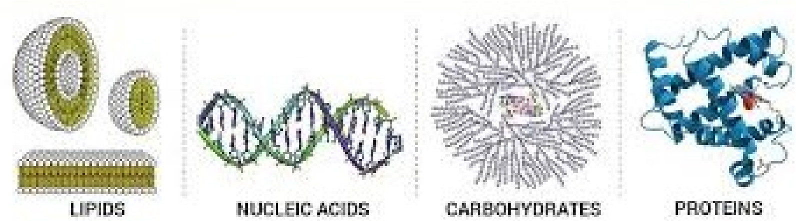
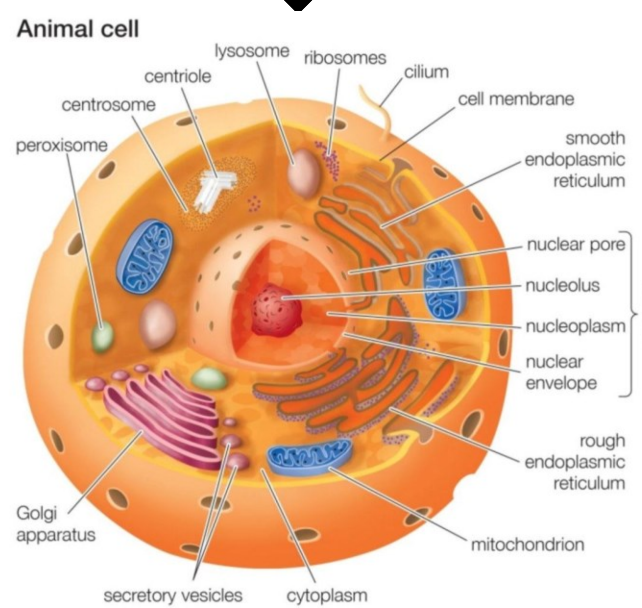
08/01/2024

Self-assembly is the autonomous organization of components into patterns or structures without human intervention.



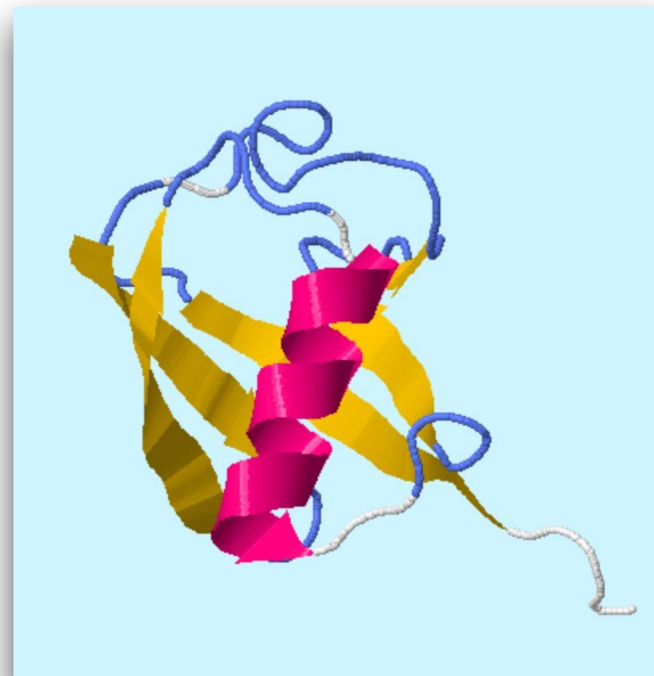
Guided Assembly

Self Assembly

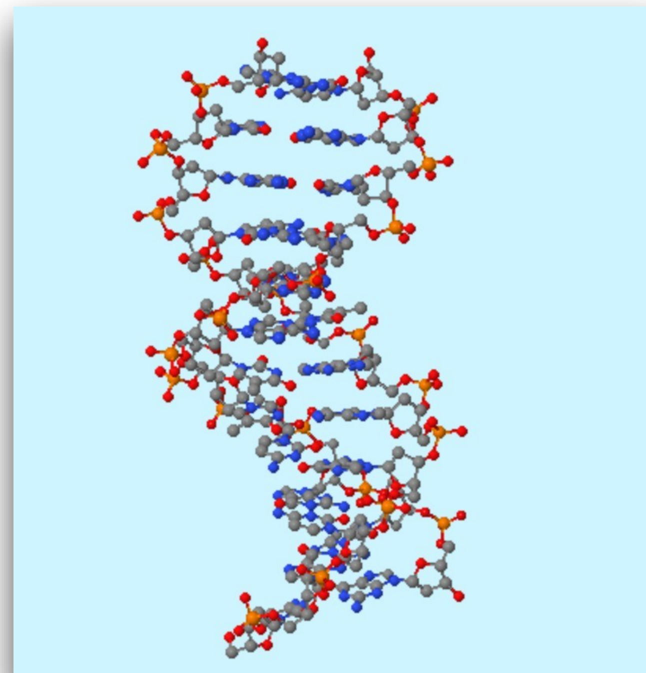


Importance of **Noncovalent Interactions**

Here are a couple of examples of how weak, noncovalent interactions influence the structures of proteins and nucleic acids.



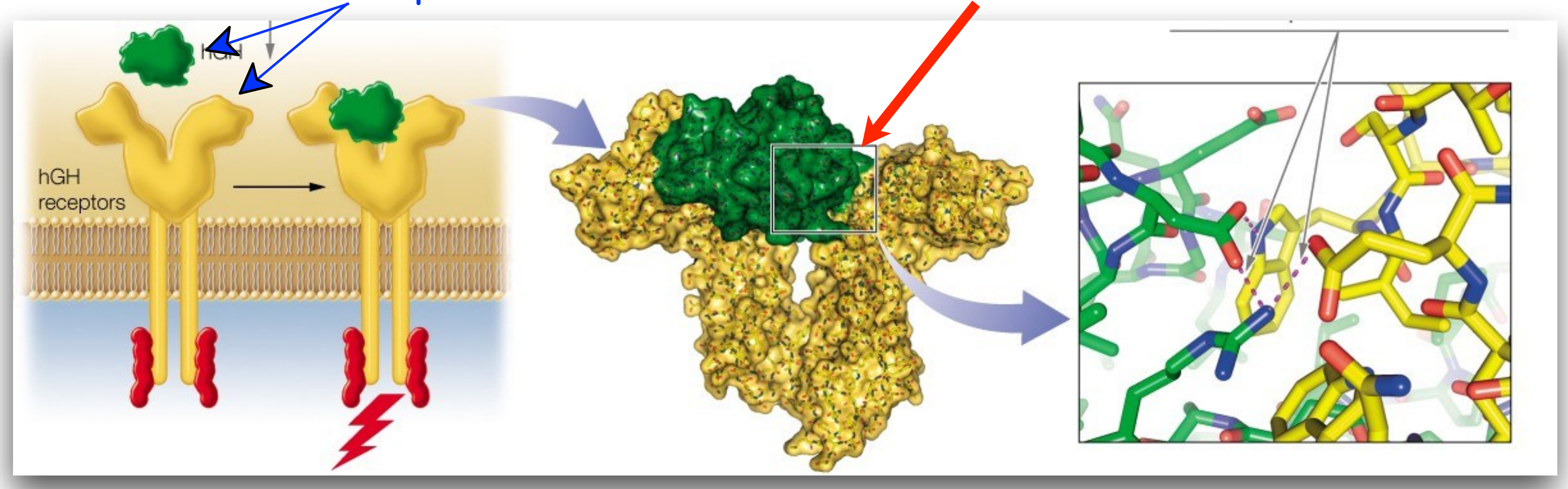
The protein ubiquitin



The nucleic acid B-DNA

Non-covalent interactions are involved in defining the structures of both the hormone and its receptor…

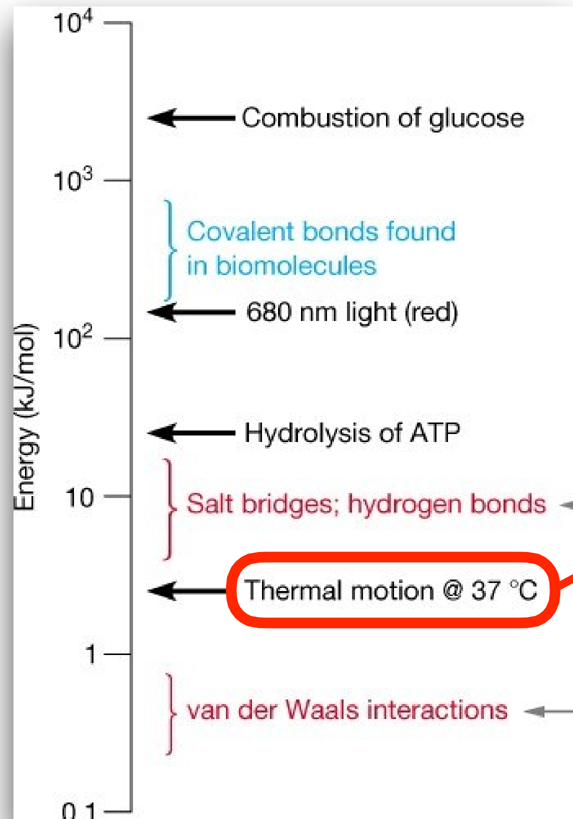
as well as the interactions that allow the hormone to bind specifically to its receptor



Human Growth Hormone (hGH) binding to its cell surface receptor and stimulating muscle growth

Importance of Non-covalent Interactions

A characteristic that distinguishes noncovalent interactions from covalent interactions (bonds) is the energy required to disrupt them.



Covalent bonds

Non-covalent interactions

TABLE 2.1 Energies of some noncovalent interactions in biomolecules

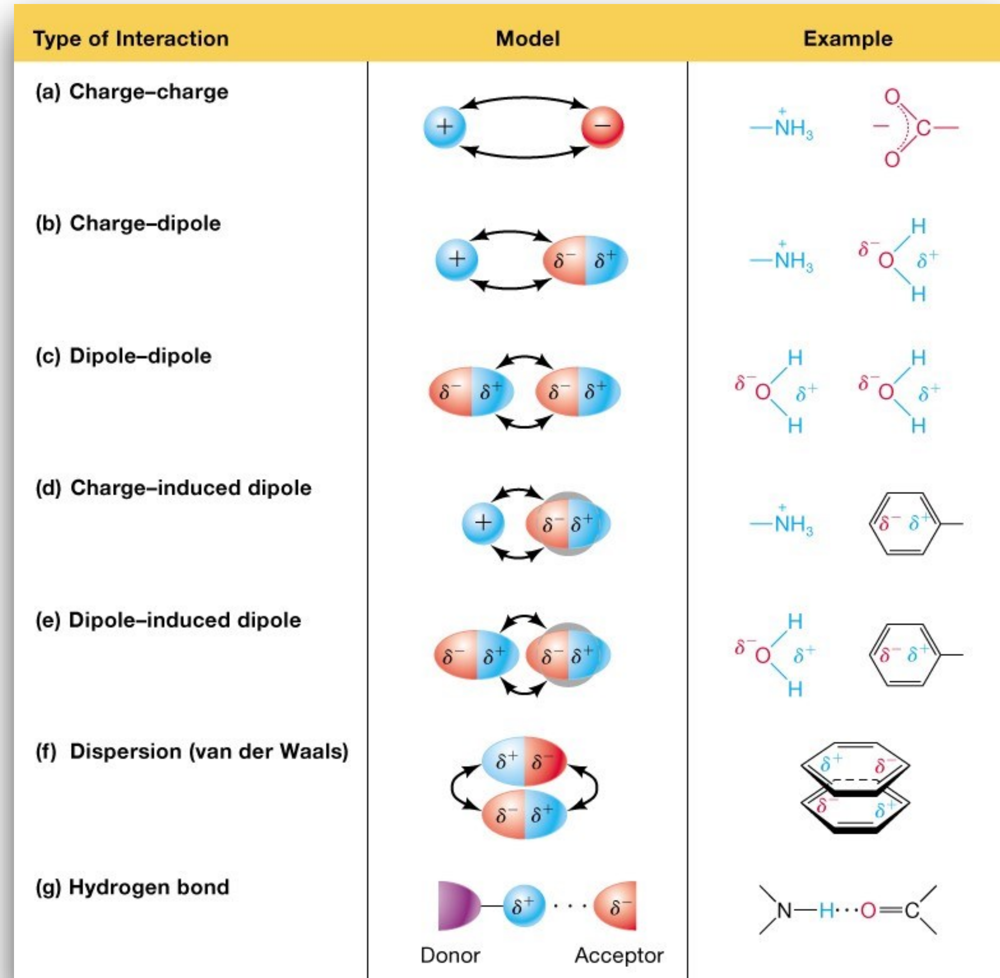
Type of Interaction	Approximate Energy (kJ/mol)
Charge–charge	13 to 17 (in water)
Hydrogen bond	2 to 21
van der Waals	0.4 to 0.8

$$RT = 8.314x10^{-3}\frac{kJ}{mol \bullet K}(37 + 273K)$$

$$= 2.5\frac{kJ}{mol}$$

Types of Noncovalent Interactions

Types of Noncovalent Interactions

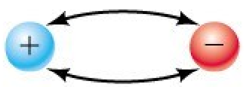
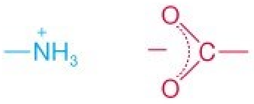
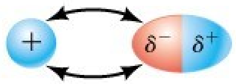
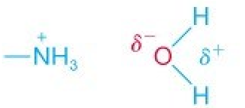
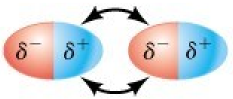
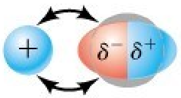
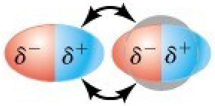
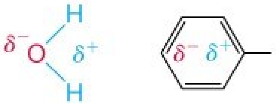
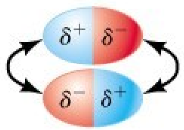
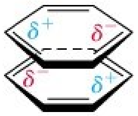


Concept: *Non-covalent interactions are fundamentally electrostatic in nature and can be described by Coulomb's law.*

δ+ = partial positive charge

δ- = partial negative charge

Types of Noncovalent Interactions

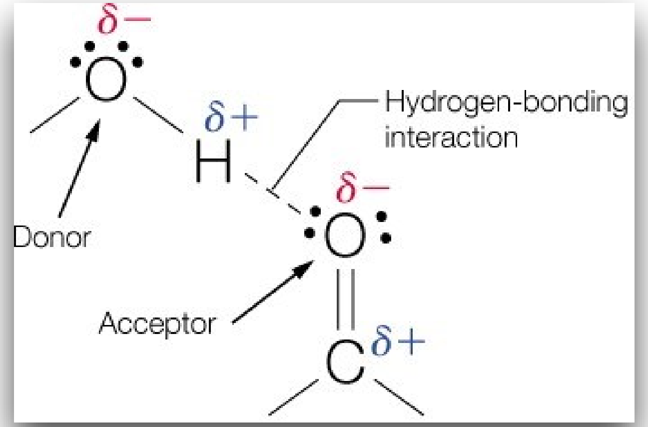
Type of Interaction	Model	Example	Dependence of Energy on Distance
(a) Charge–charge			$1/r$
(b) Charge–dipole			$1/r^2$
(c) Dipole–dipole			$1/r^3$
(d) Charge–induced dipole			$1/r^4$
(e) Dipole–induced dipole			$1/r^5$
(f) Dispersion (van der Waals)			$1/r^6$
(g) Hydrogen bond			Bond length is fixed

Hydrogen Bonding Interactions

This interaction is a special case of a dipole-dipole interaction.

