

# Chapter 8: Covalent Bonding and Molecular Structure



## Chapter In Context

In this chapter and the next, we examine chemical bonding in detail. We examined ionic bonding briefly in Chapter 2 and will do so in more detail in Chapter 11. We will also examine intermolecular forces in detail in Chapter 11. Here we will apply what you have learned about atomic structure (Chapter 6), electron configurations, and periodic trends (Chapter 7) to the chemical bonds formed between atoms and ions and the shapes of molecules and ions that contain covalent bonds.

- **Biology:** Molecular shape of enzymes specifically allow only certain reactions to occur. Drugs are developed that specifically fit into active sites in the enzyme to affect or even stop its action.

## Chapter 8

- 8.1 Interactions Between Particles: Coulomb's Law
- 8.2 Covalent Bonding Basics
- 8.3 Lewis Structures
- 8.4 Bond Properties
- 8.5 Electron Distribution in Molecules
- 8.6 Valence-Shell Electron-Pair Repulsion Theory and Molecular Shape
- 8.7 Molecular Polarity

## Chapter Goals

- Apply Coulomb's Law.
- Understand forces involved in covalent bonding.
- Write Lewis symbols and Lewis structures.
- Predict bond properties.
- Understand charge distribution in molecules.
- Use VSEPR theory.
- Identify polar and nonpolar species.

## 8.1 Interactions Between Particles: Coulomb's Law



OWL Opening Exploration  
8.1 Coulomb's Law

Matter is made up of atoms and ions that experience both attractive and repulsive forces. The strength of the force holding oppositely charged particles together in any material is described by **Coulomb's Law** (equation 8.1). According to this law, force of attraction or repulsion between two charged species is directly proportional to the magnitude of the charge on the particles ( $q_A$  and  $q_B$  in equation 8.1) and inversely proportional to the square of the distance between the two particles ( $r$  in equation 8.1).

$$\text{Force} \propto \frac{(q_A)(q_B)}{r^2} \quad (8.1)$$

For electrons,  $q = -e$ , and for nuclei,  $q = +Ze$   
 where  $e$  = magnitude of electron charge ( $1.6022 \times 10^{-19}$  C)  
 $Z$  = nuclear charge (number of protons)  
 $r$  = distance between particles A and B

All chemical attractive forces involve opposite charges, such as those between protons in a nucleus and the electrons surrounding that nucleus, and between positive and negative ions. The type and strength of these attractive forces allow us to categorize the different types of bonding found in matter (Table 8.1). In **ionic bonding**, found in ionic solids and liquids such as NaCl and CaCO<sub>3</sub>, there are strong attractive forces between positively and negatively charged ions. **Covalent bonding**, the attractive forces between electrons and nuclei on adjacent atoms within a molecule, occurs in compounds such as H<sub>2</sub>O and NH<sub>3</sub>. Another type of attraction takes place in pure metals. **Metallic bonding**, the attractive forces between electrons and nuclei in metals, occurs in metals such as Cu and Fe and will be discussed in more detail in Chapter 9. Finally, there are forces that exist between molecules, called **intermolecular forces**, which will be discussed in more detail in Chapter XX.

**Table 8.1 Types of Chemical Bonding**

Type of Interaction	Source of Attractive Forces
Ionic Bonding	Oppositely charged ions
Covalent Bonding	Nuclei and valence electrons
Metallic Bonding	Nuclei and electrons
Intermolecular Forces	Partial charges on individual, separate molecules

## 8.2 Covalent Bonding Basics



OWL Opening Exploration  
8.2

A covalent bond is characterized by the sharing of valence electrons by two adjacent atoms. This happens most often between nonmetal elements such as carbon, hydrogen, oxygen and nitrogen.

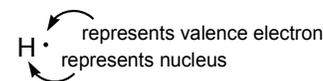
For example, consider a simple covalently bonded molecule, H<sub>2</sub>. When two isolated H atoms are at a great distance from one another, they feel no attractive or repulsive forces. However, as the atoms approach more closely, the attractive and repulsive forces between the two atoms become important.

### Chapter Goals Revisited

- Apply Coulomb's Law
- Understand relationship between charge, distance, and force of attraction or repulsion.**

### Chapter Goals Revisited

- Understand forces involved in covalent bonding.
- Identify attractive and repulsive forces between atoms.**



There are two types of repulsive forces between the two atoms. First, the nuclei repel because they are both positively charged. Second, the electrons repel because they are both negatively charged. The attractive forces between the two atoms result from the interaction between the positively charged nucleus on one hydrogen atom and the negatively charged electron on the other hydrogen atom. In summary, for two hydrogen atoms,  $H_A$  and  $H_B$ ,

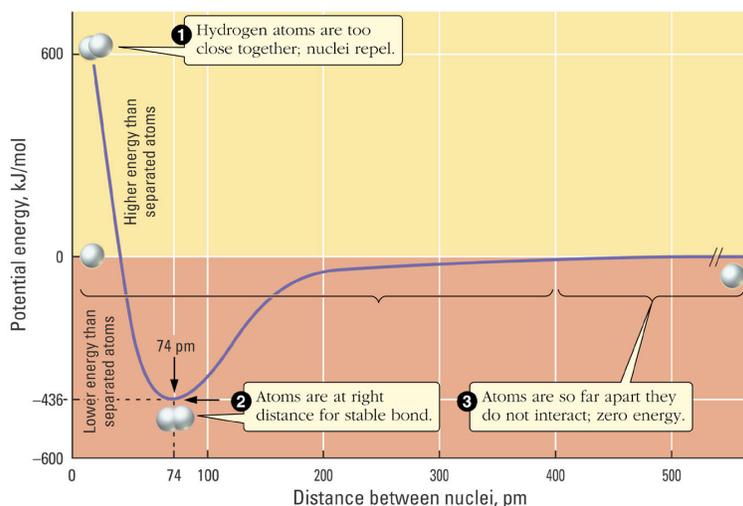
Repulsive Forces:    electron A – electron B  
                              nucleus A – nucleus B

Attractive Forces:    electron A – nucleus B  
                              electron B – nucleus A

In general, when two atoms approach each other, these repulsive and attractive forces always occur. When the attractive forces are greater than the repulsive forces, a covalent bond forms. When the repulsive forces are greater than the attractive forces, a covalent bond does not form and the atoms remain isolated.

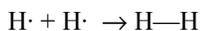


The balance between the attractive and repulsive forces in  $H_2$  is related to the distance between H atoms, as shown in Figure 8.1. At large distances, neither attractive nor repulsive forces are important and no bond forms between H atoms. At short distances, repulsive forces are stronger than attractive forces and no bond forms.



**Figure 8.1** Energy of  $H_2$  as a function of internuclear distance

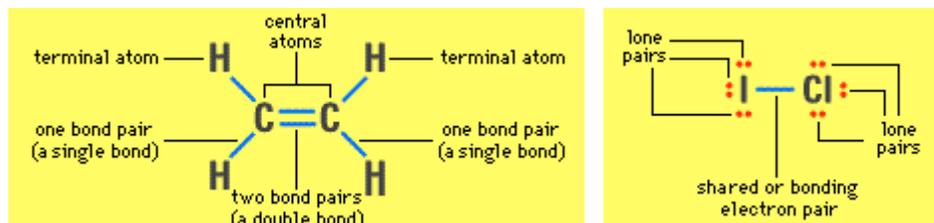
At an internuclear distance where the attractive forces are stronger than the repulsive forces, a bond forms between the H atoms. The two valence electrons “pair up” and are shared between the two hydrogen nuclei in a covalent bond that is represented by a single line connecting the H atoms.



The single line between H atoms in  $H_2$  is a very useful representation of a chemical bond, but it does not give an accurate picture of the distribution of bonding electrons in the

**Flashforward**  
9.6 Molecular Orbital Theory



Figure 8.3 Lewis structures for  $C_2H_4$  and  $ICl$ .

Lewis structures are very useful in visualizing the physical and chemical properties of compounds made up of nonmetal elements. We will begin by learning how to create Lewis dot structures, and then in the following sections use Lewis structures to explore bond properties (bond order, bond length, bond energy, bond polarity), the shapes of molecules, molecular polarity, and how the shape and polarity of molecules influence chemical properties.

