Water

Dr. Diala Abu-Hassan, DDS, PhD
Dr.abuhassand@gmail.com

Lecture 2

MD summer 2014

Life processes depend on the properties of water.

Lecture Content

- Importance of water in biological systems
- Noncovalent interactions
- Water structure
- Water properties
- Water as a solvent
- Water movement

Why water is important to our bodies?

1. ~60% of our body is water, 70-85% of the weight of a typical cell

2. A solvent of many substances our bodies need such as glucose, ions, etc.

3. Acts as a medium in which acids and bases release their chemical groups to maintain a constant cellular environment or homeostasis.

4. Essential buffer that maintain pH

5. Temperature regulation- high sppecific heat capacity.

6. A participant in many biochemical reactions.

Water distribution in body compartments

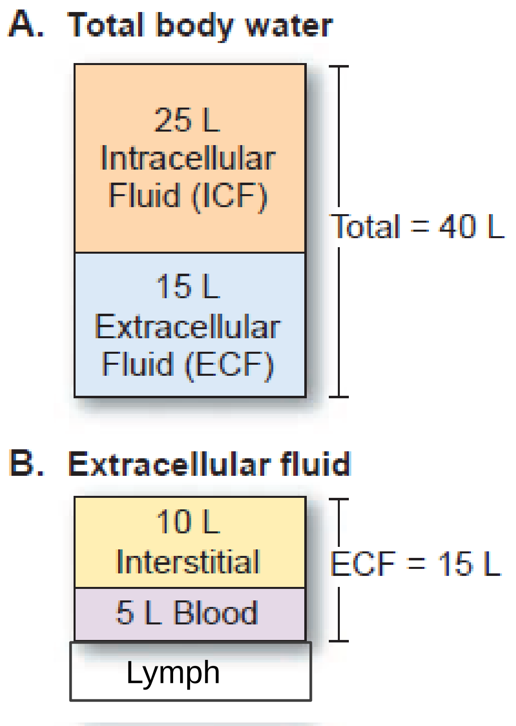


FIG. 4.2. Fluid compartments in the body based on an average 70-kg man.

Mark's 2012

Noncovalent Interactions

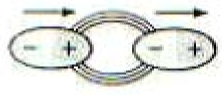
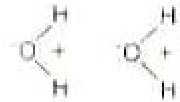
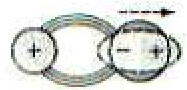
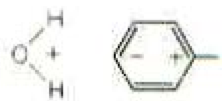
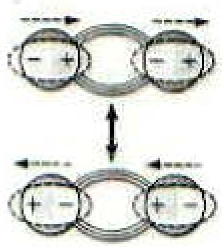
Electrostatic, or ionic interactions (salt bridges)
- Interactions between oppositely charged groups

Van der Waals forces
- Attractions between transient dipoles generated by the rapid movement of electrons of all neutral atoms. 1-5 kj/mole

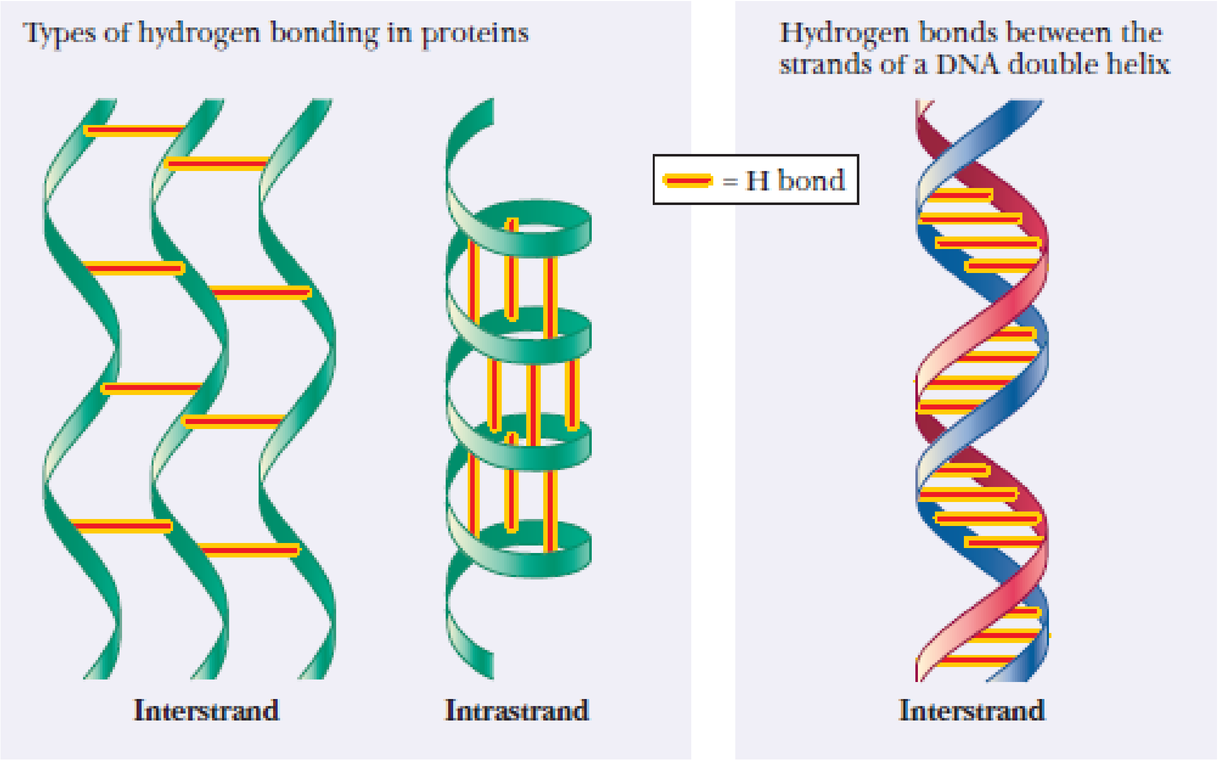
Hydrophobic interactions 5-30 kj/mole
- Self-association of nonpolar compounds in an aqueous environment.
- Minimize unfavorable interactions between nonpolar groups and water

