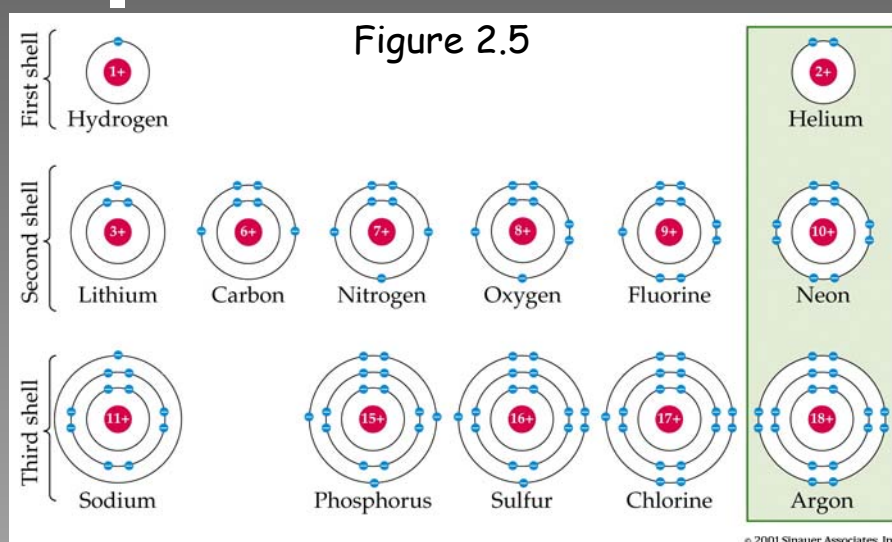


# CHAPTER 2

## Small Molecules: Structure and Behavior

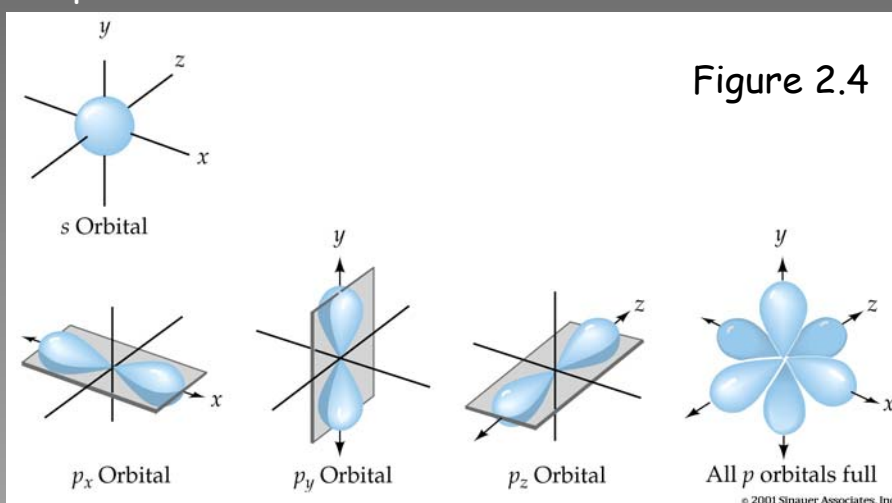
Electrons are distributed in shells of **orbitals**.  
Each **orbital** contains a maximum of two electrons.



## Chemical Bonds: Linking Atoms Together

- **Covalent bonds** form when two atomic nuclei share one or more pairs of electrons. They have spatial orientations that give molecules three-dimensional shapes. Review Figures [2.6](#), [2.7](#), Table [2.2](#)

The first shell has only an **s orbital** that is spherical in shape. The second shell has an **s orbital** and **3 p orbitals** that are shaped somewhat like dumbbells.



## Bonding properties of the most common elements in biological molecules

■  
**H:** Atomic No. 1 ==> 1 electron:  $1s^1$

1st shell needs 1 electron ==> Forms 1 covalent bond

**C:** Atomic No. 6 ==> 6 electrons:  $1s^2 2s^2 2p_x^1 2p_y^1 2p_z^0$   
 2nd shell needs 4 electrons ==> Forms 4 covalent bonds

**N:** Atomic No. 7 ==> 6 electrons: needs 3 electrons  
 ==> Forms 3 covalent bonds

**O:** Atomic No. 8 ==> 8 electrons: needs 2 electrons  
 ==> Forms 2 covalent bonds

The orbitals used by carbon to form 4 bonds to 4 different atoms are  $sp^3$  hybrid orbitals formed from the single  $2s$  and the three  $2p$  orbitals.