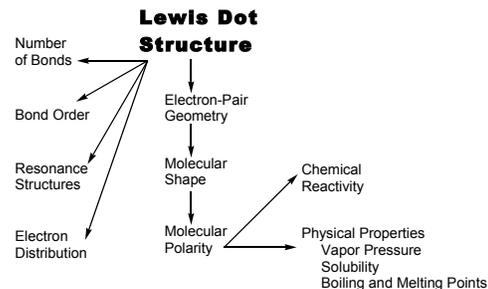
### Drawing Lewis Structures

The most important guideline to follow when drawing Lewis structures is the octet rule. The **octet rule** states that most atoms in a Lewis structures are surrounded by no more than 8 electrons (shared bonding electrons and unshared nonbonding electrons). The octet rule is related to the fact that valence shells contain a single *s* orbital and three *p* orbitals that can accommodate up to 8 electrons, and it is these orbitals that are most often involved in forming covalent bonds between nonmetals in covalent compounds. There are, however, some exceptions to the octet rule.

- Hydrogen has a single valence electron in a 1s orbital and therefore only accommodates two electrons when it forms covalent bonds. It typically forms only one chemical bond to another atom and does not have lone pairs in Lewis structures.
- Beryllium and boron often accommodate only 4 or 6 electrons, respectively, in Lewis structures.
- Elements with available empty d orbitals in the valence shell (elements in the third period and below) can accommodate more than eight electrons (often 10 or 12).

When determining if elements have satisfied octets, assign lone pairs of electrons to the element they are placed around, and divide bonding electrons equally between the two atoms that are connected by the bond.

In addition to the octet rule, it is helpful to remember that only the elements C, N, O, P, and S typically form double and triple bonds with other elements. Lewis structures are drawn by following the five steps shown in the examples below.



#### Chapter Goals Revisited

- Write Lewis symbols and Lewis structures.  
**Use octet rule to write Lewis symbols.**

	Example: PF <sub>3</sub>	Example: CO <sub>2</sub>
<b>Step 1: Count Valence Electrons</b> Count the total number of valence electrons in the molecule or ion. Anions have extra electrons, so add 1 electron for each negative charge. Cations have a deficiency of electrons, so subtract 1 electron for each positive charge.	Phosphorus has 5 valence electrons and each fluorine has 7 valence electrons. $5 + (3 \times 7) = 26$ electrons (or 13 electron pairs)	Carbon has 4 valence electrons and each oxygen has 6 valence electrons. $4 + (2 \times 6) = 16$ electrons (or 8 electron pairs)
<b>Step 2: Arrange Atoms</b> The central atom is usually the one with the lowest affinity for electrons (the one farthest from fluorine on the periodic table). Exception: H is never a central atom	F   P   F F	O   C   O
<b>Step 3: Add Single Bonds</b> Add one bond (using a line) between each terminal atom and the central atom. Each bond represents 2 electrons.	F — P — F   F 26 electrons – 6 bonding electrons = 20 electrons remaining	O — C — O 16 electrons – 4 bonding electrons = 12 electrons remaining
<b>Step 4: Add Remaining Electrons</b> Assign any remaining electrons to the terminal atoms, in pairs, until the octet rule is satisfied for each terminal atom (except hydrogen). If additional electrons remain, add them to the central atom.	:F — P — F:   :F: Each F needs 3 pairs to satisfy the octet rule, and the one remaining pair is assigned to P	:O — C — O: Each O needs 3 pairs to satisfy the octet rule. No other electrons remain to satisfy the octet rule for C.
<b>Step 5: Octet Rule Check</b> Use the octet rule to determine if multiple bonds are necessary between atoms. If there is an electron deficiency for an element, change a non-bonding electron pair (lone pair) on an adjacent atom into a bonding pair. Continue only until the octet rule is satisfied for all elements (other than the known exceptions).	:F — P — F:   :F: All elements have complete octets.	:O — C — O: ↓ :O = C = O: The central atom is sharing only 4 electrons. Use one lone pair on each oxygen to make a second bond to carbon, satisfying the octet rule.

The steps above can also be applied to the Lewis structures of ions. When drawing the Lewis structure for an ionic species, the structure is placed within square brackets and the ion charge is shown outside the brackets. For example, the steps required to draw the Lewis structure for  $\text{SO}_3^{2-}$  are shown below.

**Step 1:** Sulfur has 6 valence electrons, each oxygen has 6 valence electrons, and the 2- charge on the ion adds two more electrons

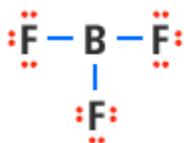
$$6 + (3 \times 6) + 2 = 26 \text{ valence electrons (or 13 pairs)}$$



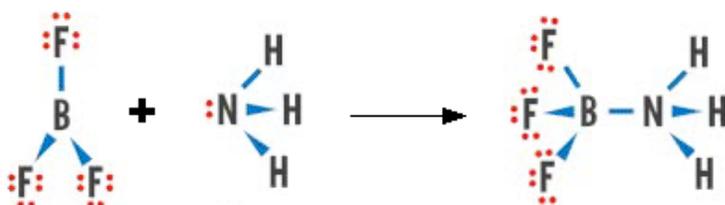
OWL Example Problems  
8.5 Drawing Lewis Structures: Tutor

### Exceptions to the Octet Rule

Beryllium and boron are often found with fewer than 8 electrons in **electron deficient** compounds, compounds in which an element has an incomplete octet. For example,  $\text{BF}_3$  is an electron deficient compound.

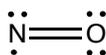


Each fluorine has a complete octet (6 nonbonding electrons + 2 bonding electrons), but boron has only 6 electrons (6 bonding electrons and no lone pairs). Changing a fluorine lone pair to a bonding pair would alleviate the electron deficiency, but neither element commonly forms multiple bonds. The electron deficiency affects the reactivity of  $\text{BF}_3$ . Consider the reaction between  $\text{BF}_3$  and  $\text{NH}_3$ ,



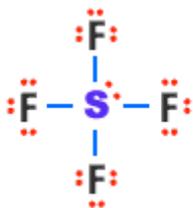
In this reaction, the lone pair on N is used to form a bond to B. Following the reaction, both N and B have full octets and the compound is not electron deficient.

A second exception to the octet rule that also involves elements with incomplete octets occurs in odd-electron molecules, also called **free radicals**. Nitrogen monoxide (nitric oxide,  $\text{NO}$ ) is an odd-electron molecule with 11 valence electrons.



Free radicals are highly reactive species because they have an unpaired electron that can react with other molecules. Pure  $\text{NO}$  reacts readily with other molecules such as the halogens,  $\text{O}_2$ , and other free radicals.

Compounds with a central atom that is an element in the third period or below in the periodic table occasionally have more than 8 electrons associated with the central atom. The central atom in these compounds have an **expanded valence**. Consider  $\text{SF}_4$ .



Each fluorine has a satisfied octet (6 nonbonding electrons + 2 bonding electrons), but the central sulfur atom has 10 electrons around it (8 bonding electrons and 2 nonbonding electrons).

#### Chapter Goals Revisited

- Write Lewis symbols and Lewis structures.  
**Recognize exceptions to octet rule when writing Lewis symbols.**

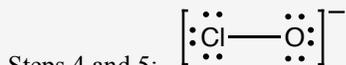
**EXAMPLE PROBLEM: Drawing Lewis Structures**

Draw the Lewis structure for

- (a)  $\text{ClO}^-$   
 (b)  $\text{IBr}_3$

**SOLUTION:**

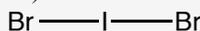
- (a) Step 1:
- $7 + 6 + 1 = 14$
- valence electrons (or 7 pairs)

Steps 2 and 3:  $\text{Cl} - \text{O}$ 

Steps 4 and 5:

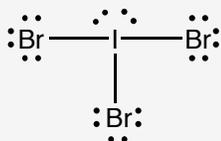
The Lewis structure includes the ion charge outside square brackets.

- (b) Step 1:
- $7 + (3 \times 7) = 28$
- valence electrons (or 14 pairs)



Steps 2 and 3:

Iodine has a lower affinity for electrons than bromine, so it is the central atom.



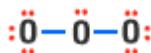
Steps 4 and 5:

Iodine is in the fifth period and therefore can have an expanded valence.

*OWL Example Problems**8.6 Exceptions to the Octet Rule: Tutor**8.7 Drawing Lewis Structures: Exercise**8.8 Drawing Lewis Structures**8.9 Free Radicals***Resonance Structures**

Some molecules have more than one valid Lewis structure. Two or more valid Lewis structures for a species that differ only in the arrangement of electrons, not the arrangement of atoms, are called **resonance structures**. A **resonance hybrid** is the actual electron arrangement for the molecule or ion, and it is intermediate between the resonance structures but not represented by any of the individual resonance structures. There is a great deal of experimental evidence to support resonance, including bond distances and angles that cannot be explained by the existence of a single Lewis structure for a molecule or ion.

