The Biochemistry of Water

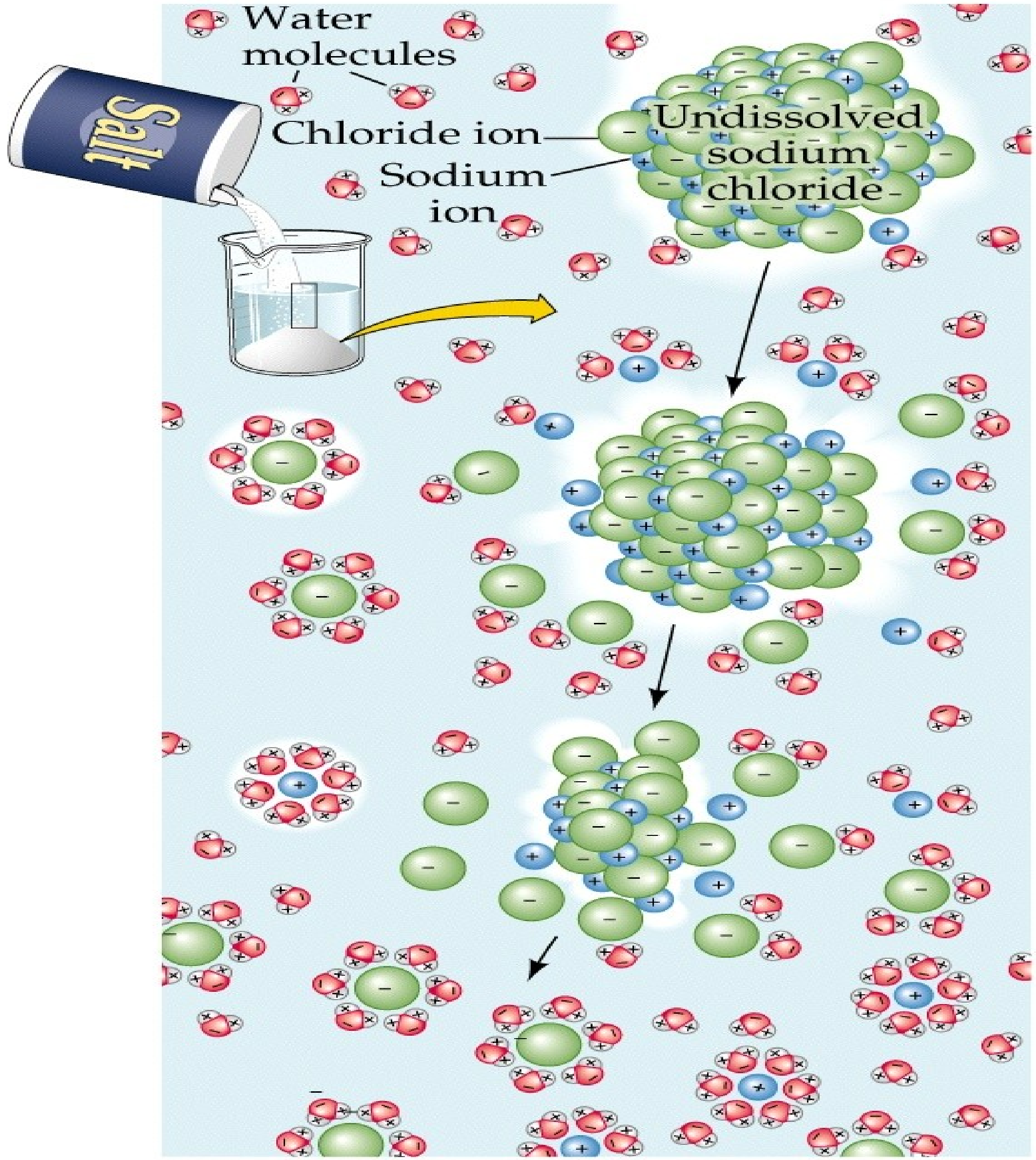
The Biochemistry of Water

- **2.3 Water, pH, and Buffers**
- Water is the solvent of life
- All organisms are composed primarily of water, such that most eukaryotic organisms are about 90 percent water while prokaryotes are about 70 percent water. No organism, not even the prokaryotes, can develop and grow without water.
- **All chemical reactions in organisms occur in liquid water**.
- Being polar, water has unique properties. These include its role as a solvent, as a chemical reactant, and as a factor to maintain a fairly constant temperature.

- Water Has Several Unique Properties
- Liquid water is the medium in which all cellular chemical reactions occur.
- Being polar, water molecules are attracted to other polar molecules and act as the universal solvent in cells.

- Take for example what happens when you put a solute like salt in water.
- The solute dissolves into separate sodium and chloride ions because water molecules break the weak ionic bonds and surround each ion in a sphere of water molecules.
- An aqueous solution, which consists of solutes in water, is essential for chemical reactions to occur

- Water molecules also are reactants in many chemical reactions. The example of the hydrolysis reaction shown at the top of this page involved water in splitting maltose into separate molecules of glucose and glucose.
- As you have learned, the polar nature of water molecules leads to hydrogen bonding.
- By forming a large number of hydrogen bonds between water molecules, it takes a large amount of heat energy to increase the temper-ature of water.
- Likewise, a large amount of heat must be lost before water decreases tem-perature.
- So, by being 70 to 90 percent water, cells are bathed in a solvent that maintains a more consistent temperature change.


Water
molecules
Salt
Chloride ion
Sodium
ion
Undissolved
sodium
chloride

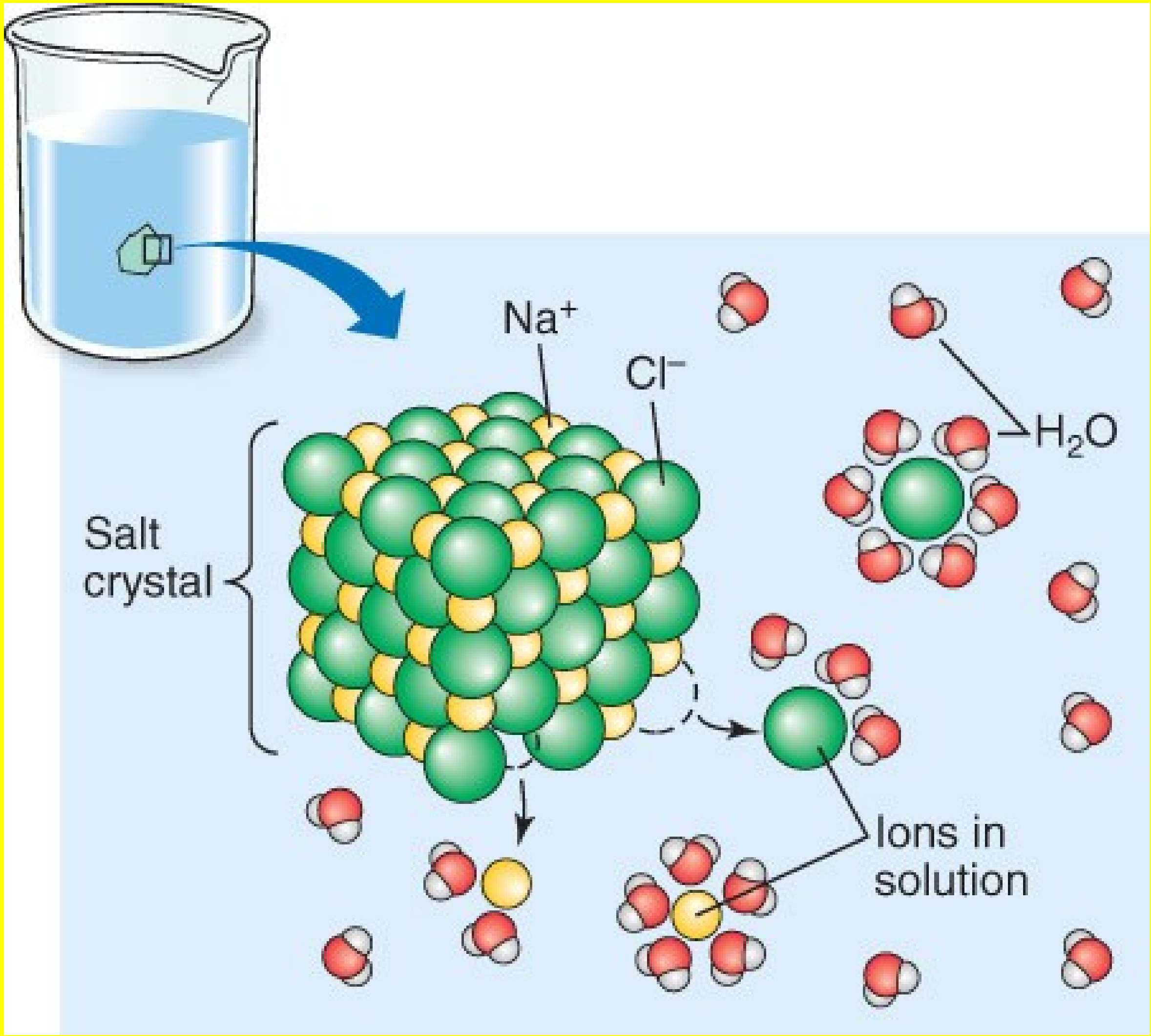
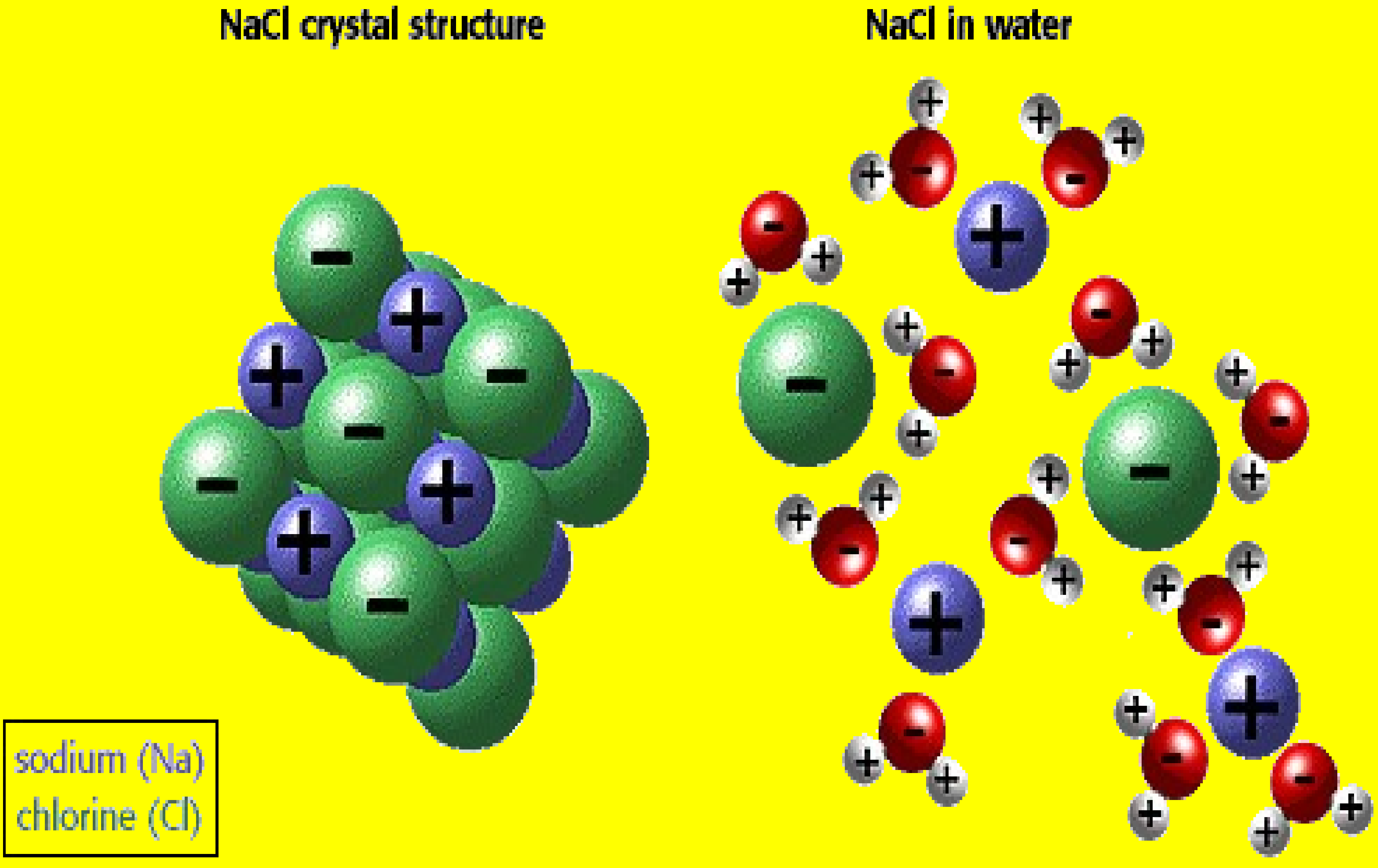