The  $sp^3$  orbitals point to the corners of a tetrahedron forming covalent bonds with 4 H atoms in methane.

This is called "Tetrahedral Geometry".  
 The angle between the bonds is 109 deg.

This type of covalent bond has electron density between the atoms and is called a  $\sigma$  bond

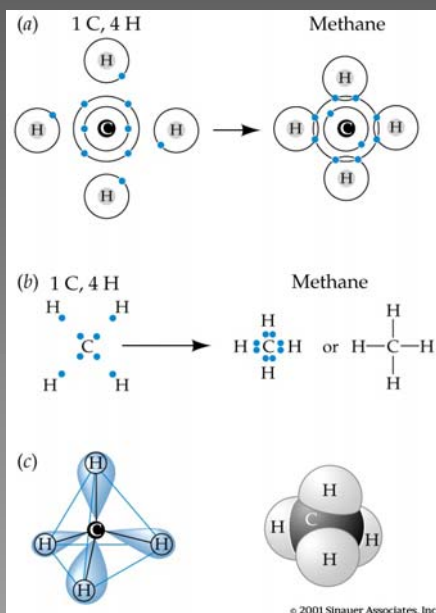
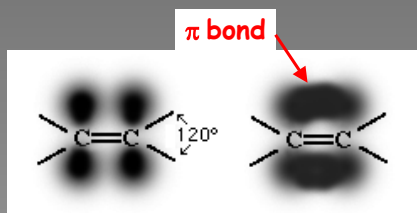
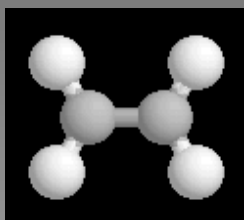


Figure 2.7

When carbon forms bonds to three different atoms, it uses **sp<sup>2</sup> hybrid orbitals** made by combining the 2s orbital and two of the 2p orbitals.

These point to the corners of a triangle and form covalent bonds with 3 different atoms, 2 H's and another C in the example of **ethene** shown below. The angle between bonds is **120** degrees.



The two C atoms in ethene form a second or **double bond** between themselves using their third 2p orbitals. The second bond is called a  **$\pi$  bond** and prevents the C atoms from rotating around the bonds connecting them.

## Chemical Bonds: Linking Atoms Together

- Nonpolar covalent bonds form when the **electronegativities** of two atoms are approximately equal. When atoms with strong electronegativity (such as oxygen) bond to atoms with weaker electronegativity (such as hydrogen), a polar covalent bond forms, in which one end is  $\delta^+$  and the other is  $\delta^-$ . Review Figure [2.8](#), Table [2.3](#)

