

Chapter 8- Bonding: General Concepts Study Guide

8.1 Types of Chemical Bonds

Chemical bonds are “forces that hold groups of atoms together and make them function as a unit.”
Bonds form because the energy of a system is lower than if the bonds did not form.

The three types of bonds:

1. Ionic Bonding-

An ion pair has energy known as **energy of interaction**. Derived from Coulomb's Law, the energy can be calculated with the formula: $E = 2.31 \times 10^{-19} \text{ J nm} [(Q_1 Q_2)/r]$

Example 8.1 Coulomb's Law

Calculate the energy of interaction (in kJ/mole) between Mg^{2+} and O^{2-} if the distance between the centers of the ions is 0.205 nm.

Solution

$$E = 2.31 \times 10^{-19} \text{ J nm} [(Q_1 Q_2)/r] = E = 2.31 \times 10^{-19} \text{ J nm} [((+2)(-2))/0.205 \text{ nm}] \\ = - 4.51 \times 10^{-18} \text{ J/ion pair} = -4.51 \times 10^{-21} \text{ kJ/ion pair}$$

- #### 2. Covalent Bonding-
- it involves the “sharing of electrons” between atoms in a molecule
Polar Covalent bonding is when there is an unequal sharing of electrons.
Non-polar Covalent bonding is when there is an equal sharing of electrons.

The nature of the bond will depend on the ability of each atom in the bond to attract electrons to itself. This is called **electronegativity**.

Problems:

1. Calculate the energy of interaction for KCl if the internuclear distance is 0.314 nm.
2. Calculate the energy of interaction between AgBr if the internuclear distance is 0.120 nm.

8.2 Electronegativity

Recall that unequal sharing of electrons in a bond results in a polar covalent bond. Ionic bonds result from the transfer of electrons between atoms. We can get a degree of ionic character of a bond by **measuring bond energies**. The more electrostatic interaction that occurs between 2 atoms, the greater will be the difference in bond energies when compared to the average of perfectly covalent bonds involving the atoms. The difference in bond energy is called Δ and is the relative **electronegativity** difference between the bonding atoms.

For the representative elements, **electronegativity decreases going down a group** and **increases going across a period**. The greater the Δ , the more ionic character a bond has. If $\Delta = 0$, the bond is perfectly covalent. There are no precise cut-offs. All bonds have some ionic and some covalent character.

Electronegativities of Elements

1A		2A										3A	4A	5A	6A	7A	<div style="display: flex; flex-direction: column; align-items: center;"> <div style="width: 15px; height: 15px; background-color: #d3d3d3; margin-bottom: 2px;"></div> 3.0-4.0 <div style="width: 15px; height: 15px; background-color: #c0c0c0; margin-bottom: 2px;"></div> 2.0-2.9 <div style="width: 15px; height: 15px; background-color: #a9a9a9; margin-bottom: 2px;"></div> 1.5-1.9 <div style="width: 15px; height: 15px; background-color: #808080; margin-bottom: 2px;"></div> <1.5 </div>
H 1.0																	
Li 0.9	Be 1.2										B 2.0	C 2.5	N 3.0	O 3.5	F 4.0		
Na 0.9	Mg 1.2	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0					As 2.0	Se 2.4	Br 2.8				
K 0.8	Ca 1.0	Sc 1.3												Te 2.1	I 2.5		
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4				Ru 2.2	Rh 2.2	Pd 2.2								
Cs 0.7	Ba 0.9	La 1.0	Hf 1.3				Os 2.2	Ir 2.2	Pt 2.2	Au 2.4				Po 2.0	At 2.2		
Fr 0.7	Ra 0.9	Ac 1.1	Th 1.3	Pa 1.4	U 1.4	Np-No 1.4-1.3											

Δ (Electronegativity Diff) (approx)	Type of Bond (In General)	Example
0.0 - 0.4	Covalent (Non-polar)	H-H (0.0)
0.4 - 1.0	Covalent (Mod. Polar)	H \leftrightarrow Cl (0.9)
1.0 - 1.9	Covalent (Very Polar)	H \leftrightarrow F (1.9)
> 1.9	Ionic	Na (+) Cl (-) (2.1)

Problems:

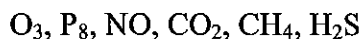
- Using a periodic table, order the following from lowest to highest electronegativity.
 - Fr, Mg, Rb
 - B, Al, C, N
 - P, As, Ga, O
 - Cl, S, P
- Using the periodic chart of the elements, place the following in order from the lowest to the highest electronegativity: F, Nb, N, Si, Rb, Ca, Pt
- Using the table above, calculate the difference in electronegativity (Δ) for each of the following bonds:
 - Cl - Cl
 - K - Br
 - Fe - O
 - H - O

6. Indicate whether the bonds between the following would be primarily covalent, polar covalent or ionic.



7. Place the following in order of increasing polarity: NaBr, I₂, H₂O, MnO₂, CN

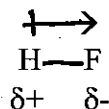
8. Which of the following molecules contain polar covalent bonds? List in order of increasing bond polarity.