Figure 02.06: Solutes dissolve in water

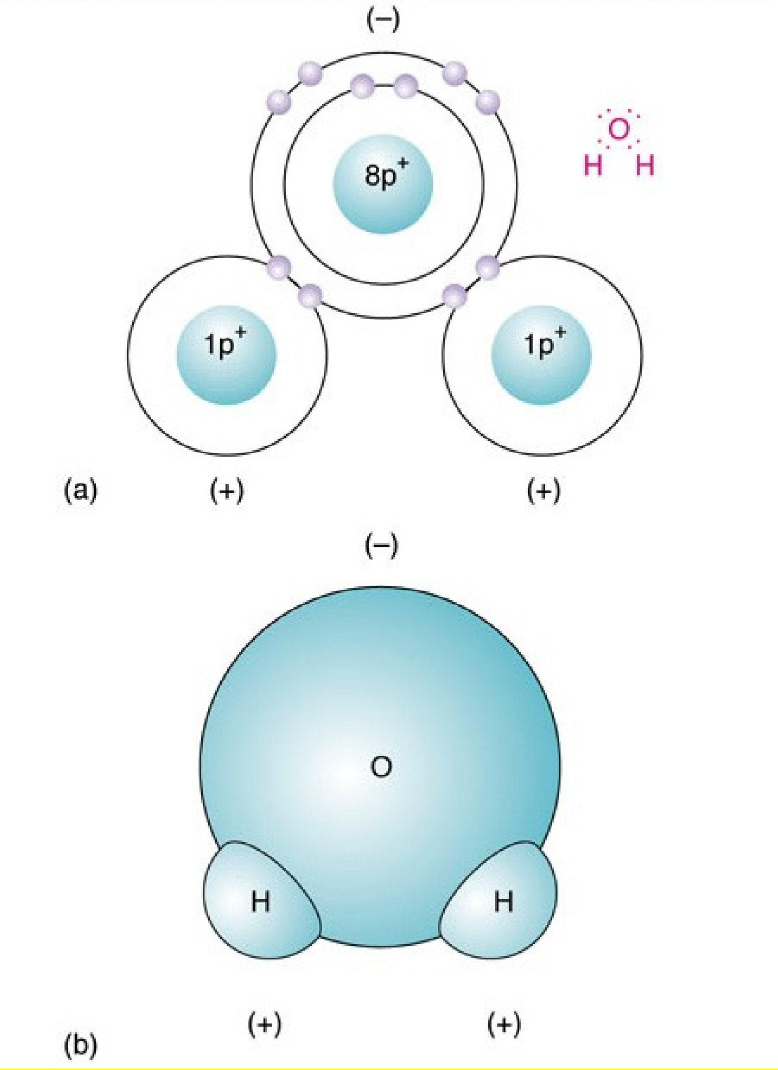
Dissolution of NaCl in H_2O



Water

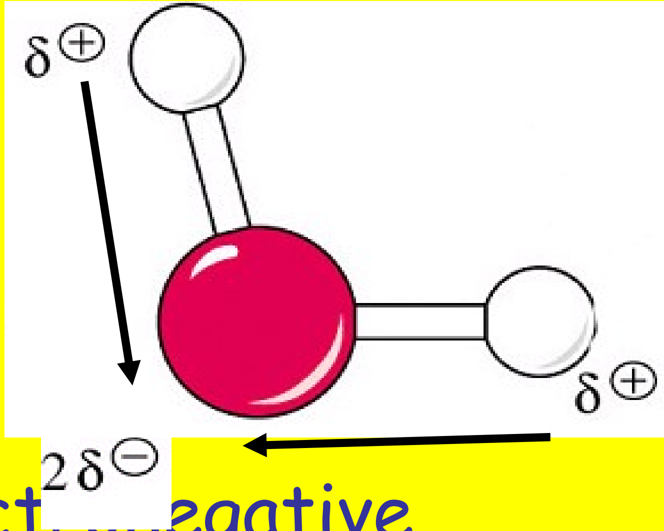
- Water **contains polar covalent bonds because oxygen and hydrogen do not share electrons equally**
- Oxygen exerts a greater pull on the electrons and gains a negative charge
- Hydrogen as a result has a positive charge
- As a result – the water molecule has a positive end (the hydrogen atoms)
- **The oxygen is slightly negative**
- **This forms a dipole – a polar covalent molecule**

H_2O – a polar molecule



Properties of water

- Very polar



- Oxygen is highly electronegative
- H-bond donor and acceptor
- High b.p., m.p., heat of vaporization, surface tension