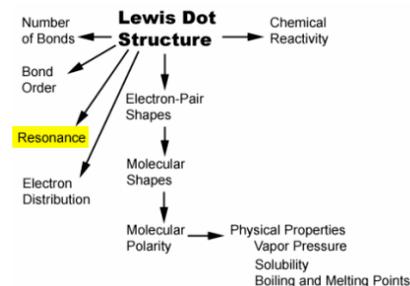
Consider the case of ozone,  $\text{O}_3$ . Completing the first four steps of drawing its Lewis structure results in the following structure for ozone.



To complete the Lewis structure, the central oxygen needs one more pair of electrons. Both terminal oxygens have lone pairs that can be changed to shared bonding pairs, completing the octet for the central oxygen. There are therefore two possible Lewis structures for  $\text{O}_3$ , and they are drawn separated by a double-headed arrow.

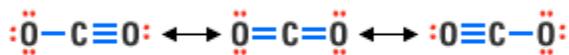


The two resonance structures for ozone suggest that the oxygen-oxygen bonds in this molecule are not single bonds or double bonds, but something in between. The resonance hybrid, which is not represented by either resonance structure, has oxygen-oxygen bonds that have equivalent properties such as length and energy.

**Chapter Goals Revisited**

- Write Lewis symbols and Lewis structures.
- Understand relationship between resonance structures and resonance hybrid.**

The ozone resonance structures are equivalent to one another because they contain the same number and type of chemical bonds. Not all resonance structures are equivalent, however. For example, carbon dioxide has three resonance structures and they are not all equivalent.



The first and third resonance structures are equivalent because each contains one carbon-oxygen triple bond and one carbon-oxygen single bond. The middle resonance structure is unique because it has two carbon-oxygen double bonds. Later in this chapter we will look more closely at the electron distribution in molecules and will see how to use that information to determine the most likely resonance structure for a molecule or ion

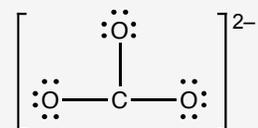
**Flashforward**  
8.5 Electron Distribution

#### EXAMPLE PROBLEM: Resonance Structures

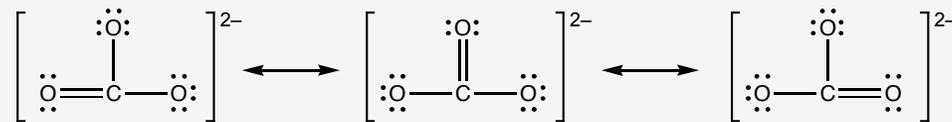
Draw all resonance structures for the carbonate ion,  $\text{CO}_3^{2-}$ .

#### SOLUTION:

The incomplete Lewis structure (octet rule not satisfied for carbon) is



The electron deficiency for carbon is corrected by changing a lone pair on an adjacent oxygen into a bonding pair. There are three oxygen atoms with lone pairs that can correct the carbon electron deficiency, so there are three equivalent resonance structures for the carbonate ion.



*OWL Example Problems*  
8.10 Resonance Structures: Tutor  
8.11 Resonance Structures

## 8.4 Bond Properties

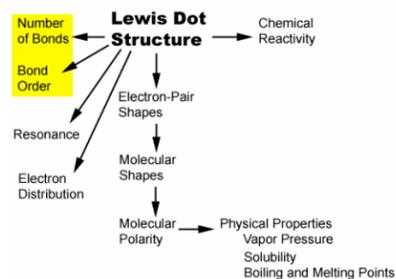


*OWL Opening Exploration*  
8.12

The properties of the chemical bonds in a molecule affect its chemical and physical properties. For example, nitrogen,  $\text{N}_2$ , is very unreactive because of the strong triple bond between nitrogen atoms. Hydrazine,  $\text{N}_2\text{H}_4$ , has a weaker nitrogen-nitrogen single bond that contributes to its high reactivity and its use as a rocket fuel. One factor that has a great influence on bond properties is **bond order**, the number of bonding electron pairs between two bonded atoms. The bond order of a carbon-carbon single bond is 1, for example, while a carbon-carbon double bond has a bond order of 2 and a carbon-carbon triple bond has a bond order of 3.

### Bond Length

As we saw earlier, chemical bonds form when attractive forces between atoms are stronger than repulsive forces. The distance between the atomic nuclei when energy is minimized is the **bond length** (Figure 8.4).



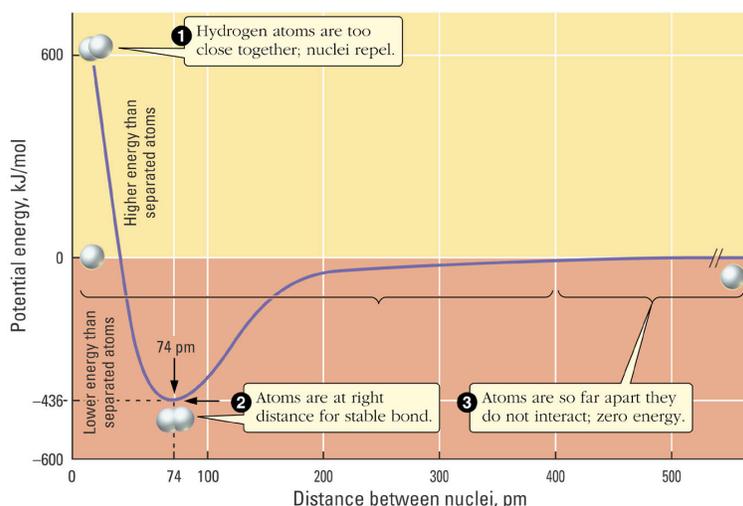


Figure 8.4 H—H bond formation

Accurate bond distances are determined from careful measurements using techniques such as X-ray crystallography. Bond lengths between two different elements vary slightly between compounds. For that reason, average bond lengths are reported in tables such as the one shown below (Table 8.2).

Table 8.2. Average Bond Lengths

Single Bond Lengths, pm											
	H	C	N	O	F	Si	P	S	Cl	Br	I
H	74	110	98	94	92	145	138	132	127	142	161
C		154	147	143	141	194	187	181	176	191	210
N			140	136	134	187	180	174	169	184	203
O				132	130	183	176	170	165	180	199
F					128	181	174	168	163	178	197
Si						234	227	221	216	231	250
P							220	214	209	224	243
S								208	203	218	237
Cl									200	213	232
Br										228	247
I											266

Multiple Bond Lengths, pm			
C=C	134	C≡C	121
C=N	127	C≡N	115
C=O	122	C≡O	113
N=O	115	N≡O	108

The data in Table 8.2 demonstrate two general trends in bond lengths. First, bond lengths increase with increasing atom size. Consider the trend in H—X bond lengths (where X is a halogen). Halogen atomic radii increase moving down the periodic table ( $F < Cl < Br < I$ ), and therefore the H—X bond lengths increase as the halogen radius increases.



The second trend demonstrated in Table 8.x is the relationship between bond length and bond order. As bond order increases, there is an increase in electron density between two

#### Chapter Goals Revisited

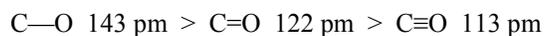
- Predict bond properties.
- Relate bond length to atom size and bond order.

The bond lengths in Table 8.2 have units of picometers ( $1 \text{ pm} = 10^{-12} \text{ m}$ ). Other common units for bond lengths are nanometers ( $1 \text{ nm} = 10^{-9} \text{ m}$ ) and Ångströms ( $1 \text{ Å} = 10^{-10} \text{ m}$ ).

#### Flashback

7.4 Properties of Atoms

nuclei. This results in stronger attractive forces between electrons and nuclei, decreasing the distance between the nuclei. A carbon-carbon single bond has a bond order of 1 and is longer than a carbon-carbon double bond with a bond order of 2. In general, for a series of bonds that differ only in bond order, an increase in bond order results in a decrease in bond length.



### Bond Energy

As shown previously in Figure 8.x, a chemical bond forms when the attractive and repulsive forces between atoms results in an energy minimum. **Bond energy** is the energy required to break a chemical bond in a gas-phase molecule. For example, the bond energy of an H—H bond is 436 kJ/mol (at 298 K). This means that 436 kJ of energy is required to break one mole of H—H bonds, forming two moles of H atoms.



Breaking bonds is an endothermic process, therefore bond energies are always positive values. Conversely, bond formation is an exothermic process that always releases energy. Just as bond lengths vary between compounds, so do bond energies. Some average bond energies are shown in Table 8.3.

