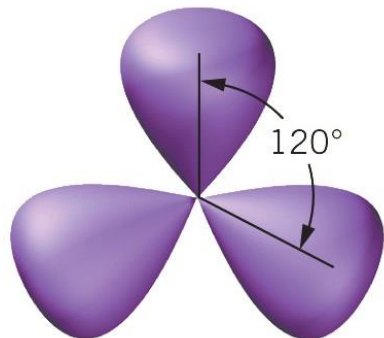
Two *sp*
hybrids



180° angle

Linear

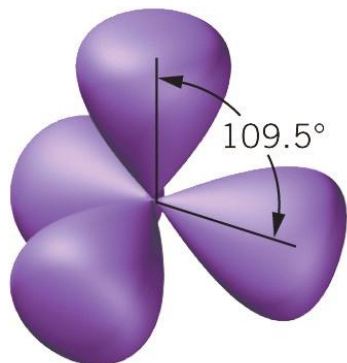
Three *sp*²
hybrids



All angles
120°

**Planar
Triangular**

Four *sp*³
hybrids



All angles
109.5°

Tetrahedral

Your Turn!

What is the hybridization of oxygen in OCl_2 ?

A. sp

B. sp^3

C. sp^2

D. No hybridization

Your Turn!

What is the hybridization of the carbon atom in carbon disulfide?

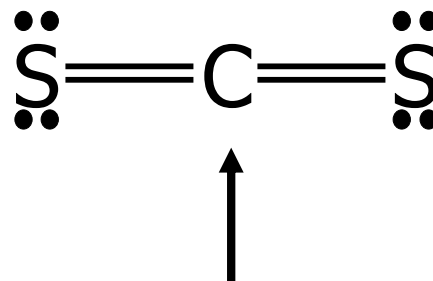
A. sp

B. sp^3

C. sp^2

D. sp^3d

D. sp^3d^2



Two electron domains and
 180° bond angle: sp hybrid orbitals

Expanded Octet Hybridization

Hybridization When Central Atom has More Than Octet

- If there are more than four equivalent bonds on central atom, then must add *d* orbitals to make hybrid orbitals

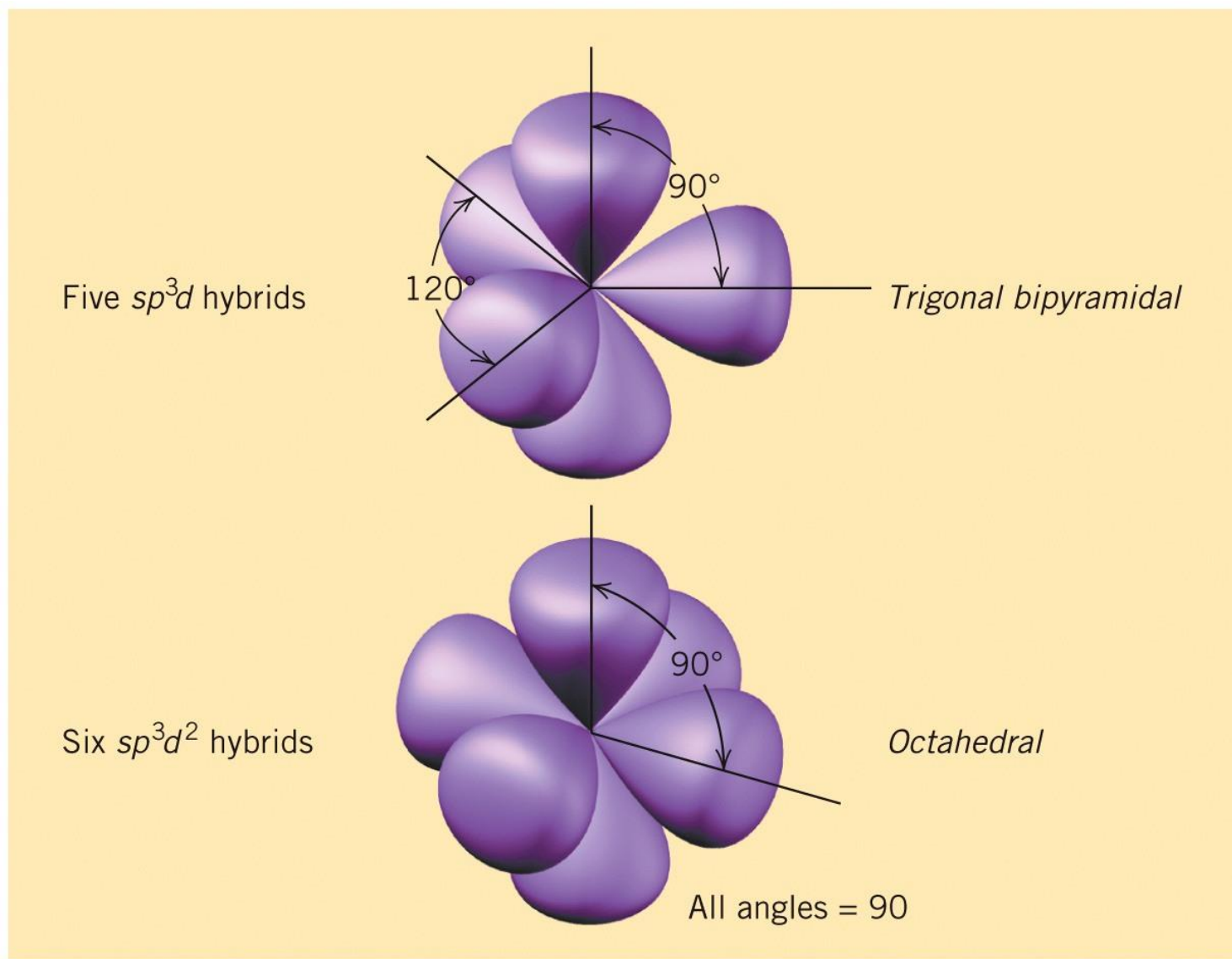
Why?