Hydrogen bonds
- The two strands of the DNA helix. 10-30 kj/mole

Types of noncovalent interactions

TYPE OF INTERACTION	MODEL	EXAMPLE	DEPENDENCE OF ENERGY ON DISTANCE	COMMENT
(a) Charge–charge			$1/r$	Longest-range force, nondirectional
(b) Charge–dipole			$1/r^2$	Depends on orientation of dipole
(c) Dipole–dipole			$1/r^3$	Depends on *mutual* orientation of dipoles
(d) Charge–induced dipole			$1/r^4$	Depends on polarizability of molecule in which dipole is induced
(e) Dipole–induced dipole			$1/r^5$	Depends on polarizability of molecule in which dipole is induced
(f) Dispersion			$1/r^6$	Involves mutual synchronization of fluctuating charges
(g) Hydrogen bond	DONOR—H···· ACCEPTOR		Length of bond fixed	Depends on donor–acceptor pair

Noncovalent Interactions



Properties of Noncovalent Interactions

1. Reversible

2. Relatively weak. 1-30 kj/mole vs. 350 kj/mole in C─C bond

3. Molecules interact and bind specifically.

Covalent vs Noncovalent bonds

Table 2.3

Some Bond Energies

		Energy	
	Type of Bond	**($kJ\ mol^{-1}$)**	**($kcal\ mol^{-1}$)**
Covalent Bonds	O—H	460	110
(Strong)	H—H	416	100
	C—H	413	105
Noncovalent Bonds	Hydrogen bond	20	5
(Weaker)	Ion–dipole interaction	20	5
	Hydrophobic interaction	4–12	1–3
	Van der Waals interactions	4	1

*Note that two units of energy are used throughout this text. The kilocalorie (kcal) is a commonly used unit in the biochemical literature. The kilojoule (kJ) is an SI unit and will come into wider use as time goes on. The kcal is the same as the "Calorie" reported on food labels.