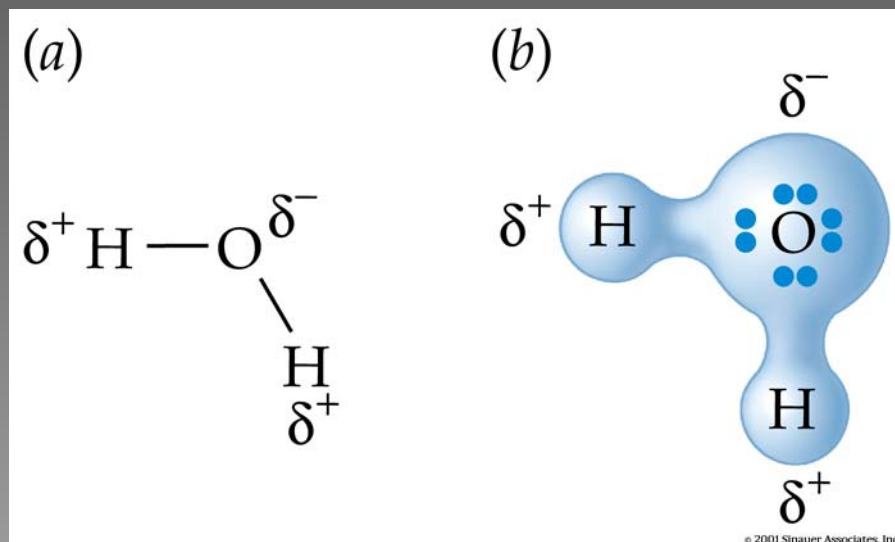


Figure 2.8

## 2.3 Some Electronegativities

ELEMENT	ELECTRONEGATIVITY
Oxygen	3.5 ← High
Chlorine	3.1
Nitrogen	3.0 ← High
Carbon	2.5 ←
Phosphorus	2.1
Hydrogen	2.1 ←
Sodium	0.9
Potassium	0.8

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Table 2.3

## Chemical Bonds: Linking Atoms Together

- **Hydrogen bonds** form between a  $\delta^+$  hydrogen atom in one molecule and a  $\delta^-$  nitrogen or oxygen atom in another molecule or in another part of a large molecule. Review Figure [2.9](#)

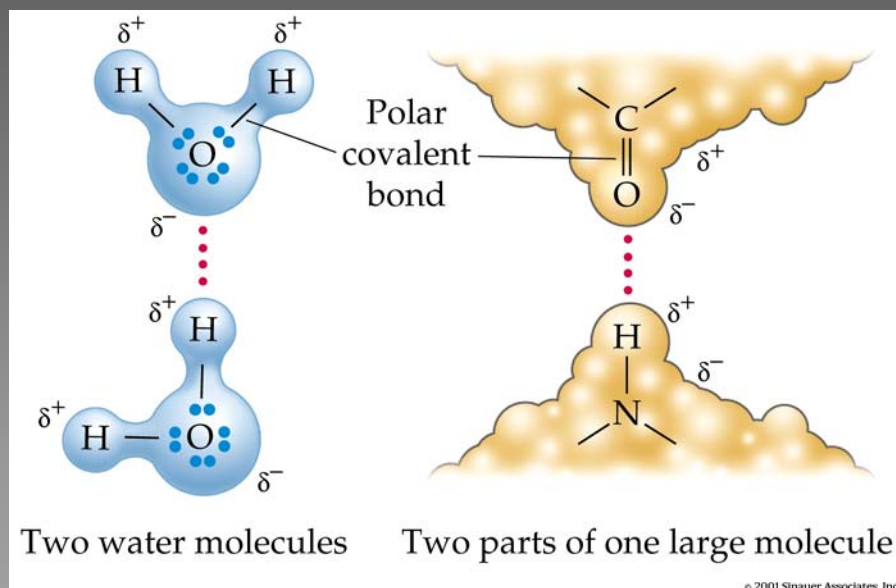


Figure 2.9

## Chemical Bonds: Linking Atoms Together

- Ions, electrically charged bodies, form when an atom gains or loses one or more electrons. **Ionic bonds** are electrical attractions between oppositely charged ions. Review Figures [2.10](#), [2.11](#)

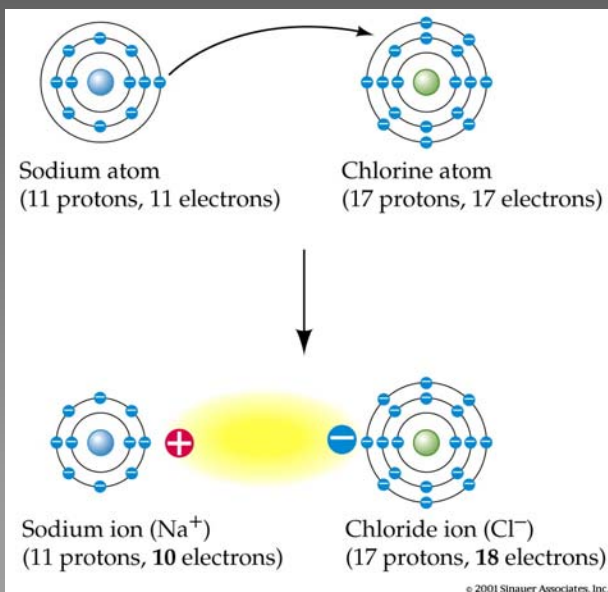


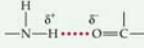

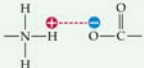



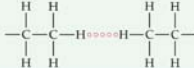



Figure 2.10

## Chemical Bonds: Linking Atoms Together

- Nonpolar molecules do not interact directly with polar substances. They are attracted to each other by very weak bonds called van der Waals forces. Review Figure [2.12](#)