It occurs when one of the dipoles involves a hydrogen atom covalently bonded to an electronegative atom (**the donor**).

The other dipole includes an electronegative atom with a non-bonding pair of electrons (**the acceptor**)



The Role of Water

Fig. 3-1

Water plays a major role in biological systems

Water comprises approximately 70% of the mass for most living cells.

We have also seen that with its high dielectric constant it can, when present, greatly mitigate the strength of most of the non-covalent interactions.

The Structure and Properties of Water

- Water displays some very unique and unusual properties.

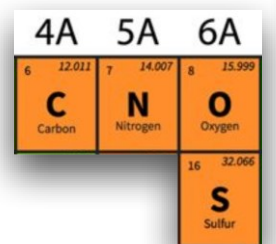


TABLE 2.4 Properties of water compared to those of some other hydrogen-containing, low-molecular-weight compounds

Compound	Molecular Weight	Melting Point (°C)	Boiling Point (°C)	Heat of Vaporization (kJ/mol)
CH_4	16.04	−182	−164	8.16
NH_3	17.03	−78	−33	23.26
H_2O	18.02	0	+100	40.71
H_2S	34.08	−86	−61	18.66

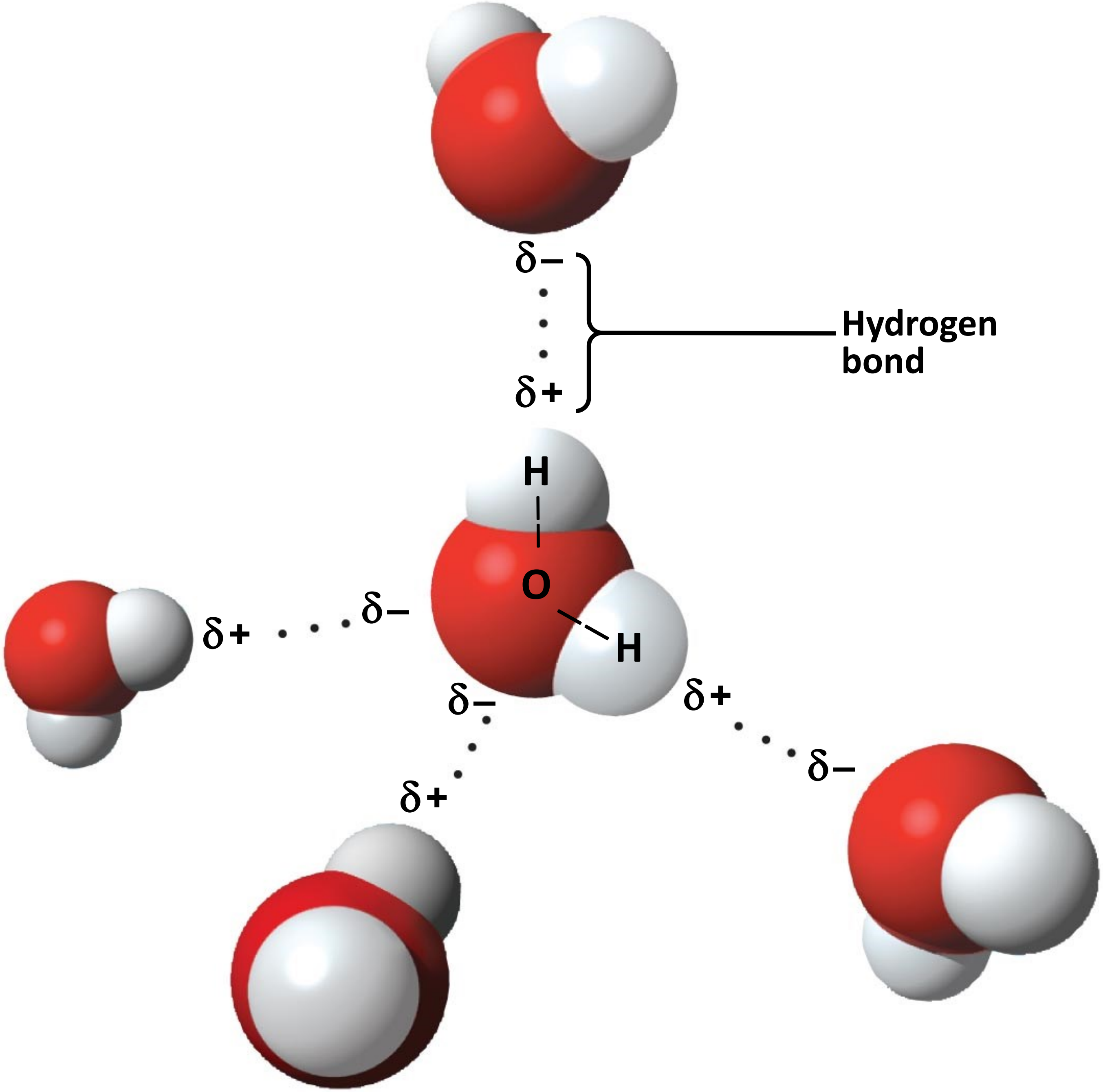
In general, the strength of the dispersion interaction scales with the molecular weight of a molecule.

Melting points and boiling points trend with the number and strengths of the non-covalent interactions

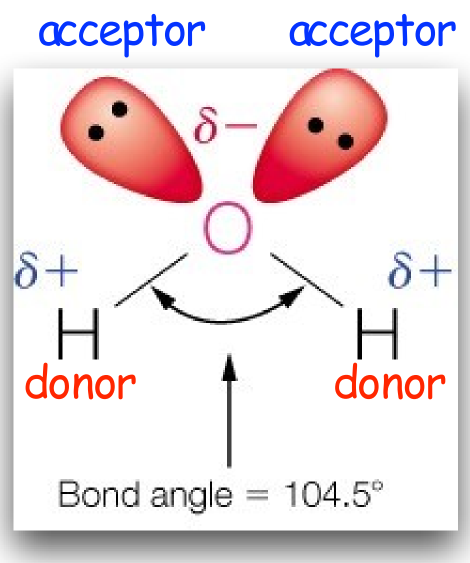
The polarity of water molecules results in hydrogen bonding

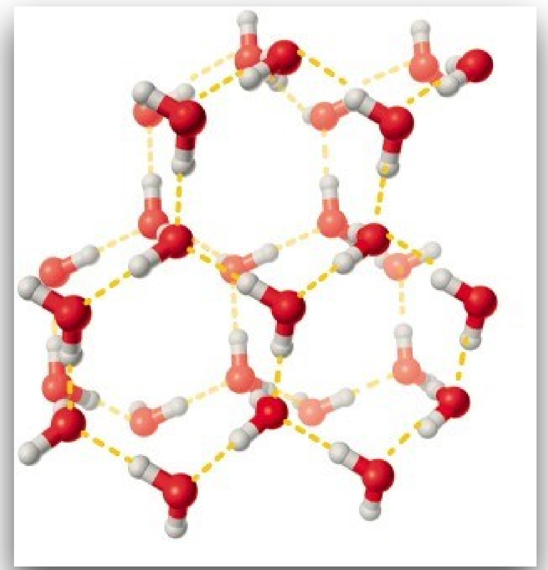
- The water molecule is a **polar molecule**: The opposite ends have opposite charges
- Polarity allows water molecules to form hydrogen bonds with each other

Fig. 3-2



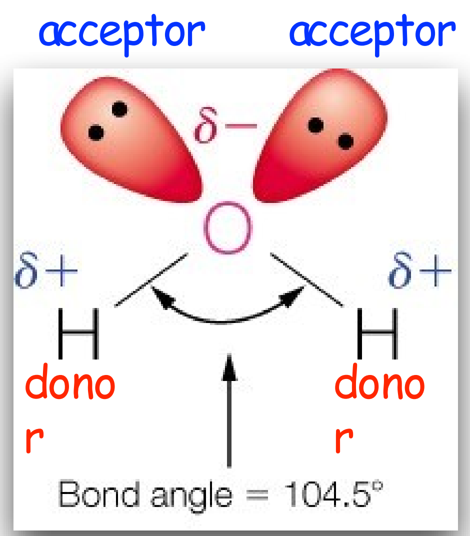
These unique properties arise from water's polarity, but also from its ability to simultaneously form 4 hydrogen bonding interactions with its neighbors.

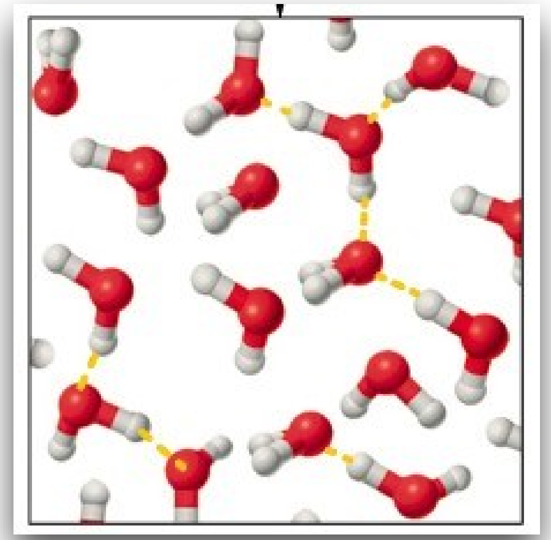




In ice (solid water), each water molecule is hydrogen bonded to 4 neighboring water molecules

- These unique properties arise from water's polarity, but also from its ability to simultaneously form 4 hydrogen bonding interactions with its neighbors.





In liquid water, each water molecule is still hydrogen bonded to approximately 3.4 neighboring water molecules.

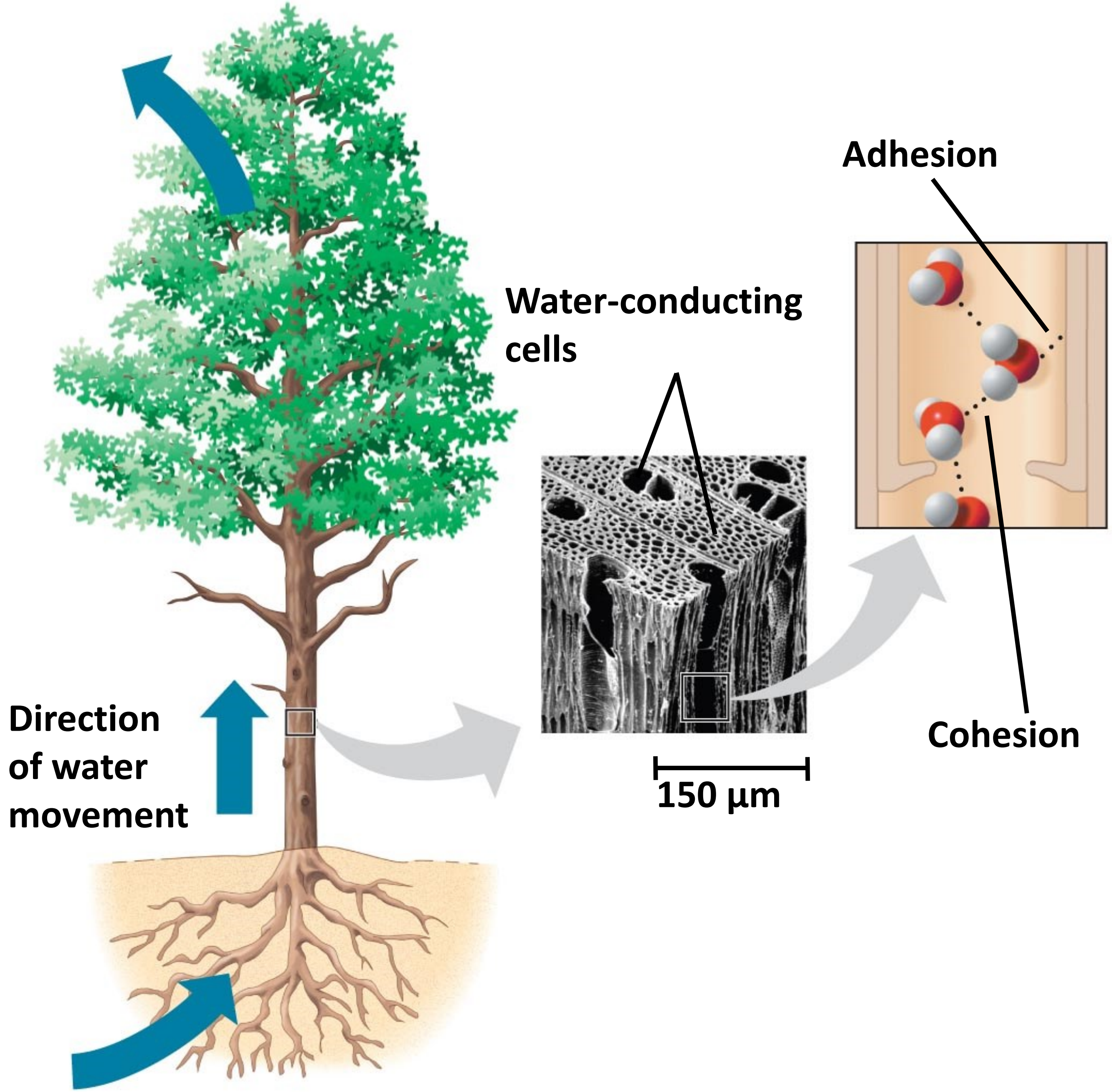
Four emergent properties of water contribute to Earth's fitness for life

- Four of water's properties that facilitate an environment for life are:
  - Cohesive behavior
  - Ability to moderate temperature
  - Expansion upon freezing
  - Versatility as a solvent

Cohesion

- Collectively, hydrogen bonds hold water molecules together, a phenomenon called **cohesion**
- Cohesion helps the transport of water against gravity in plants
- **Adhesion** is an attraction between different substances, for example, between water and plant cell walls