- One *s* and three *p* orbitals means that four equivalent orbitals is the most you can get using *s* and *p* orbitals alone

Expanded Octet Hybridization

- So, only atoms in third row of the periodic table and below can exceed their octet
 - These are the only atoms that have empty *d* orbitals of same *n* level as *s* and *p* that can be used to form hybrid orbitals
- One *d* orbital is added for each pair of electrons in excess of standard octet

Expanded Octet Hybrid Orbitals

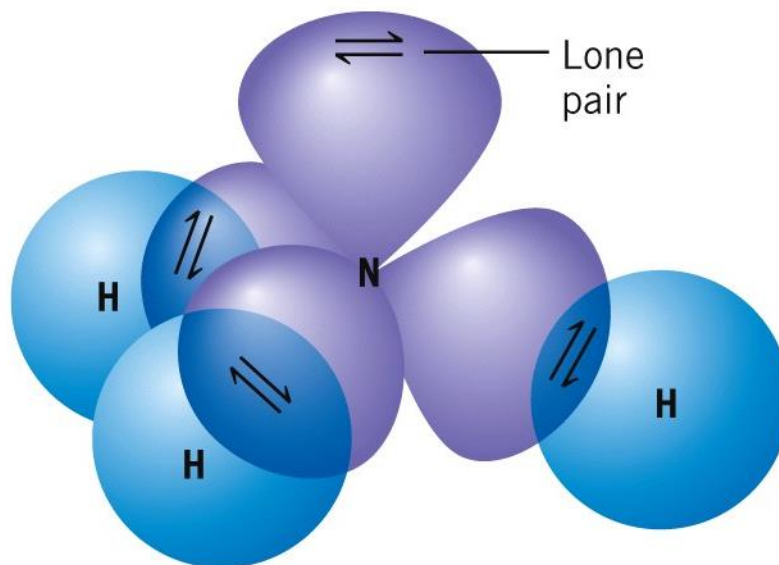
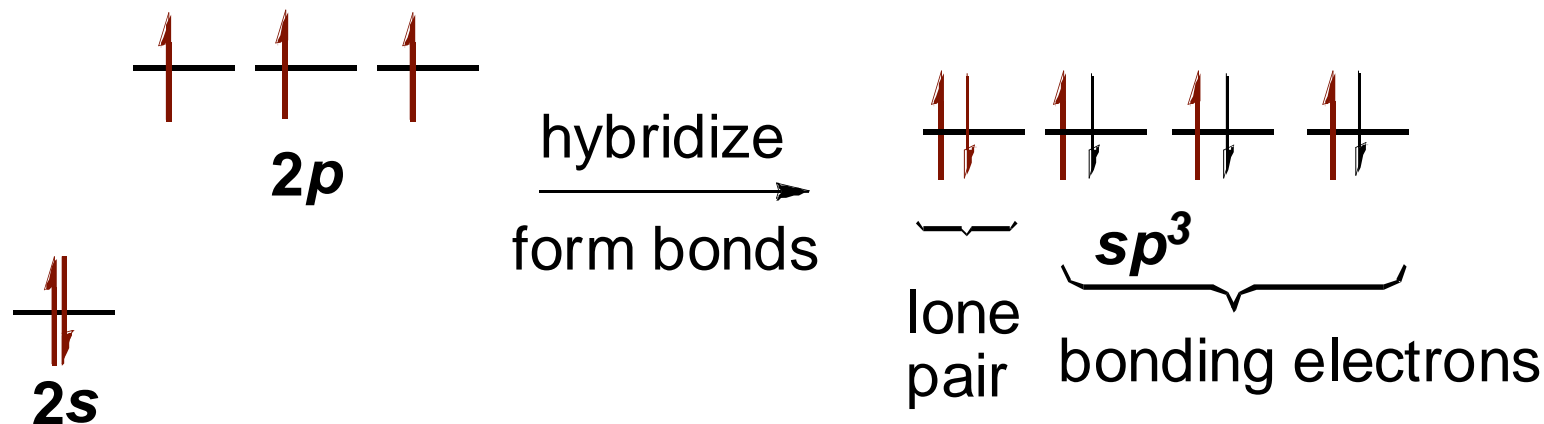