Campbell 6th edition

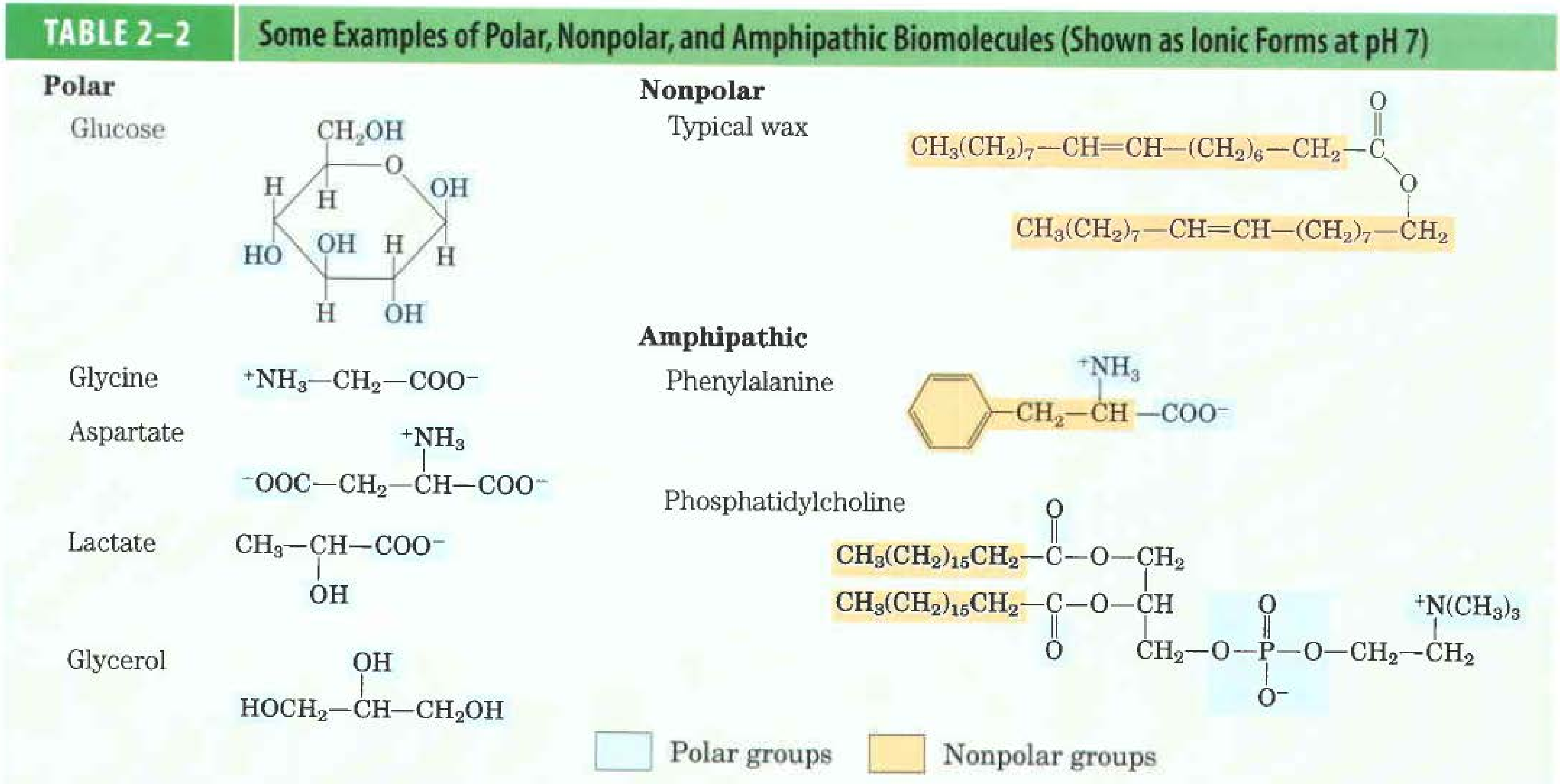
Noncovalent Interactions

-Noncovalent forces significantly contribute to the structure, stability, and functional competence of macromolecules in living cells.

- Can be either attractive or repulsive,

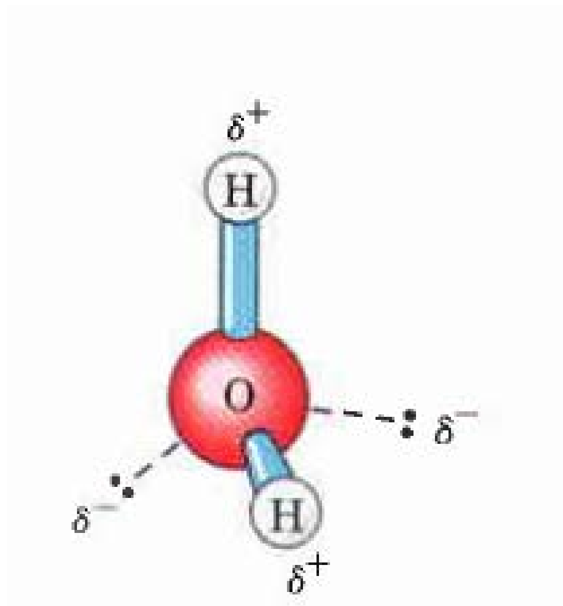
-Involve interactions both within the biomolecule and between it and the water of the surrounding environment.