Table 8.3 Average Bond Energies

Single Bond Energies, kJ/mol											
	H	C	N	O	F	Si	P	S	Cl	Br	I
H	436	414	389	464	569	293	318	339	431	368	297
C		347	293	351	439	289	264	259	330	276	238
N			159	201	272		209		201	243?	
O				138	184	368	351		205		201
F					159	540	490	285	255	197?	
Si						176	213	226	360	289	
P							213	230	331	272	213
S								213	251	213	
Cl									243	218	209
Br										192	180
I											151
Multiple Bond Energies, kJ/mol											
			N=N	418		C=C					611
			N≡N	946		C≡C					837
			C=N	615		C=O (in O=C=O)					803
			C≡N	891		C=O (as in H <sub>2</sub> C=O)					745
			O=O (in O <sub>2</sub> )	498		C≡O					1075

A clear trend that can be observed from the data in Table 8.x is the relationship between bond energy and bond order. As shown below, bond energy increases with increasing bond order.



As bond order increases, the stronger attractive forces between bonding electrons and nuclei mean that more and more energy is required to separate the bonded nuclei.

### Resonance Structures, Bond Order, Bond Length, Bond Energy

As shown earlier, compounds with resonance structures often have chemical bonds that are not easily described as single, double, or triple bonds. In order to describe the bond

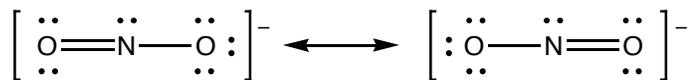
For a series of bonds between like atoms, as bond order increases, bond length decreases.

#### Chapter Goals Revisited

- Predict bond properties. **Relate bond energy to bond order.**

For a series of bonds between like atoms, as bond order increases, bond energy increases.

order, bond energy and bond length of these bonds, the number of resonance structures and bonding pairs must be taken into account. Consider the nitrite ion,  $\text{NO}_2^-$ , which has two equivalent resonance structures.



Because neither resonance structure represents the actual electron arrangement, the nitrogen-oxygen bonds in this ion are not single bonds (bond order = 1) or double bonds (bond order = 2). Instead,  $\text{NO}_2^-$  has two equivalent NO bonds where the three pairs of bonding electrons are distributed between the two equivalent NO bond locations. The best way to describe the bonding in the resonance hybrid is with a fractional bond order:

$$\text{Each NO bond order} = \frac{\text{total number of NO bonding pairs}}{\text{number of NO bond locations}} = \frac{3}{2} = 1.5$$

The NO bonds in the nitrite ion have a bond order that is intermediate between a single and a double bond. The bond length and bond energy of the NO bonds in the nitrite ion are also intermediate between average NO single and double bond lengths and bond energies.

Bond	Bond length	Bond energy
N—O	136 pm	201 kJ/mol
NO in $\text{NO}_2^-$	125 pm	174 kJ/mol
N=O	115 pm	143 kJ/mol

#### Chapter Goals Revisited

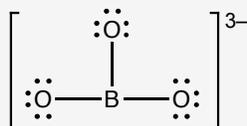
- Predict bond properties.  
**Predict bond properties of the resonance hybrid.**

#### EXAMPLE PROBLEM: Bond Order, Length, Strength

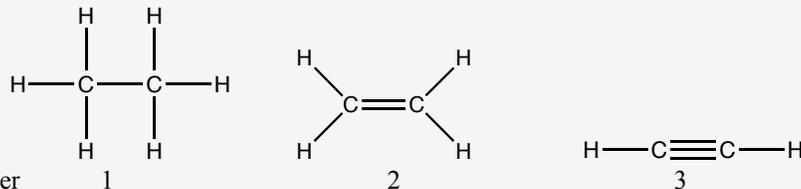
- (a) What is the bond order of the boron-oxygen bonds in the borate ion,  $\text{BO}_3^{3-}$ ?  
 (b) Which molecule has the shortest CC bond,  $\text{C}_2\text{H}_4$ ,  $\text{C}_2\text{H}_2$ , or  $\text{C}_2\text{H}_6$ ?  
 (c) Which ion has stronger nitrogen-oxygen bonds,  $\text{NO}_3^-$  or  $\text{NO}_2^-$ ?

#### SOLUTION:

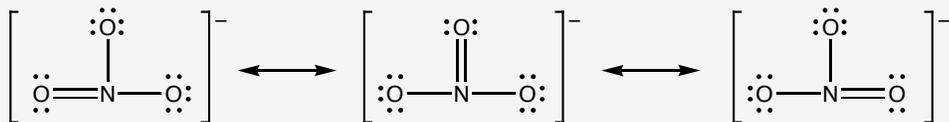
- (a) The Lewis structure for the borate ion shows three boron-oxygen single bonds. Each B—O bond has a bond order of 1.



- (b) Bond length decreases with increasing bond order.  $\text{C}_2\text{H}_4$  has the highest carbon-carbon bond order and the shortest carbon-carbon bond.



- (c) Bond energy increases with increasing bond order.  $\text{NO}_2^-$  has the highest nitrogen-oxygen bond order and the strongest nitrogen-oxygen bond.



$$\text{NO bond order in } \text{NO}_3^- = \frac{4 \text{ NO bonding pairs}}{3 \text{ NO bond locations}} = 1.3$$



$$\text{NO bond order in } \text{NO}_2^- = \frac{3 \text{ NO bonding pairs}}{2 \text{ NO bond locations}} = 1.5$$



*OWL Example Problems*  
8.13 Bond Order, Length, Strength

### Bond Energy and Enthalpy of Reaction

Bond energy values can be used to calculate the enthalpy change for gas-phase reactions. First assume all chemical bonds are broken in reactant molecules, creating isolated atoms. Next, rearrange the atoms to form products and new chemical bonds. The first step involves breaking bonds and is an endothermic process, and the second step involves forming bonds and is an exothermic process. The bond energies are summed as shown in equation 8.2.

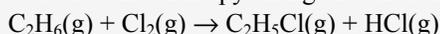
$$\Delta H^\circ = \Sigma(\text{energies of bonds broken}) - \Sigma(\text{energies of bonds formed}) \quad (8.2)$$

#### Chapter Goals Revisited

- Predict bond properties.  
**Use bond energy to calculate reaction enthalpy.**

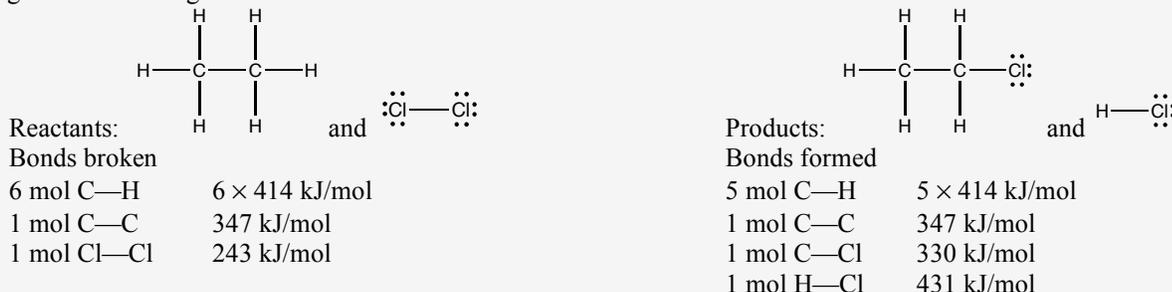
#### EXAMPLE PROBLEM: Bond Energy and Enthalpy of Reaction

Calculate the enthalpy change for the following gas-phase reaction.



#### SOLUTION:

Draw Lewis structures for reactants and products and use them to list all reactant bonds broken and product bonds formed, along with bond energies from Table 8.x.



Use equation 8.x to calculate  $\Delta H^\circ$  for the reaction.

$$\begin{aligned} \Delta H^\circ &= [6 \text{ mol}(414 \text{ kJ/mol}) + 1 \text{ mol}(243 \text{ kJ/mol}) + 1 \text{ mol}(347 \text{ kJ/mol})] \\ &\quad - [5 \text{ mol}(414 \text{ kJ/mol}) + 1 \text{ mol}(347 \text{ kJ/mol}) + 1 \text{ mol}(330 \text{ kJ/mol}) + 1 \text{ mol}(431 \text{ kJ/mol})] \\ &= -104 \text{ kJ} \end{aligned}$$

Notice that five of the C—H bonds and the C—C bond in  $\text{C}_2\text{H}_6$  are unchanged in the reaction. The enthalpy of reaction can also be calculated using only the energies of the bonds that are broken (1 mol C—H and 1 mol Cl—Cl) and the bonds that are formed (1 mol C—Cl and 1 mol H—Cl).

$$\begin{aligned} \Delta H^\circ &= [1 \text{ mol}(414 \text{ kJ/mol}) + 1 \text{ mol}(243 \text{ kJ/mol})] - [1 \text{ mol}(330 \text{ kJ/mol}) + 1 \text{ mol}(431 \text{ kJ/mol})] \\ &= -104 \text{ kJ} \end{aligned}$$



*OWL Example Problems*  
8.14 Bond Energy and Enthalpy of Reaction: Simulation  
8.15 Bond Energy and Enthalpy of Reaction

## 8.5 Electron Distribution in Molecules



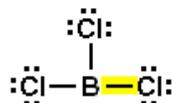
*OWL Opening Exploration*  
8.X

Lewis structures give chemists one method for visualizing the valence electron arrangement in molecules and ions. However, these structures do not fully represent the way electrons are distributed. Calculated formal charge and electronegativity are two

tools chemists use, in addition to a Lewis structure, to more accurately describe the electron distribution in a molecule.