Hybridization in Molecules That Have Lone Pair Electrons

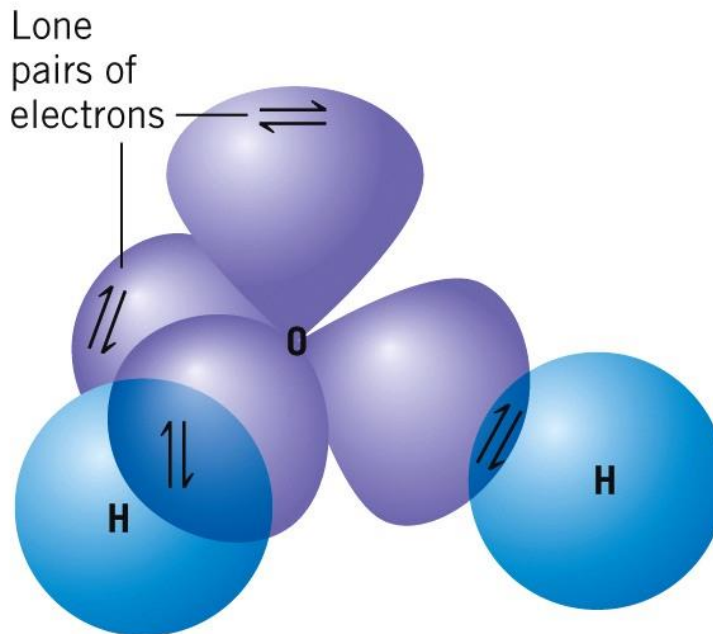
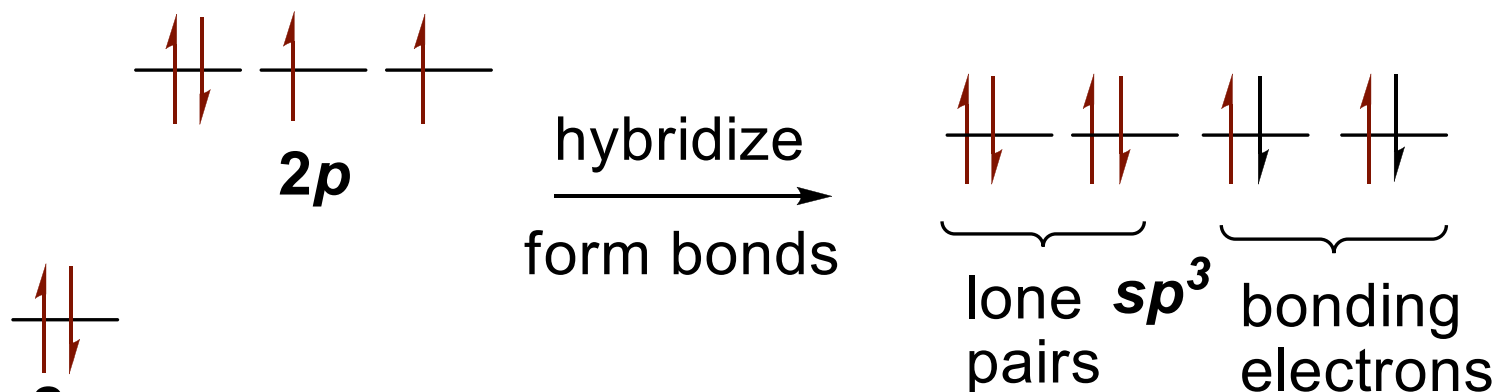
CH ₄	<i>sp</i> ³	tetrahedral geometry	109.5°	bond angle
NH ₃			107°	bond angle
H ₂ O			104.5°	bond angle

- Angles suggest that NH₃ and H₂O both use *sp*³ hybrid orbitals in bonding
- Not all hybrid orbitals used for bonding e⁻
 - Lone pairs can occupy hybrid orbitals
- Lone pairs must always be counted to determine geometry

Hybridization in Molecules That Have Lone Pair Electrons – NH_3



Hybridization in Molecules that Have Lone Pair Electrons – H₂O



Your Turn!

For the species ClF_2^+ , determine the following:

1. electron domain geometry
 2. molecular geometry
-
- A. tetrahedral, trigonal planar
 - B. pentagonal, tetrahedral
 - C. tetrahedral, bent
 - D. trigonal planar, bent

Your Turn!

For the species ClF_2^+ , determine the following:

1. hybridization around the central atom
 2. Polarity
-
- A. sp^3 , polar
 - B. sp^3 , non-polar
 - C. sp^3 , polar
 - D. sp^2 , non-polar

Your Turn!

For the species XeF_4O , determine the following:

1. electron domain geometry
 2. molecular geometry
-
- A. octahedral, square pyramidal
 - B. trigonal bipyramidal, distorted tetrahedral
 - C. square pyramidal, octahedral
 - D. trigonal bipyramidal, planar

Your Turn!

For the species XeF_4O , determine the following:

1. hybridization around the central atom
 2. the molecular polarity
-
- A. sp^3d , polar
 - B. sp^3d^2 , polar
 - C. sp^3d , nonpolar
 - D. sp^3d^2 , nonpolar

Double and Triple Bonds

- So where do extra electron pairs in multiple bonds go?
 - Not in hybrid orbitals
 - Remember VSEPR, multiple bonds have no effect on geometry
- Why don't they effect geometry?

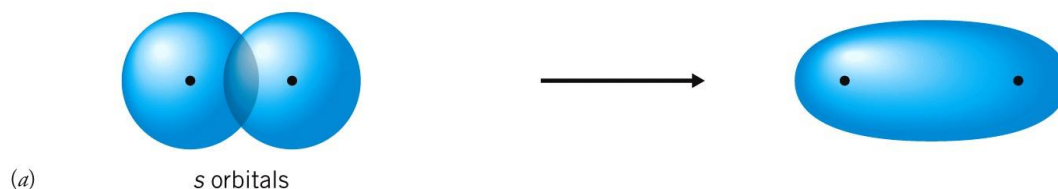
Two types of bond result from orbital overlap

- Sigma (σ) bond
 - Accounts for first bond
- Pi (π) bond
 - Accounts for second and third bonds