9. How will the charge be distributed on each of the following molecules: HF, NO, CO and HCl?

8.3 Bond Polarity & Dipole Moments

Remember that you can determine the polarity of a bond by the size of the Δ . In the molecule HF, it is polar covalent with fluorine being the more electronegative atom. A partial negative charge (δ^-) resides on the fluorine atom and a partial positive charge (δ^+) resides on the hydrogen atom.



The arrow points to the center of the negative charge while the tail is at the center of the positive charge. A **dipole moment** means that the molecule has two poles.

The situation is clear-cut with HF. It becomes more difficult with 3 or more atoms in a molecule because the individual dipoles can cancel each other out. **Look at Table 8.2 in your book.** This shows how individual bond polarities can cancel each other out to yield a molecule with no dipole moment. Although you will be able to derive the geometries later on, you should memorize them for now.

Example 8.3A Dipole Moment

Does CHCl₃ (a tetrahedral molecule with carbon at the center) have a dipole moment? If so, show the orientation of the dipole moment.

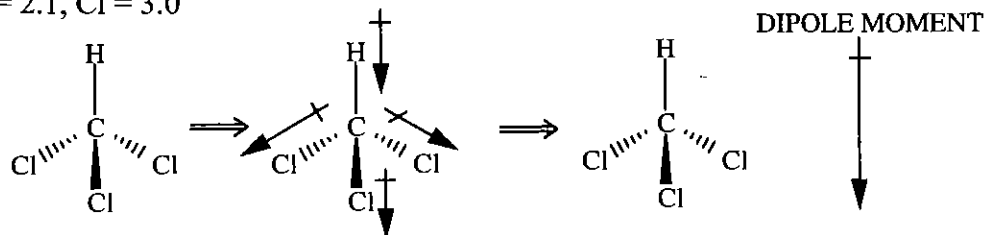
Strategy

Perform the following steps:

- Look up electronegativity of each atom.
- Draw the molecule in a 3-D space.
- Determine the polarity of each bond and the net polarity on each atom.
- Draw the dipoles and determine the direction (if any) of the molecule dipole moment.

Solution

C = 2.5, H = 2.1, Cl = 3.0

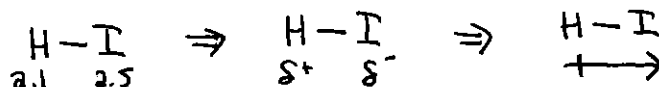
**Example 8.3B Practice with Dipole Moments**

For each of the following, determine the orientation of the dipole moment (if any).

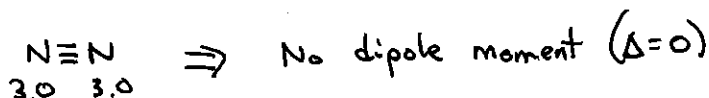
a. HI

b. N₂c. CCl₂F₂ (carbon is central atom)**Solution**

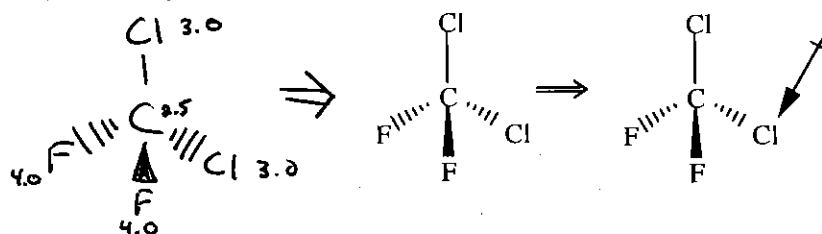
a. H = 2.5, I = 2.1



b. N = 3.0



c. C = 2.5, Cl = 3.0, F = 4.0

**Problems:**

10. Determine the orientation of the dipole of the following, if any:

a. AlCl₃ (planar w/ aluminum in the center)b. CH₃F (tetrahedral w/ carbon at center)c. N₂O (linear w/ N-N-O structure)d. AgCl₄ (planar molecule w/ Ag at center, Ag-Cl bonds 90° apart)

8.4 Ions: Electron Configurations & Sizes

Your textbook deals only w/ nonmetals, representative metals and ionic bonds in this discussion. It has been observed that atoms that form bonds in stable compounds have a **noble gas configuration**. (Each is **isoelectric** with the closest noble gas).

To determine the formula of a binary ionic compound, remember that chemical compounds are electrically neutral. For examples, the formula of the ionic compound formed from magnesium (Mg^{2+}) and chlorine (Cl^-) to form MgCl_2 .