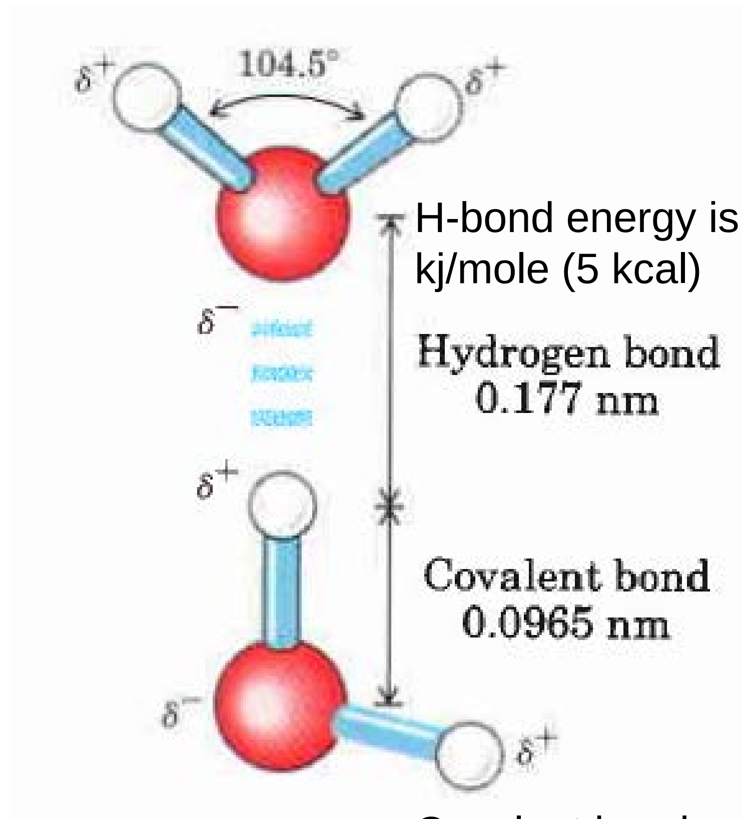
- Amphipathic molecules



Lehninger 5th edition

Water structure





H-bond energy is 20 kj/mole (5 kcal)

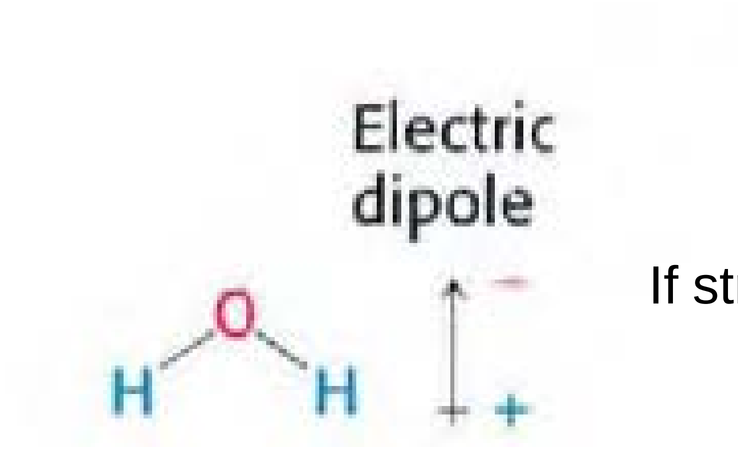
Electronegativity of O atom is 3.5
Electronegativity of H atom is 2.1

Water is electrically neutral (net charge is zero)
Bent geometry → dipole

Covalent bond energy is 460 kj/mole (110 kcal)

Lehninger 5th edition

Polarity



If straight?

CO_2 has polar bonds but is nonpolar

δ- δ+ δ-

O ═ C ═ O

Linear- no dipole moment

Water and Hydrogen Bonds (H-bonds)

-A hydrogen bond is a weak noncovalent interaction between the H of one molecule and the more electronegative atom of an acceptor molecule.

-A dipolar molecule with an uneven distribution of electrons between the hydrogen and oxygen atoms.

- Forms H-bonds with other polar molecules, thus acts as a solvent.