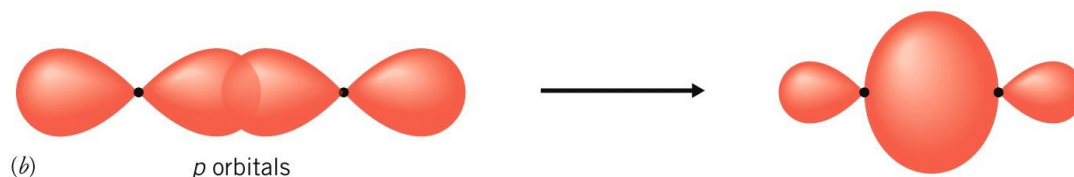
Sigma (σ) Bonds

- Head on overlap of orbitals
- Concentrate electron density concentrated most heavily between nuclei of two atoms
- Lie along imaginary line joining their nuclei

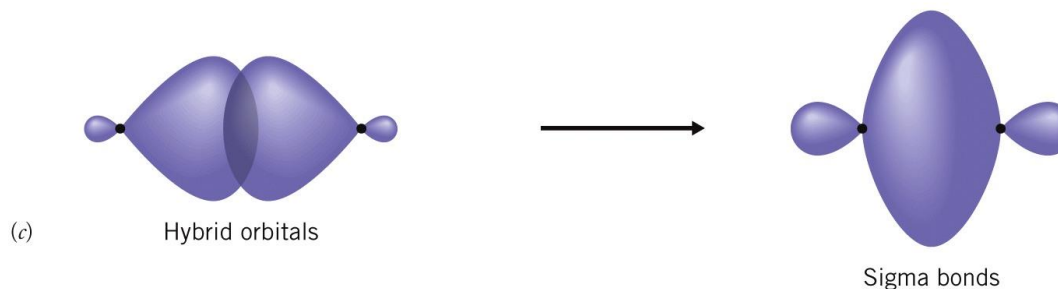
$s + s$



$p + p$

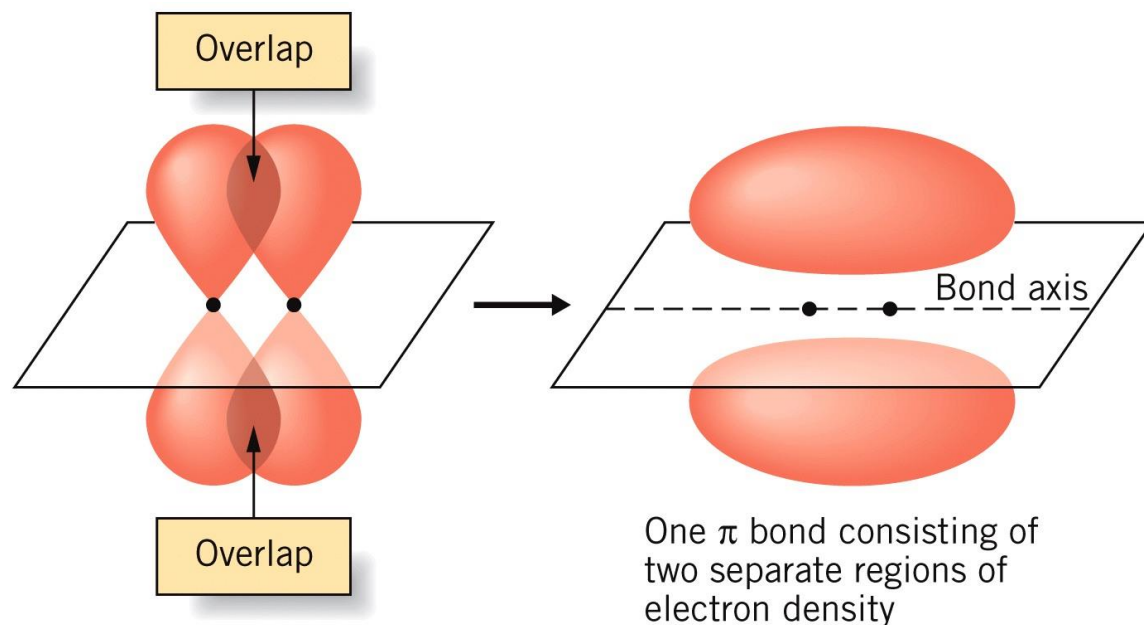


$sp + sp$



Pi (π) Bonds

- Sideways overlap of unhybridized p orbitals
- Electron density divided into two regions
 - Lie on opposite sides of imaginary line connecting two atoms
- Electron density above and below σ bond.
- No electron density along σ bond axis
- π bond consists of both regions
- Both regions = one π bond



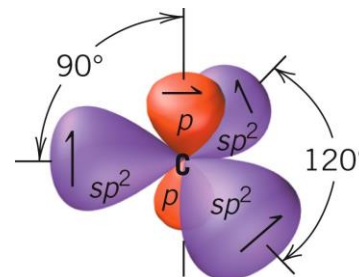
Pi (π) Bonds

- Can never occur alone
 - Must have σ bond
- Can form from unhybridized p orbitals on adjacent atoms after forming σ bonds
- π bonds allow atoms to form double and triple bonds

Bonding in Ethene (C_2H_4)