We discussed in chapter 7, as we go down a group, ion size increases (higher energy levels have a larger average distance). Because the ratio of protons to electrons becomes greater, **cations are smaller than their neutral atoms**. Because of electron-electron repulsion and less effective shielding **anions are always larger than their neutral atoms**. The larger the charge, the more pronounced the effect. Basically, **the higher the nuclear charge, the smaller the ion**.

Problems

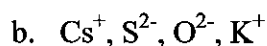
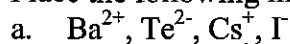
11. Determine the most stable ion for each of the following atoms and indicate which element they would be isoelectric with if they lost or gained electrons.
 - a. O
 - b. Be
 - c. I
 - d. Te
 - e. Na

12. List the four ions that are isoelectric with argon and have charges from -2 to +2. Arrange those in order of increasing atomic radius.

13. Determine the formula of the binary compound from the following sets of atoms.
 - a. Ca and O
 - b. K and Cl
 - c. Rb and S
 - d. Ba and P

14. Using shorthand notation, list the core electron configurations for the ions in the compounds in problem 13.

15. Place the following in an order of increasing atomic size.



8.5 Formation of Binary Ionic Compounds

The theme of this section is that there are many separate processes that go into forming an ionic solid. As we have said before, the ionic compound forms because its energy is lower than if its elements remained separated. However, not every part of the process is energetically favorable. Your book points out that **lattice energy**, the energy released when an ionic solid is formed from its gaseous ions, that is the most favorable, and more than makes up for some parts of the process that are energetically unfavorable. Let's examine the formation of the **KCl** ionic solid from $\text{K}(\text{s})$ and $\text{Cl}_2(\text{g})$.

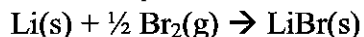
Processes that Must Occur

1. $\text{K}(\text{s})$ must form $\text{K}(\text{g})$: Energy of Sublimation = + 64 KJ
2. $\text{K}(\text{g})$ must form $\text{K}^+(\text{g})$: First Ionization Energy = +419 KJ
3. $1/2\text{Cl}_2$ must form $\text{Cl}(\text{g})$: Bond Energy $\times 1/2 = 120$ KJ
4. $\text{Cl}(\text{g})$ must form $\text{Cl}^-(\text{g})$: Electron Affinity = -349 KJ
5. $\text{K}^+(\text{g})$ must combine with $\text{Cl}^-(\text{g})$ to form $\text{KCl}(\text{s})$: Lattice Energy = -690 KJ

The net energy of formation equals the sum of the energy changes, -436 kJ. So you see that the value for any of the processes that make up salt formation can be obtained if you understand the processes involved, and are given suitable data.

Problem

16. Given the following data, determine the ΔH_f for LiBr from the equation



1. $\text{Li}(\text{s})$ must form $\text{Li}(\text{g})$: Energy of Sublimation = + 161 KJ
2. $\text{Li}(\text{g})$ must form $\text{Li}^+(\text{g})$: First Ionization Energy = +520 KJ
3. Br_2 must form $\text{Br}(\text{g})$: Bond Energy = 193 KJ
4. $\text{Br}(\text{g})$ must form $\text{Br}^-(\text{g})$: Electron Affinity = -324 KJ
5. $\text{Li}^+(\text{g})$ must combine with $\text{Br}^-(\text{g})$ to form $\text{LiBr}(\text{s})$: Lattice Energy = -787 KJ

The remainder of the section makes the point that the higher the charge on each ion, the greater the lattice energy will be. This value counteracts the higher endothermic ionization energies, thus resulting in a more energetically stable crystal.

8.8 Covalent Bond Energies and Chemical Reactions

In the beginning of this section, it is calculated that the average bond energy for a C – H bond for methane (CH₄). Assumptions made were:

1. that the energy needed to break each C – H bond was the same (413 kJ), and
2. that each of the bonds was not sensitive to its environment.

Table 8.4 in your book gives **average bond energies** for many covalent bonds. Notice that **multiple bonds** (bonds that involve sharing more than 2 electrons between atoms) require more energy to break than single bonds.

You can determine the heat of a reaction by knowing the individual bond energies. It is simply:

$$\Delta H = \Sigma D (\text{bonds broken}) - ED (\text{bonds formed})$$

where ΔH = heat of reaction and D = bond energy per mole of bonds

The key to calculating the heat of reaction from the average bond energy is to **carefully list all bonds broken and all bonds formed**. Also, recognize that it takes energy to break bonds (endothermic, $\Delta H = +$) while energy is released when bonds are formed (exothermic, $\Delta H = -$).

Example 8.8 Heat of Reaction from Bond Energy

Using data from Table 8.4 in your book, calculate ΔH for the following reaction.



Solution:

First, make a list of bonds broken and bonds formed.