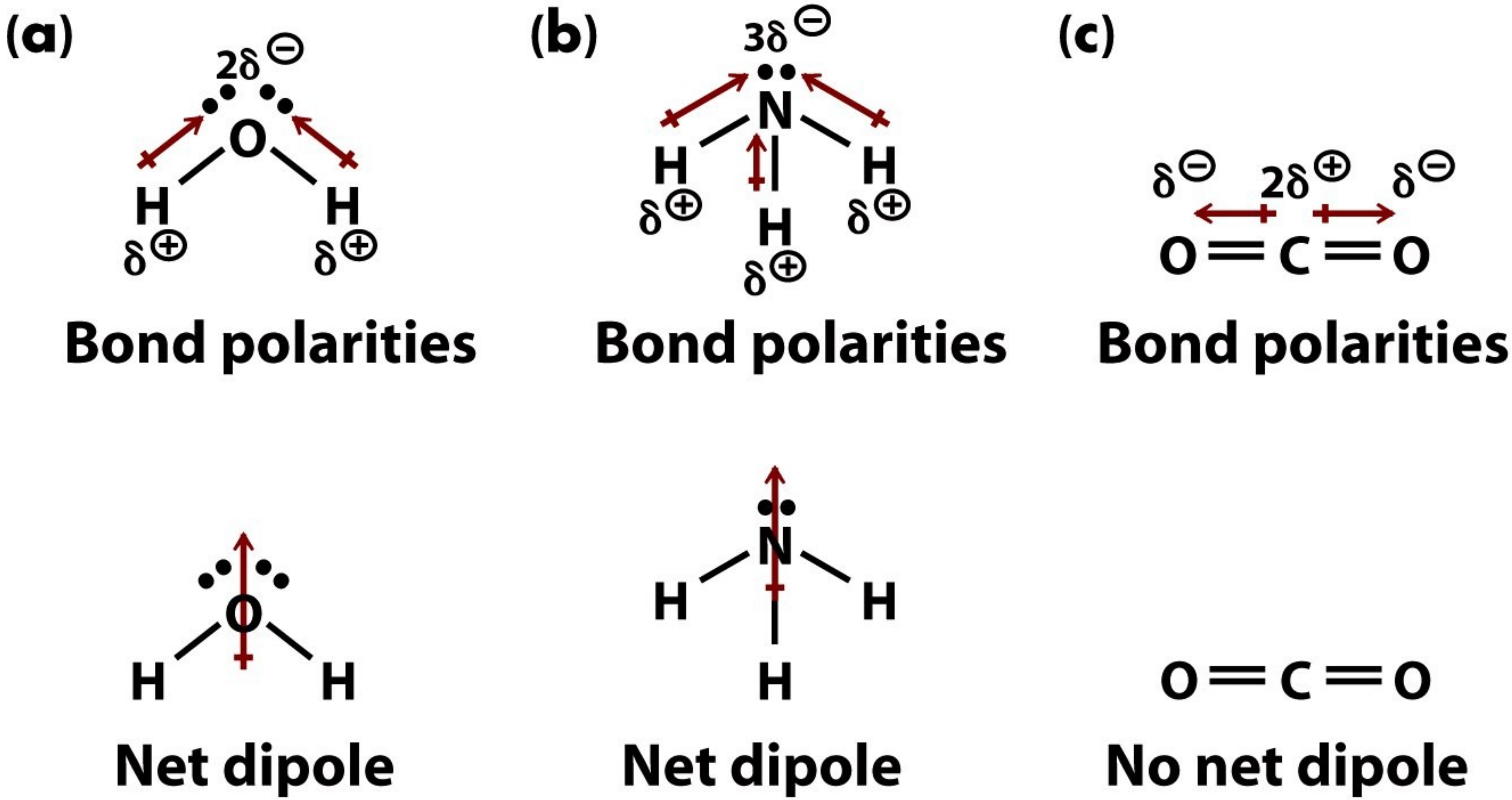


Figure 2-2 Principles of Biochemistry, 4/e

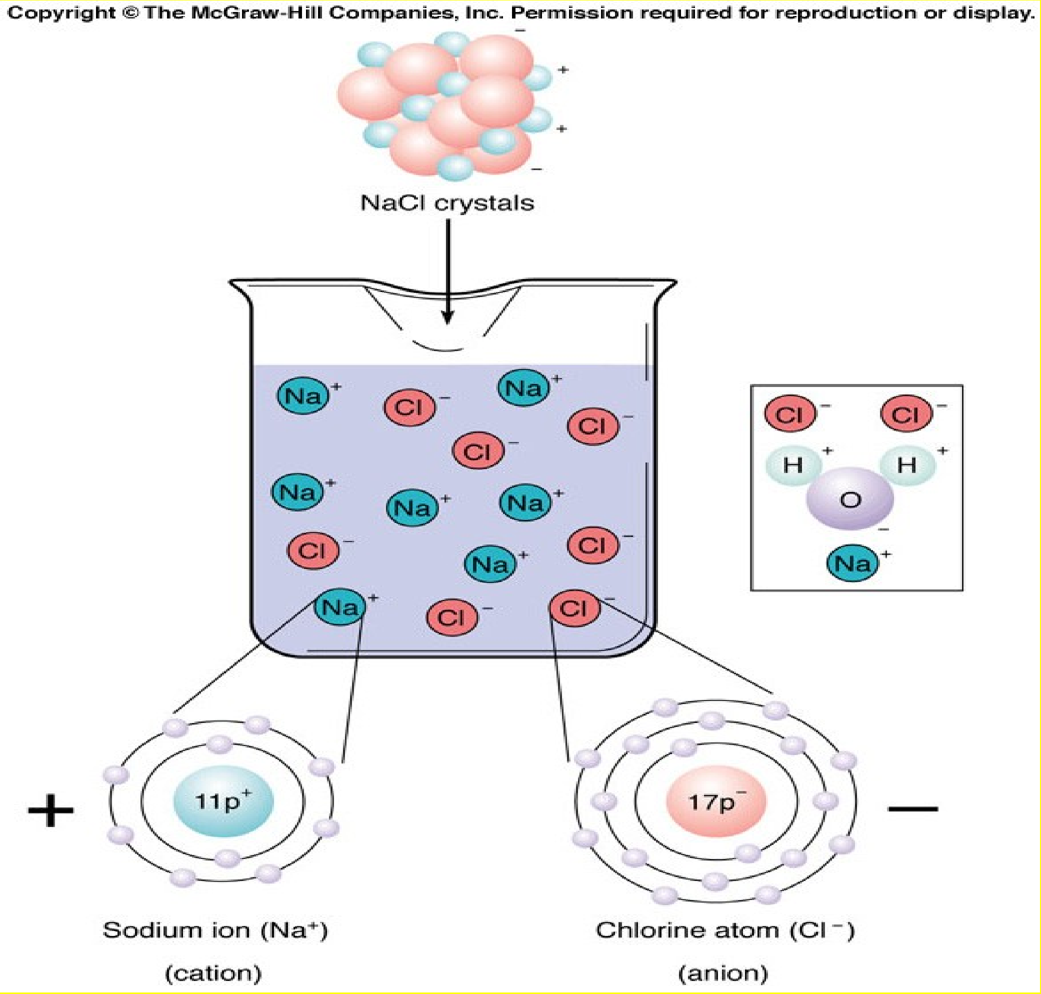
- **Properties of Water**
- Water Has Several Unique Properties
- **Water exists in three states (Liquid** – aquatic environment outside us and inside us), solid (ice) and gas (steam)
- **1. Surface Tension-** cell membranes moist, protection.
- Ex. Capillary action in plant roots, attraction to glass-meniscus.
- **2. Cohesion-** water molecules stick to each other held together by H-bonds.
- **3. Adhesion-** water molecules stick to unlike surfaces such as glass or plastic due to H-bonds between water and other polar compounds.
- **4. High Specific Heat-** water can absorb **or** release large amounts of heat energy with little temp change. E.g. Water stabilizes temp. in cells and ecosystems.

- **5. _High Heat of Vaporization-** many H-bonds must be broken before water can evaporate.
- **6. _Lower Density of Ice-** water molecules in an ice crystal are further apart because of H-bonding.
- **7 Water is Polar-** a good solvent; surrounds ions and other polar molecules. E.g.Transport of nutrients in organisms- plasma, cytoplasm, and xylem.
- **8 Medium for Chemical Reactions-** hydration/dehydration reactions.

Water as the universal solvent

- Most biological activities occur in **aqueous (water-based) solutions.**
- Water is able to dissolve small non polar covalent molecules, ionic compounds, and other polar covalent molecules
- **Water soluble molecules are described as hydrophilic (**water loving)**. Hydrophilic** molecules dissolve in water.
- **Those molecules that are not soluble in water are hydrophobic (**water hating or fearing)**. Hydrophobic** molecules – repel water.
- **Amphipathic** molecules -have both hydrophilic and hydrophobic properties

Solution – a mixture of one or more substances called **solutes**, dispersed in a dissolving medium called a **solvent**