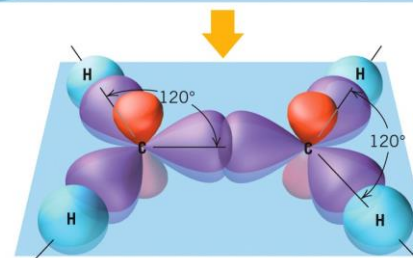
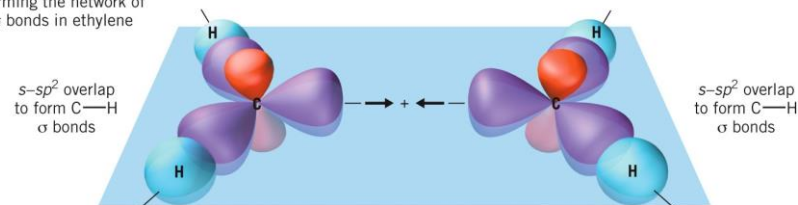
- Each carbon is
 - sp^2 hybridized (**violet**)
 - has one unhybridized p orbital (**red**)
- $C=C$ double bond is
 - one σ bond ($sp^2 - sp^2$)
 - one π bond ($p - p$)

$p-p$ overlap forms a $C-C$ π bond

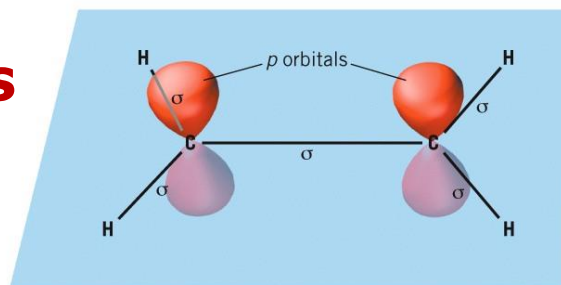


The three sp^2 hybrid orbitals and the unhybridized p orbital at each carbon in ethylene

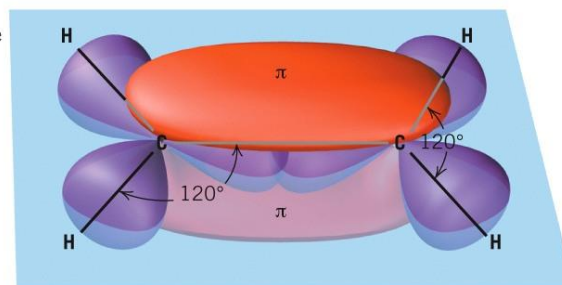
Forming the network of σ bonds in ethylene