### Formal Charge

The **formal charge** of an atom in a molecule or ion is the charge it would have if all bonding electrons were shared equally. Formal charge is a “bookkeeping” method of showing electron distribution in a Lewis structure and while it does not give a completely accurate picture of charge distribution, it is helpful in identifying regions with a large positive or negative charge buildup. Consider the Lewis structure for  $\text{BCl}_3$ , and in particular the electrons represented by one of the B-Cl bonds.



The formal charge on the chlorine atom in the B—Cl bond is a measure of the relationship between the chlorine valence electrons (its group number) and the number of bonding and nonbonding electrons assigned to chlorine in the Lewis structure. In calculating formal charge, we assume that all bonding electrons are shared equally between the atoms in the bond and therefore that each atom gets half of them (Equation 8.3).

$$\text{Formal charge} = (\text{number of valence electrons}) - [(\text{number of nonbonding electrons}) + \frac{1}{2}(\text{number of bonding electrons})] \quad (8.3)$$



Imagine each bond is split in half and the bonding electrons are shared equally between bonded atoms.

$$\text{Cl formal charge} = (7) - [6 + \frac{1}{2}(2)] = 0$$

$$\text{B formal charge} = (3) - [0 + \frac{1}{2}(6)] = 0$$

In  $\text{BCl}_3$ , all atoms have a formal charge of zero and we predict that there is no buildup of positive or negative charge in the molecule. Formal charge, however, assumes all bonding electrons are shared equally. As you will see in the following section, other methods that take into account the unequal sharing of bonding electrons can give a more accurate picture of electron distribution in a molecule.

The sum of the formal charges for all atoms in a molecule or ion is equal to the charge on the molecule or ion, as shown in the following example.

#### EXAMPLE PROBLEM: Formal Charge

Use the formal charge for each atom in the cyanide ion,  $\text{CN}^-$ , to predict whether  $\text{H}^+$  is more likely to attach to carbon or nitrogen when forming hydrocyanic acid.

#### SOLUTION:

First draw the Lewis structure of  $\text{CN}^-$ .



Use equation 8.x to calculate the formal charge for carbon and nitrogen.

$$\text{C formal charge} = (4) - [2 + \frac{1}{2}(6)] = -1$$

$$\text{N formal charge} = (5) - [2 + \frac{1}{2}(6)] = 0$$

Notice that the sum of the formal charges is equal to the overall charge on the ion ( $-1$ ).

When  $\text{H}^+$  attaches to  $\text{CN}^-$ , it is more likely to attach to the atom with the negative formal charge, carbon, forming  $\text{H}-\text{C}\equiv\text{N}$ .

#### Chapter Goals Revisited

- Understand charge distribution in molecules. **Calculate formal charge.**



OWL Example Problems  
8.18 Formal Charge: Tutor

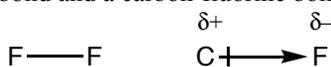
## Bond Polarity

In a covalent bond, electrons are attracted to two nuclei, but sometimes one nucleus attracts the electrons more strongly than the other. When one nucleus attracts the electrons more strongly, the bonding electrons are located closer to one nucleus than the other. This creates an uneven distribution of bond electron density and a **polar bond** (or **polar covalent bond**). When electrons experience the same attractive force to both nuclei, the bond is **nonpolar**.

The term “polar” refers to the existence of a **dipole**, a separation of partial positive (symbolized  $\delta^+$ ) and partial negative (symbolized  $\delta^-$ ) charge within a bond or a molecule. The partial charges are due to an uneven distribution of electron density, not a transfer of electrons between atoms to form ions. A dipole is indicated using an arrow that points at the negative end of the dipole and has a cross to indicate the positive end of the dipole.



Consider a fluorine-fluorine bond and a carbon-fluorine bond.

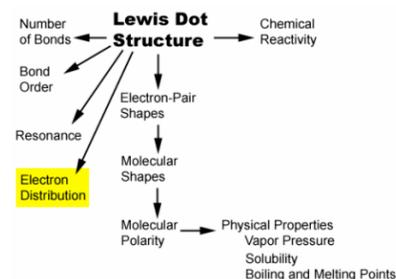


In the fluorine-fluorine bond, the bonding electrons are attracted equally to both fluorine nuclei. The electron density is therefore evenly distributed between the fluorine atoms and the bond is nonpolar. The carbon-fluorine bond, in contrast, is polar because the bonding electrons are attracted more strongly to fluorine than to carbon. This results in electron density that is closer to fluorine than to carbon. Recall that fluorine has a higher effective nuclear charge than carbon and its valence atomic orbitals are lower in energy than those of carbon. A partial negative charge occurs at fluorine due to this uneven electron density distribution, and a corresponding partial positive charge happens at the electron deficient carbon.

The ability of an atom in a molecule to attract electrons to itself is its **electronegativity**,  $\chi$  (Figure 8.5). Electronegativity, a concept first proposed by Linus Pauling in 1932, is a relative scale where the most electronegative element (fluorine) is assigned a value of 4.0.

IA																	VIIIA						
1 H 2.1																	2 He						
3 Li 1.0	4 Be 1.5																	5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	9 F 4.0	10 Ne
11 Na 1.0	12 Mg 1.2																	13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0	18 Ar
19 K 0.9	20 Ca 1.0	21 Sc 1.3	22 Ti 1.4	23 V 1.5	24 Cr 1.6	25 Mn 1.6	26 Fe 1.7	27 Co 1.7	28 Ni 1.8	29 Cu 1.8	30 Zn 1.6	31 Ga 1.7	32 Ge 1.9	33 As 2.1	34 Se 2.4	35 Br 2.8	36 Kr						
37 Rb 0.9	38 Sr 1.0	39 Y 1.2	40 Zr 1.3	41 Nb 1.5	42 Mo 1.6	43 Tc 1.7	44 Ru 1.8	45 Rh 1.8	46 Pd 1.8	47 Ag 1.6	48 Cd 1.6	49 In 1.6	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	53 I 2.5	54 Xe						
55 Cs 0.8	56 Ba 1.0	57 La 1.1	72 Hf 1.3	73 Ta 1.4	74 W 1.5	75 Re 1.7	76 Os 1.9	77 Ir 1.9	78 Pt 1.8	79 Au 1.9	80 Hg 1.7	81 Tl 1.6	82 Pb 1.7	83 Bi 1.8	84 Po 1.9	85 At 2.1	86 Rn						
87 Fr 0.8	88 Ra 1.0	89 Ac 1.1																					
			58 Ce 1.1	59 Pr 1.1	60 Nd 1.1	61 Pm 1.1	62 Sm 1.1	63 Eu 1.1	64 Gd 1.1	65 Tb 1.1	66 Dy 1.1	67 Ho 1.1	68 Er 1.1	69 Tm 1.1	70 Yb 1.0	71 Lu 1.2							
			90 Th 1.2	91 Pa 1.3	92 U 1.5	93 Np 1.3	94 Pu 1.3	95 Am 1.3	96 Cm 1.3	97 Bk 1.3	98 Cf 1.3	99 Es 1.3	100 Fm 1.3	101 Md 1.3	102 No 1.3	103 Lr 1.5							

Figure 8.5 Electronegativity Values



### Chapter Goals Revisited

- Understand charge distribution in molecules. Use electronegativity to predict bond polarity.

### Flashback

7.4 Properties of Atoms

Notice in Figure 8.5 that

- the noble gases (Group 8A) are not assigned electronegativity values (most of these elements do not form covalent bonds);
- electronegativity values increase moving left to right and decrease moving down the periodic table;
- hydrogen does not follow the periodic trend and has an electronegativity similar to that of carbon;
- metals generally have low electronegativity values and nonmetals generally have high electronegativity values; and
- fluorine, oxygen, nitrogen and chlorine are the most electronegative elements.

