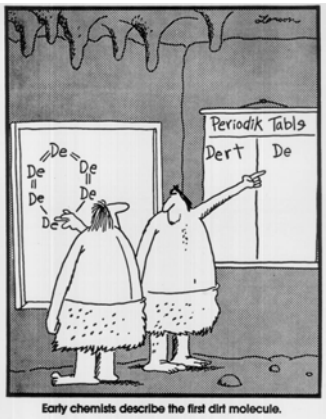
Lecture Series 2

Small Molecules: Structure and Function

A. Atoms: The Constituents of Matter

- An element is made up of only one kind of atom.
- The number of protons identifies the element.
- Isotopes differ in the number of neutrons.



Early chemists describe the first dirt molecule.

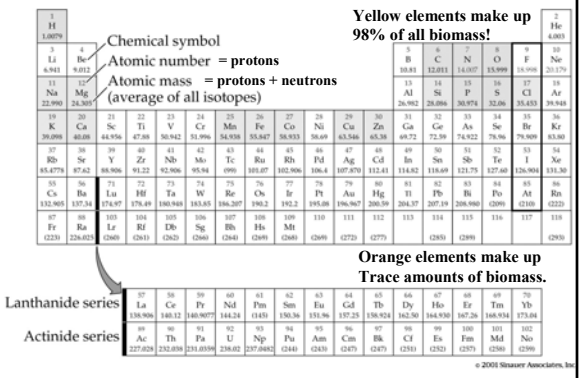


Figure 2.1

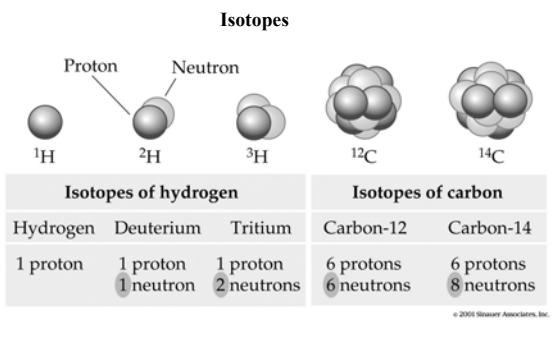


Figure 2.2

A. Atoms: The Constituents of Matter

- Electron behavior determines chemical bonding.
- Electrons are distributed in shells of "orbitals" containing a maximum of two.
  - Octet Rule: stable molecules have 8 electrons in outer shell.

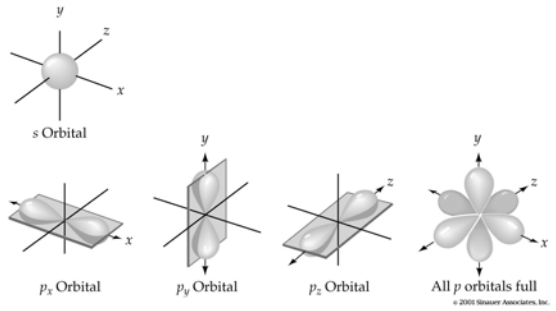


Figure 2.4

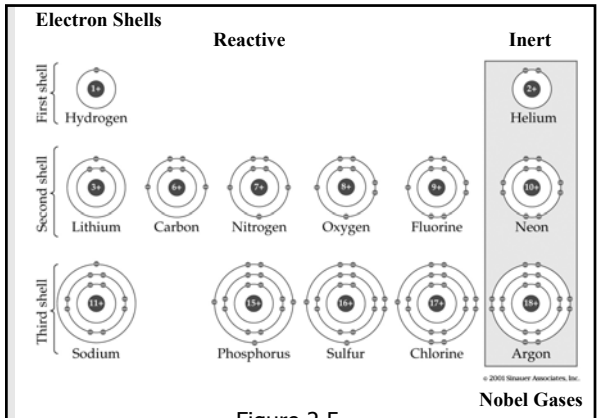


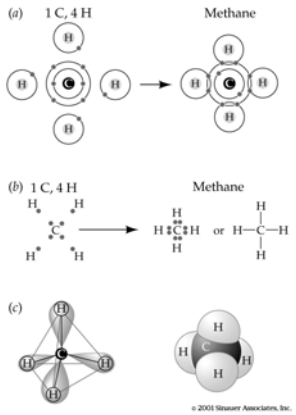
Figure 2.5

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.