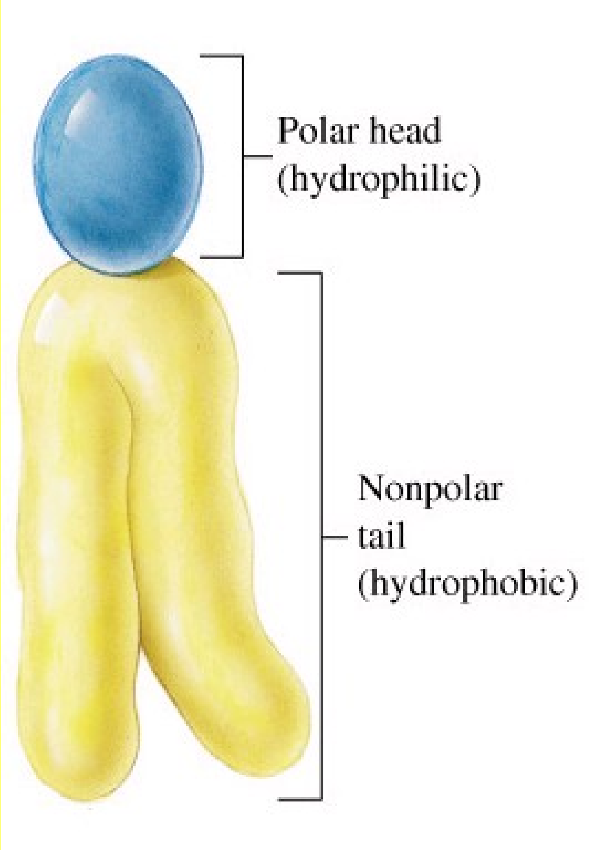


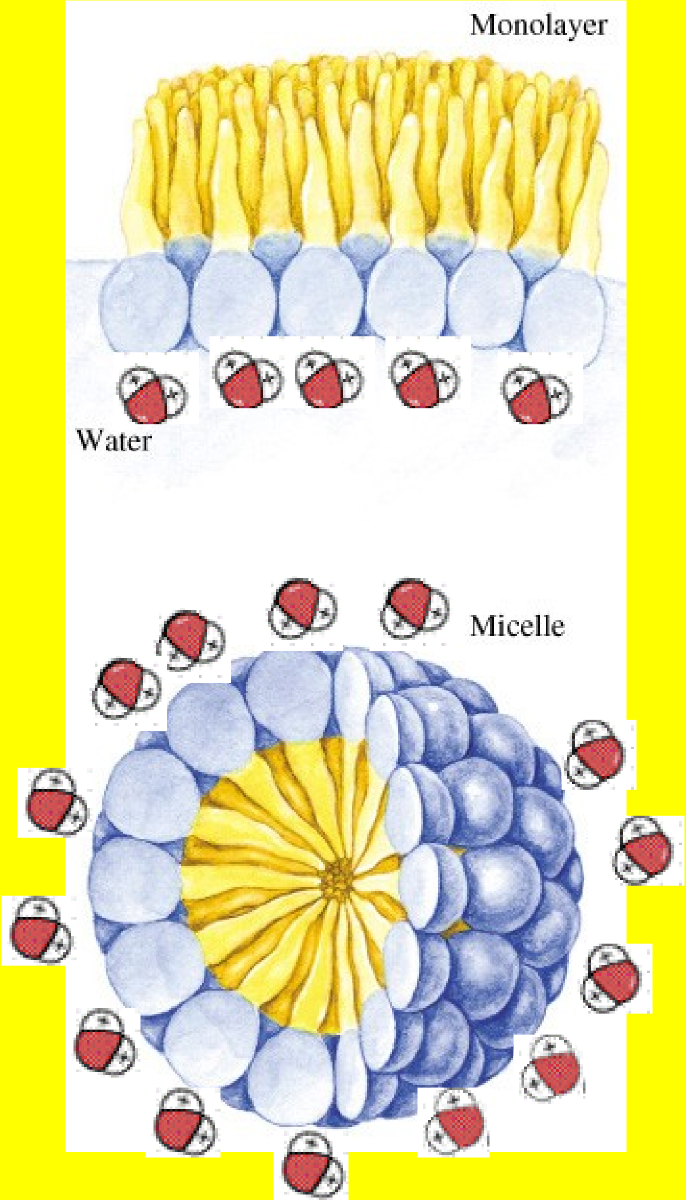
Solutes – Na+ & Cl-

Solvent – H_2O

Non-polar substances are insoluble in water

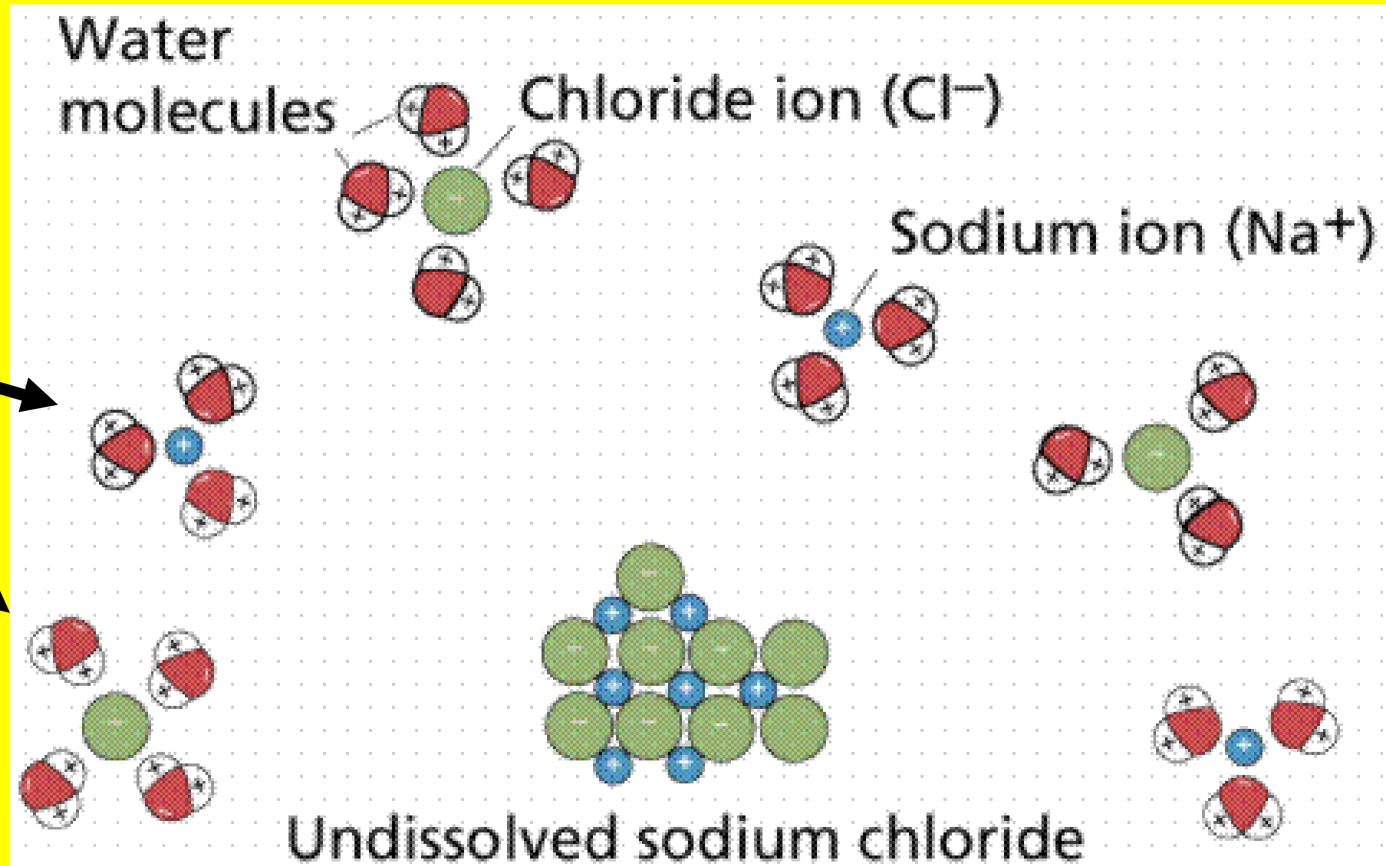
Many lipids are amphipathic

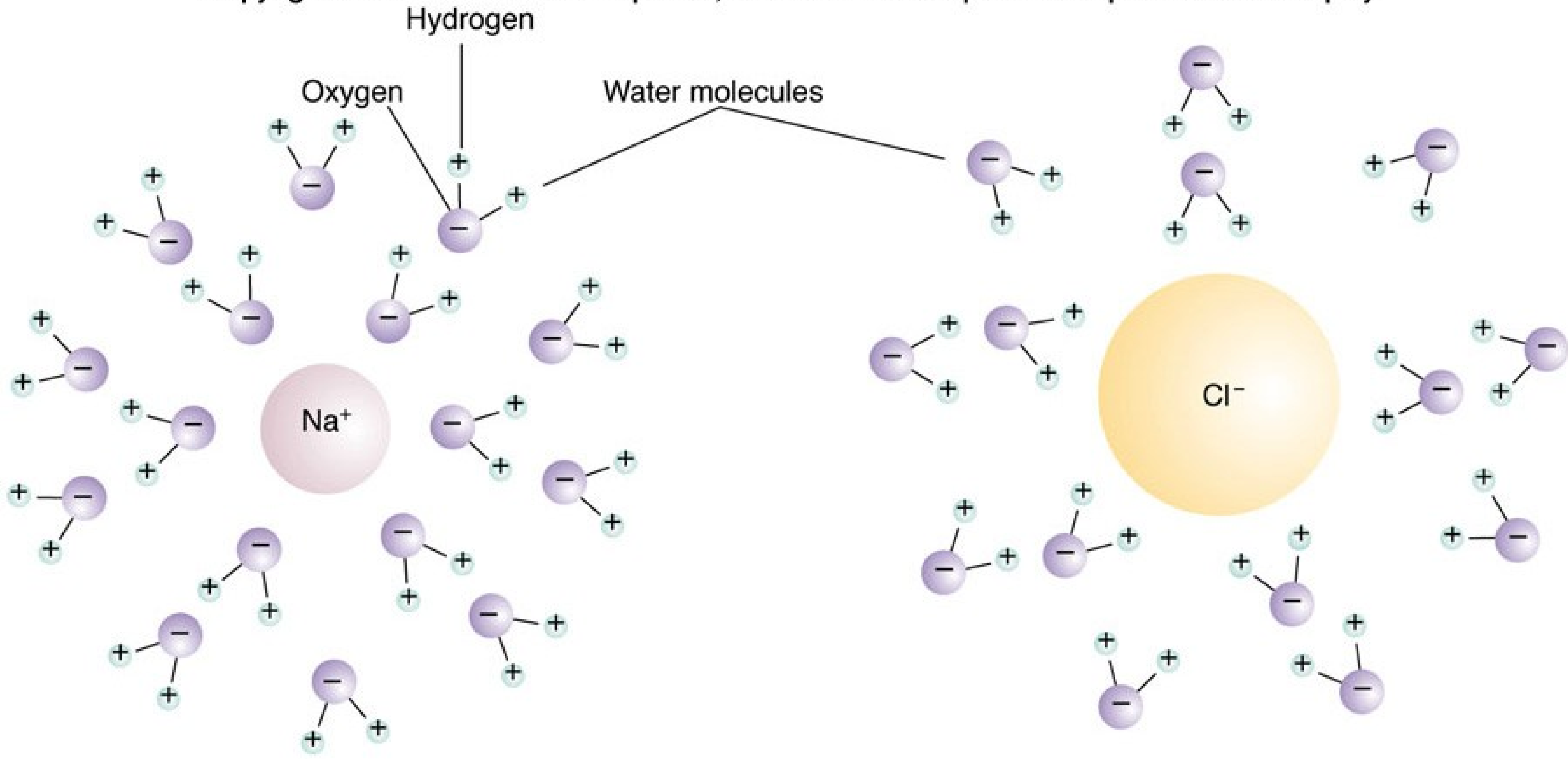




Water dissolves polar compounds

solvation shell
or
hydration shell




Hydrogen
Oxygen
Water molecules
Na⁺
Cl⁻

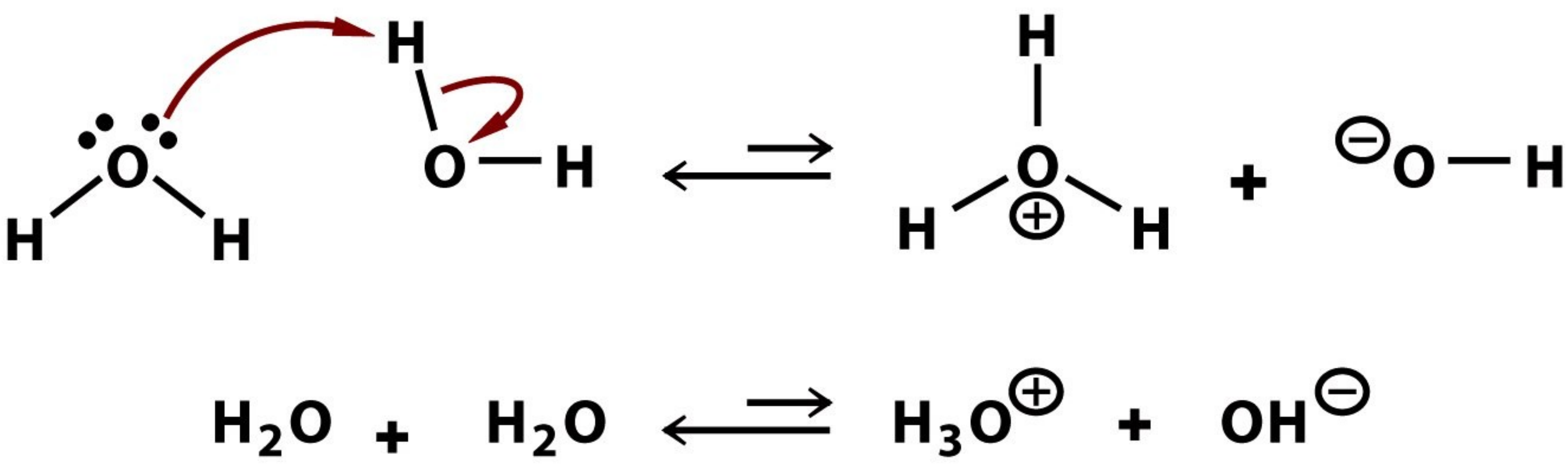
Solvation and Hydration shells

- Depending on the pH of a solution, macromolecules such as proteins which contain many charged groups, will carry substantial net charge, either positive or negative.
- Cells of the body and blood contain many polyelectrolytes (molecules that contain multiple same charges, e.g. DNA and RNA) and polyampholytes that are in close proximity.
- The close association allows these molecules to interact through opposing charged groups.

- The presence, in cells and blood, of numerous small charged ions (e.g. Na^+, Cl^-, Mg^{2+}, Mn^{2+}, K^+) leads to the interaction of many small ions with the larger macroions.
- This interaction can result in a shielding of the electrostatic charges of like-charged molecules.

- This electrostatic shielding allows macroions to become more closely associated than predicted based upon their expected charge repulsion from one another.
- The net effect of the presence of small ions is to maintain the solubility of macromolecules at pH ranges near their pI.
- This interaction between solute (e.g. proteins, DNA, RNA, etc.) and solvent (e.g. blood) is termed solvation or hydration.
- The opposite effect to solvation occurs when the salt (small ion) concentration increases to such a level as to interfere with the solvation of proteins by H_2O. This results from the H_2O forming hydration shells around the small ions.

Ionization of Water



Unnumbered figure pg 38 Principles of Biochemistry, 4/e

Ionization of Water

$$H_20 + H_20 \rightleftharpoons H_3O^+ + OH^-$$

$$H_20 \rightleftharpoons H^+ + OH^-$$

$$K_{eq} = \frac{[H^+]\,[OH^-]}{[H_2O]}$$

$K_{eq} = 1.8 \times 10^{-16} M$

$[H_2O] = 55.5\ M$

$$[H_2O]\,K_{eq} = [H^+]\,[OH^-]$$

$$(1.8 \times 10^{-16} M)(55.5\ M) = [H^+]\,[OH^-]$$

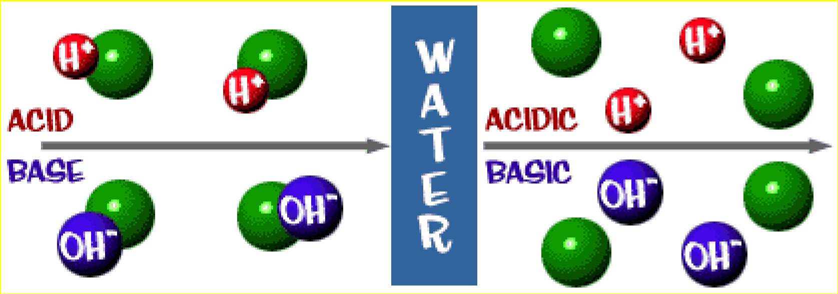
$$1.0 \times 10^{-14}\ M^2 = [H^+]\,[OH^-] = K_w$$

If $[H^+]=[OH^-]$ then $[H^+] = 1.0 \times 10^{-7}$

- Ionization of H_2O releases hydrogen ions [H^+] & hydroxyl ions [OH^-]
- pH scale – ranges from 0 to 14, expresses the concentration of H^+ ions
  - pH is the negative logarithm of the concentration of H+ ions.
- pH 6 = 0.000001 moles H^+/ l
- pH 9 = 0.000000001 moles H^+/ l

Water and hydrogen ions

- http://www.biology.arizona.edu/biochemistry/p



- **Acids and Bases Must Be Balanced in Cells**
- **Cell chemistry is sensitive to pH changes**
- An acid is a chemical substance that donates a H+ to a solution; a base accepts the H+