The polarity of a chemical bond is related to the difference in electronegativity ( $\Delta\chi$ ) of the two elements that make up the bond. For covalent bonds between nonmetals, a  $\Delta\chi$  greater than zero indicates that the bond is polar and a zero  $\Delta\chi$  indicates a nonpolar bond. For example, the C—F bond described earlier has  $\Delta\chi = (4.0 - 2.5) = 1.5$ . It is a polar bond.

When  $\Delta\chi$  is very large, the interaction between elements has more ionic character than covalent character. For example, sodium and fluorine have very different electronegativities [ $F(4.0) - Na(1.0) = 3.0$ ]. When sodium and fluorine react, electrons are transferred resulting in the formation of  $Na^+$  and  $F^-$ .

There is not a defined electronegativity difference that separates ionic from polar bonds. Instead, there is a continuum moving between these two extremes. All polar bonds have some “ionic character” and some “covalent character.”

#### EXAMPLE PROBLEM: Electronegativity and Bond Polarity

(a) Which of the following bonds are nonpolar?

C-Cl    H-Cl    H-H    F-F    P-H    S-O    B-F

(b) Which of the following bonds is most polar?

C-Cl    H-Cl    H-I    H-F    P-H    S-O    B-F

#### SOLUTION:

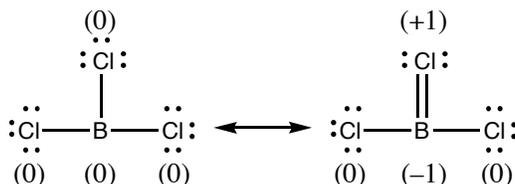
- (a) H-H, F-F and P-H bonds are nonpolar. Any bond between two like atoms is nonpolar because  $\Delta\chi = 0$ . The P-H bond is nonpolar by the coincidence that both P and H have the same electronegativity value of 2.1. C-Cl, H-Cl, S-O, and B-F bonds are polar because when two different elements are bonded, the bond is almost always polar.
- (b) The B-F bond has the greatest  $\Delta\chi$  ( $4.0 - 2.0 = 2.0$ ) so it is the most polar bond.



OWL Example Problems  
8.17 Electronegativity and Bond Polarity

#### Resonance Structures, Formal Charge, and Electronegativity

When nonequivalent resonance structures exist, the most likely resonance structure is the one with formal charges closest to zero. A general rule of chemical stability is that the localization of positive or negative charges within a molecule is destabilizing. Consider the two possible inequivalent resonance structures for  $BCl_3$  shown below along with calculated formal charges.

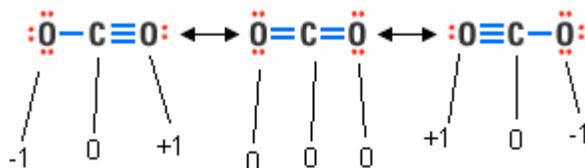


#### Chapter Goals Revisited

- Understand charge distribution in molecules. **Use charge distribution to evaluate resonance structures.**

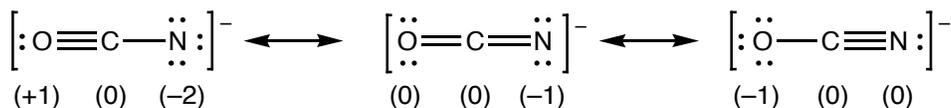
The resonance structure on the right is less likely than the one on the left because it has localized formal charges of +1 and -1. In addition, chlorine ( $\chi = 3.0$ ) is more electronegative than boron ( $\chi = 2.0$ ), so a resonance structure that has a positive formal charge on the more electronegative element (and a negative formal charge on the less electronegative element) is probably not stable.

The three nonequivalent resonance structures of  $\text{CO}_2$  are shown below along with calculated formal charges.



The central structure is the most likely resonance structure for  $\text{CO}_2$  because it has formal charges of zero on each atom, while both of the other resonance structures have formal charges of +1 and -1 on the O atoms.

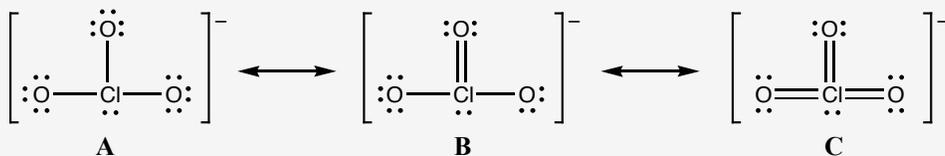
The cyanate ion,  $\text{OCN}^-$ , has three nonequivalent resonance structures.



None of the three resonance structures have formal charges of zero on all atoms. The first resonance structure is not very likely due to the large formal charges (+1 and -2). The other two resonance structures, however, each have small formal charges. In this case, electronegativity can help determine the best resonance structure. The electronegativity of oxygen (3.5) is greater than that of nitrogen (3.0). Therefore, oxygen is more likely to carry a negative formal charge in a Lewis structure, and according to formal charges, the resonance structure on the right is most likely.

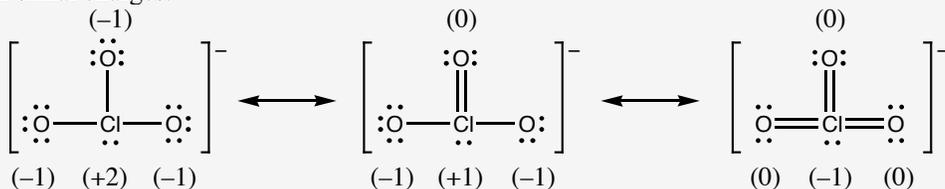
#### EXAMPLE PROBLEM: Resonance Structures and Formal Charge

Three inequivalent resonance structures for the chlorate ion are shown below. Assign formal charges to all atoms in the resonance structures and identify the more likely resonance structure.



#### SOLUTION:

Formal charges:



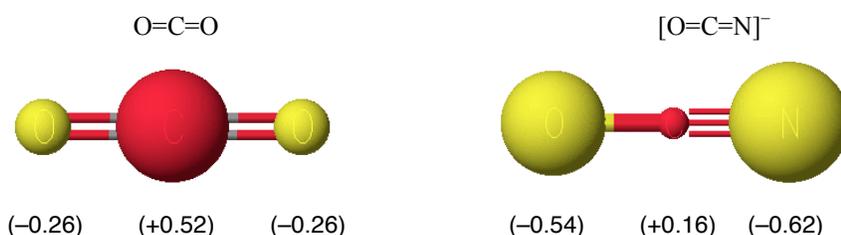
Structure **B** is the most likely resonance structure. The formal charges in **B** are close to zero and the highly electronegative oxygen atom carries a -1 formal charge. Structure **A** is unlikely because of the large positive formal charge on chlorine. Structure **C** is unlikely because the least electronegative element in the ion (chlorine) has a negative formal charge while the most electronegative element in the ion (oxygen) has a formal charge of zero.



*OWL Example Problems*  
8.19 Resonance Structures and Formal Charge

### Partial Charge

Calculated formal charges and relative electronegativities are useful tools for assigning charge distribution in a Lewis structure because they help identify likely resonance structures and regions with a buildup of positive or negative charge in molecules and ions. They do not, however, give an accurate picture of the actual electron distribution in molecules. Modern computer modeling programs calculate **partial charges** on atoms that give a more accurate picture of electron distribution. For example, the calculated partial charges on the atoms in carbon dioxide and the cyanate ion are shown below. Red spheres indicate positive partial charge and yellow spheres indicate negative partial charge. The size of the sphere is proportional to the magnitude of the partial charge. As was true with formal charge, the sum of partial charges is equal to the charge on the molecule or ion.



In CO<sub>2</sub>, each oxygen carries a negative partial charge and the carbon has a positive partial charge. This reflects the fact that oxygen is more electronegative than carbon but does not reflect the calculated formal charges of zero in the most likely resonance structure for CO<sub>2</sub>. However, the fact that both oxygen atoms have negative calculated partial charges suggests that the two resonance structures that have a positive formal charge on oxygen are very unlikely. The calculated partial charges also show that the CO bonds are polar, results that are supported by electronegativity values but not by formal charge calculations.

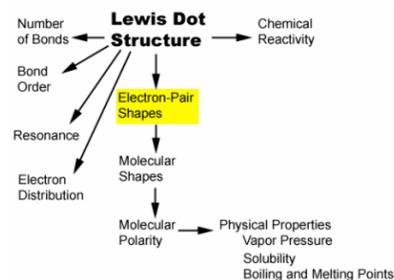
In the cyanate structure, both oxygen and nitrogen carry approximately the same negative partial charge and carbon has a slightly positive formal charge. None of the three OCN<sup>-</sup> resonance structures show a negative formal charge on both nitrogen and oxygen, but two of the resonance structures have a -1 formal charge on either nitrogen or oxygen. The calculated partial charges for OCN<sup>-</sup> suggest that both of the resonance structures with -1 formal charges on nitrogen and oxygen are important and both contribute to the resonance hybrid for OCN<sup>-</sup>.