Fig. 3-3


Adhesion
Water-conducting cells
Direction of water movement
150 µm
Cohesion

Moderation of Temperature

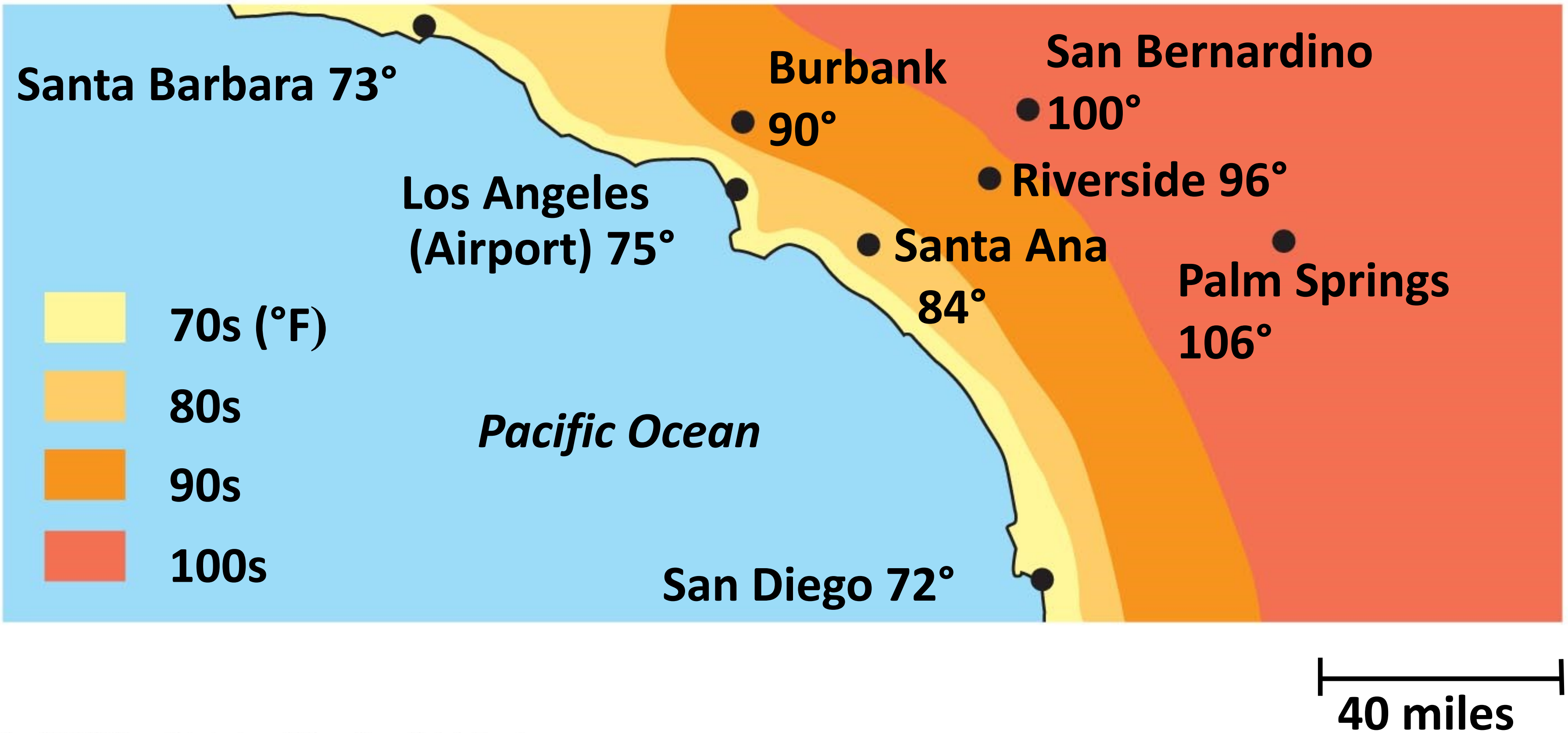
- Water absorbs heat from warmer air and releases stored heat to cooler air
- Water can absorb or release a large amount of heat with only a slight change in its own temperature

Water's High Specific Heat

- The **specific heat** of a substance is the amount of heat that must be absorbed or lost for 1 g of that substance to change its temperature by 1°C
- The specific heat of water is 1 cal/g/°C
- Water resists changing its temperature because of its high specific heat

- Water’s high specific heat can be traced to hydrogen bonding
  - Heat is absorbed when hydrogen bonds break
  - Heat is released when hydrogen bonds form
- The high specific heat of water minimizes temperature fluctuations to within limits that permit life

Fig. 3-5



Santa Barbara 73°
Burbank
90°
San Bernardino
100°
Riverside 96°
Los Angeles
(Airport) 75°
Santa Ana
84°
Palm Springs
106°
70s (°F)
80s
90s
100s
Pacific Ocean
San Diego 72°
40 miles

Evaporative Cooling

- *Evaporation* is transformation of a substance from liquid to *gas*
- **Heat of vaporization** is the heat a liquid must absorb for 1 g to be converted to *gas*
- *As* a liquid evaporates, its remaining surface cools, a process called **evaporative cooling**
- Evaporative cooling of water helps stabilize temperatures in organisms and bodies of water

Insulation of Bodies of Water by Floating Ice

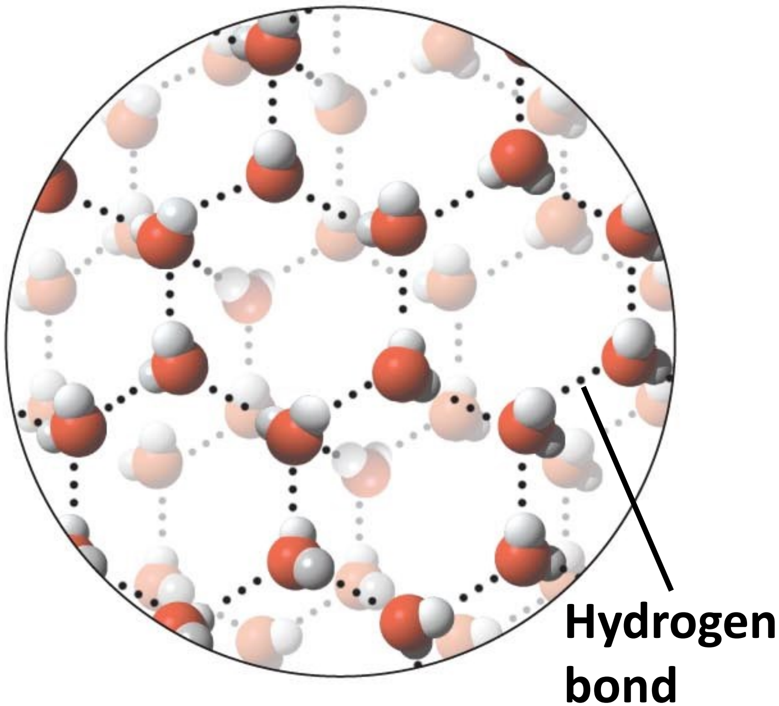
- Ice floats in liquid water because hydrogen bonds in ice are more "ordered," making ice less dense
- Water reaches its greatest density at 4°C
- If ice sank, all bodies of water would eventually freeze solid, making life impossible on Earth

Fig. 3-6

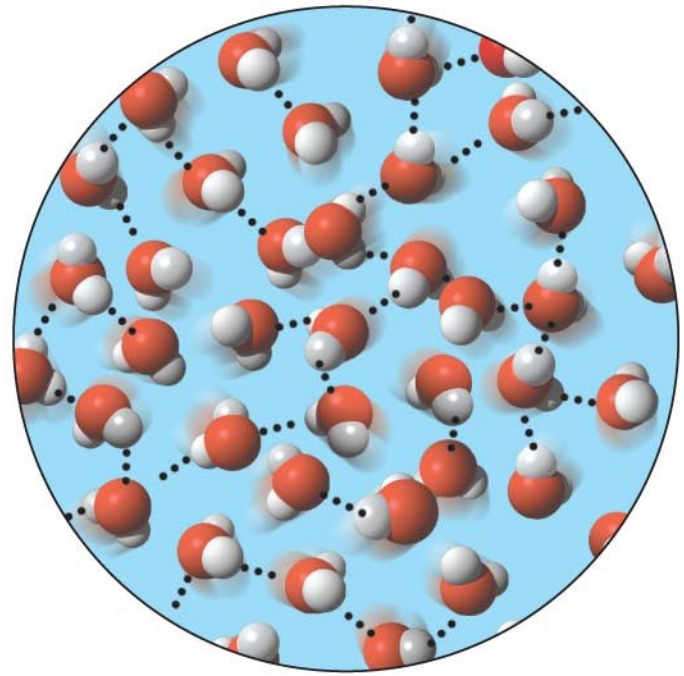
Ice
Hydrogen bonds are stable

Liquid water
Hydrogen bonds break and re-form

Fig. 3-6a



Ice
Hydrogen bonds are stable



Liquid water
Hydrogen bonds break and re-form

- Water is a versatile solvent due to its polarity, which allows it to form hydrogen bonds easily
- When an ionic compound is dissolved in water, each ion is surrounded by a sphere of water molecules called a **hydration shell**
- Water can also dissolve compounds made of nonionic polar molecules
- Even large polar molecules such as proteins can dissolve in water if they have ionic and polar regions

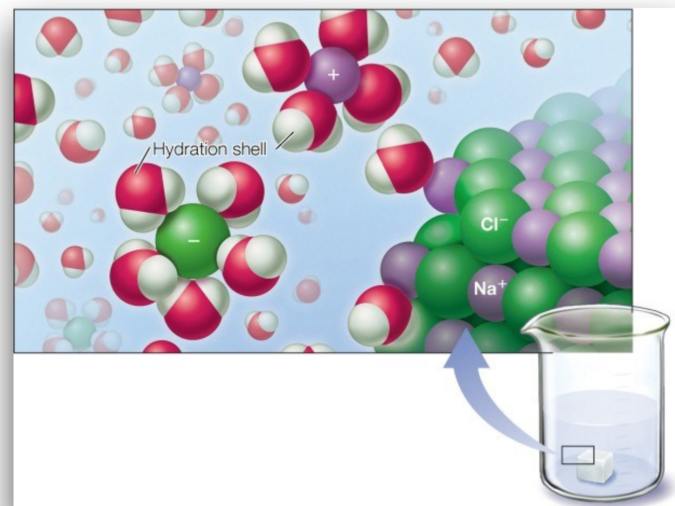
Hydrophilic and Hydrophobic Substances

- A **hydrophilic** substance is one that has an affinity for water
- A **hydrophobic** substance is one that does not have an affinity for water
- Oil molecules are hydrophobic because they have relatively nonpolar bonds
- A **colloid** is a stable suspension of fine particles in a liquid

Water as a Solvent

Concept: *Water is an excellent solvent for polar molecules and many salts because of its hydrogen-bonding potential and its polar nature.*

- Substances that dissolve readily in water are said to be hydrophilic.



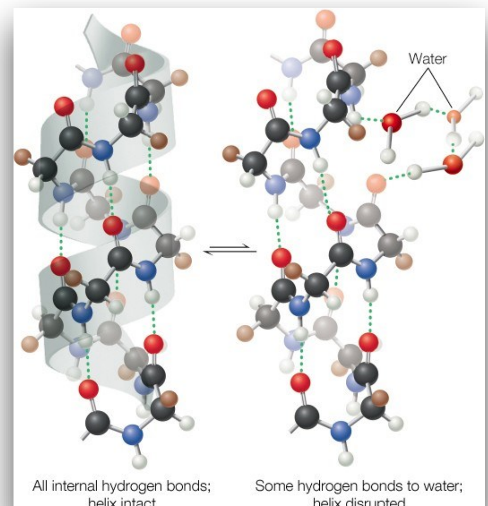
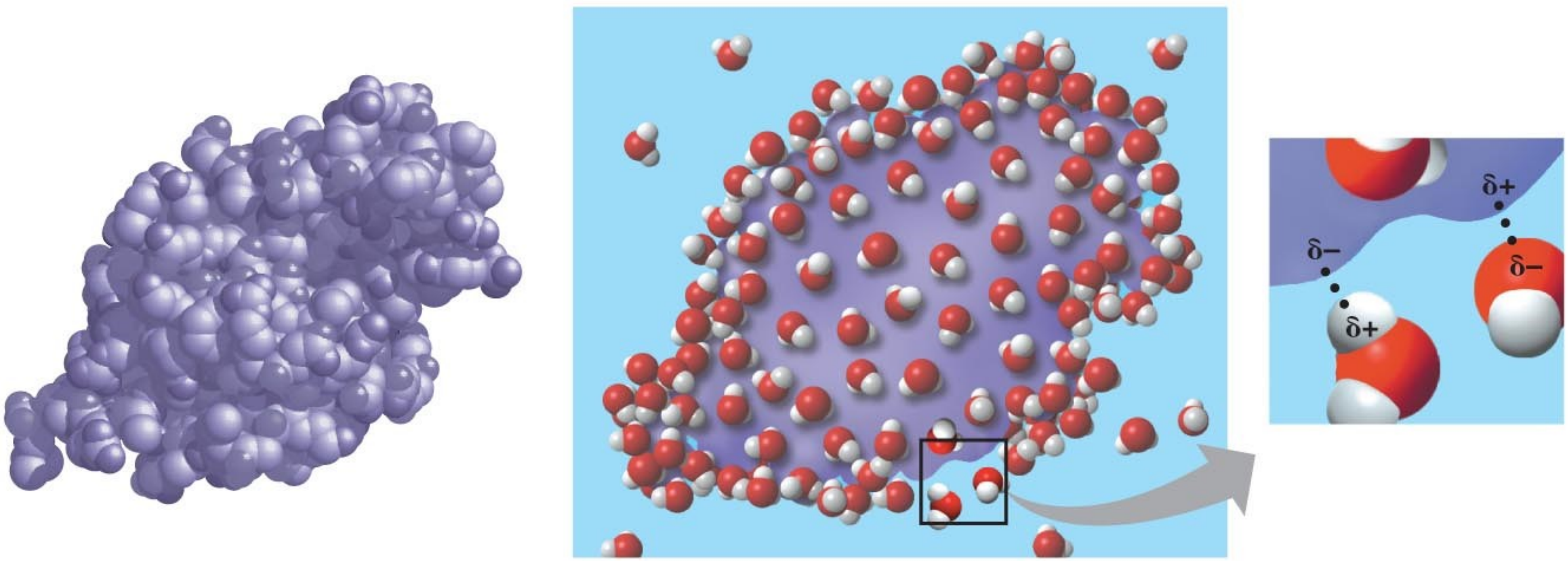


Fig. 3-8

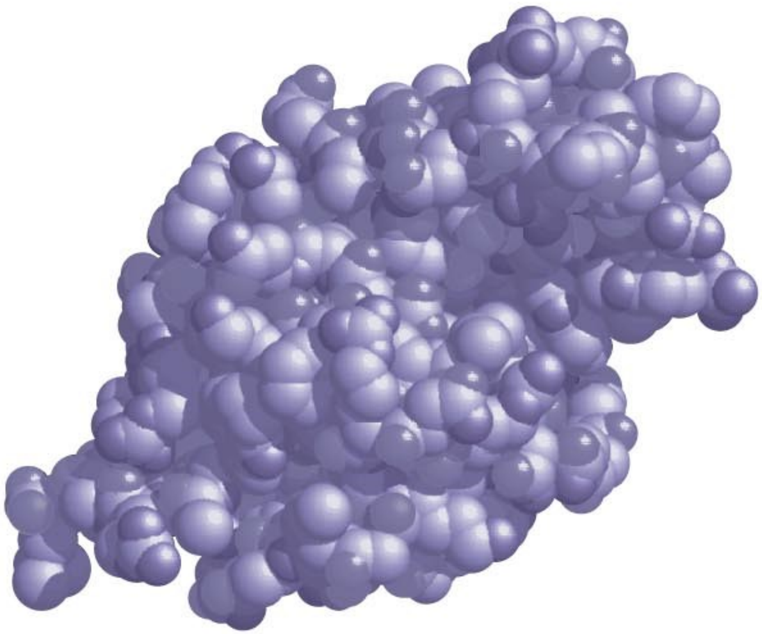


(a) Lysozyme molecule in a nonaqueous environment

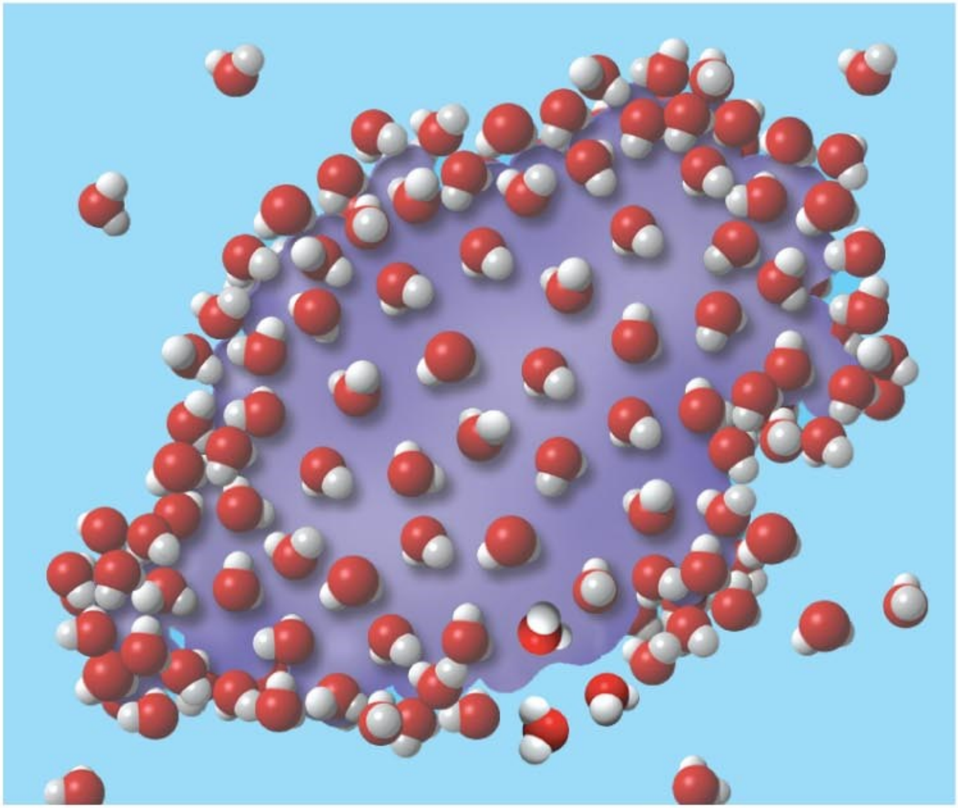
(b) Lysozyme molecule (purple) in an aqueous environment

(c) Ionic and polar regions on the protein's surface attract water molecules.