Table 2.1



Covalent Bonding with Carbon

Figure 2.7

2.2 Covalent Bonding Capabilities of Some Biologically Important Elements

ELEMENT	NUMBER OF COVALENT BONDS
Hydrogen	1
Oxygen	2
Sulfur	2
Nitrogen	3
Carbon	4
Phosphorus	5

Table 2.2

B. 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 δ^+ and the other is δ^-.
- Covalent bonds involve sharing of electrons.

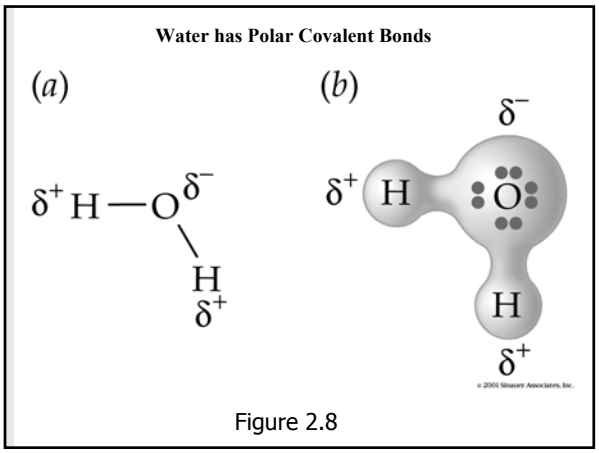


Figure 2.8

2.3 Some Electronegativities

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

Table 2.3

B. Chemical Bonds: Linking Atoms Together

- Hydrogen bonds form between a δ^+ hydrogen atom in one molecule and a δ^- nitrogen or oxygen atom in another molecule or in another part of a large molecule.
- Some sharing at work.

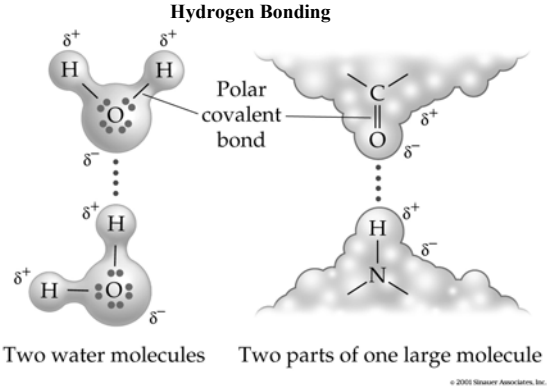


Figure 2.9

B. 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.
- No sharing involved!

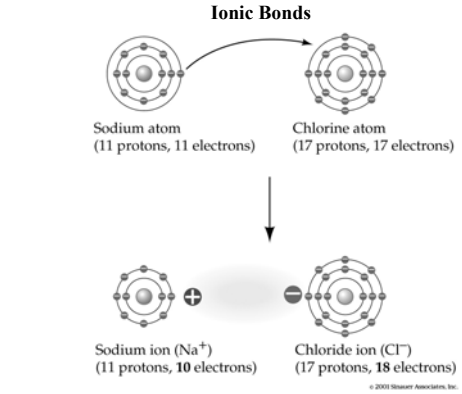
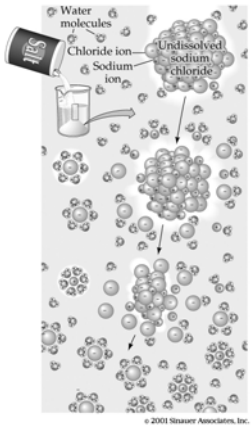


Figure 2.10



Water forms Hydration Spheres around ions

Figure 2.11

B. Chemical Bonds: Linking Atoms Together

- Nonpolar molecules have no attraction for polar substances. They are attracted to each other by very weak bonds called van der Waals forces.
- These are very important for membranes.
  - Hydrophobic vs. hydrophilic molecules.