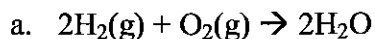
<u>Bonds Broken</u>	<u>Energy per bond (kJ)</u>	<u>Total Energy (kJ)</u>
4 C – H	413 x 4 =	1652
4 F – F	154 x 4 =	616
Total Energy to break bonds	=	2268 kJ

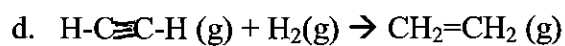
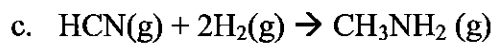
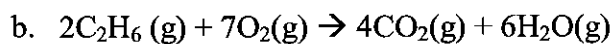
<u>Bonds Formed</u>	<u>Energy per bond (kJ)</u>	<u>Total Energy (kJ)</u>
4 C – F	485 x 4 =	1940
4 H – F	565 x 4 =	2260
Total Energy to form bonds	=	4200 kJ

$$\Delta H = (\text{Energy to break bonds}) - (\text{Energy to form bonds}) = 2268 \text{ kJ} - 4200 \text{ kJ} = -1932 \text{ kJ (exothermic)}$$

Problems

17. Using bond energy values from Table 8.4 in your book, calculate the ΔH for the following reactions:





18. Compare the values obtained in part "d" of problem 17 to ΔH values calculated from ΔH_f° data in Appendix 4 of your book.

8.9 The Localized Electron Bonding Model

If you can answer the following review questions, you understand the important ideas in this brief section.

1. What are the two covalent bonding models?

2. What is the difference in the basic assumptions about electron position in these models?
3. Why is the MO model somewhat unsuitable for use with larger molecules?
4. What information can the MO model give us that the LE model doesn't?
5. What are lone pairs and bonding pairs?
6. What are the parts of the LE model?

8.10 Lewis Structures

Lewis structures are often used to depict bonding pairs and lone pairs in molecules. We are concerned only with valence electrons because these are the ones (for period 1 and 2 atoms) that are involved in bond making and breaking.

Individual atoms are represented with Lewis structures by putting valence electrons (as dots or circles) around the atomic symbol. For example, magnesium ($[\text{Ne}]3s^2$) would be represented as: $\bullet\text{Mg}\bullet$. Mg^{2+} would be simply Mg. It no longer has valence electrons. Chlorine ($[\text{Ne}]3s^23p^5$) would be $\bullet\ddot{\text{Cl}}\bullet$ and Cl^- would be $\text{:}\ddot{\text{Cl}}\text{:}$.

Problem

19. Draw Lewis dot structures for the following atoms or ions.

- a. N b. N^{3-} c. I d. Ba e. Ba^{2+}

EVERY PERIOD 1 AND 2 ELEMENT (with the exception of H, He, B, and Be) CAN FORM COMPOUNDS OF LOWEST ENERGY IF THEIR HIGHEST ENERGY LEVELS ARE FILLED (s^2p^6). THIS IS CALLED THE OCTET RULE. If an ion or atom observes the octet rule, we will say that it is "happy." Hydrogen is "happy" if its 1s orbital is filled. We will discuss boron and beryllium later on.

Your book discusses a strategy for drawing Lewis structures. Here is a different approach. Use the one you feel more comfortable with.

Strategy for Writing Lewis Structures

- 1. Total number of valence electrons in the system:** Sum the number of valence electrons on all the atoms. Add the total negative charge if you have an anion. Subtract the charge if you have a cation.

Ex. CO_3^{2-}	C has 4 valence electrons	= 4
	O has 6 valence electrons x 3 atoms	= 18
	Charge on ion is -2 so add	= 2
	Electrons in system	= 24

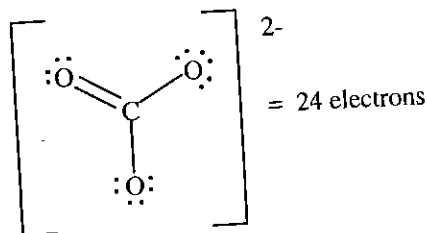
- 2. Number of electrons if each atom is to be "happy":** Atoms in our examples will need 8 electrons (octet rule) or 2 electrons (hydrogen).

	C needs 8 electrons	= 8
	O needs 8 electrons x 3 atoms	= 24
	Electrons for happiness	= 32

- 3. The number of bonds in the system:** Covalent bonds are made by sharing electrons. You need 32 electrons and you have 24. You are 8 electrons deficient. If you make 4 bonds (with 2 electrons per bond), you will make up the deficiency. Therefore,

$$\# \text{ of bonds} = \frac{\text{happiness electrons} - \text{system electrons}}{2} = \frac{32 - 24}{2} = 4 \text{ bonds}$$

- 4. Draw the structure.** The central atom is carbon. The oxygen atoms surround it. Because there are 4 bonds, there will be two single bonds and one double bond. Each bond accounts for two electrons. Then, complete the octets by putting electrons around each atom. Double-check your results by counting the total electrons in the system.