- Acids donate hydrogen ions to a solution while bases remove hydrogen ions from a solution.
- The pH scale indicates the number of hydrogen ions in a solution and denotes the relative acidity of a solution.

- **Acids and Bases Must Be Balanced in Cells**
- **KEY CONCEPT Cell chemistry is sensitive to pH changes.**
- In an aqueous solution, **most of the water molecules remain intact, but some can dissociate into hydrogen ions (H+) and (OH-) only to rapidly recombine in a reversible reaction** represented thus:
- H2O <=> H+ + OH-
- For the chemical reactions in all cells to work properly, there must be a correct balance of H+ and OH-
- Besides water, other compounds in cells can release H+ or OH- and affect cell function

- For our purposes, an acid is a chemical that donates H+ to water or another solution.
- By contrast, a base (or alkali) is a substance that accepts hydrogen ions in solution, often by combining them with the hydroxyls of the base.

- Acids are distinguished by their sour taste. Some common examples are acetic acid in vinegar, citric acid in citrus fruits, and lactic acid in sour milk products.
- **Strong acids can donate large numbers of hydrogen ions to a solution.** Hydrochloric acid (HC1), sulfuric acid (H2SO4), and nitric acid (HNO3) are examples.
- Weak acids, typified by carbonic acid (HaCO3), donate a smaller number of hydrogen ions.
- Bases have a bitter taste. Strong bases take up numerous hydrogen ions from a solution leaving the solution with an excess of hydroxyl ions. Potassium hydroxide (KOH), a material used to make soap, is among them.
- Acids and bases frequently react with each other because of their opposing chemical characteristics. An exchange reaction involving hydrochloric acid (HCl) and sodium hydroxide (NaOH) is one example:
- HCl + NaOH -» NaCl + H2O

- To indicate the degree to which a solution is acidic, the Danish chemist Soren P. L. Sorensen introduced the symbol pH (potential hydrogen) and the pH scale.
- The scale extends from 0 (extremely acidic; high H+) to 14 (extremely basic; low H+) and is based on actual calculations of the number of hydrogen ions present when a substance mixes with water.
- Realize that **every time the pH changes by one unit, the hydrogen ion concentration changes 10 times**.
- A substance with a pH of 7,such as pure water, is said to be neutral; it is
- neither acidic nor basic because it has equal numbers of H+ and OH-.
- Figure 2”7 summarizes the pH values of several common substances.
- The greatest diversity of microorganisms occurs in environments where the pH is near neutral, although there are some spectacular exceptions
- In fact, the acidic soils of the Amazon rain forest contain less than half as many bacterial species as do the neutral soils of the deserts in the American Southwest.