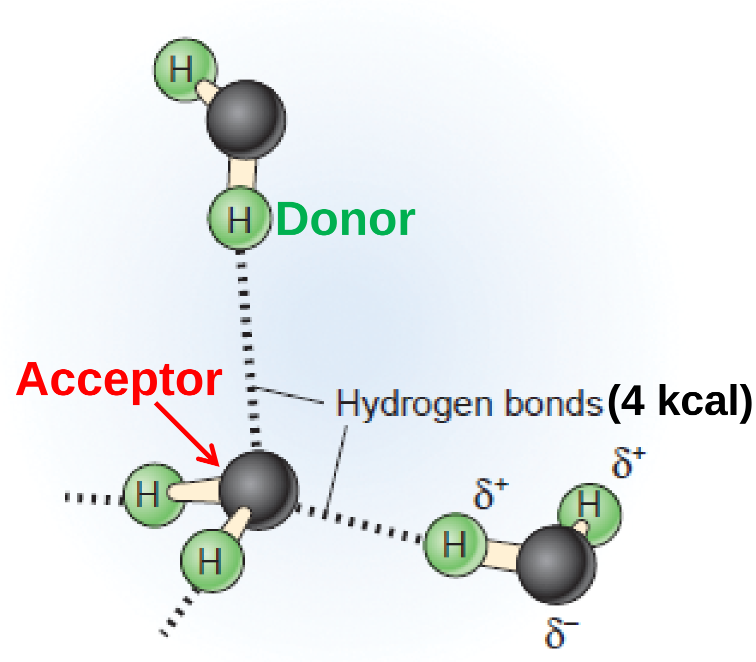


FIG. 4.3. Hydrogen bonds between water molecules. The oxygen atoms are shown in *black*.

Mark's 2012

Hydrogen Bonds (H-bonds)