2.1 Chemical Bonds and Interactions			
NAME	BASIS OF INTERACTION	STRUCTURE	BOND ENERGY* (KCAL/MOL)
Covalent bond	Sharing of electron pairs		50-110 
Hydrogen bond	Sharing of H atom		3-7 
Ionic interaction	Attraction of opposite charges		3-7 
van der Waals interaction	Interaction of electron clouds		1 
Hydrophobic interaction	Interaction of nonpolar substances		1-2 

\*Bond energy is the amount of energy needed to separate two bonded or interacting atoms under physiological conditions.

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 High Energy

 Low Energy

 Very Low Energy

Table 2.1

## Water: Structure and Properties

- Water's molecular structure and capacity to form hydrogen bonds give it unusual properties significant for life. Review Figure [2.15](#)

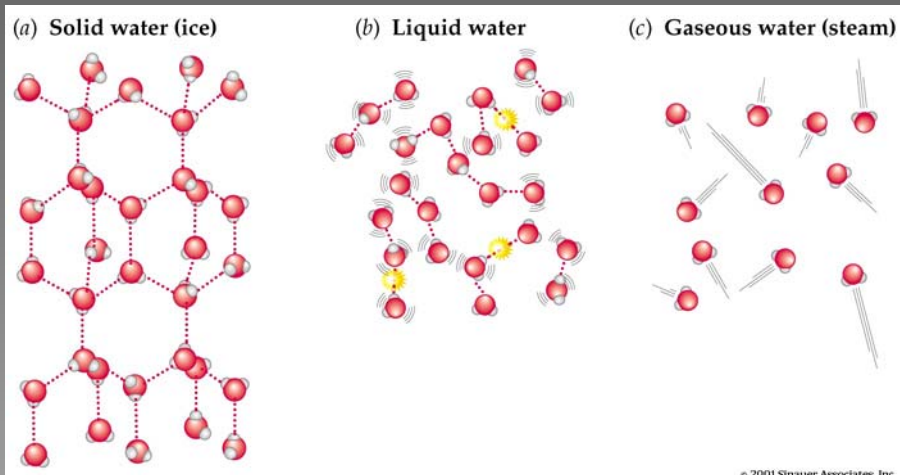
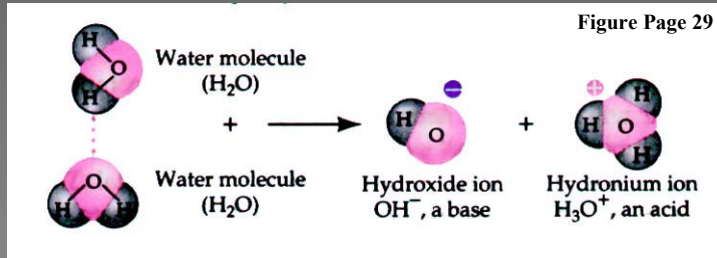


Figure 2.15

O and N can form an "extra" bond by using their nonbonding electron pair  
 $H_2O + H^+ \rightarrow H_3O^+$  or  $NH_3 + H^+ \rightarrow NH_4^+$