## 8.6 Valence-Shell Electron-Pair Repulsion Theory and Molecular Shape



*OWL Opening Exploration*  
8.20 Exploring Geometry 1  
8.21 Exploring Geometry 2

Lewis electron dot structures show the atom connectivity and number of bonds and lone pairs in a molecule or ion but do not provide information about the three-dimensional shapes of molecules. For example, numerous experiments have shown that water, H<sub>2</sub>O, has a bent (non-linear) shape. The Lewis structure, however, can be drawn to show a linear arrangement of atoms.





The shape of a molecule or ion is one of its most important characteristics because it controls many other properties such as melting and boiling points and chemical reactivity. A variety of experimental techniques such as X-ray crystallography and spectroscopy are used to determine precise atom distances, bond angles, and the shape of a molecule. However, predicting the shape of a molecule or ion from its Lewis structure is one of the most useful tools a chemist has.

The **valence shell electron pair repulsion (VSEPR)** theory allows chemists to easily predict the shapes of molecules and ions made up of nonmetals. According to VSEPR theory,

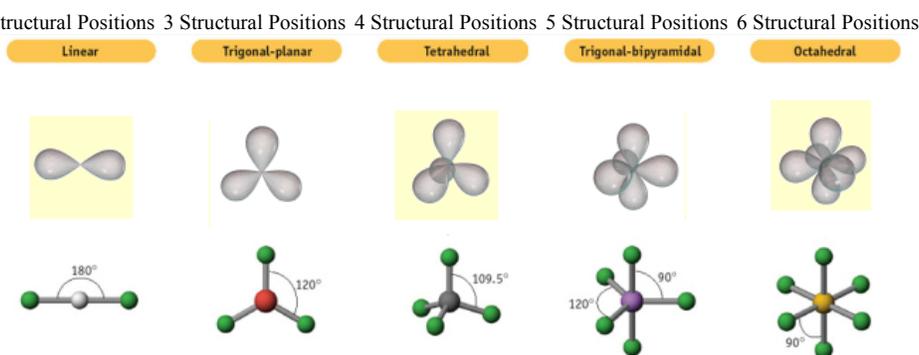
- positions around a central atom are occupied by either *nonbonding electrons* (single or pairs of electrons are counted as one nonbonding position) or *bonding electrons* (single or multiple bonding pairs are counted as one bonding position);
- the number of **structural positions** around a central atom is equal to the total number of nonbonding and bonding positions occupied around the atom;
- the electrons in structural positions repel each other and are arranged so as to avoid one another as best as possible;
- the **electron-pair geometry** is the arrangement of the structural positions around the central atom; and
- the **shape** (also called **molecular geometry**) is the arrangement of atoms around the central atom (ignoring the nonbonding positions on the central atom).

#### Chapter Goals Revisited

- Use VSEPR theory  
Identify **electron-pair geometry**.

### Electron-Pair Geometry

The **electron-pair geometry** is defined by the electrons (bonding and nonbonding) around the central atom. In large molecules with multiple central atoms, we will describe the electron-pair geometry around each central atom. When two, three, four, five, or six pairs of electrons are arranged around a central atom, the electrons are arranged in one of the following ideal electron-pair geometries (Figure 8.6).



**Figure 8.6** Ideal Electron-Pair Geometries

Figure 8.6 also shows the bond angles that are characteristic for each ideal electron-pair geometry. **Bond angle** is the angle formed by the nuclei of two atoms with a central atom at the vertex. The bond angles shown in Figure 8.6 are ideal angles and most molecules have bond angles that are very close to these values.

To determine the electron-pair geometry of a molecule with a single central atom,

1. Draw the Lewis structure.
2. Sum the number of structural positions (the total number of nonbonding and bonding positions) around the central atom.
3. Use this total number of structural positions to identify the electron-pair geometry using the ideal geometries shown in Figure 8.6.

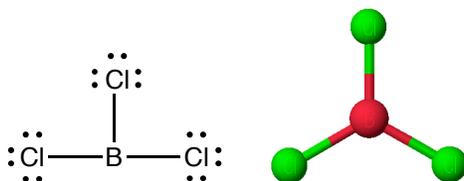


*OWL Example Problems*  
8.22 Ideal Electron Pair Shapes: Tutor

### Shape (Molecular Geometry)

The **shape** of a molecule (its **molecular geometry**) is defined by the atom positions in a molecule. The shape is the same as the electron-pair geometry when all structural positions are occupied by bonding electrons.

For example, boron trichloride ( $\text{BCl}_3$ ) has a trigonal planar electron-geometry and a trigonal planar shape. There are three structural positions around the central boron atom and all are occupied by bonding electrons.



Carbon dioxide,  $\text{CO}_2$ , has a linear electron-geometry and a linear shape. There are two structural positions around the central carbon atom and both are occupied by bonding electrons.



here are many molecules for which the shape that is not the electron-pair geometry. For example, ozone ( $\text{O}_3$ ) has a trigonal planar electron-pair geometry and a bent shape. There are three structural positions around the central oxygen atom, but two are occupied by bonding electrons and one is occupied by nonbonding electrons. Because shape is defined by the positions of the atoms in a molecule not the electrons, ozone has a bent shape and not a trigonal planar shape.

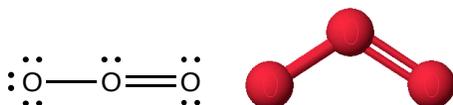
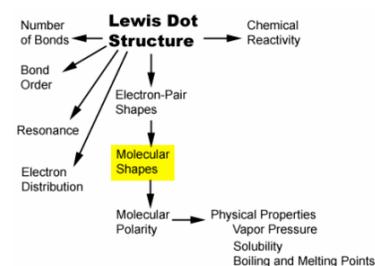


Figure 8.7 shows the shapes for molecules with 3–6 structural positions and varying numbers of nonbonding electron pairs on the central atom.



Notice that a Lewis structure is not always drawn to show the shape of the molecule or the correct bond angles.

#### Chapter Goals Revisited

- Use VSEPR theory to **Identify molecular geometry**.

		Number of Nonbonding Positions			
		0	1	2	3
Number of Structural Positions	3	Trigonal planar 	Bent 		
	4	Tetrahedral 	Trigonal-pyramidal 	Bent 	
	5	Trigonal bipyramidal 	Seesaw $SF_4$ 4 bond pairs 1 lone pair 	T-shaped $ClF_3$ 3 bond pairs 2 lone pairs 	Linear $XeF_2$ 2 bond pairs 3 lone pairs 
	6	Octahedral 	Square-pyramidal $BrF_5$ 5 bond pairs 1 lone pair 	Square-planar $XeF_4$ 4 bond pairs 2 lone pairs 	

Figure 8.7 Shapes of Molecules With 3–6 Structural Positions

**EXAMPLE PROBLEM: Determining Molecular Shapes**

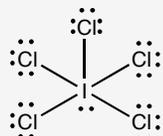
Determine the shape of

- (a)  $ICl_5$   
 (b)  $SO_3^{2-}$

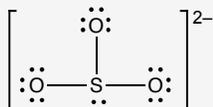
**SOLUTION:**

Draw the Lewis structure of each species and use Figure 8.x to determine the shape.

- (a) Square pyramid.  $ICl_5$  has 6 structural positions around the central atom. Five are occupied by bonding electrons and one is occupied by nonbonding electrons.



- (b) Trigonal pyramid.  $SO_3^{2-}$  has 4 structural positions around the central atom. Three are occupied by bonding electrons and one is occupied by nonbonding electrons.