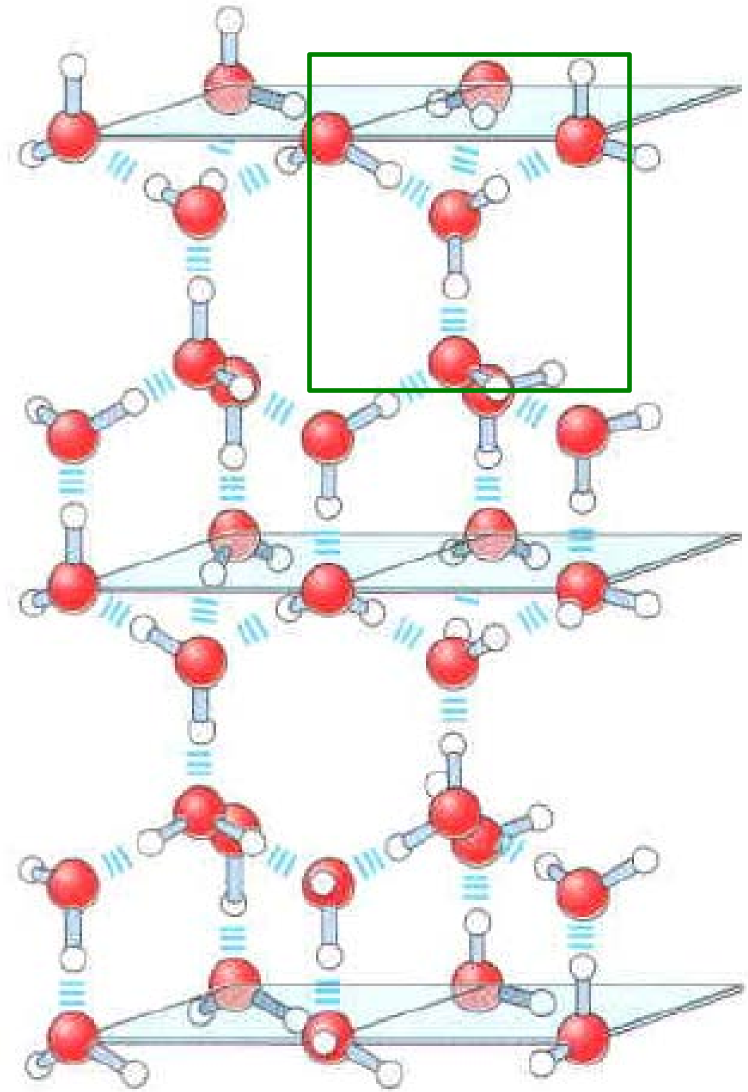
H-bond is stronger if

X–H .... A

A is O, N or F
X is O, N or F

Average number of H-bond
in liquid water at 10°C is 3.4
in ice crystals is 4

Number of H-bonds decrease
with higher temperatures



Lehninger 5th edition

H-bonding gives water its unusual properties

Higher melting and boiling points

Heat of vaporization

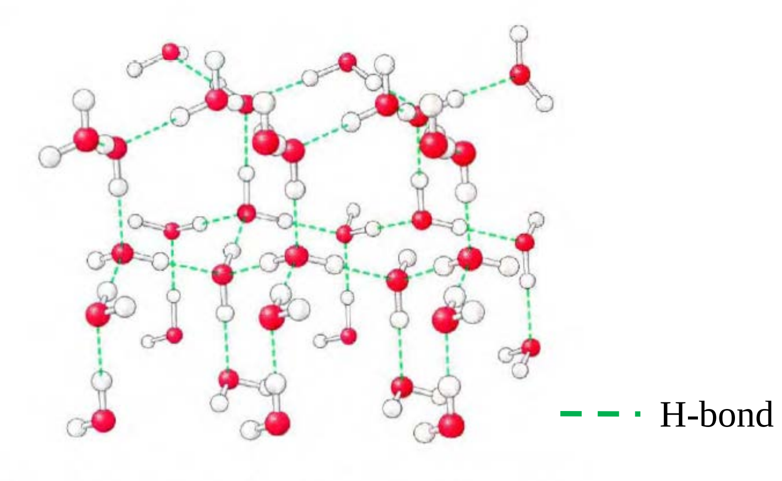
Higher freezing point

Surface tension

H-bond has:

A bond energy of 20 kj/mole

Life time 1x 10^{-9} second



Highly cohesive (ice)

Berg 2006

Physical properties of water

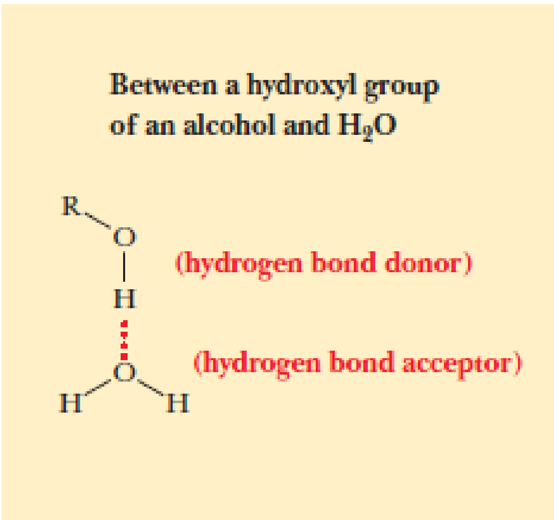
TABLE 2–1 Melting Point, Boiling Point, and Heat of Vaporization of Some Common Solvents

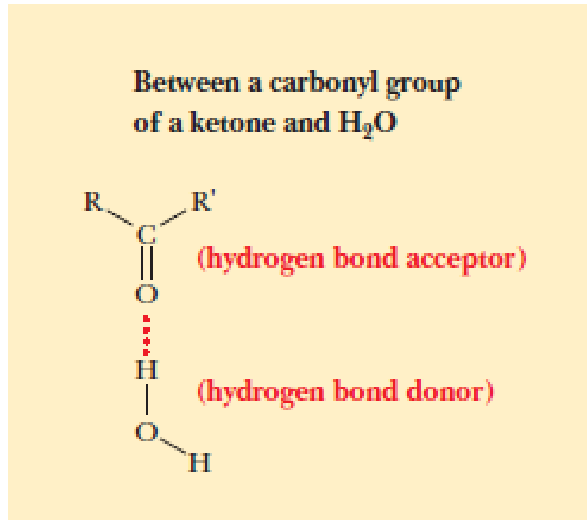
	Melting point (°C)	Boiling point (°C)	Heat of vaporization (J/g)*
Water	0	100	2,260
Methanol (CH_3OH)	−98	65	1,100
Ethanol (CH_3CH_2OH)	−117	78	854
Propanol ($CH_3CH_2CH_2OH$)	−127	97	687
Butanol ($CH_3(CH_2)_2CH_2OH$)	−90	117	590
Acetone (CH_3COCH_3)	−95	56	523
Hexane ($CH_3(CH_2)_4CH_3$)	−98	69	423
Benzene (C_6H_6)	6	80	394
Butane ($CH_3(CH_2)_2CH_3$)	−135	−0.5	381
Chloroform ($CHCl_3$)	−63	61	247

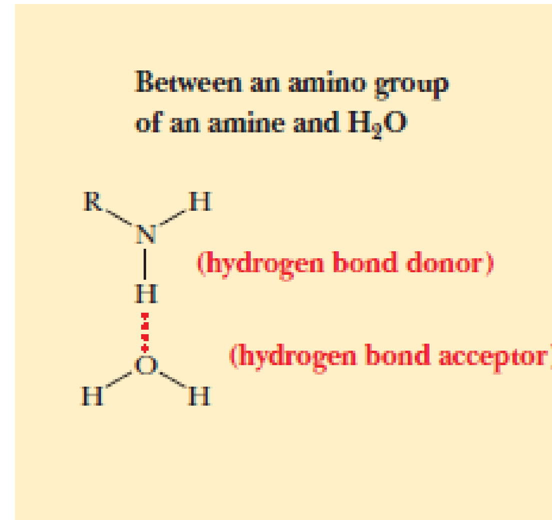
*The heat energy required to convert 1.0 g of a liquid at its boiling point and at atmospheric pressure into its gaseous state at the same temperature. It is a direct measure of the energy required to overcome attractive forces between molecules in the liquid phase.