This reaction is frequently abbreviated as:  $H_2O = H^+ + OH^-$

The  $K_w = [H^+][OH^-] = 1.0 \times 10^{-14} M^2$  at 25°C

In pure water,  $[H^+] = [OH^-] = 1.0 \times 10^{-7} M$

$pH = -\log[H^+] = 7$  in pure water at 25°C = neutral pH

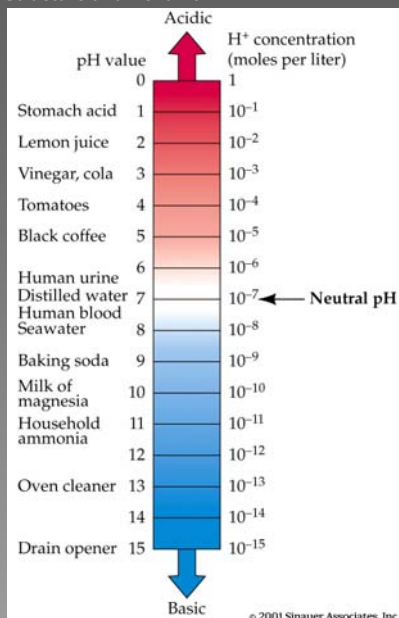


Figure 2.18

## Acids and Bases

■ **Acid:** Increases the  $[H^+]$  of a solution (decreases the pH)

**Base:** Decreases the  $[H^+]$  of a solution (increases the pH)

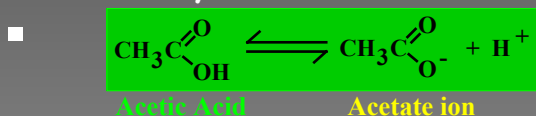
**Strong Acids** dissociate completely to produce  $H^+$



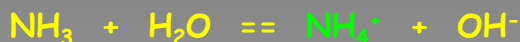
**Strong Bases** dissociate completely to produce  $OH^-$   
this reduces the  $[H^+]$



**Weak Acids** partially dissociate producing  $H^+$   
==> they are **Proton Donors**



**Weak Bases** bind  $H^+$  from  $H_2O$  molecules  
==> they are **Proton Acceptors**



**Note:** The equilibrium constants for these reactions are generally small. The  $K_a = 1.8 \times 10^{-5} M$  for the first reaction;  $K_b = 1.8 \times 10^{-5} M$  for the second

**Note also:** The product of the dissociation of a **weak acid**, **acetate ion** in this example is a **weak base**, and the product of the reaction of a **weak base** with water, **ammonium ion** in this example, is a **weak acid**.

## Buffers

The negative logarithm of the  $K_a$  of a weak acid is called the  $pK_a$ . For example, the  $pK_a$  of Acetic Acid is  $-\log(1.8 \times 10^{-5}) = 4.7$ .

Solutions of weak acids and their conjugate bases stabilize the pH around the value of the  $pK_a$



These solutions are called **Buffers**

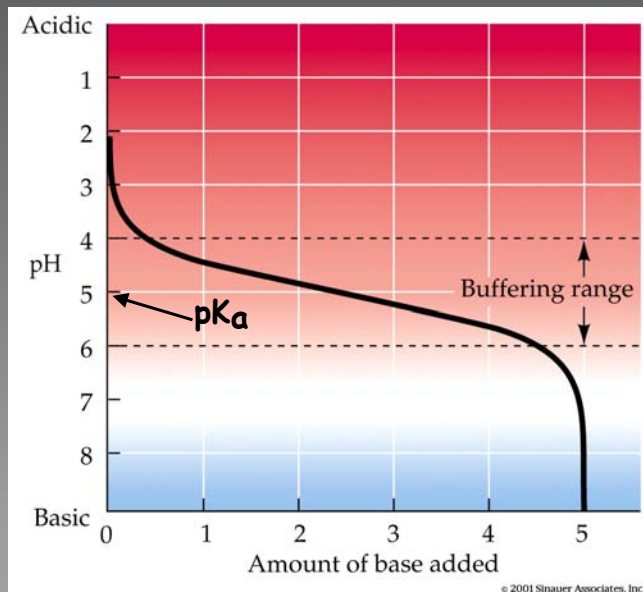
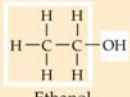
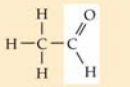

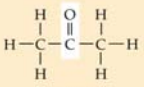
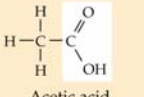


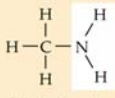
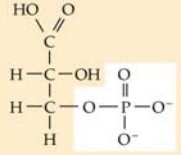
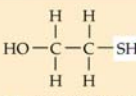
Figure 2.19

Organic compounds can contain atoms other than C and H; these form **"Functional Groups"** characterized by the types of atoms present and the way they are bonded giving these groups special properties.