Fig. 3-8ab

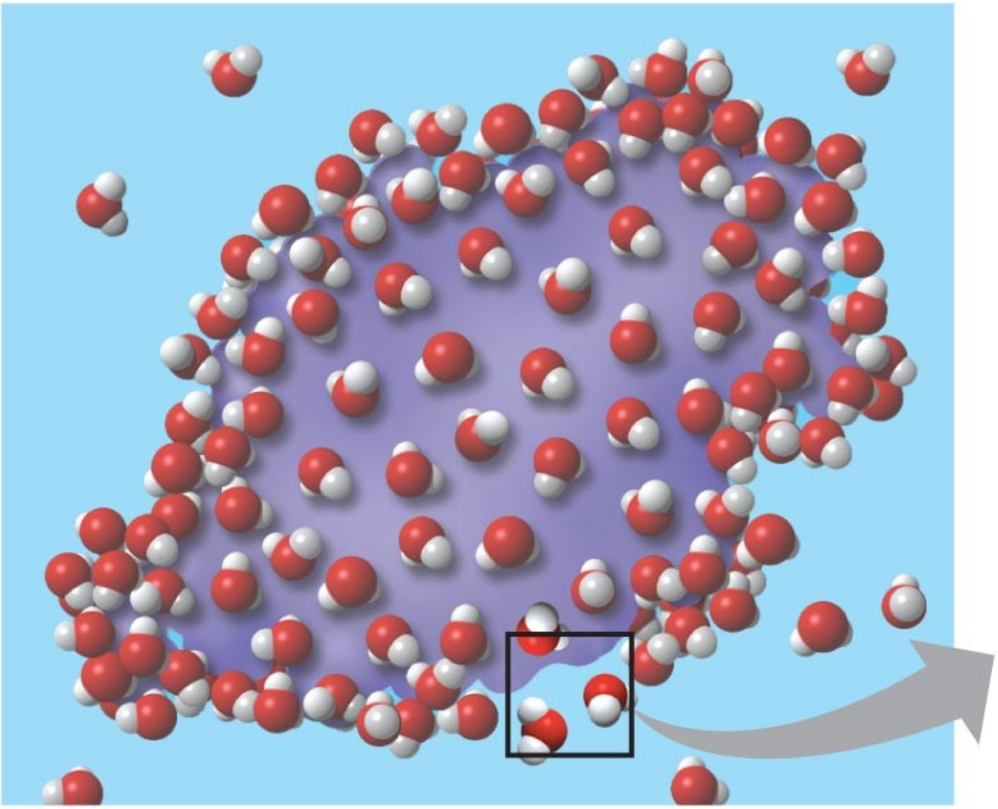


(a) Lysozyme molecule in a nonaqueous environment

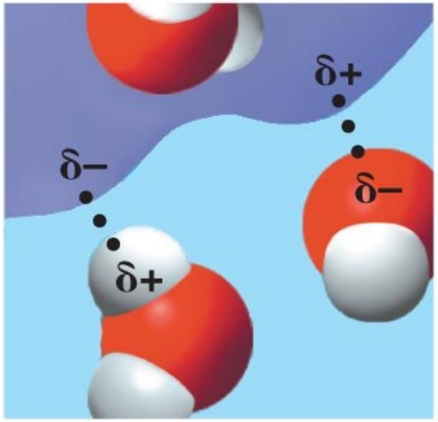


(b) Lysozyme molecule (purple) in an aqueous environment

Fig. 3-8bc



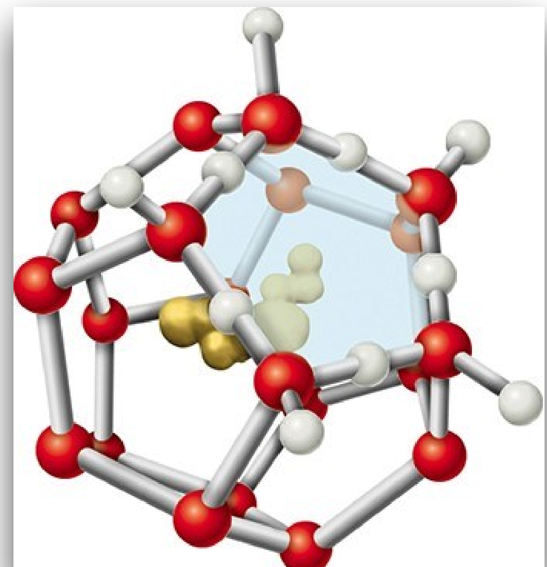
(b) Lysozyme molecule (purple) in an aqueous environment



(c) Ionic and polar regions on the protein's surface attract water molecules.

Hydrophobic Molecules in Aqueous Solution

- Molecules that do not interact favorably with water and therefore do not not dissolve well in water are said to be *hydrophobic*.
  - Non-polar, organic molecules are a prime examples.
  - When water cannot interact favorable with a molecule, it will form highly organized *clathrate* structures around the molecule.
  - Because of the loss of entropy for these water molecules, dissolving non-polar molecules in water becomes thermodynamically unfavorable.

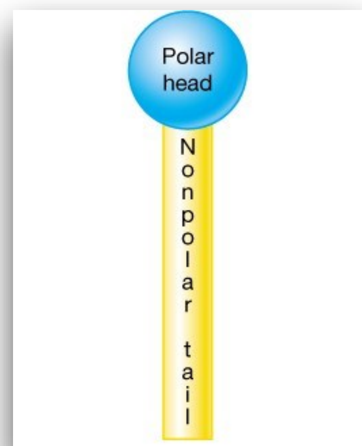


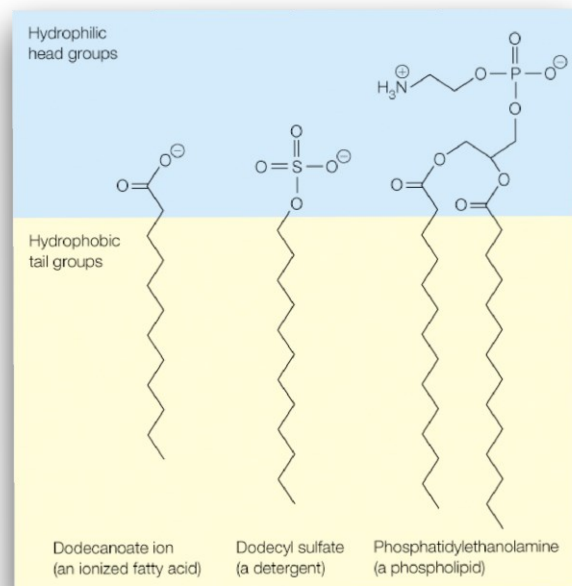
Amphipathic Molecules

A molecule is amphipathic if some parts of its molecular surface are significantly hydrophilic while other parts are significantly hydrophobic.

Examples include

- soaps
- detergents
- membrane phospholipids

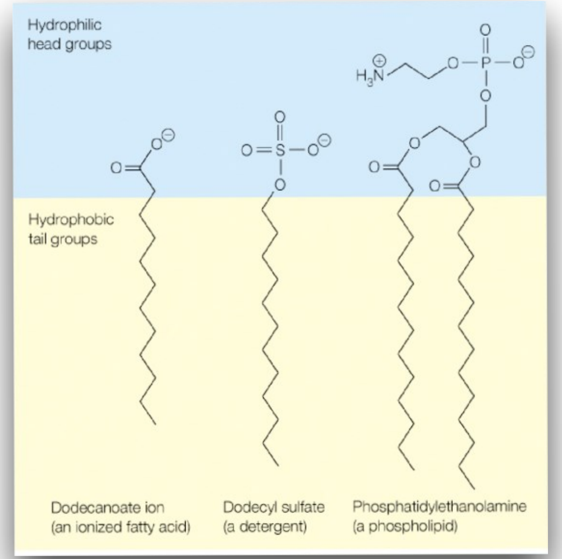


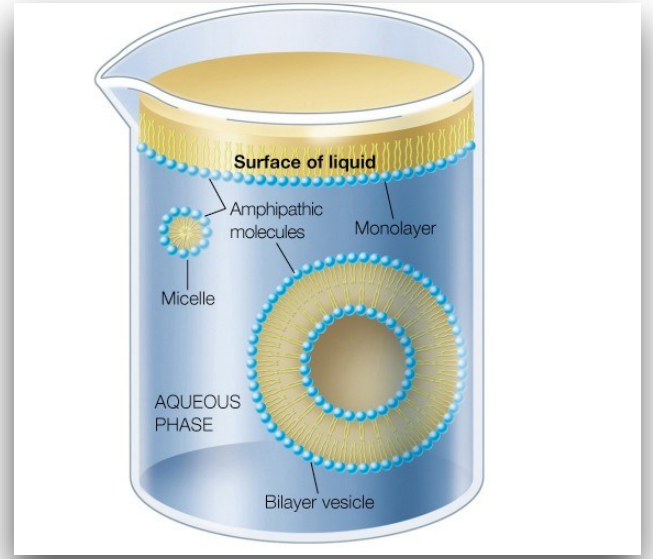


Amphipathic Molecules in Aqueous Solution

When placed in water, amphipathic molecules, such as soaps, detergents and phospholipids, will aggregate to form micelles (soaps & detergents) and bilayer vesicles (phospholipids).

The do this as a strategy to simultaneously expose their hydrophilic parts to water while removing the hydrophobic parts from water.



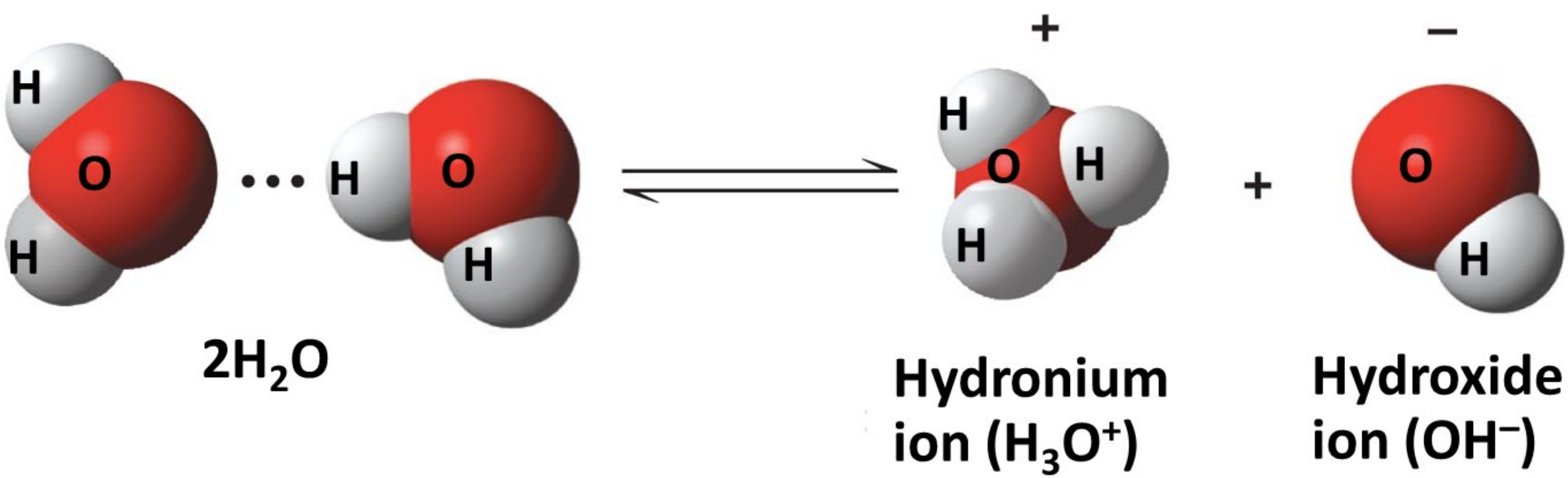


Solute Concentration in Aqueous Solutions

- Most biochemical reactions occur in water
- Chemical reactions depend on collisions of molecules and therefore on the concentration of solutes in an aqueous solution

Acidic and basic conditions affect living organismsa

- A hydrogen atom in a hydrogen bond between two water molecules can shift from one to the other:
  - The hydrogen atom leaves its electron behind and is transferred as a proton, or **hydrogen ion** (H^+)
  - The molecule with the extra proton is now a **hydronium ion** (H_3O^+), though it is often represented as H^+
  - The molecule that lost the proton is now a **hydroxide ion** (OH^-)
  - Water is in a state of dynamic equilibrium in which water molecules dissociate at the same rate at which they are being reformed



Effects of Changes in pH

- Concentrations of H^+ and OH^- are equal in pure water
- Adding certain solutes, called acids and bases, modifies the concentrations of H^+ and OH^-
- Biologists use something called the pH scale to describe whether a solution is acidic or basic (the opposite of acidic)