Lehninger 5th edition

Water forms H-bonds with other polar molecules







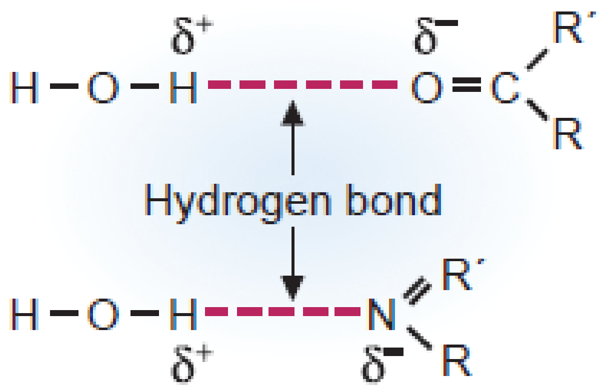
- H-bonds are not unique only for water

- H atoms bonded to O, N or any electronegative atom can form H-bond

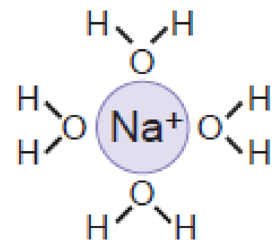
- H atoms bound to carbon atoms, which are not electronegative, do not form H-bonds

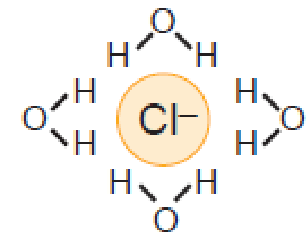
Campbell 6th edition

Water as a solvent



H-bonds between water and polar molecules. *R denotes additional atoms.*





Hydration shells surrounding anions and cations.

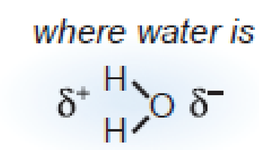
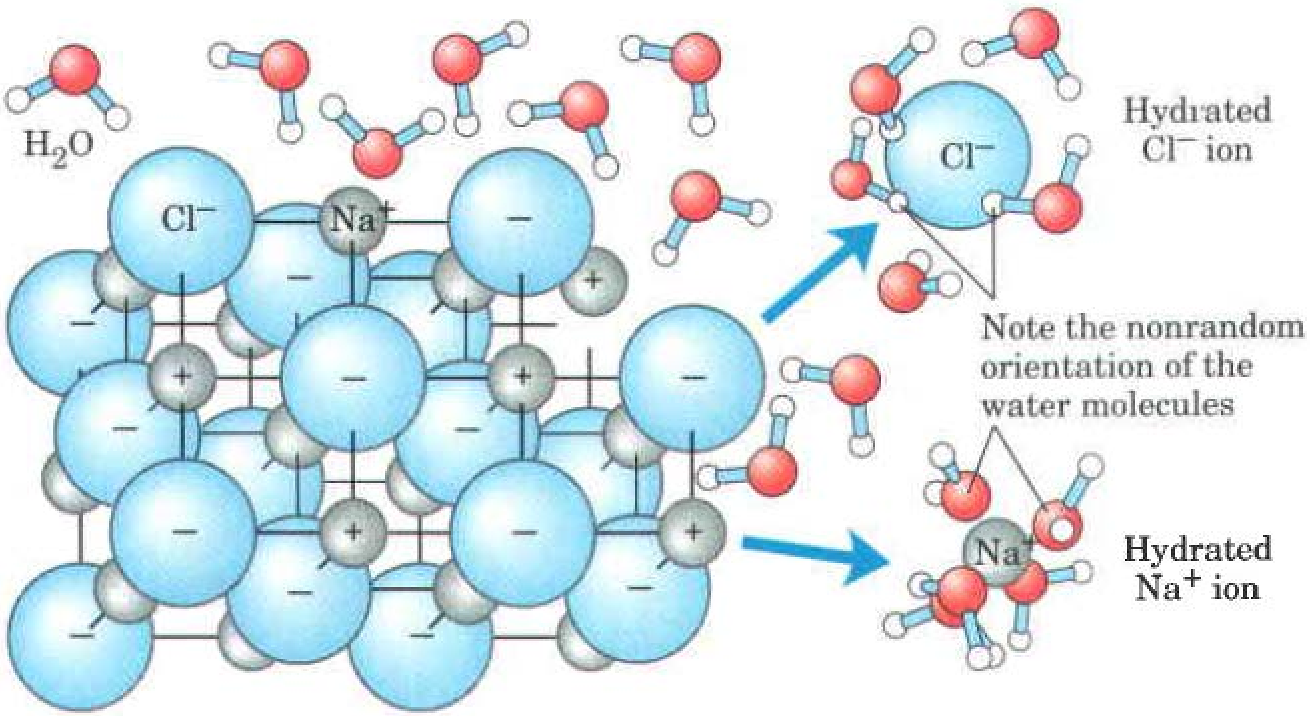