We will discuss resonance in this system later on.

Problems

- Write the Lewis Structure for the following molecules and polyatomic ions. (All which obey the octet rule.)
 - OCl^-

b. CH_3OH (C is central atom with $-\text{OH}$)

c. AsO_4^{3-}

d. SO_2

e. N_2

21. Draw Lewis structures for the following species (the skeleton is indicated by the way the molecule is written):

a. $\text{H}_2\text{N}-\text{OH}$

b. $\text{H}_2\text{C}-\text{CO}$

c. $\text{H}_2\text{C}-\text{N}-\text{N}$

8.11 Exceptions to the Octet Rule

Although your book deals with boron and beryllium in this section, we will focus on the more general case of **central atoms that can exceed the octet rule**. This can happen because there are **empty d orbitals** that shared electrons can occupy. This can happen with the third period elements.

Writing Lewis Structures for Octet Rule Exceptions

To determine if you have an exception to the rule, proceed as if your molecule obeys the octet rule. Let's use ICl_3 as an example.

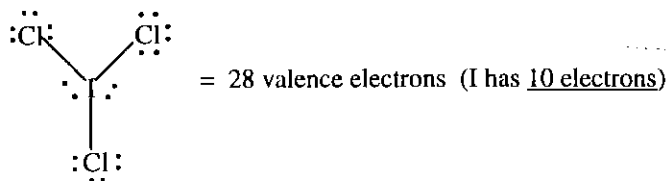
$$\begin{array}{rcl} 1. \text{ Total valence electrons} & = 7 \text{ for the I} & = 7 \\ & \underline{7 \text{ per Cl} \times 3 = 21} & \\ \text{valence } e^- & & = 28 \end{array}$$

$$\begin{array}{rcl} 2. \text{ Total if happy} & = 8 \text{ for the I} & = 8 \\ & \underline{8 \text{ per Cl} \times 3 = 24} & \\ e^- \text{ if happy} & & = 32 \end{array}$$

$$3. \text{ \# of bonds} = (32-28)/2 = 2 \text{ bonds}$$

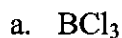
CAUTION! We have 2 bonds for 3 chlorine atoms! **There are not enough bonds to account for all the atoms!** This is how you know we have an exception to the octet rule.

To write Lewis structure of exceptions, draw the structure with one bond to each ligand, complete the octets, and add any extra electrons with the central atom. With ICl_3 ,

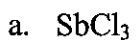


Problems

22. Draw Lewis structures for the following:

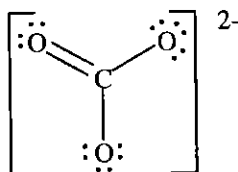


23. Draw Lewis structures for the following:

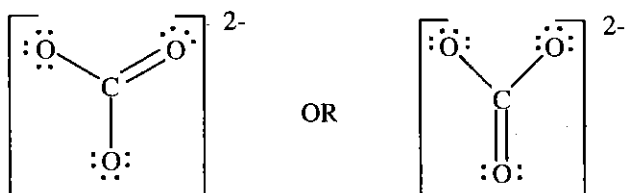


8.12 Resonance

Recall the example of CO_3^{2-} that we did at the beginning of Section 8.10. We determined the Lewis structure to be:



However, the double bond could have been placed on any of the three oxygens.



Measurements in bond lengths suggest that all three C – O bonds are equivalent. Electrons move around the entire molecule. There, the actual structure is a time-average of all these structures. These structures are called **resonance** structures. The Lewis structure of the molecule can be drawn any of the three ways. The double bond seems to resonate between the carbon and oxygen atoms.

Formal Charge and Resonance

Formal charge is “the difference between the number of valence electron on the free atom and the number of valence electrons assigned to the atom in a molecule. Formal charge is a computational device based on a localized electron (LE) model, and as such is not perfect. To determine a formal charge, we need to know:

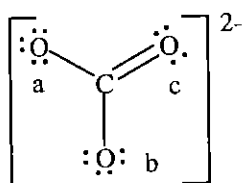
1. How many electron an atom “owns.”

Electrons owned = (# of valence electrons around the atom + # of bonds)
(# of bonds = $\frac{1}{2}$ # of shared electrons)

2. The formal charge on an atom.

Formal Charge = # of valence electrons on the neutral atom - # of electrons owned based on the resonance structure you drew.

Lets look at CO_3^{2-} again.