Polar and Nonpolar Molecules

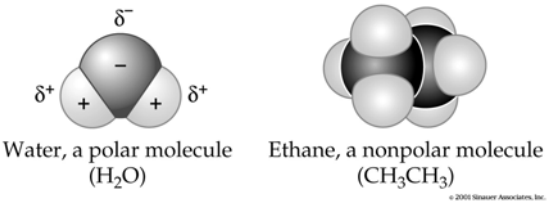


Figure 2.12

C. Eggs by the Dozen: Molecules by the Mole

- Calculate the number of molecules by weighing: Avogadro's # = 6.023×10^{23}
- This is the weight in grams equal to a molecules combined atomic weight.
- Useful as in Biology, most reactions take place in solutions, which yields units of Molarity.

Moles

D. Chemical Reactions: Atoms Change Partners

- In chemical reactions, substances change their atomic compositions and properties. Energy is either released or added. Matter and energy are not created or destroyed, but change form.
- Conservation of Mass & Energy.

D. Chemical Reactions: Atoms Change Partners

- Combustion reactions are oxidation-reduction aka "redox" reactions.
- Fuel is converted to carbon dioxide and water, while energy is released as heat and light.
- In living cells, these reactions occur in multiple steps.

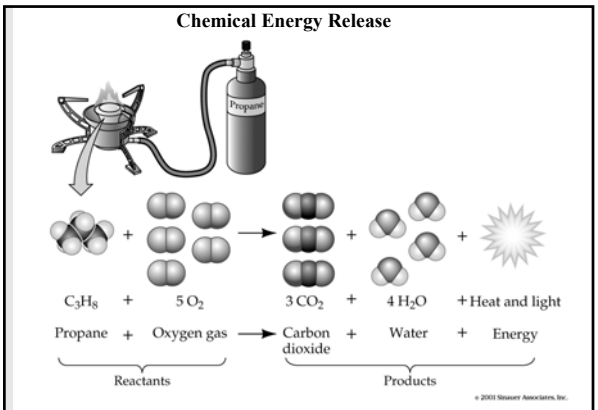


Figure 2.13

E. Water: Structure and Properties

- Water's molecular structure and capacity to form hydrogen bonds give it unusual and special properties significant for life.
- These include: Phase change avoidance, Specific Heat, Cohesive and Adhesive Strength, Latent Heat of Vaporization.
- Rare Ion formation (1 in 5 x10^8) or pH 7.0

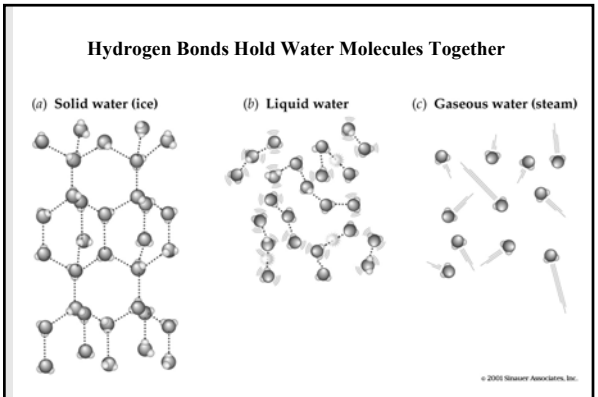


Figure 2.15

Ice floats and frozen benzene sinks

E. Water: Structure and Properties

- "Cohesion" of water molecules results in a high surface tension.
- Water's high "heat of vaporization" assures cooling when it evaporates.
- Wide range of "Reynold's Numbers" encountered by organisms.