- Acids and Bases Must Be Balanced in Cells
  - An acid is a chemical substance that donates a H+ to a solution; a base accepts the H+
  - The pH scale indicates the acidity or alkalinity of a solution
  - Cell chemistry is very sensitive to changes in pH

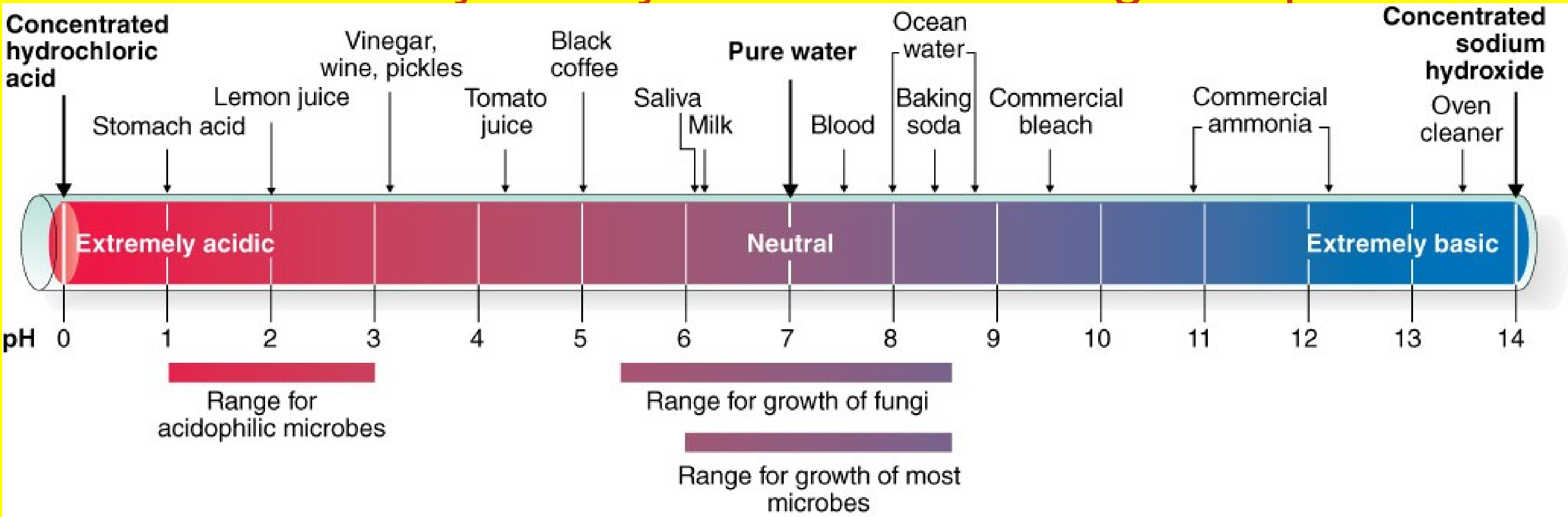


Figure 2.7, page 51

Acid and Base

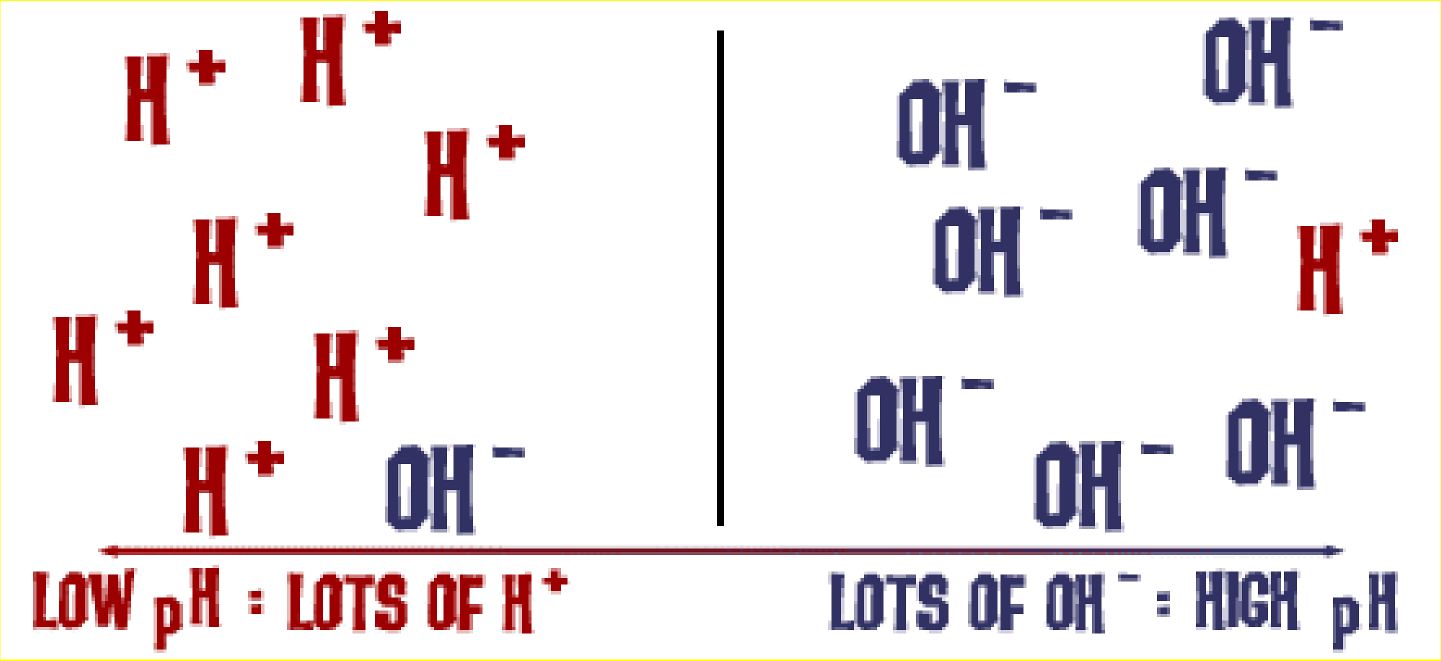
- Acids are hydrogen donors or proton donors

$COOH \rightarrow COO^- + H^+$

- Bases are hydrogen acceptors or proton acceptors

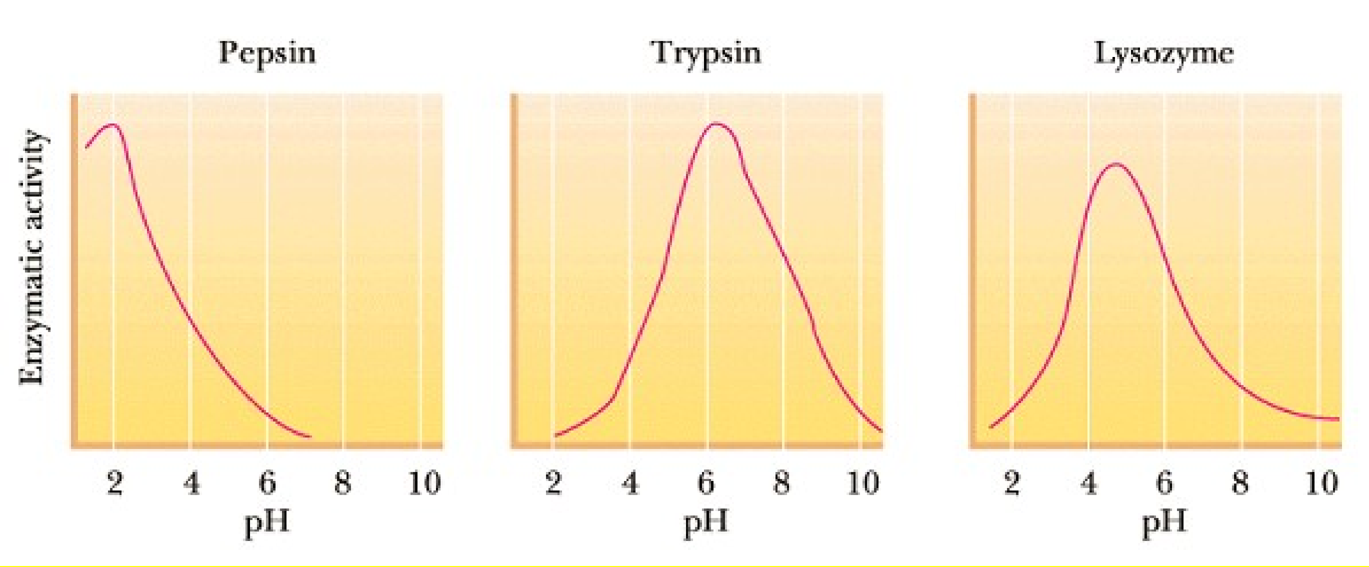
$NH_2 \rightarrow NH_3^+$

Acids and Bases



Weak Acids and Bases Equilibria

- **Strong acids / bases** – disassociate completely
- **Weak acids / bases** – disassociate only partially
- Enzyme activity sensitive to pH
- weak acid/bases play important role in protein structure/function



Acid/conjugate base pairs

$$HA + H_2O \rightleftharpoons A^- + H_3O^+$$

$$HA \rightleftharpoons A^- + H^+$$

HA = acid (donates H^+)(Bronstad Acid)

A^- = Conjugate base (accepts H^+)(Bronstad Base)

$$K_a = \frac{[H^+][A^-]}{[HA]}$$

K_a & pK_a value describe tendency to loose H^+

large K_a = stronger acid

small K_a = weaker acid

$$pK_a = -\log K_a$$

Carboxylic acids
(Organic acids)

- The acidic functional group in organic acids is the carboxl group
- The carboxyl group is a proton donor
- $COOH \longrightarrow COO^-$ in water solution

Organic bases

- Proton acceptors – gain a hydrogen and become positively charged in water solution
- The amino group - NH_2 becomes NH_3^+

pH

- The pH scale **indicates the acidity or alkalinity of a solution.**
- **Cell chemistry is very sensitive to changes in pH**