sp^2-sp^2 overlap to form a $C-C$ σ bond

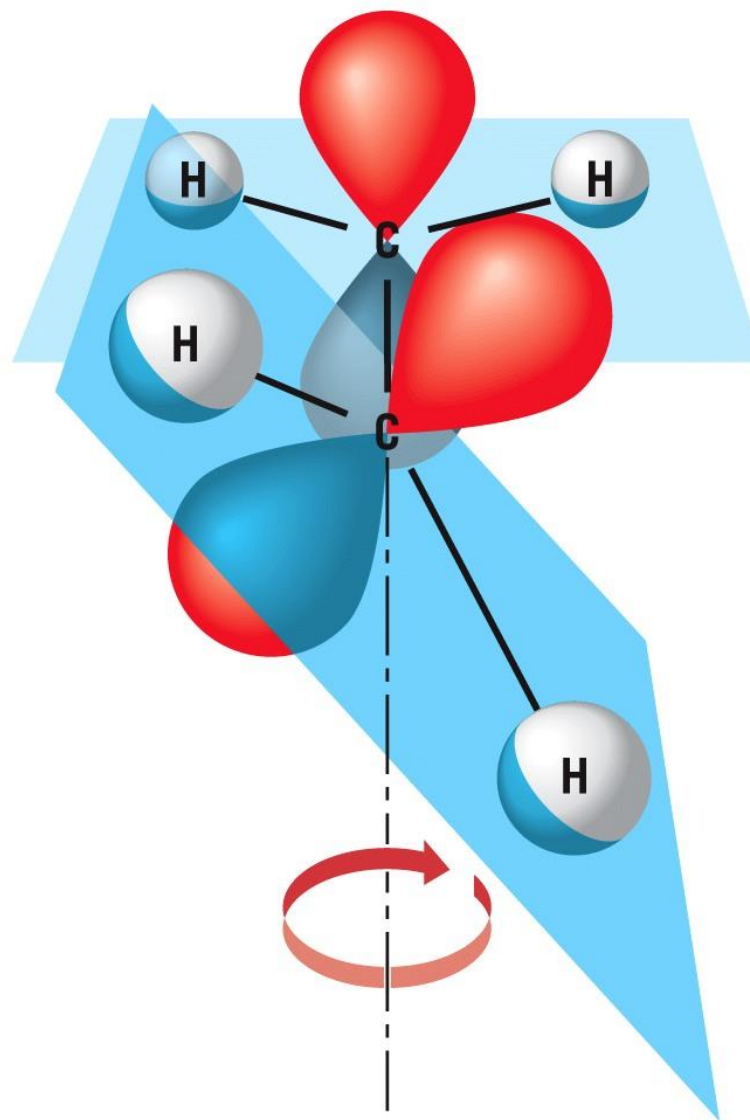


Forming the π bond in ethylene



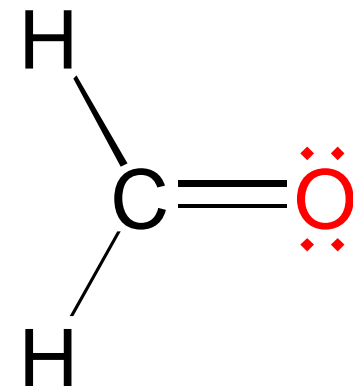
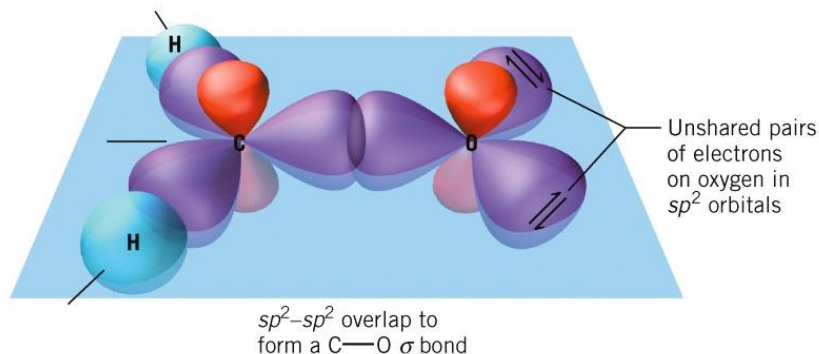
Properties of π -Bonds

- Can't rotate about double bond
- π bond must first be broken before rotation can occur



Bonding in Formaldehyde

- C and O each
 - sp^2 hybridized (**violet**)
 - Has one unhybridized p orbital (**red**)

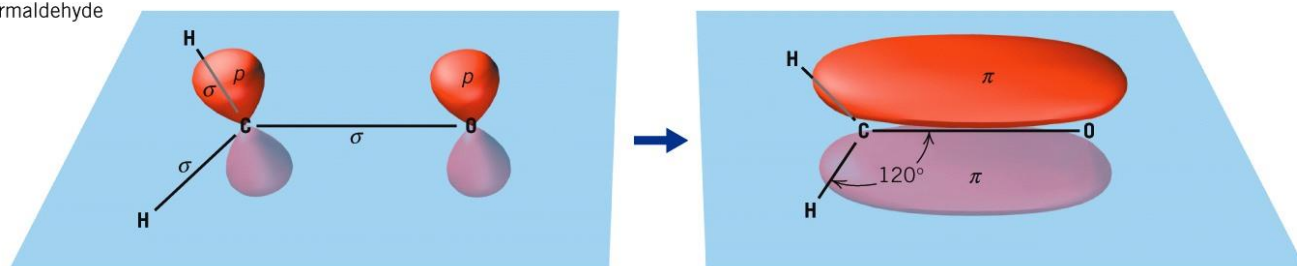


Unshared pairs of electrons on oxygen in sp^2 orbitals

- C=O double bond is

- one σ bond ($sp^2 - sp^2$)
- one π bond ($p - p$)