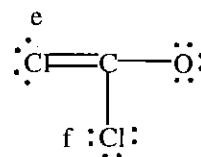
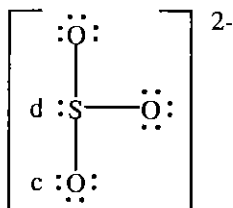
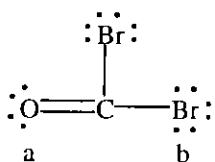


- Carbon owns 4 electrons (4 bonds). The formal chare on carbon = 4 valence electron on neutral atom minus 4 electrons owned = 0.
- Oxygen_a has 6 valence electrons and 1 bond. It owns 7 total valence electrons. The formal charge = 6 valence electrons on the neutral atom minus 7 electrons owned = -1.
- Oxygen_b has the same formal charge as oxygen_a = -1.
- Oxygen_c has 4 valence electrons and 2 bonds. It owns 6 total valence electrons. The formal charge = 6 valence electrons on the neutral atom minus 6 electrons owned = 0.

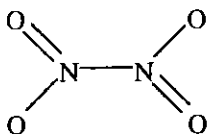
The sum of the formal charges, $0 + (-1) + (-1) + 0 = -2$, must always equal the charge on the ion (or molecule, if that what you're dealing with. Your book states you can write nonequivalent Lewis structures (different # of single and double bonds) for a molecule or ion, those with formal charges closest to zero and with any negative formal charges on the most electronegative atoms are considered to best describe the bonding.

Problems

24. Assign formal charges to each of the labeled atoms.



25. Draw the remaining resonance forms for N_2O_4 .



26. Hydrazine, N_2H_4 , is used as a propellant on the Space Shuttle. Draw all reasonable structures for N_2H_4 and assign formal charges.

27. Draw a Lewis structure and any resonance forms of benzene, C_6H_6 . Benzene consists of a ring of 6 carbon atoms with single hydrogen bonded to each carbon.

8.13 Molecular Structure: The VSEPR Model

The Valence Shell Electron Pair Repulsion (VSEPR) model assumes that atoms will orient themselves so as to minimize electron pair repulsions around the central atom.

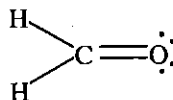
Memorize the information in Table 8.6 in your book. Each lone pair or bond around the central atom occupies a position in space. The effect of lone pairs around the central atom is to squeeze bonded pairs closer together (see your book's discussion regarding bond angles in CH_4 , NH_3 , and H_2O). Multiple bonds are counted as "one bonding pair" in the VSEPR model, because the double bonds are constrained in space. Let's determine the VSEPR structure of formaldehyde, H_2CO , together.

Step 1: Determine the Lewis Structure.

Total valence electrons = 12

Total if happy = 20

of bonds = 4



Step 2: Count the number of bonds and lone pairs on the central atom.

$$2 \text{ C-H} + 1 \text{ C=O} = 3 \text{ bonds}$$

Step 3: Determine the geometry based on Table 8.6 in your book.

$$3 \text{ "electron pairs"} = \text{trigonal planar}$$

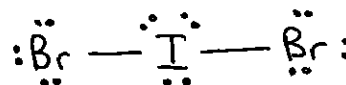
Now, let's try Ibr_2

Step 1: Determine the Lewis Structure.

Total valence electrons = 22

Total if happy = 24

of bonds = 1 **EXCEPTION TO OCTET RULE!!!!**

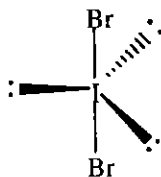


Step 2: Count the number of bonds and lone pairs on the central atom.

There are 2 bonds and 3 lone pairs around the central atom for a total of 5 electron pairs.

Step 3: Determine the geometry based on Table 8.6 in your book.

5 "electron pairs" = trigonal bipyramidal. The electron pairs will orient in the equatorial positions first, (see discussion in the book) and the bonding pairs will make up the remaining positions.

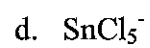
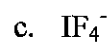
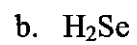
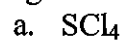


The molecule will be linear.

(Note that when we draw VSEPR structures, we are only concerned with the central atom. We often omit valence electrons around the ligands.)

Problems

28. Using VSEPR model, determine the molecular geometry for each of the following molecules:



Polarity of Molecules

Covalent bonds and molecules held together by such bonds may be

polar. As a result of unsymmetrical distributions of electrons, the bond or molecule contains a positive and a negative pole and is therefore a *dipole*.

nonpolar. A symmetrical distribution of electrons leads to a bond or a molecule with no positive or negative poles.

It is easy to determine if a bond is polar or nonpolar. Simply consult a table of electronegativity values. Calculate the electronegativity difference (ΔEN) between the two atoms involved in the bond. If the ΔEN is greater than 0.4, the bond is considered to be polar. The atom with the greater electronegativity value is the negative pole in the bond.