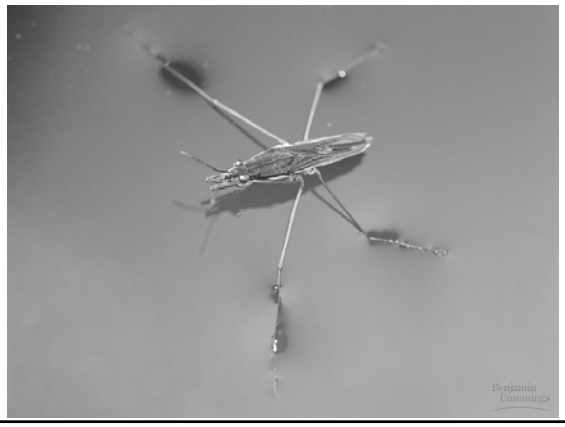


TABLE 6.2. REYNOLDS NUMBERS—EXAMPLES

Bacterium swimming	0.000001
Pollen grain falling, or sperm swimming	0.01
Fruit fly (fuselage) in flight	100
Small bird flying	100,000
Squid fast jetting	1,000,000
Large whale swimming	200,000,000

Re = Reynold's Number

Re = Inertial Forces / Viscous Forces

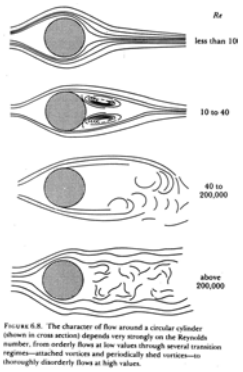
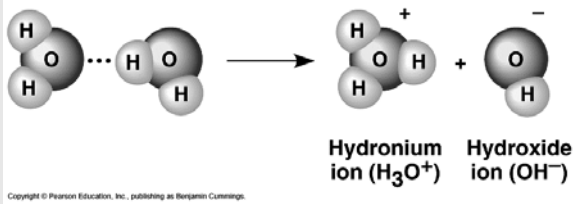


FIGURE 6.8. The character of flow around a circular cylinder (shown in cross section) depends very strongly on the Reynolds number, from orderly flows at low values through several transition regimes—attached vortices and periodically shed vortices—to thoroughly disorderly flows at high values.

F. Acids, Bases, & pH Scale

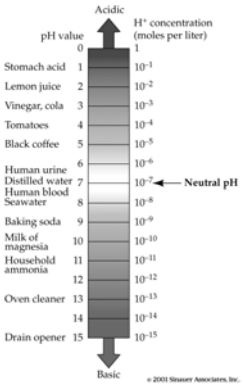
- Acids are substances that donate hydrogen ions. Bases are those that accept hydrogen ions.

Chemical reaction: hydrogen bond shift



F. Acids, Bases, & pH Scale

- The pH of a solution is the negative logarithm of the hydrogen ion concentration. $pH = -\log[H^+]$
- pH scales range from 0 to 14 as $[H^+][OH^-] = 1 \times 10^{-14}$
- Most biological solutions are between the pH range of 6 to 8.



pH Scale

Figure 2.18

F. Acids, Bases, & pH Scale

- Buffers are systems of weak acids and bases that limit the sudden change in pH when hydrogen ions are added or removed.
- Examples are Bicarbonate or Phosphate Buffers.

Buffers

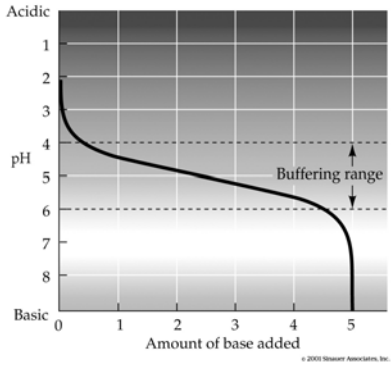
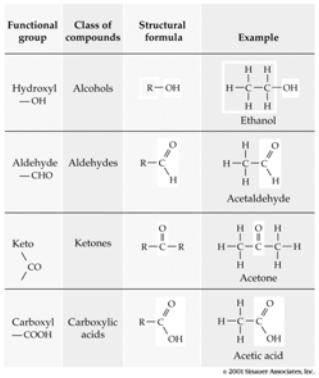


Figure 2.19

G. Properties of Molecules

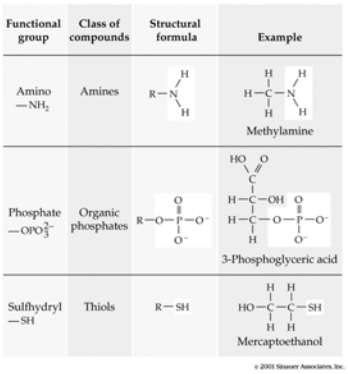
- Molecules vary in size, shape, reactivity, solubility, and other chemical properties.
- Functional groups make up part of a larger molecule and provide specific chemical properties.