Forming the π bond in formaldehyde

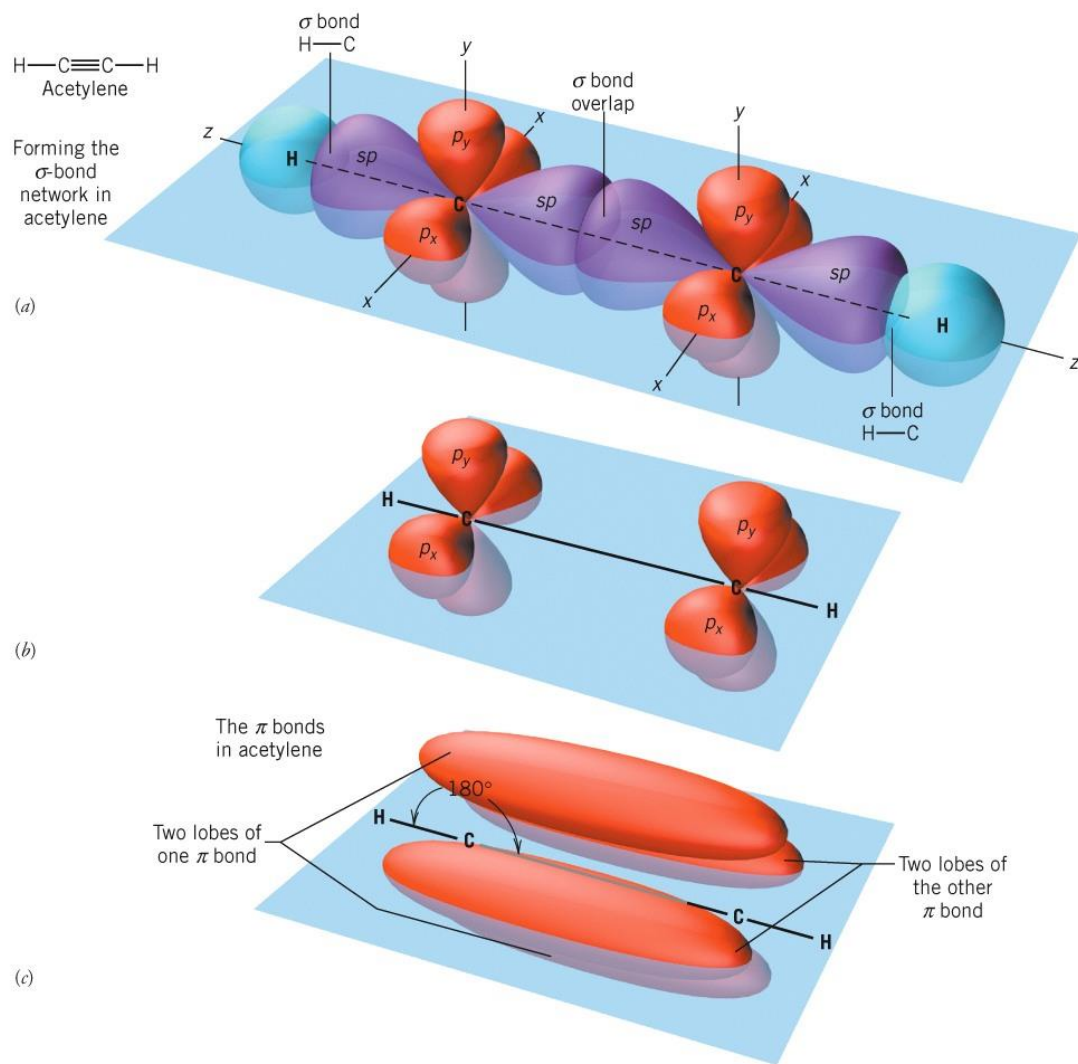


sp^2-sp^2 overlap to form C—O σ bond

Bonding in Ethyne (Acetylene)

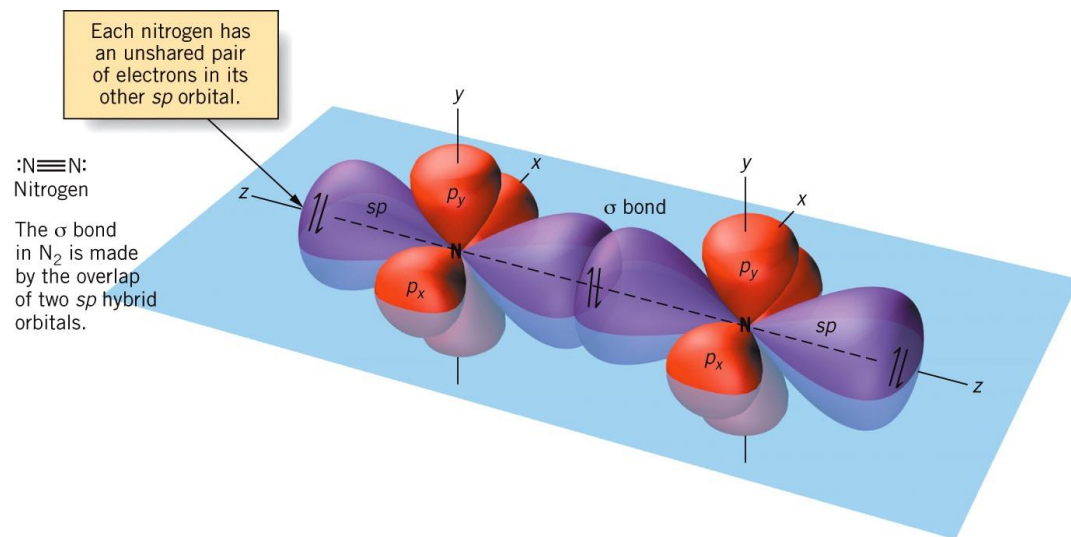


- Each carbon
 - is sp hybridized (violet)
 - Has two unhybridized p orbitals, p_x and p_y (red)
- $\text{C}\equiv\text{C}$ triple bond
 - one σ bond
 - $sp - sp$
 - two π bonds
 - $p_x - p_x$
 - $p_y - p_y$



Bonding in N₂

- Each nitrogen
 - *sp* hybridized (**violet**)
 - Has two unhybridized *p* orbitals, *p_x* and *p_y* (**red**)