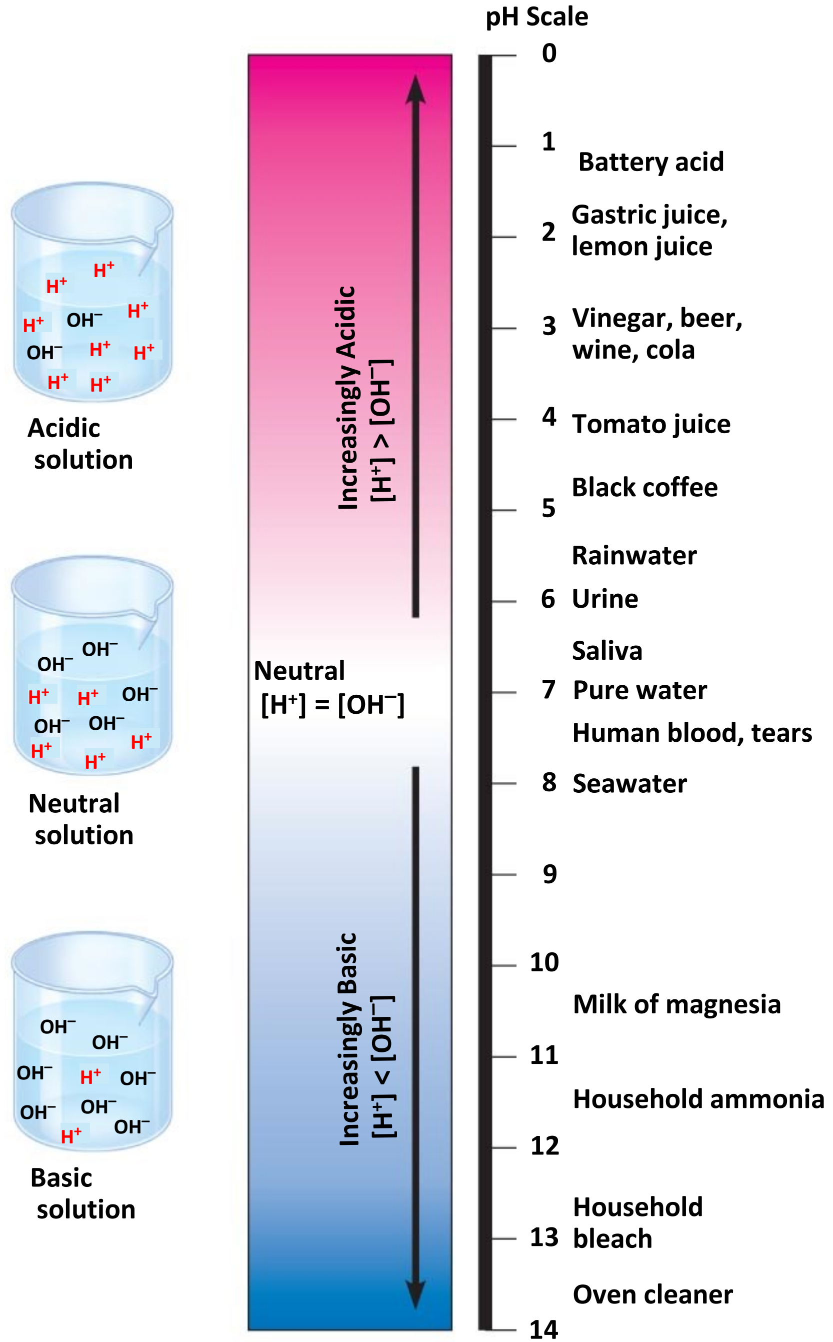
Acids and Bases

- An **acid** is any substance that increases the H^+ concentration of a solution
- A **base** is any substance that reduces the H^+ concentration of a solution

The pH Scale

- In any aqueous solution at 25°C the product of H^+ and OH^- is constant and can be written as
  $$[H^+][OH^-] = 10^{-14}$$
- The **pH** of a solution is defined by the negative logarithm of H^+ concentration, written as $pH = -\log [H^+]$
- For a neutral aqueous solution
  $[H^+]$ is $10^{-7} = -(-7) = 7$
- Acidic solutions have pH values less than 7
- Basic solutions have pH values greater than 7
- Most biological fluids have pH values in the range of 6 to 8

Fig. 3-9


pH Scale
0
1 Battery acid
2 Gastric juice, lemon juice
3 Vinegar, beer, wine, cola
4 Tomato juice
Black coffee
5
Rainwater
6 Urine
Saliva
7 Pure water
Human blood, tears
8 Seawater
9
10
Milk of magnesia
11
Household ammonia
12
Household bleach
13
Oven cleaner
14
Increasingly Acidic
[H+] > [OH−]
Neutral
[H+] = [OH−]
Increasingly Basic
[H+] < [OH−]
Acidic solution
Neutral solution
Basic solution
H+
OH−

10/01/2023

Distinguishing features of living organisms

- A high degree of chemical complexity and microscopic organization.
- Systems for extracting, transforming, and using energy from the environment.
- Defined functions for each of an organism's components and regulated interactions among them.

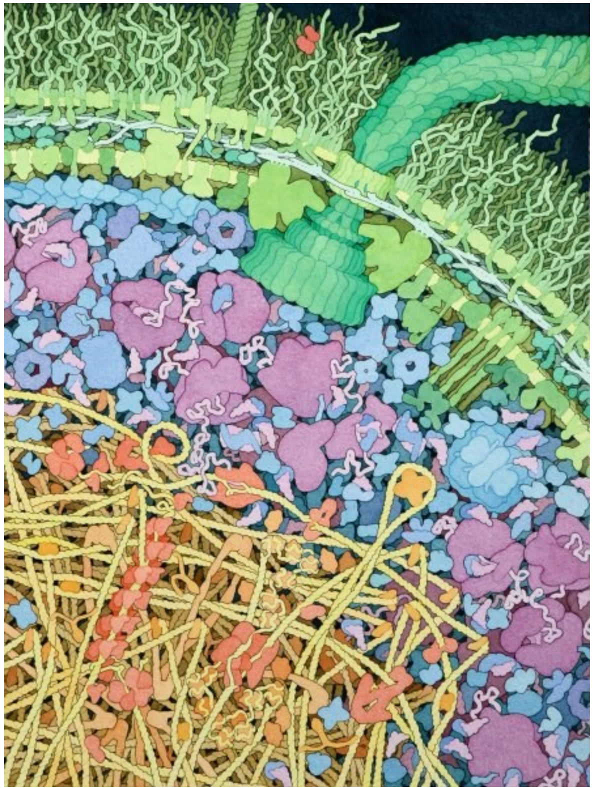
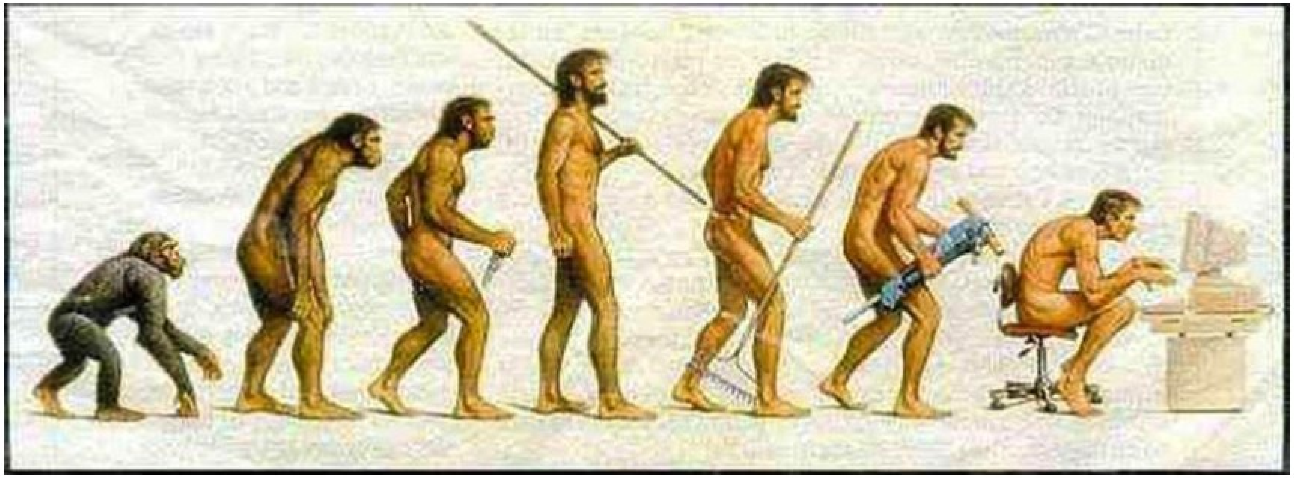


Image taken from http://mgl.scripps.edu/people/goodsell/books/MoL2-preview.html

Distinguishing features of living organisms

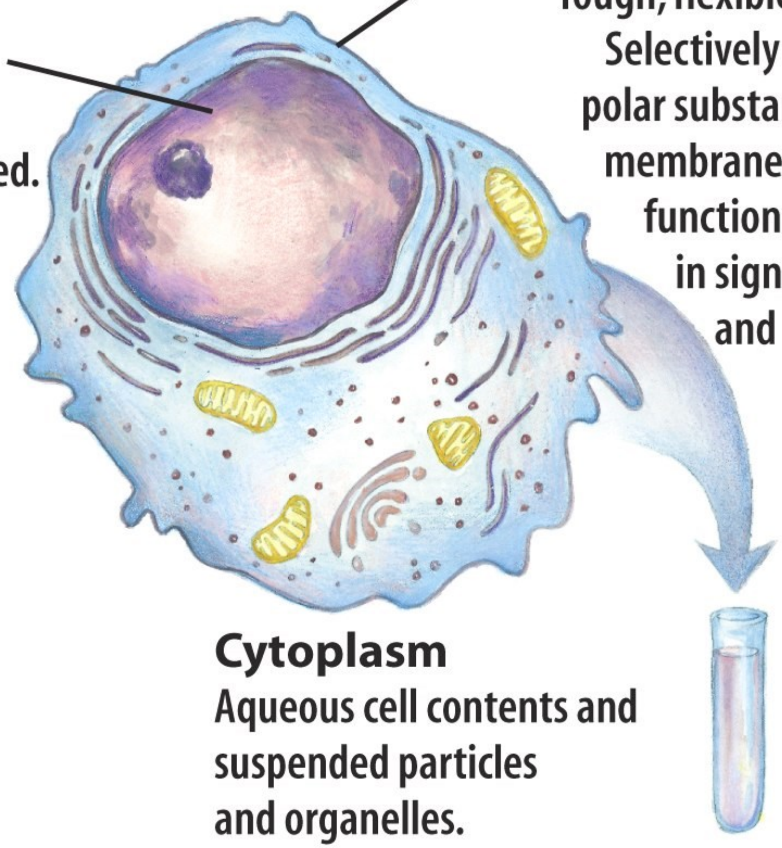
- Mechanisms for sensing and responding to alterations in their surroundings.
- A capacity for precise self-replication and self-assembly.
- A capacity to change over time by gradual evolution.



Taken from: http://hydrodictyon.eeb.uconn.edu/courses/EEB210/evolution.jpg

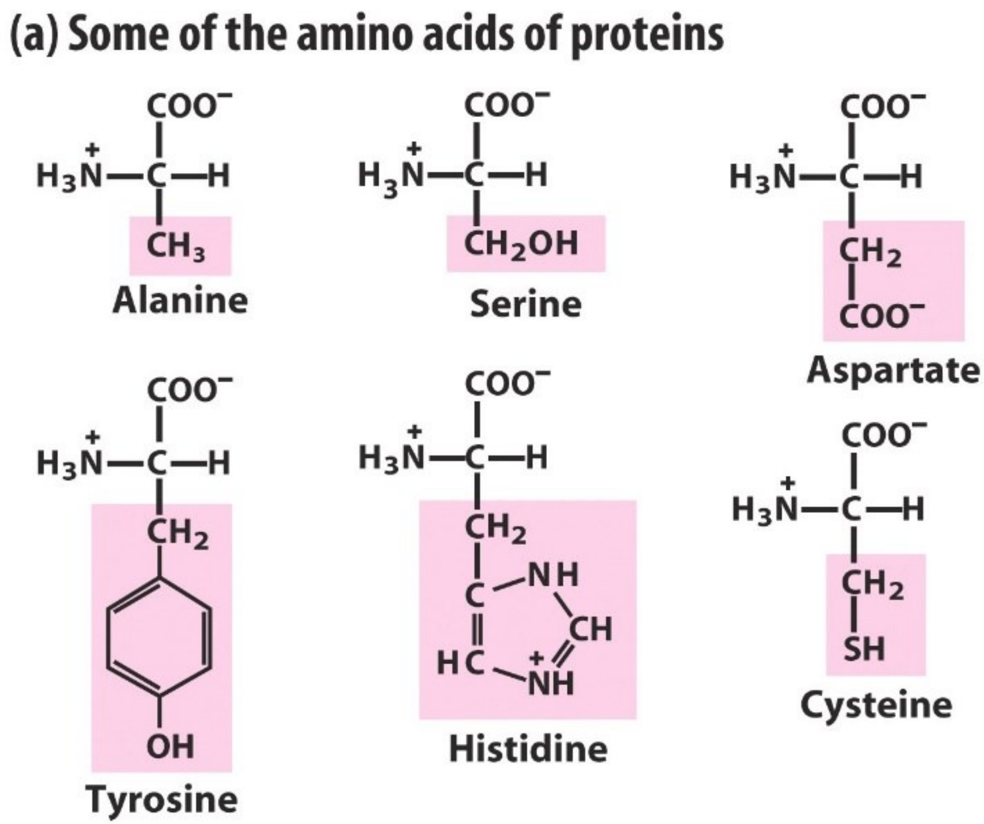
1.1 Cellular foundations

Cells are structural and functional units of all living organisms



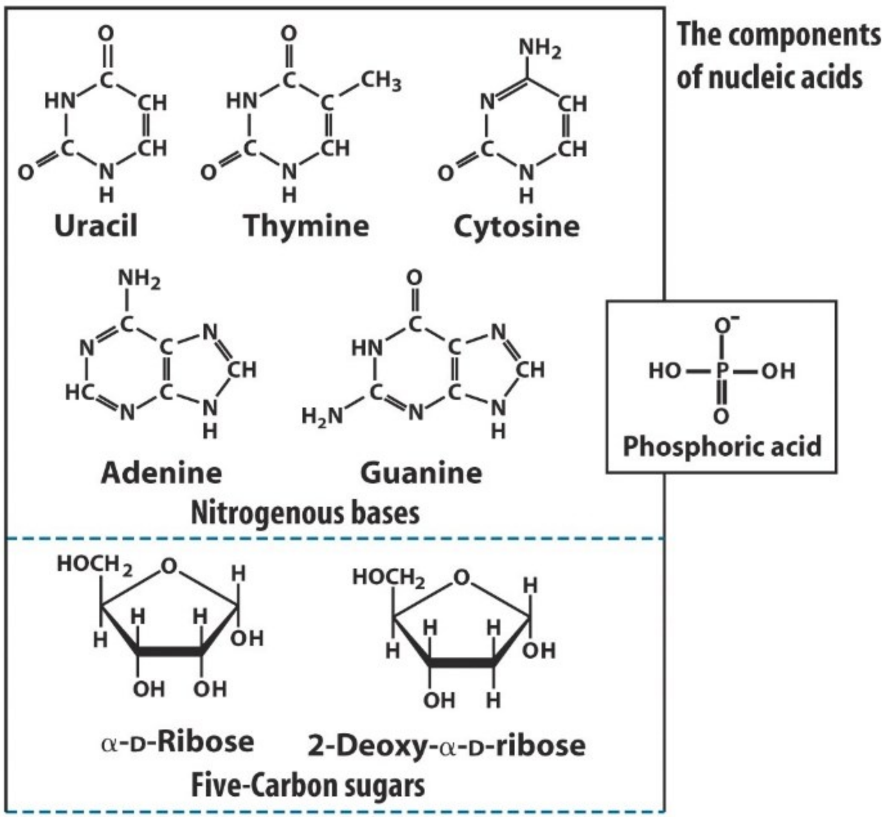
Cells build macromolecular structures from simple organic compounds