Functional group	Class of compounds	Structural formula	Example
Hydroxyl —OH	Alcohols	$R-OH$	 Ethanol
Aldehyde —CHO	Aldehydes	$R-\overset{O}{\parallel}C-H$	 Acetaldehyde
Keto 	Ketones	$R-\overset{O}{\parallel}C-R$	 Acetone
Carboxyl —COOH	Carboxylic acids	$R-\overset{O}{\parallel}C-OH$	 Acetic acid

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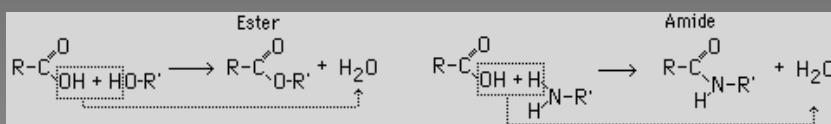
Figure 2.20 - Part 1

Functional group	Class of compounds	Structural formula	Example
Amino —NH <sub>2</sub>	Amines	$R-\overset{H}{\underset{H}{ }{N}}$	 Methylamine
Phosphate —OPO <sub>3</sub> <sup>2-</sup>	Organic phosphates	$R-O-\overset{O}{\parallel}P-O^-$	 3-Phosphoglyceric acid
Sulfhydryl —SH	Thiols	$R-SH$	 Mercaptoethanol

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Figure 2.20 - Part 2

Two organic molecules with certain functional groups can be joined by a covalent bond formed when a molecule of water is removed; this allows the creation of new types of organic molecules.

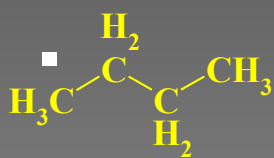


An **ester** is formed by combining an **alcohol** and a **carboxylic acid**.

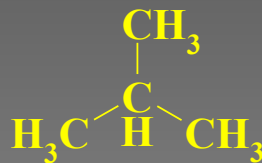
An **amide** is formed by combining an **amine** and a **carboxylic acid**.

## The Properties of Molecules

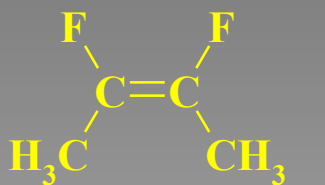
- Structural and optical isomers have the same kinds and numbers of atoms, but differ in their structures and properties. Review Figure [2.21](#)



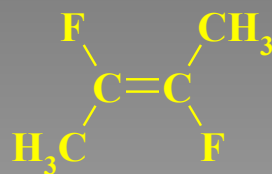
butane



isobutane



*cis*-difluoroethene



*trans*-difluoroethene

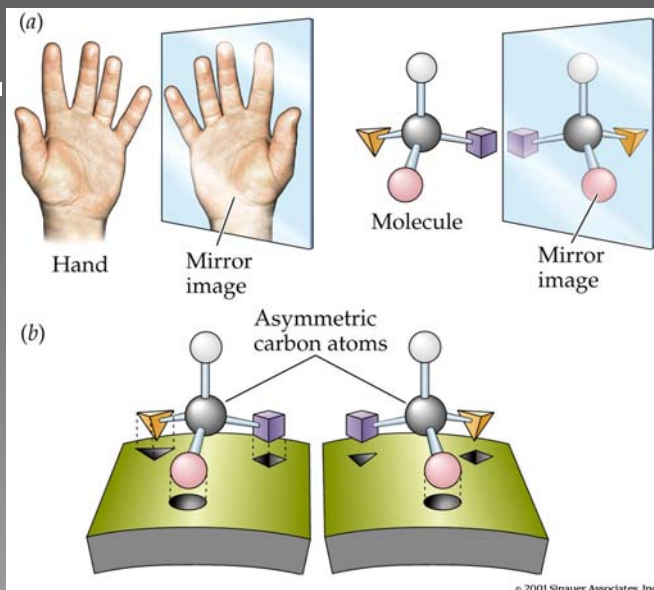


Figure 2.21