A polar molecule contains positive and negative poles. If a molecule is diatomic, it is easy to decide whether it is polar or nonpolar. However, if a molecule contains more than two atoms, it is not so easy to determine whether it is polar or nonpolar. In this case, not only bond polarity but also molecular geometry determines polarity.

There are two criteria for determining polarity of a molecule; bond polarity and molecular geometry. *If the polar A-X bonds and electron pairs in a molecule AX_mE_n are arranged symmetrically around the central atom A, the molecule is nonpolar.*

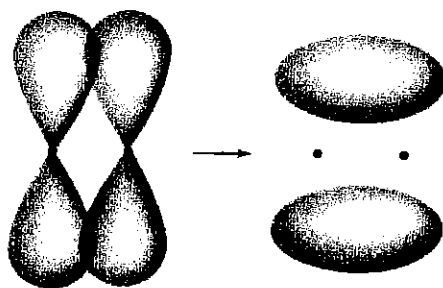
Note: It is possible for a molecule to have polar bonds and NOT be a polar molecule (i.e. dipole). An example of this is CO_2 (see previous table).

Multiple Bonds: Sigma (σ) and Pi (π) Bonds

It was noted that, in counting the number of electron pairs surrounding an atom in determining hybridization, double and triple bonds were treated as a single electron pair. What happened to those electrons? Where are they?

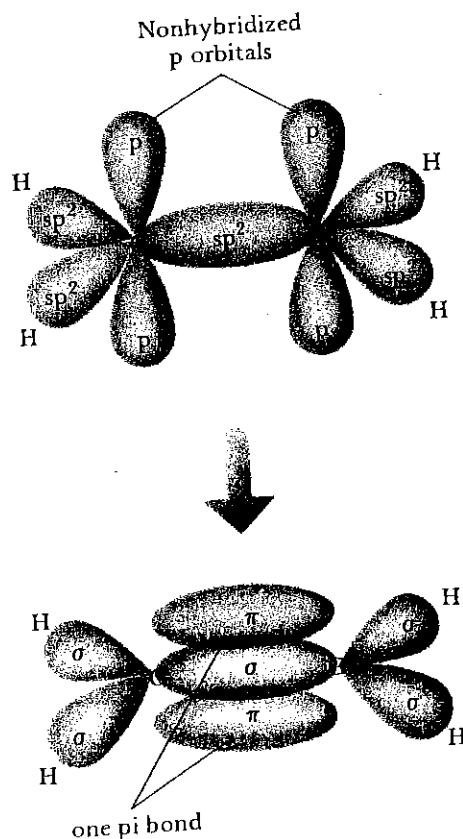
To answer this question, it is necessary to consider the shape or spatial arrangement of the orbitals filled by bonding electrons in molecules. From this point of view, two different types of bonding orbitals can be distinguished. The first, and by far the most common, is called a **sigma** (σ) bonding orbital. Hybrid orbitals involved in bonds are of this type. A sigma bonding orbital consists of a single lobe in which the electron density is concentrated in the region directly between the two atoms.

Multiple bonds use not only hybridized orbitals but also unhybridized p orbitals in their formation. Bonds using unhybridized p orbitals are called pi (π) bonding orbitals and have a quite different shape.



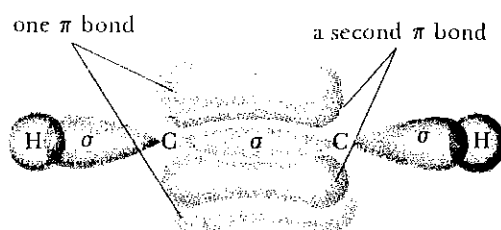
In a pi bond, the electron density is concentrated in two lobes, one above the bond axis, the other below it. Pi bonds are formed when two p orbitals overlap side-to-side.

The geometries of bonding orbitals in ethylene (C_2H_4), and acetylene (C_2H_2) are shown below.



The nature of the π bond in C_2H_4 prohibits rotation around the carbon-carbon bond. The π bond consists of two lobes, one above the bond axis and the other below it. Along the bond axis itself, the electron density is zero. The π bond is in a fixed position in the plane of the paper. The geometry around each carbon atom is trigonal planar.

In C_2H_2 , the two π bonding orbitals, both of which consists of two lobes, are orientated at right angles to each other. This is difficult to show in a two-dimensional figure. In effect, the four lobes of the two π bonds are wrapped around the central σ bond like a bun around a hot dog.



Bonding in acetylene,
 C_2H_2 .