- Amino acids ---> Proteins

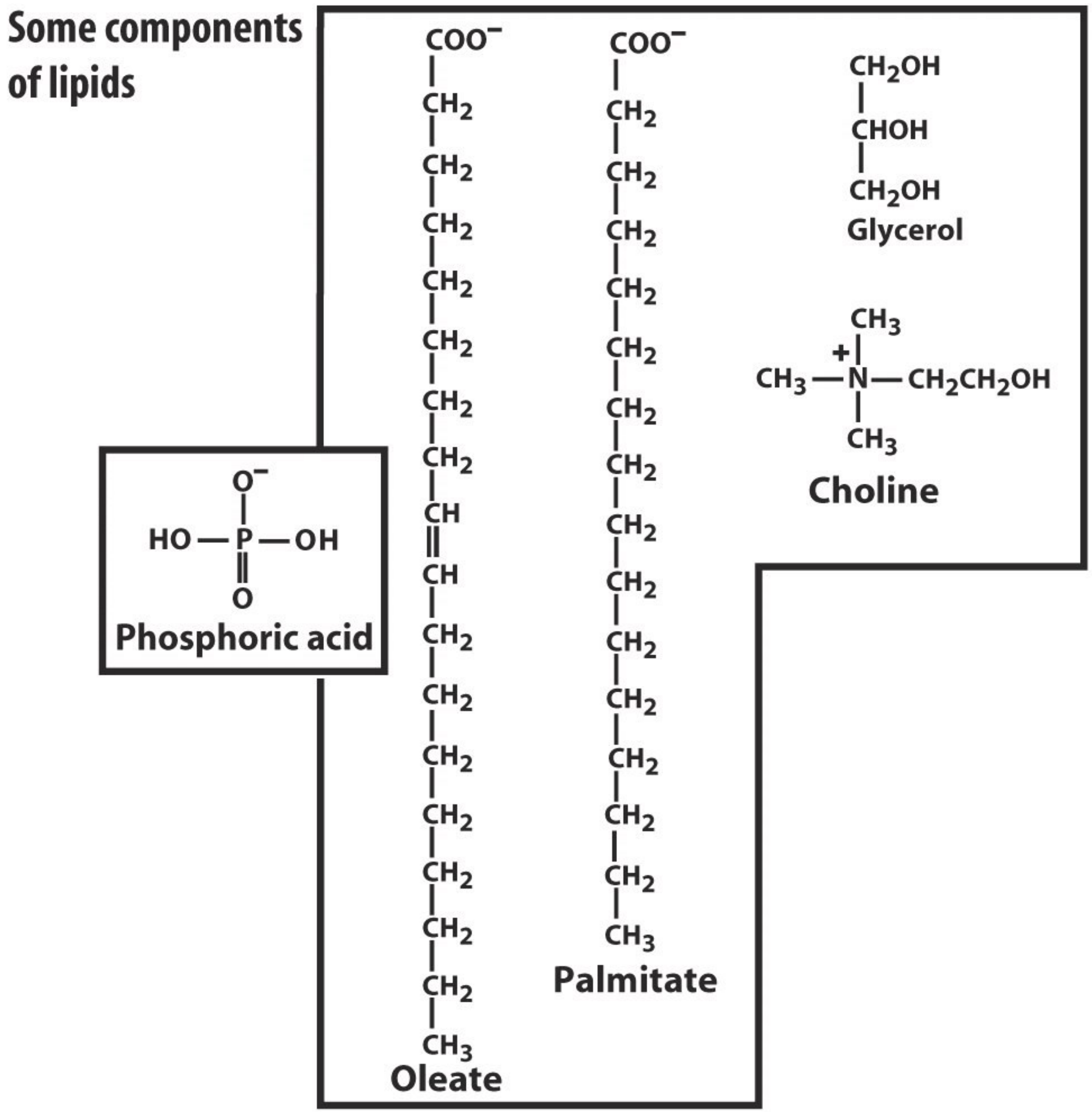


Cells build macroamolecular structures from simple organic compounds

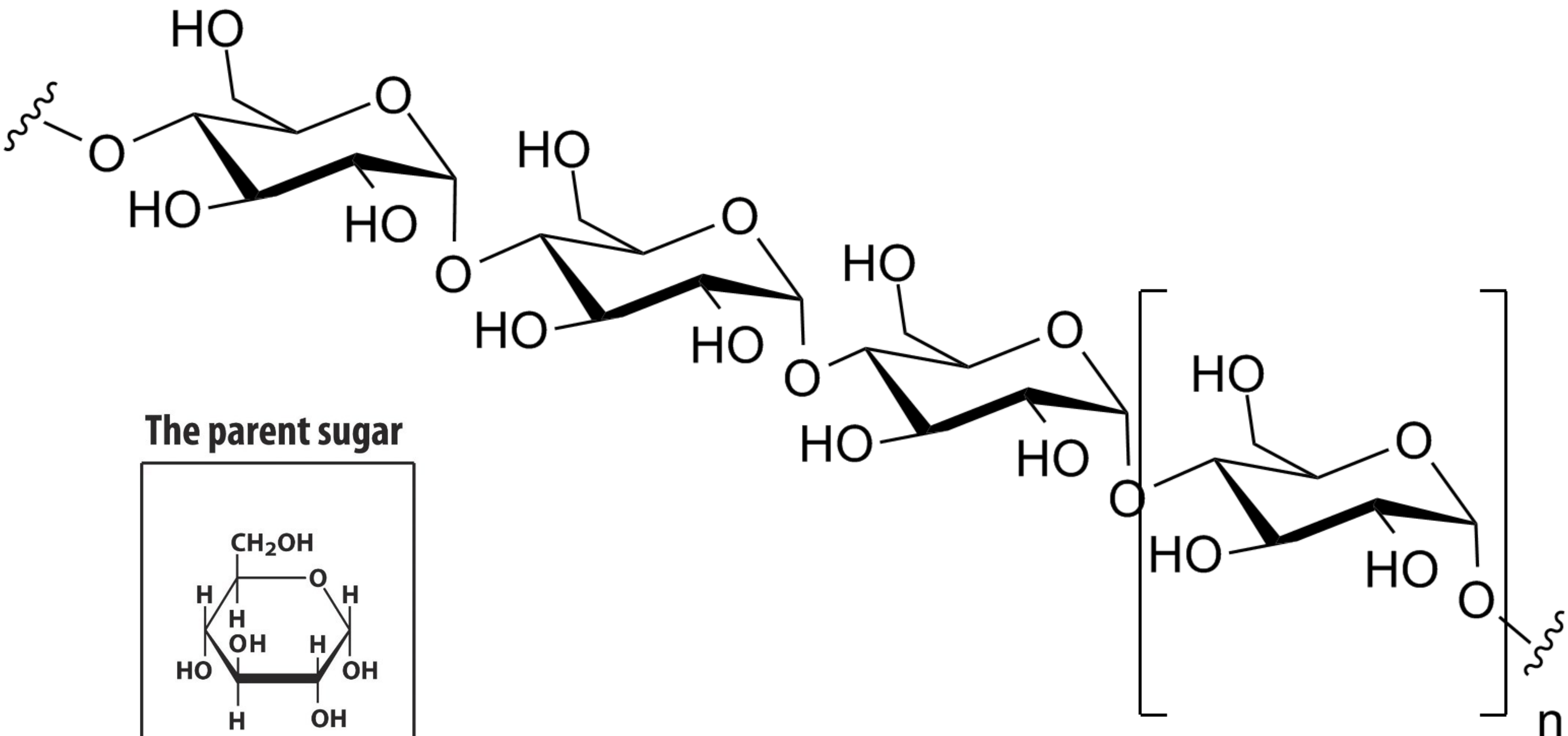
- Nucleotides---> DNA & RNA



- Fatty acid derivatives ---> Lipids



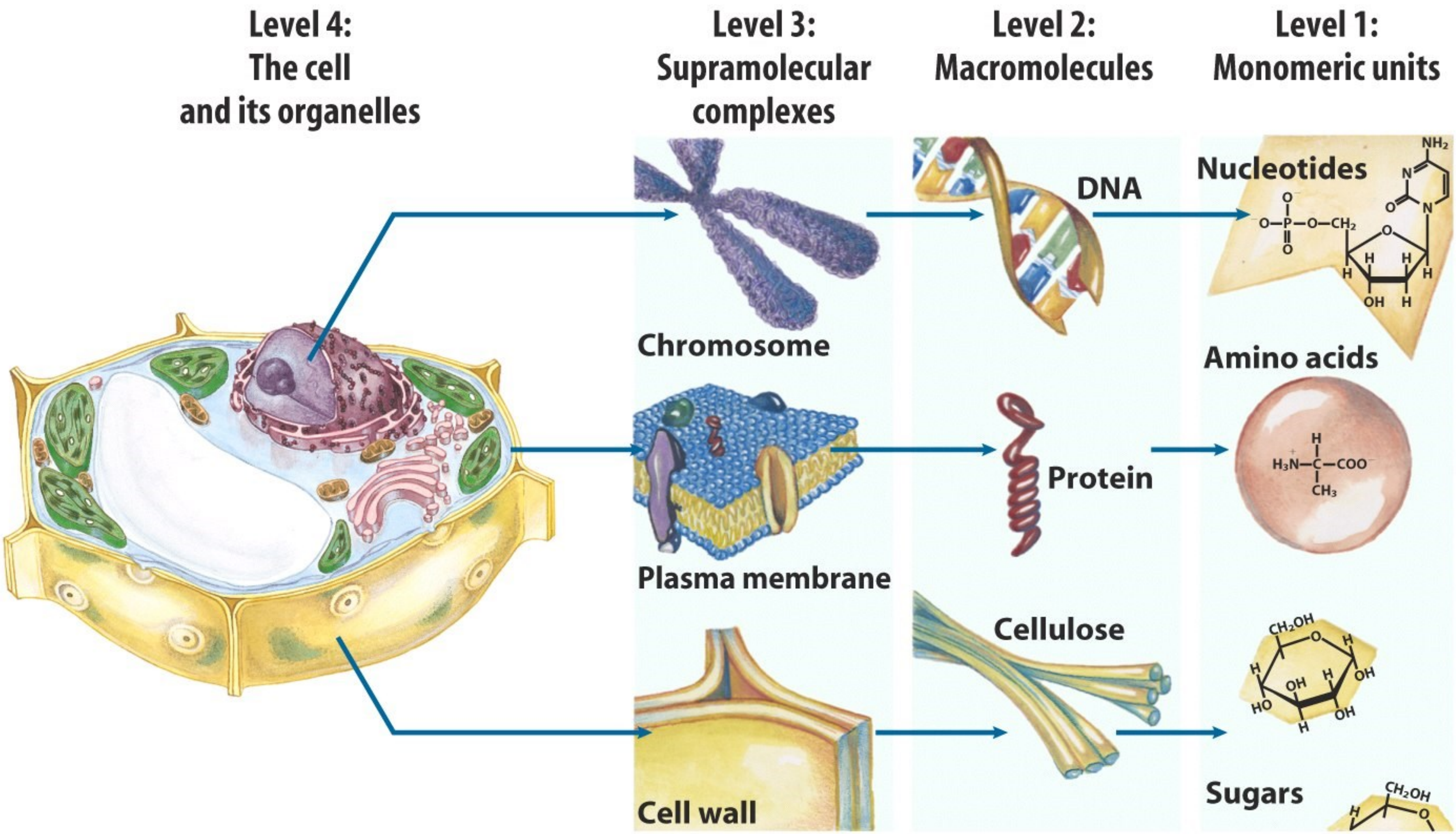
• Sugars ---> polysaccharides



The parent sugar

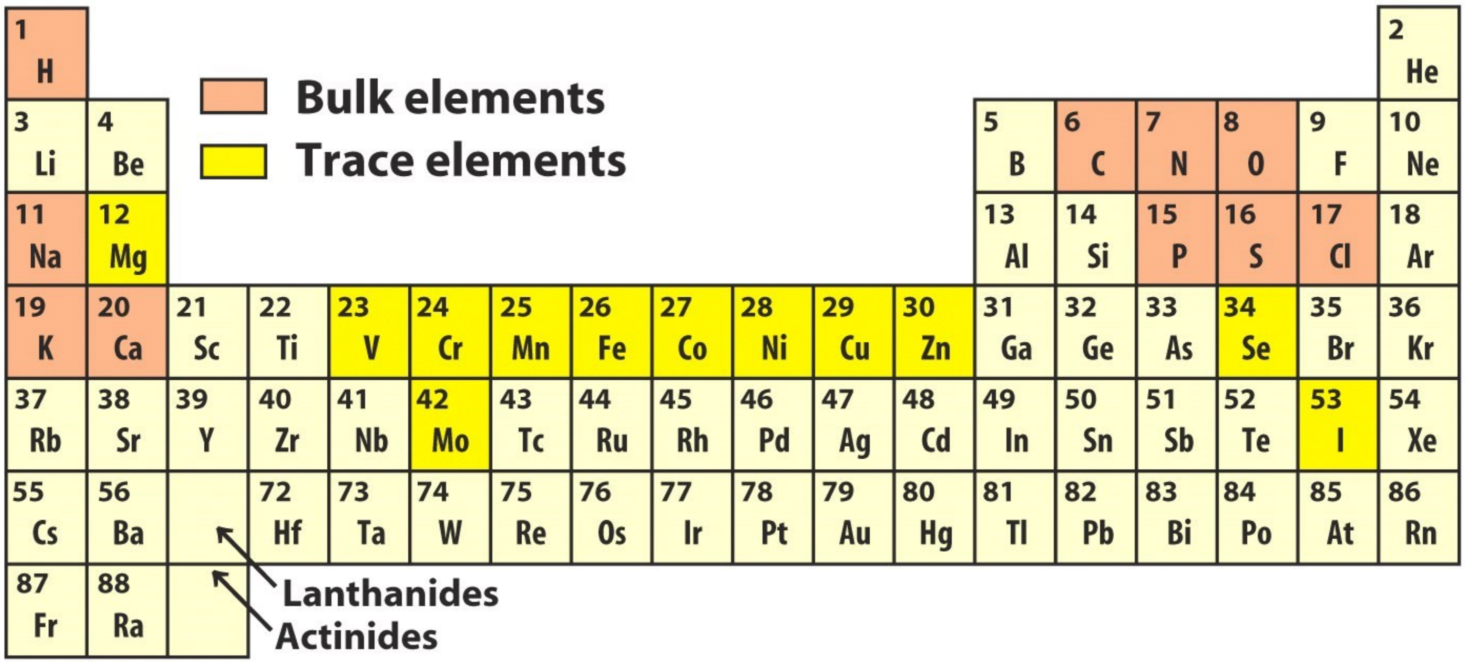
α-D-**Glucose**

Structural hierarchy in the molecular organization of cells



1.2 Chemical Foundations

Biochemist's periodic table



- Four most abundant elements in living organisms: H, O, N, C, 99% of the mass of most cells.
- The trace elements are essential to the function of specific proteins.