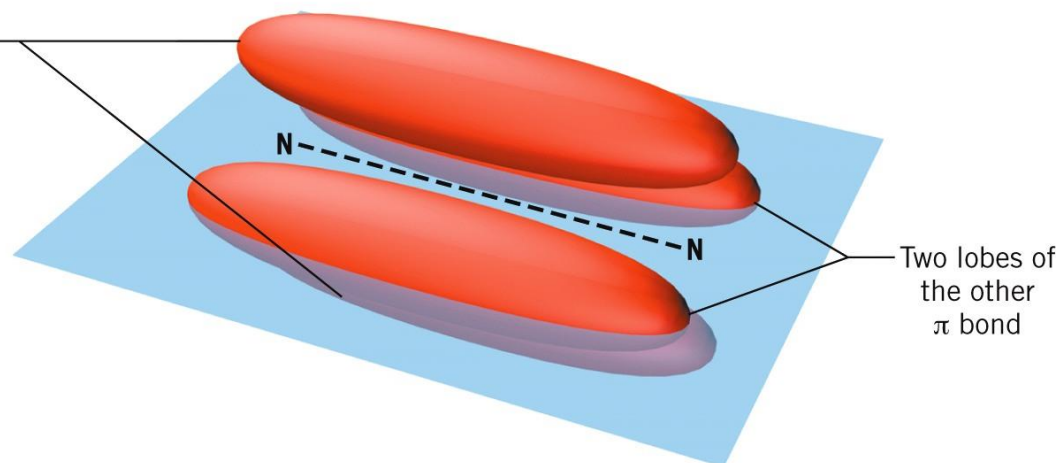


N \equiv N triple bond

- one σ bond
 - *sp* – *sp*
- two π bonds
 - *p_x* – *p_x*
 - *p_y* – *p_y*

The π bonds in N₂

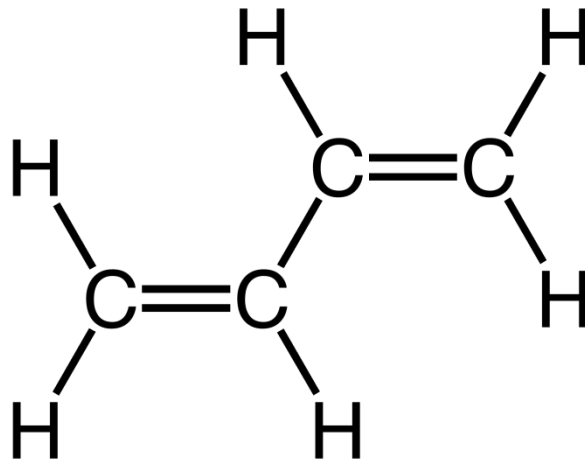
Two lobes of one π bond



Your Turn!

How many σ and π bonds are there in $\text{CH}_2\text{CHCHCH}_2$, and what is the hybridization around the carbon atoms?

- A. 7, 1, sp
- B. 8, 2, sp^3
- C. 9, 2, sp^2
- D. 9, 3, sp^2
- E. 8, 2, sp



Your Turn!

How many σ and π bonds are there in carbon monoxide and what is the hybridization of the C and O atoms?

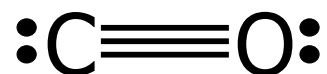
A. 1, 2, both sp

B. 2, 2, both sp

C. 0, 3, both sp^2

D. 3, 0, sp^2 and sp

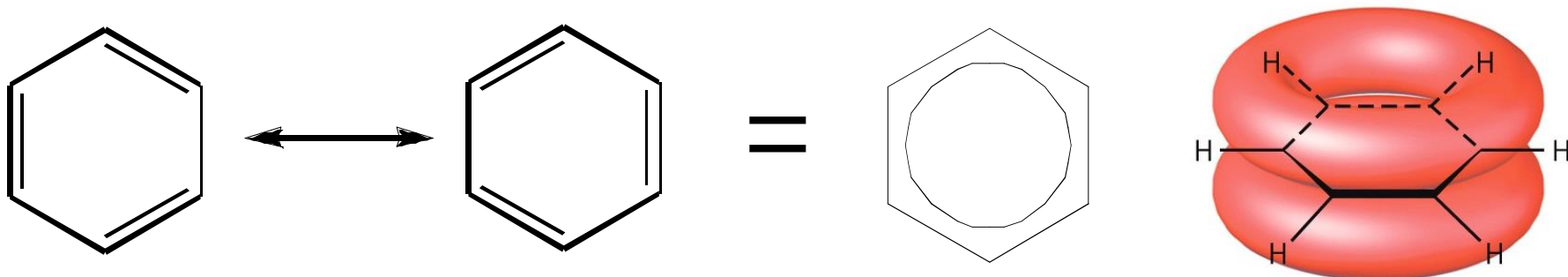
E. 3, 2, sp^2 and sp



Successes of VB Theory

- Based on simple Lewis structures and related geometric figures
- Three dimensional structures based on electron domains without massive calculations
- Simple hybrid orbitals invoked where experimental evidence shows the need
- Integer bond orders are often correct

Benzene, In Valence Bond Terms

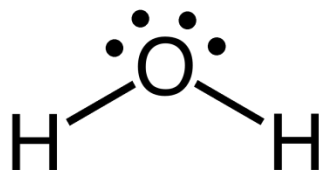


- Can write benzene as two resonance structures
- But actual structure is composite of these two
- Electrons are **delocalized**
- Have three pairs of electrons delocalized over six C atoms
- Extra stability is **resonance energy**
- Functionally, resonance and delocalization energy are the same thing

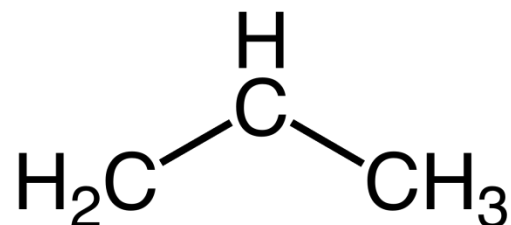
Your Turn!

Which of the following species exhibits resonance?

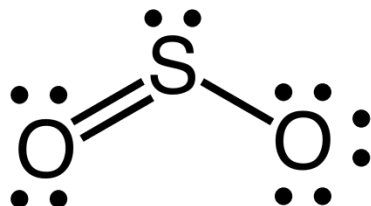
A.



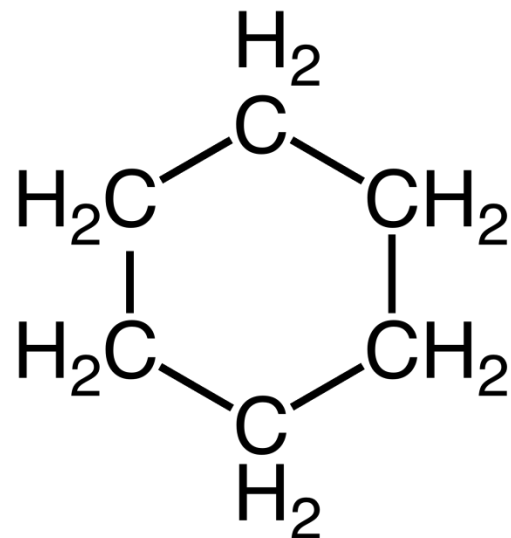
D.



B.



E.



C.