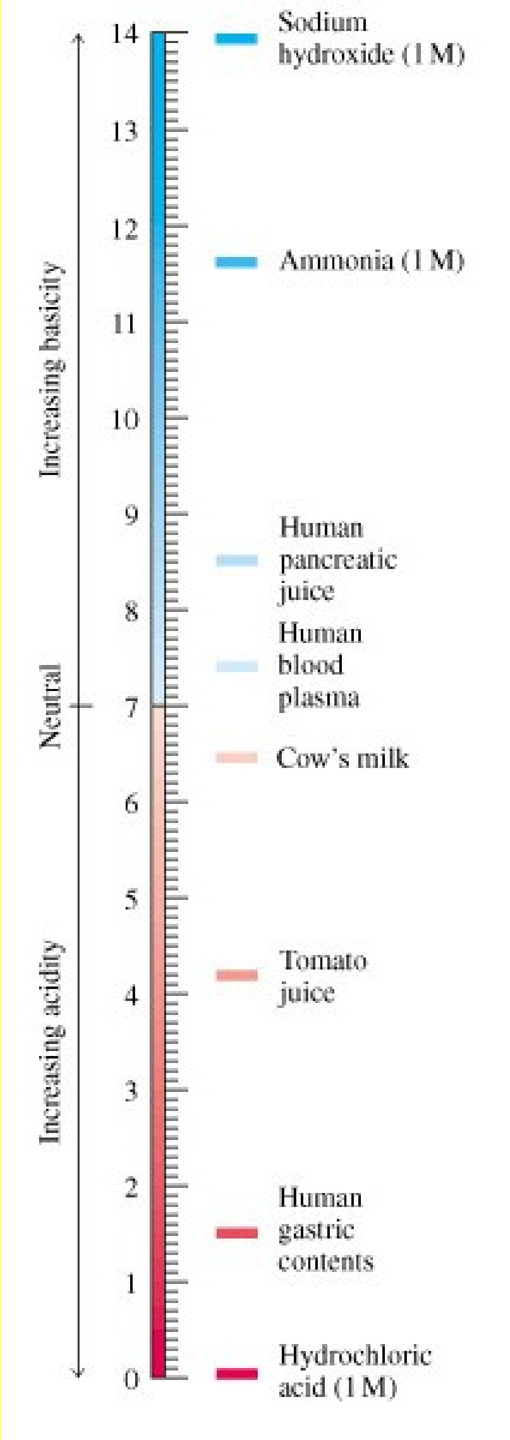
pH

- pH = **The concentration of H+ ions**
- **The negative logarithm of the hydrogen ion concentration in an aqueous solution**.

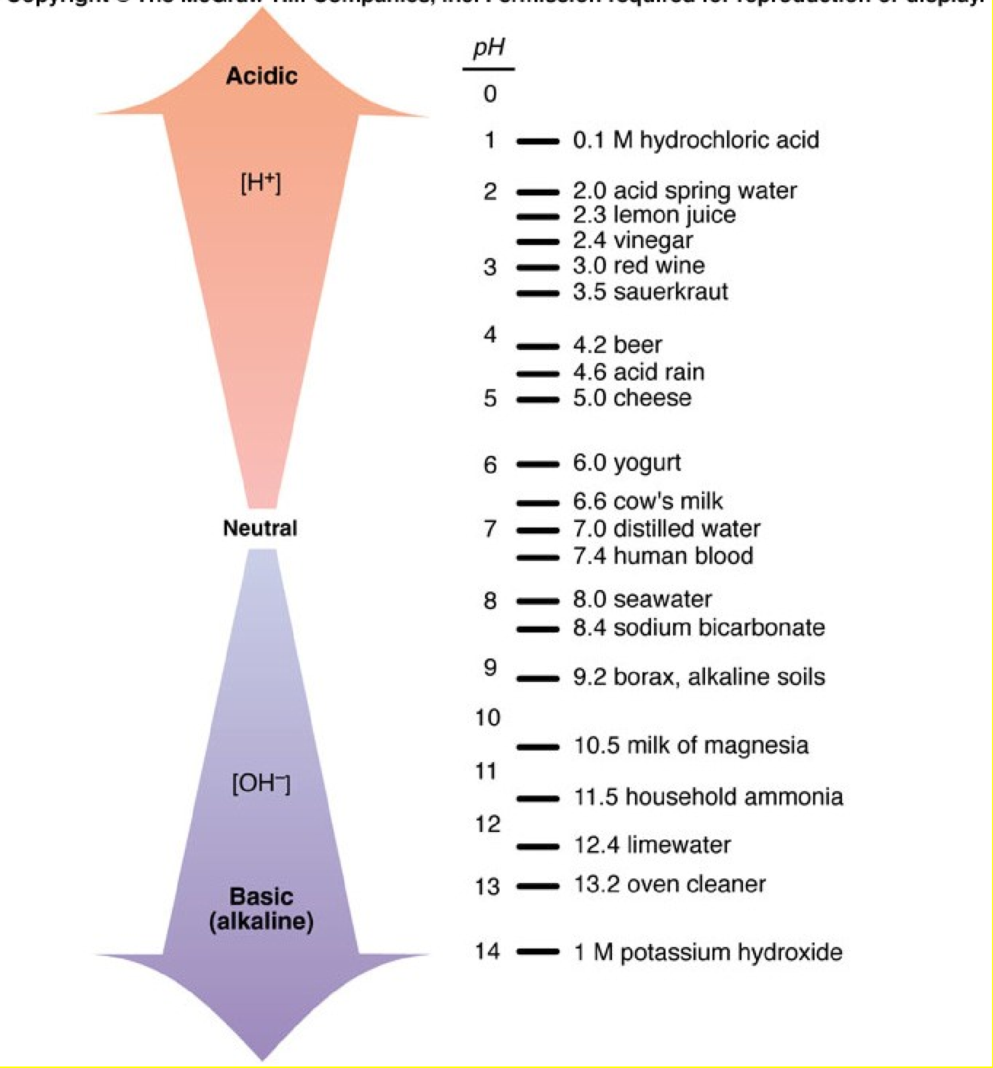
- $pH = -\log[H_30^+]$

pH Scale

- Devised by Sorenson (1902)
- [H+] can range from 1M and 1 X 10^{-14}M
- using a log scale simplifies notation
- pH = -log [H^+]
- Neutral pH = 7.0



pH scale



Acidic
[H+]
Neutral
[OH−]
Basic
(alkaline)
pH
0
1 0.1 M hydrochloric acid
2 2.0 acid spring water
2.3 lemon juice
2.4 vinegar
3 3.0 red wine
3.5 sauerkraut
4 4.2 beer
4.6 acid rain
5 5.0 cheese
6 6.0 yogurt
6.6 cow's milk
7 7.0 distilled water
7.4 human blood
8 8.0 seawater
8.4 sodium bicarbonate
9 9.2 borax, alkaline soils
10
10.5 milk of magnesia
11
11.5 household ammonia
12
12.4 limewater
13 13.2 oven cleaner
14 1 M potassium hydroxide

	Environmental Effects	pH Value	Examples
ACIDIC		pH = 0	Battery acid
		pH = 1	Sulfuric acid
		pH = 2	Lemon juice, Vinegar
		pH = 3	Orange juice, Soda
	All fish die (4.2)	pH = 4	Acid rain (4.2-4.4) Acidic lake (4.5)
	Frog eggs, tadpoles, crayfish, and mayflies die (5.5)	pH = 5	Bananas (5.0-5.3) Clean rain (5.6)
NEUTRAL	Rainbow trout begin to die (6.0)	pH = 6	Healthy lake (6.5) Milk (6.5-6.8)
		pH = 7	Pure water
		pH = 8	Sea water, Eggs
		pH = 9	Baking soda
		pH = 10	Milk of Magnesia
		pH = 11	Ammonia
		pH = 12	Soapy water
		pH = 13	Bleach
BASIC		pH = 14	Liquid drain cleaner

- pH and measurement- pHydrion paper
- pH measurement – pH meter

Buffers

- **Buffers Are a Combination of a Weak Acid and Base**
- Buffers prevent pH shifts
- **Buffers are aqueous systems that resist changes in pH when small amounts of a strong acid or base are added.**
- **A buffered system consist of a weak acid and its conjugate base.**
- **The most effective buffering occurs at the region of minimum slope on a titration curve**

  (i.e. around the pKa).
- **Buffers are effective at pHs that are within +/-1 pH unit of the pKa**

- Buffers are a mixture of a weak acid and a weak base that maintain acid/base balance in cells. Excess hydrogen ions can be absorbed by the base and too few hydrogen ions can be provided by the acid.

- As microorganisms—and all organisms—take up or ingest nutrients and undergo metabolism, chemical reactions occur that use up or produce H+.
- It is important for all organisms to balance the acids and bases in their cells because chemical reactions and organic compounds are very sensitive to pH shifts.
- Proteins are especially vulnerable. If the internal cellular pH is not maintained, these proteins may be destroyed.
- Likewise, when most microbes grow in a microbiological nutrient medium, the waste products produced may lower the pH of the medium, which could kill the organisms.
- To prevent pH shifts, cells and the growth media contain **buffers,** which are compounds that maintain a specific pH. The buffer does not necessarily maintain a neutral pH, but rather whatever pH is required for that environment.
- Most biological buffers consist of a weak acid and a weak base
- If an excessive number of H+ are produced (potential pH drop), the base can absorb them. Alternatively, if there is a decrease in the hydrogen ion concentration (potential pH increase), the weak acid can dissociate, replacing the lost hydrogen ions.