Element	Dry Weight (%)	Element	Dry Weight (%)
C	**61.7**	Ca	5.0
N	**11.0**	K	3.3
O	**9.3**	S	1.0
H	**5.7**	Cl	0.7
		Na	0.7
		Mg	0.3

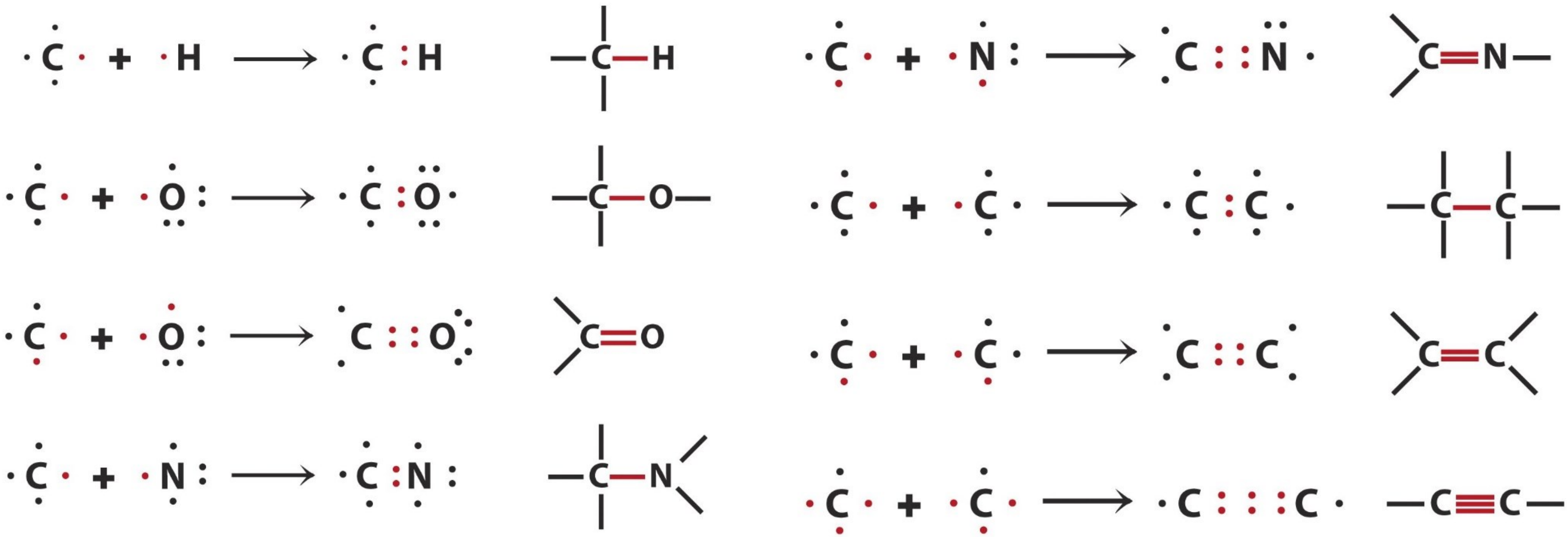
- What property unites H, O, C and N and renders these atoms so appropriate to the chemistry of life?

- Answer: Their ability to form covalent bonds by electron-pair sharing. They are the lightest elements capable of efficiently forming stable one, two, three and four covalent bonds.

Why carbon based life?

- Covalently linked carbon atoms in biomolecules can form linear chains, branched chains, and cyclic structures. It seems likely that the bonding versatility of carbon, with itself and with other elements, was a major factor in the selection of carbon compounds for the molecular machinery of cells during the origin and evolution of living organisms. No other chemical element can form molecules of such widely different sizes, shapes, and composition.

Versatility of carbon bonding

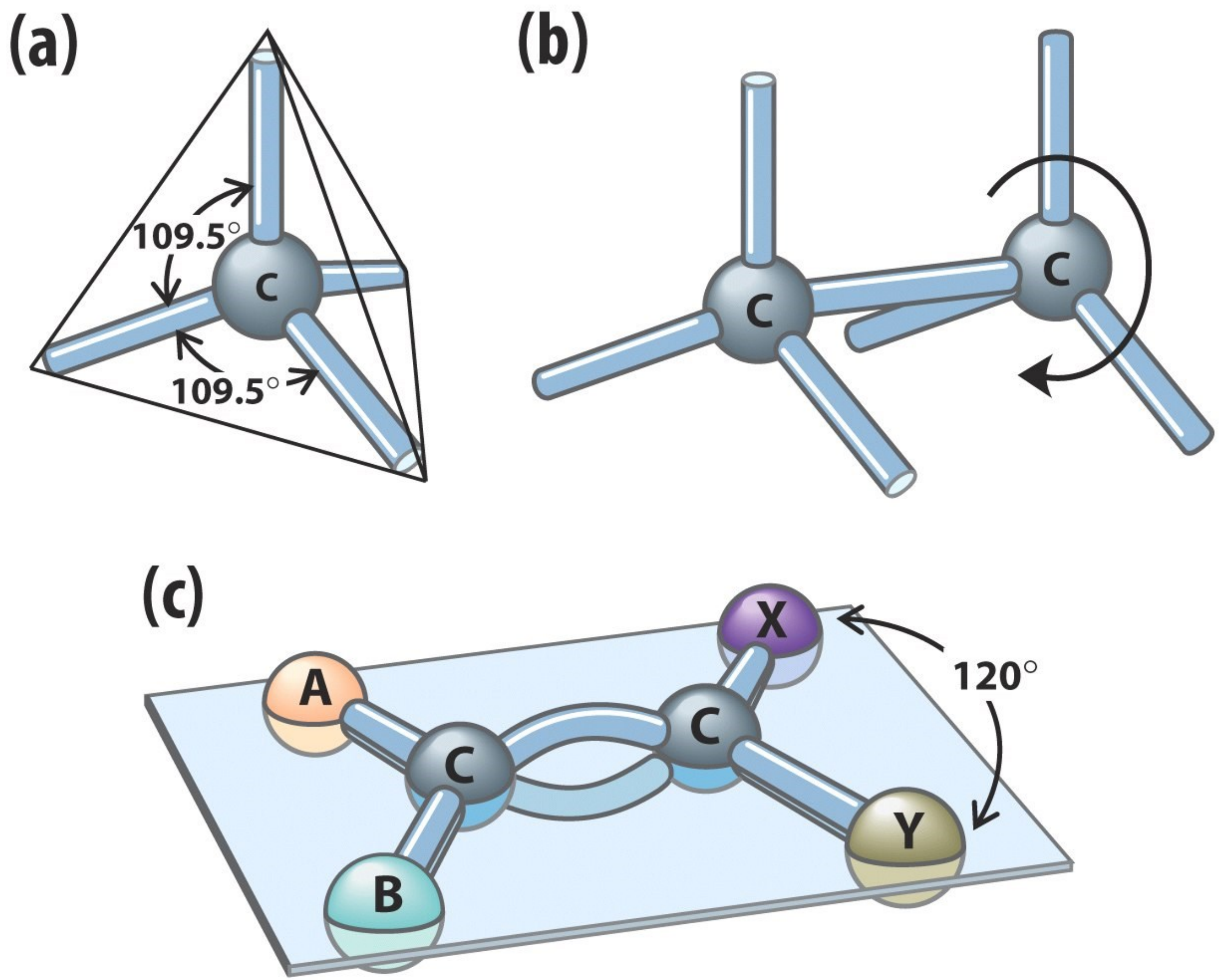


What are the bond energies of covalent bonds?

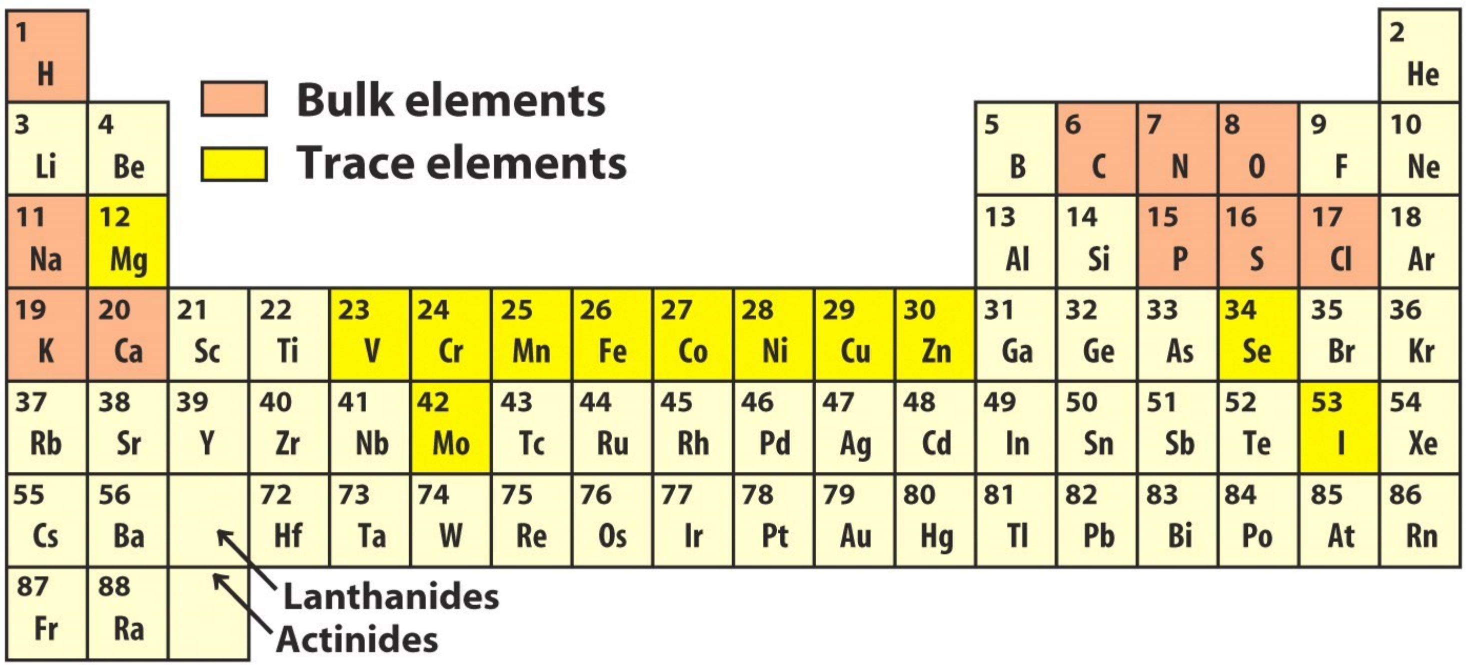
Bond	Energy (kJ/mol)
H-H	436
C-H	414
C-C	343
C-O	351

H, C, N and O form the strongest covalent bonds.
P and S are also covalent-bond forming

Geometry of carbon bonding

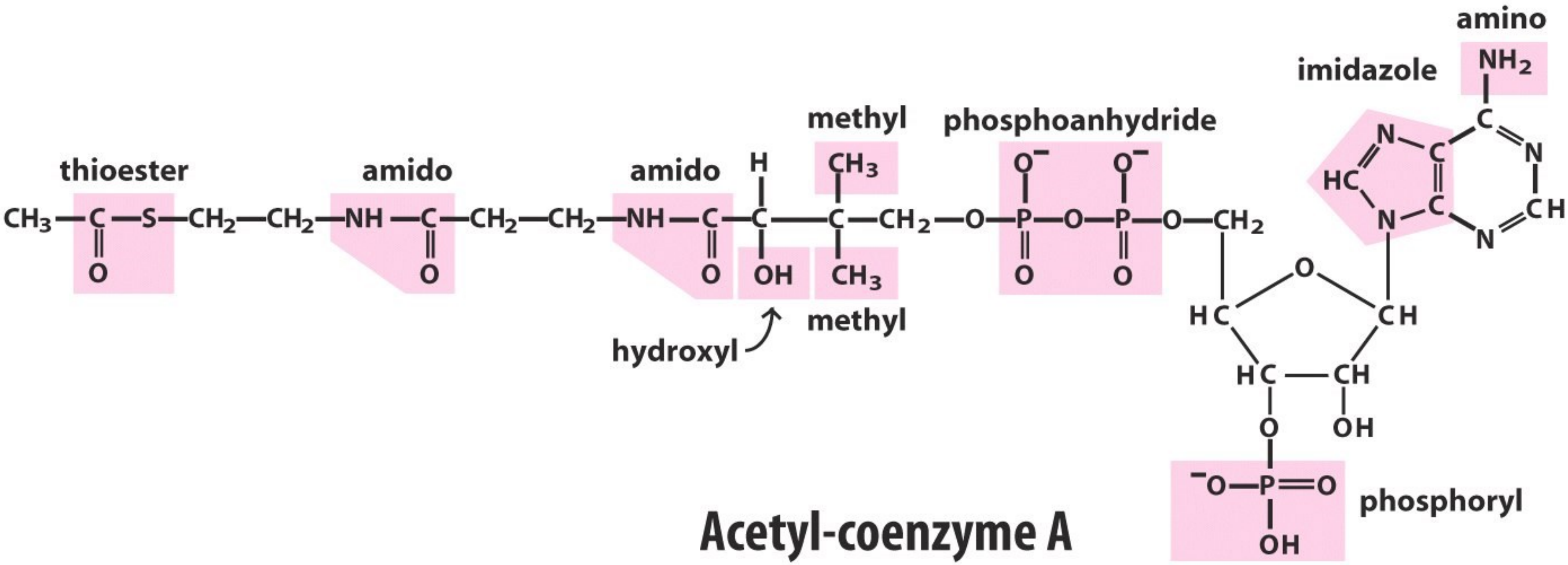


Why not Si based life



Why not silicon based life?

- Long chains of silicon atoms are not readily synthesized, thus the polymeric macromolecules necessary for more complex functions would not readily form.
- Oxygen disrupt bonds between two silicon atoms, so silicon based life-forms would be unstable in an oxygen-containing atmosphere. Once formed, the bonds between silicon and oxygen are extremely stable and difficult to break, which would prevent the degradation and synthesis of biomolecules.



An example of several common functional groups in a single biomolecule

Cells contain universal set of small molecules

- A collection of perhaps a thousand different small organic molecules (Molecular weight (Mr ~100 to 500). These molecules are conserved during evolution, serve as central metabolites in the cell life. They include the common amino acids, nucleotides, sugars, etc.

- These small molecules are trapped in the cell because the plasma membrane is impermeable to them.

- Besides the universal small molecules, there are other small biomolecules specific to only certain types of cells or organisms. They are called secondary metabolites.