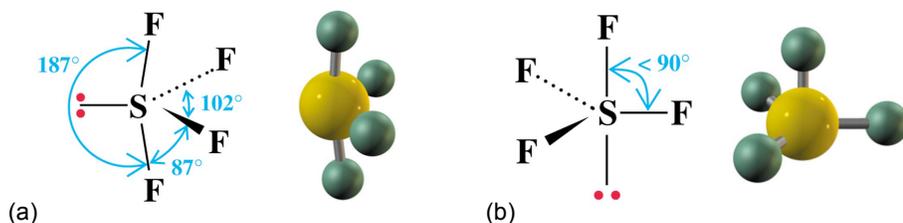
*OWL Example Problems*

8.23 Determining Molecular Shapes: Tutor

8.24 Determining Molecular Shapes: Exercise

8.23 Determining Molecular Shapes

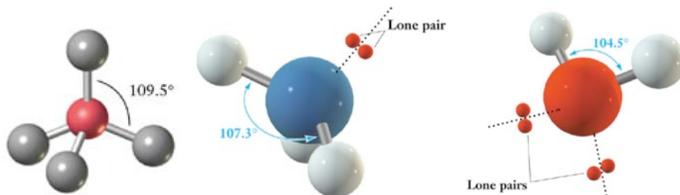
When determining the shape of a molecule with lone pairs in structural positions, it is important to note the different steric requirements of lone pairs and bonding pairs. Lone pairs are diffuse because they are attracted to a single nucleus, while bonding pairs are localized between and attracted to two nuclei. Lone pairs therefore occupy more space around a central atom than bonding pairs. Consider  $\text{SF}_4$ , which has four structural positions occupied by bonding pairs and one occupied by a lone pair. The five structural positions are arranged in a trigonal bipyramid. The lone pair occupies an equatorial position because this minimizes repulsive forces between the larger, diffuse lone pair and the bonding pairs (Figure 8.8(a)). If the lone pair occupies an axial position (Figure 8.8(b)), the close contact ( $90^\circ$  angles) between the lone pair and bonding pairs increases repulsive forces making this configuration less favorable.



**Figure 8.8**  $\text{SF}_4$  shape with the lone pair in (a) equatorial and (b) axial position

Thus lone pairs occupy equatorial positions in a trigonal bipyramidal electron-pair geometries. Similarly, because lone pairs occupy positions opposite each other in an octahedron because this also minimizes repulsive forces.

Molecular shapes predicted using the VSEPR ideal electron pair shapes are usually very close to the shapes measured by experiment, especially when all terminal atoms are identical. However, when lone pairs are present on the central atom, bond angles in particular differ from predicted values. Consider the bond angles in  $\text{NH}_3$  and  $\text{H}_2\text{O}$  (Figure 8.9). Both molecules have the same electron-pair geometry (tetrahedral) but they differ in the number of lone pairs on the central atom. As the number of lone pairs on the central atom increases, the H-X-H bond angle decreases.



**Figure 8.9** H-X-H bond angles  $\text{CH}_4$ ,  $\text{NH}_3$ , and  $\text{H}_2\text{O}$

## 8.7 Molecular Polarity



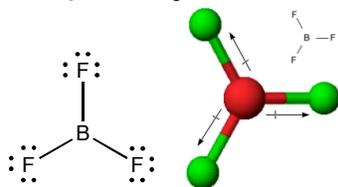
### OWL Opening Exploration 8.27

As we saw earlier, covalent bonds are polar when there is an uneven attraction for electrons between the bonded atoms. Polar bonds in a molecule can result in a polar molecule, which affects the physical properties of a compound. For example, polar molecules are often very soluble in water while nonpolar molecules are not.

For a molecule to be polar, it must contain polar bonds and those bonds must be arranged so that there is an uneven charge distribution. The following steps are used to predict whether a molecule is polar.

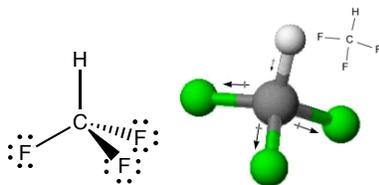
1. Draw the Lewis structure.
2. Determine the shape.
3. If the molecule has polar bonds, indicate them on the molecule.
4. Use the shape and bond dipoles to determine if there is an uneven distribution of bond electron density in the molecule.

For example, boron trifluoride,  $\text{BF}_3$ , is a nonpolar molecule that has polar bonds.

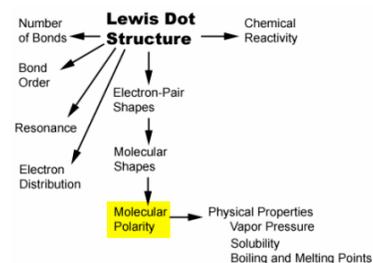
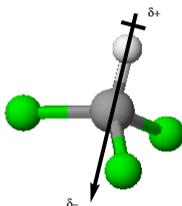


The shape of  $\text{BF}_3$  is trigonal planar and the B—F bonds are polar (fluorine is the negative end of the bond dipole). As shown above, the three bond dipoles are arranged symmetrically in the molecule and do not result in an uneven distribution of electron density.  $\text{BF}_3$  is therefore nonpolar.

Trifluoromethane is a polar molecule.



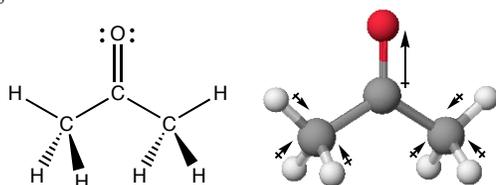
The shape of  $\text{CHF}_3$  is tetrahedral and the C—F and C—H bonds are polar. Carbon is the negative end of the C—H bond dipole, and fluorine is the negative end of each C—F bond dipole. When we draw in the individual bond dipoles, we see that there is a net movement of bond electron density away from hydrogen and toward the fluorine atoms. This uneven electron density distribution means that  $\text{CHF}_3$  is polar, and the molecule has a net dipole with the positive end near hydrogen and the negative end near the fluorine atoms.



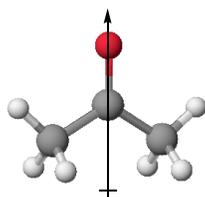
### Chapter Goals Revisited

- Identify polar and nonpolar species.  
**Predict molecular polarity using molecular shape and electron distribution.**

This method is also useful for larger, more complex molecules. For example, consider acetone,  $\text{CH}_3\text{COCH}_3$ .



The carbon-carbon bonds in acetone are nonpolar, the carbon-hydrogen bonds are slightly polar (carbon is the negative end of the bond dipole) and the carbon-oxygen bond is polar (oxygen is the negative end of the bond dipole). There is a net shift of electron density towards oxygen, so the molecule is polar. The net molecular dipole is shown below.



#### EXAMPLE PROBLEM: Determining Polarity of Molecules

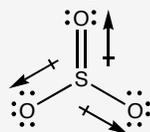
Determine if each of the following is polar.

- (a)  $\text{SO}_3$   
 (b)  $\text{BrF}_3$

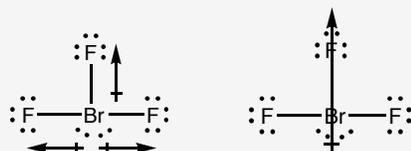
#### SOLUTION:

Draw the Lewis structure for each molecule, determine the shape, and label any polar bonds. Use shape and bond polarity to determine if the molecule is polar.

- (a) Nonpolar.  $\text{SO}_3$  has a trigonal planar shape and all three SO bonds are polar. The three bond dipoles are arranged symmetrically in the molecule, so the molecule is not polar.



- (b) Polar.  $\text{BrF}_3$  has a T-shaped shape and all three BrF bonds are polar. The three bond dipoles are not arranged symmetrically around the molecule, so the molecule is polar. The bromine is the positive end of the net dipole and one of the fluorine atoms is the negative end of the bond dipole.



*OWL Example Problems*  
 8.28 Determining Polarity of Molecules: Exercise  
 8.28 Determining Polarity of Molecules

## Chapter Review



*OWL Summary Assignments*

*8.29 Chapter Review*

*8.30 Challenge Problems*

### Key Equations

$$\text{Force} \propto \frac{(q_A)(q_B)}{r^2} \quad (8.1)$$

$$\Delta H^\circ = \Sigma(\text{energies of bonds broken}) - \Sigma(\text{energies of bonds formed}) \quad (8.2)$$

$$\text{Formal charge} = (\text{number of valence electrons}) - [(\text{number of nonbonding electrons}) + \frac{1}{2}(\text{number of bonding electrons})] \quad (8.3)$$

### Key Terms

#### 8.1 Interactions Between Particles: Coulomb's Law

Coulomb's Law  
ionic bonding  
Covalent bonding  
Metallic bonding  
intermolecular forces

#### 8.3 Lewis Structures

Lewis structure  
Lewis symbol  
lone (electron) pairs  
single bond  
double bond  
triple bond  
octet rule  
electron deficient  
free radicals  
expanded valence  
resonance structures  
resonance hybrid

#### 8.4 Bond Properties

bond order  
bond length  
bond energy

#### 8.5 Electron Distribution in Molecules

formal charge  
polar bond  
polar covalent bond  
nonpolar  
dipole  
electronegativity,  $\chi$   
partial charges  
valence shell electron pair repulsion (VSEPR)  
structural positions  
electron-pair geometry  
shape (molecular geometry)  
electron-pair geometry  
bond angle