Functional group	Class of compounds	Structural formula	Example
Hydroxyl —OH	Alcohols	R—OH	Ethanol
Aldehyde —CHO	Aldehydes		Acetaldehyde
Keto	Ketones		Acetone
Carboxyl —COOH	Carboxylic acids		Acetic acid

Functional Groups

Figure 2.20 – Part 1

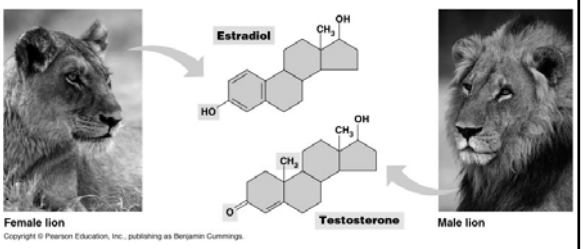


Functional group	Class of compounds	Structural formula	Example
Amino —NH_2	Amines		Methylamine
Phosphate —OPO_3^{2-}	Organic phosphates		3-Phosphoglyceric acid
Sulfhydryl —SH	Thiols	R—SH	Mercaptoethanol

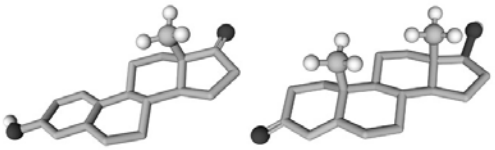
Functional Groups

Figure 2.20 – Part 2

A comparison of functional groups of female (estradiol) and male (testosterone) sex hormones



Estradiol and Testosterone



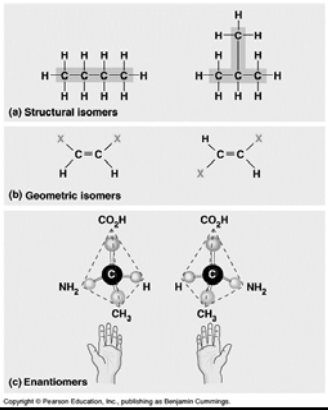
G. Properties of Molecules

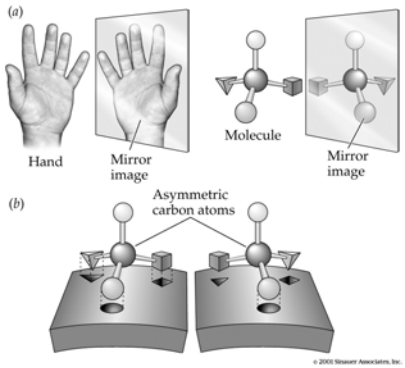
- Structural, geometric and optical isomers have the same kinds and numbers of atoms, but differ in their structures and properties.

G. Properties of Molecules

- Structural isomers: variation in covalent bond arrangement such as butane and isobutane.
- Geometric isomers: variation in the arrangement about a double bond such as with cis or trans configurations.
- Optical isomers: variation in the spatial arrangement around an asymmetric carbon, resulting molecules that are mirror images.

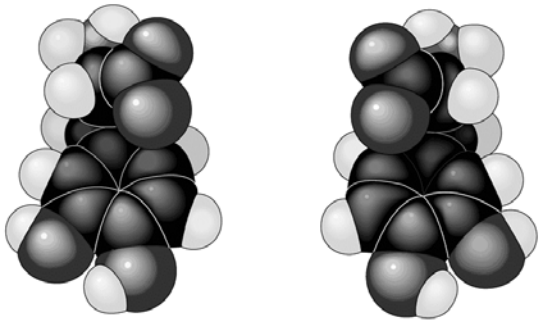
Three types of isomers





Optical Isomers aka Enantimers Figure 2.21

The pharmacological importance of enantiomers



L-Dopa
(effective against Parkinson's disease)

D-Dopa
(biologically inactive)