In general, to find the number of σ and π bonds in a molecule, remember that:

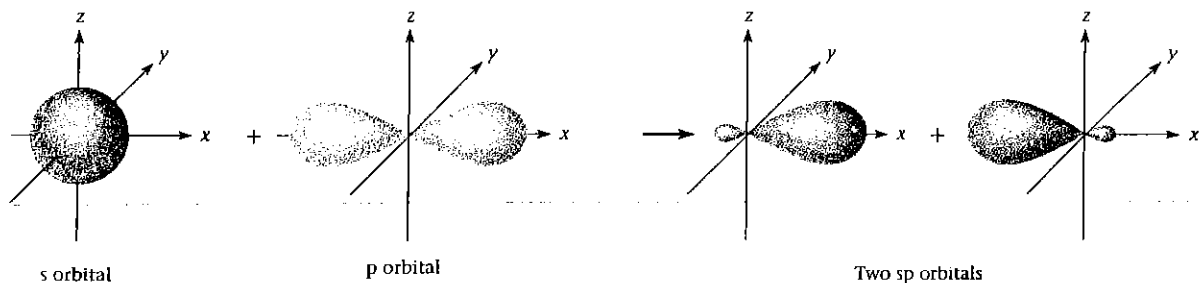
1. All single bonds are sigma bonds using hybrid orbitals.
2. If the molecule has a double bond, one of the bonds is a sigma bond using hybrid orbitals and the other is a pi bond using unhybridized p orbitals.
3. If the molecule has a triple bond, one of the bonds is sigma using hybridized orbitals and the other two are pi using unhybridized p orbitals.

Chemical Bonding

Molecular Geometry and Properties of Molecules

Hybridization

When atoms approach to form a chemical bond, the atomic orbitals of each atom undergo a significant change. Atomic orbitals are mixed or *hybridized* to form new bonding orbitals which have a characteristic shape as shown below.



Formation of sp hybrid orbitals. The mixing of an s orbital with a p orbital gives two sp hybrid orbitals.

Hybridization occurs with s , p and the d orbitals. The d orbital sublevel does not appear until the filling of the third energy level (row 3 of the periodic table).

The number of hybrid orbitals formed is equal to the number of atomic orbitals mixed.

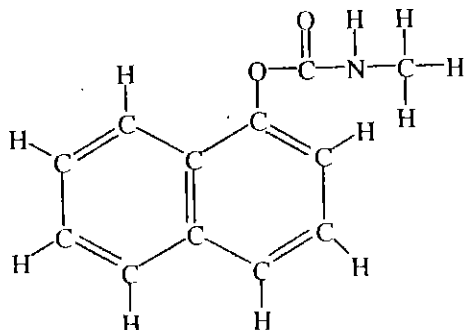
In general, it is found that both *unshared as well as shared electron pairs are located in hybrid orbitals*. In determining the number of hybrid orbitals surrounding an atom in a molecule, simply draw the Lewis structure and count all the electron pairs (shared and unshared) surrounding the individual atom. *Note: In determining the number of electron pairs, double and triple bonds are treated as a single pair.*

Hybrid Orbitals and Their Geometries

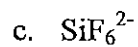
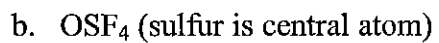
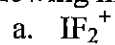
Number of Electron Pairs	Atomic Orbitals	Hybrid Orbitals	Orientation	Examples
2	s, p	sp	linear	$\text{BeF}_2, \text{CO}_2$
3	$s, \text{ two } p$	sp^2	triangular planar	BF_3, SO_3
4	$s, \text{ three } p$	sp^3	tetrahedron	$\text{CH}_4, \text{NH}_3, \text{H}_2\text{O}$
5	$s, \text{ three } p, d$	sp^3d	triangular bipyramid	$\text{PCl}_5, \text{SF}_4, \text{ClF}_3$
6	$s, \text{ three } p, \text{ two } d$	sp^3d^2	octahedron	$\text{SF}_6, \text{ClF}_5, \text{XeF}_4$

Problems:

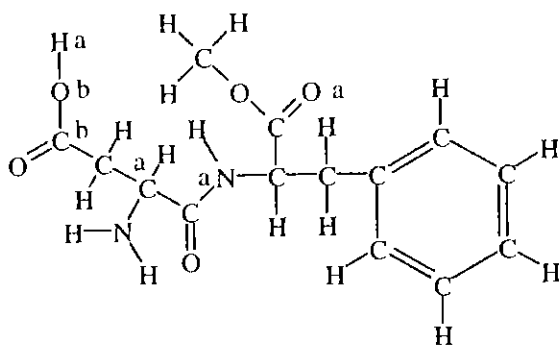
1. How many σ bonds are there in the commercial insecticide, "Sevin" shown below? How many π bonds?



2. Give the hybridization and predict the geometry of each of the atoms in the following molecules or ions.



3. Answer the following questions regarding Aspartame (Nutra-sweet).



- How many σ bonds are in the molecule?
- How many π bonds?
- What is the hybridization on carbon "a"? Carbon "b"?
- What is the hybridization on nitrogen "a"? Oxygen "a"?
- What is the $C_b-O_b-H_a$ bond angle?