Macromolecules are the major constituents of cells

	% of Total Weight of Cell	Approximate Number of Different Molecular Species
Water	70	1
Protein	15	3,000
Nucleic Acids		
DNA	1	1
RNA	6	>3,000
Polysaccharides	3	5
Lipids	2	20
Monomeric Subunits and Intermediates	2	500
Inorganic Ions	1	20

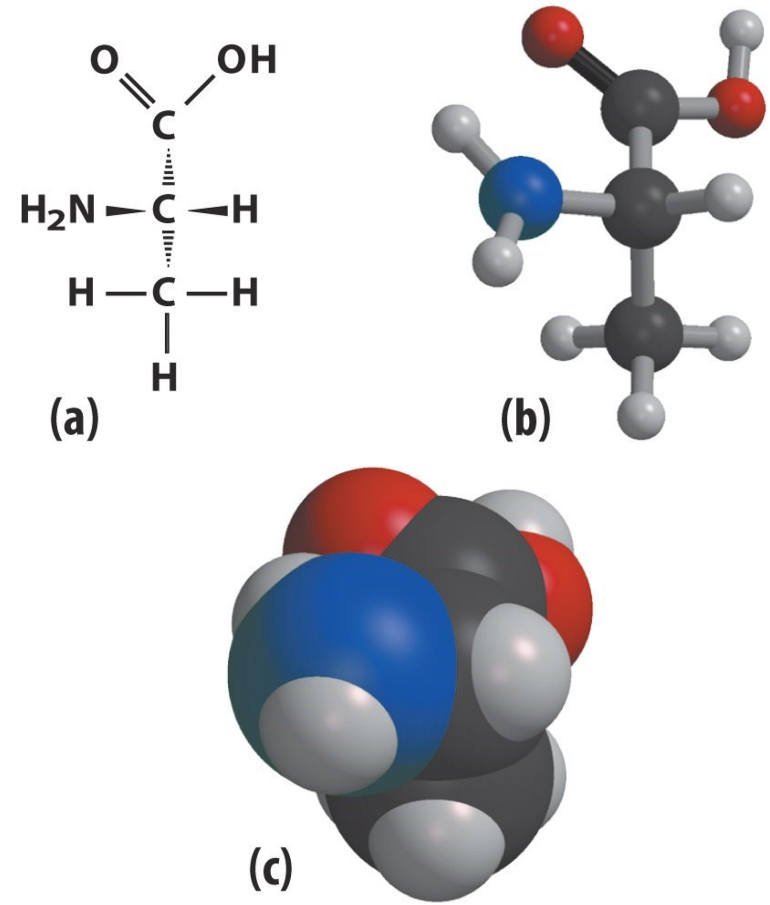
Molecular Components of an E. coli Cell

A review: Three-dimensional structures is Described by configuration and conformation

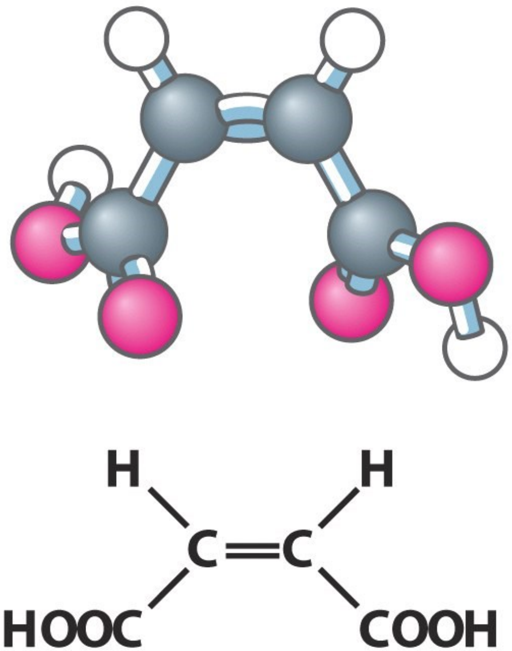
Solid wedge:
Bond project out of the plane of the screen.

Dotted wedge:
Bond project behind of the plane of the screen.

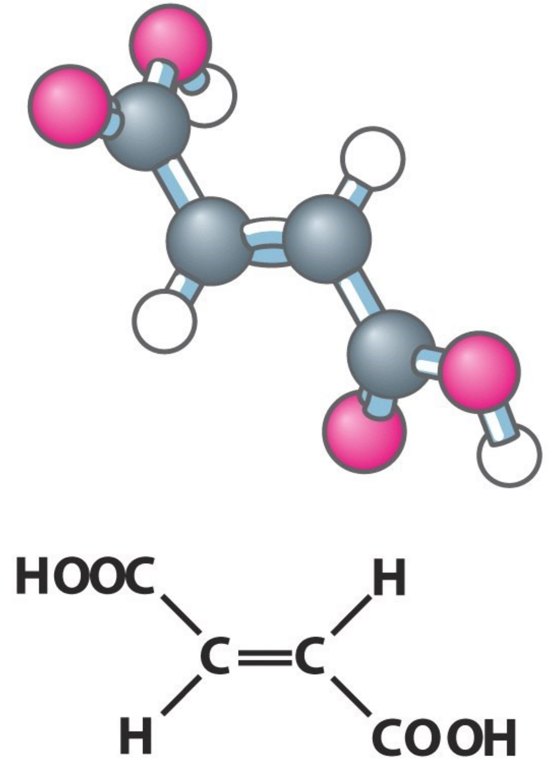
Blue ball: Nitrogen
Black ball: Carbon
Red ball: Oxygen
White: Hydrogen
Orange: Phosphate



Ways to illustrate configuration (stereochemistry) of molecules



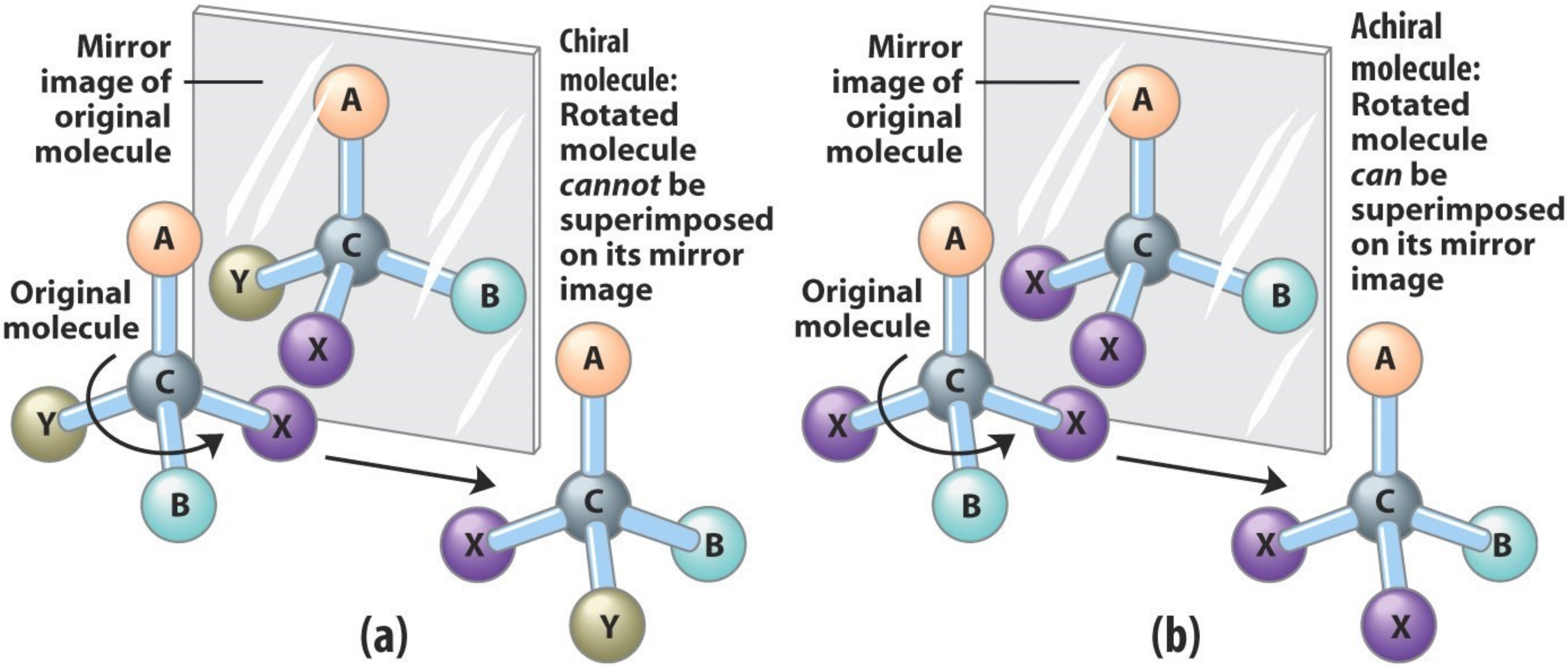
Maleic acid (cis)



Fumaric acid (trans)

Geometric isomers, or Cis-trans isomers

Differ in the arrangement of their substituent groups with respect to the nonrotating double bond

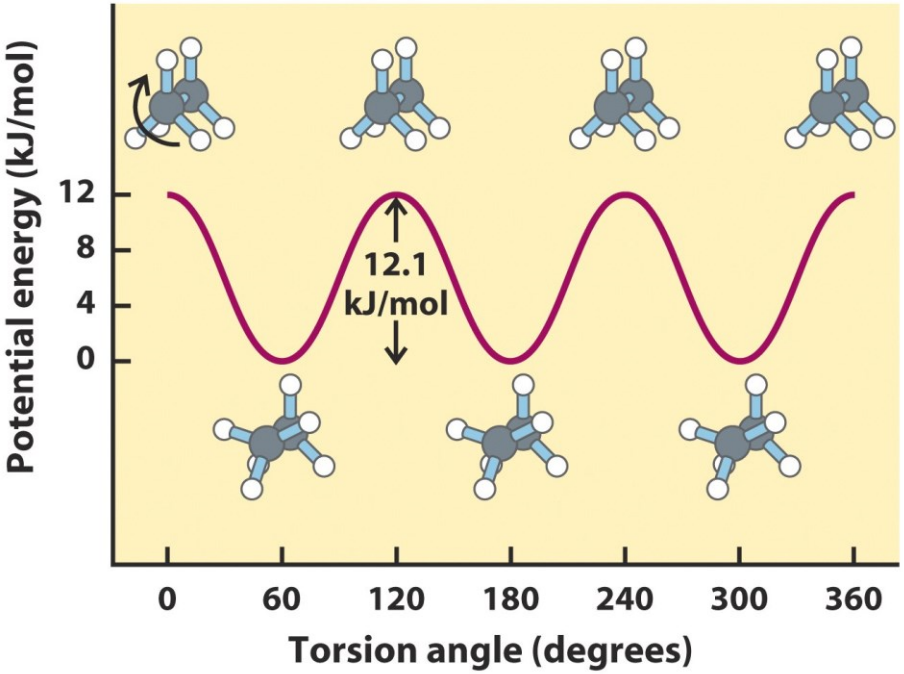


Enantiomers are stereoisomers That are mirror image of each other

A pair of molecules, or compounds that are mirror images of each other but are not identical, and that rotate the plane of polarized light equally, but in opposite directions.

conformation

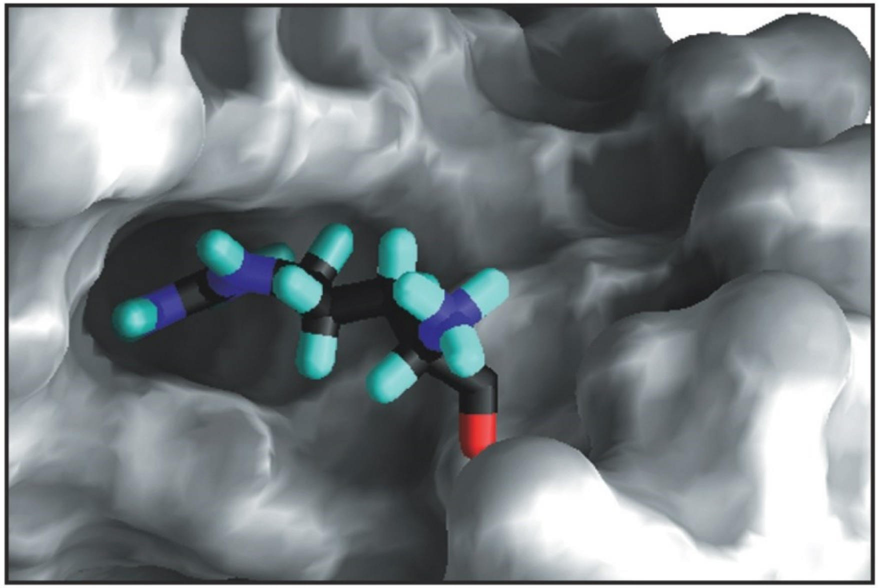
Conformation: the spatial arrangement of substituent groups that, without breaking any bonds, are free to assume different positions in space because of the freedom of rotation about single bonds.



A biomolecule will stay in a specific conformation under certain condition.

Biomolecules Have Characteristic *Three-Dimensional Architecture*

Interaction between biomolecules are stereospecific



When biomolecules interact, the "fit" between them must be stereochemically correct. Stereospecificity, the ability to distinguish between stereoisomers, is a property of enzymes and other proteins and a characteristic feature of the molecular logic of living cells.

1.3 Physical foundations

Living organisms exist in a dynamic **steady state**, never at **equilibrium** with their surroundings.

Examples:
Small molecules, macromolecule, supermolecular complexes are continuously synthesized and broken down in chemical reactions that involves a constant flux of mass and energy through the system.

Hemoglobin-O2
glucose

Organisms transform energy and matter from their surroundings

Isolated system (the system exchanges neither matter nor energy with its surroundings)

Closed system (exchanges energy but not matter)

Open system (exchange both energy and matter)

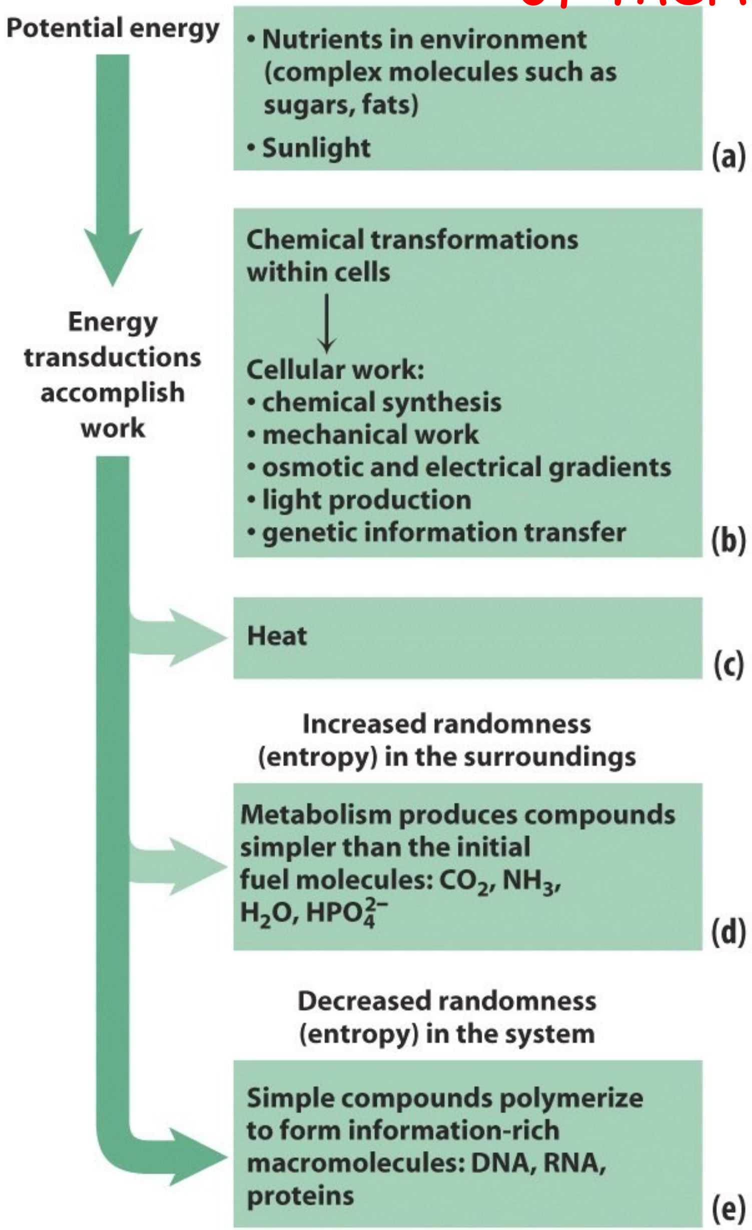
A living organism is an open system.

Organisms derive energy from surroundings in two ways:

(1) taking up chemical fuels (such as glucose) from the environment and extract energy by oxidizing them.

(2) absorbing energy directly from sunlight.

Energy interconversions in living organisms follow the laws of thermodynamics



During metabolic energy transductions, the randomness of the system plus surroundings (entropy) increases as the potential energy of the complex nutrient molecule decreases.