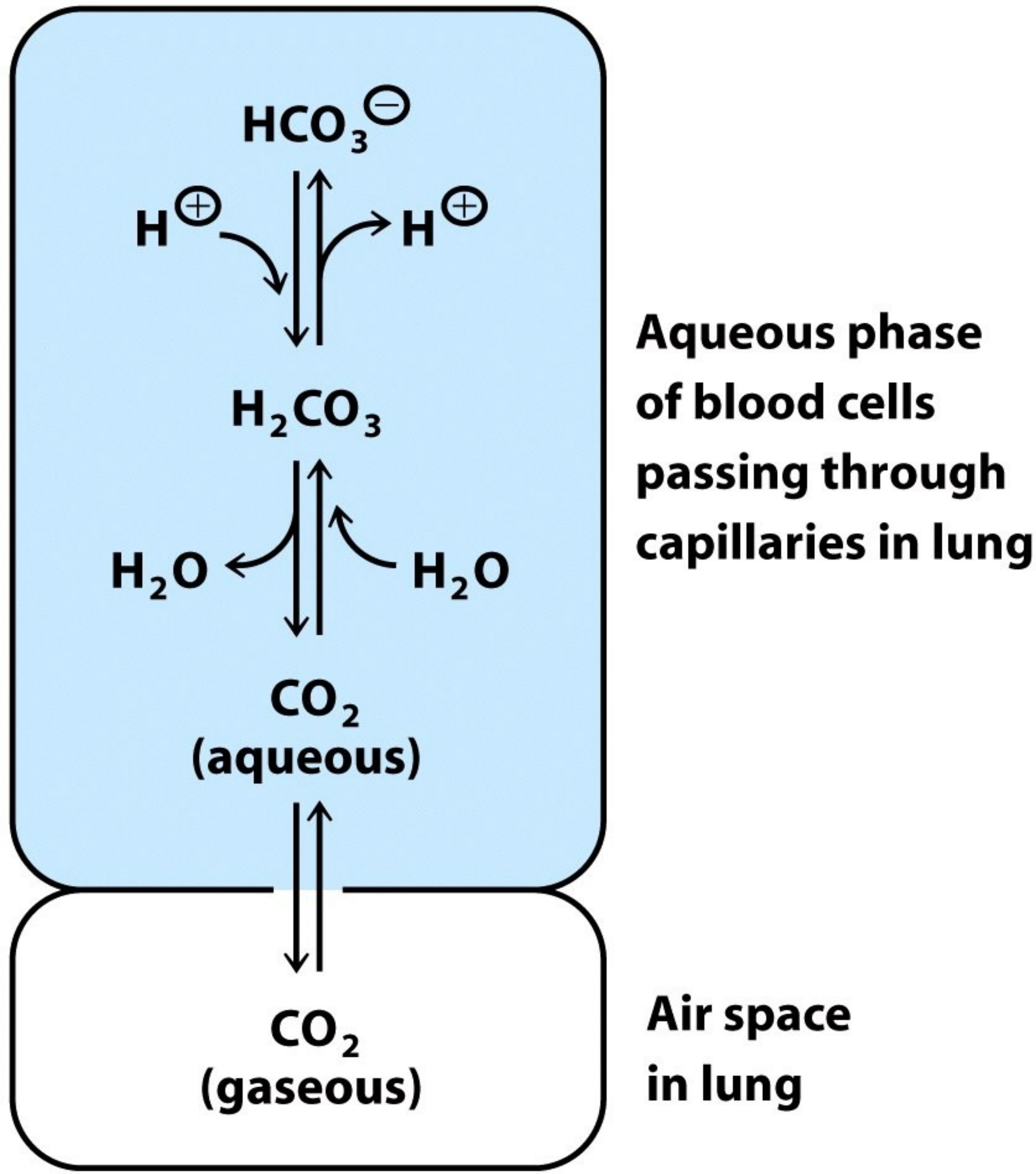
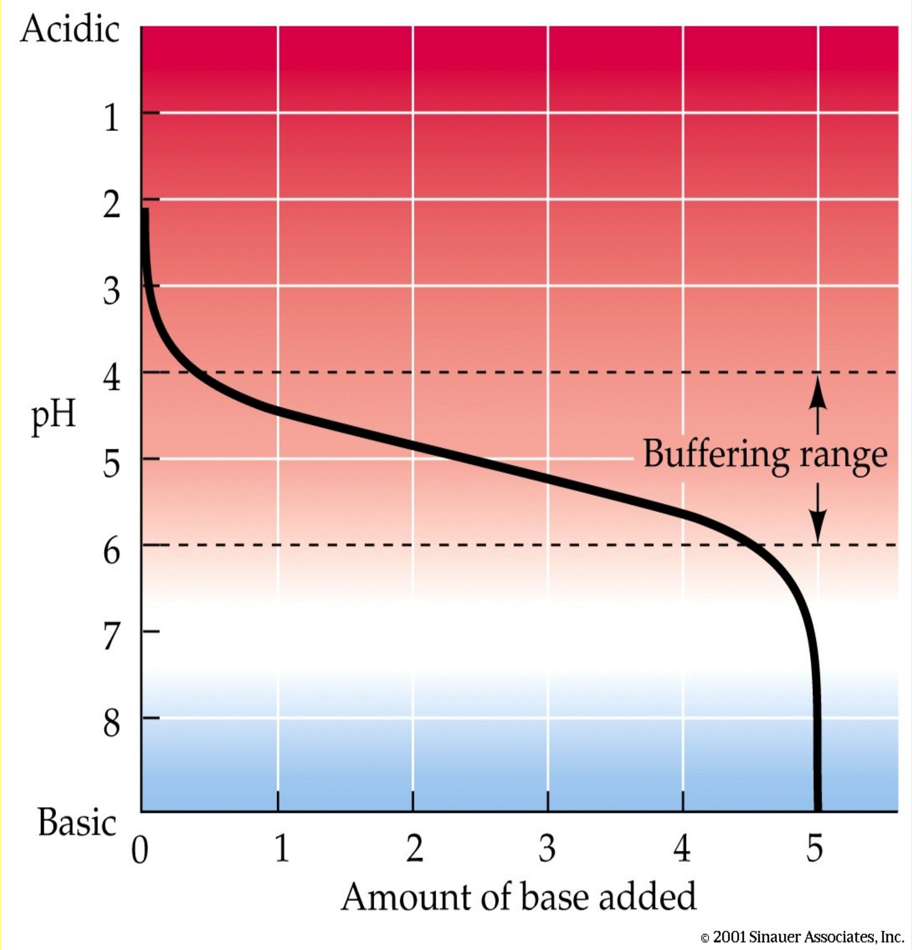


Figure 2-20 Principles of Biochemistry, 4/e

Buffering capacity



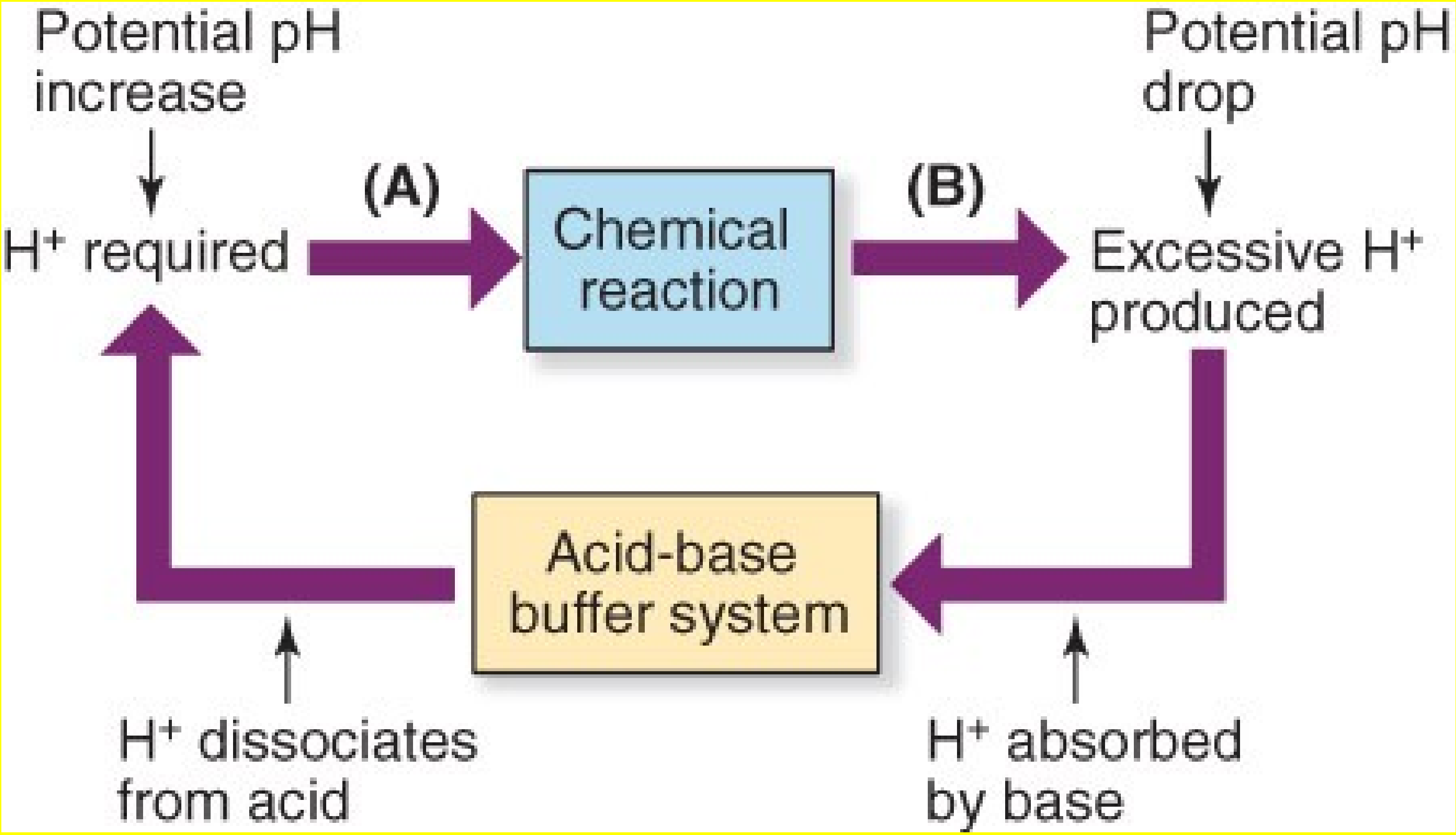


Figure 2.8, page 52

- Buffers Are a Combination of a Weak Acid and Base
  - Buffers prevent pH shifts