Table 4.1 Distribution of Ions in Body Fluids

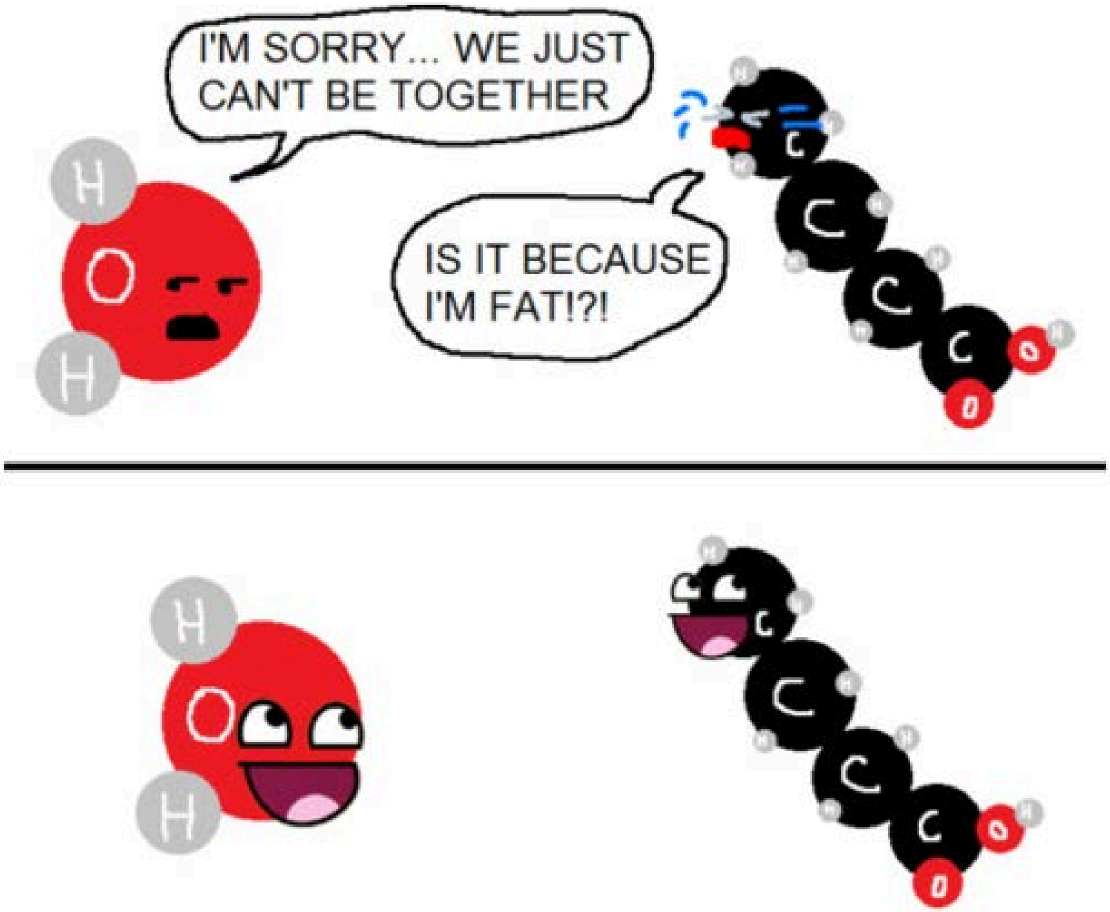
	ECF[a] (mmol/L)	*ICF (mmol/L)*
Cations		
Na^+	145	12
K^+	4	150
Anions		
Cl^-	105	5
HCO_3^-	25	12
Inorganic phosphate	2	100

ECF, extracellular fluid; *ICF*, intracellular fluid.
[a]The content of inorganic ions is very similar in plasma and interstitial fluid, the two components of the ECF.

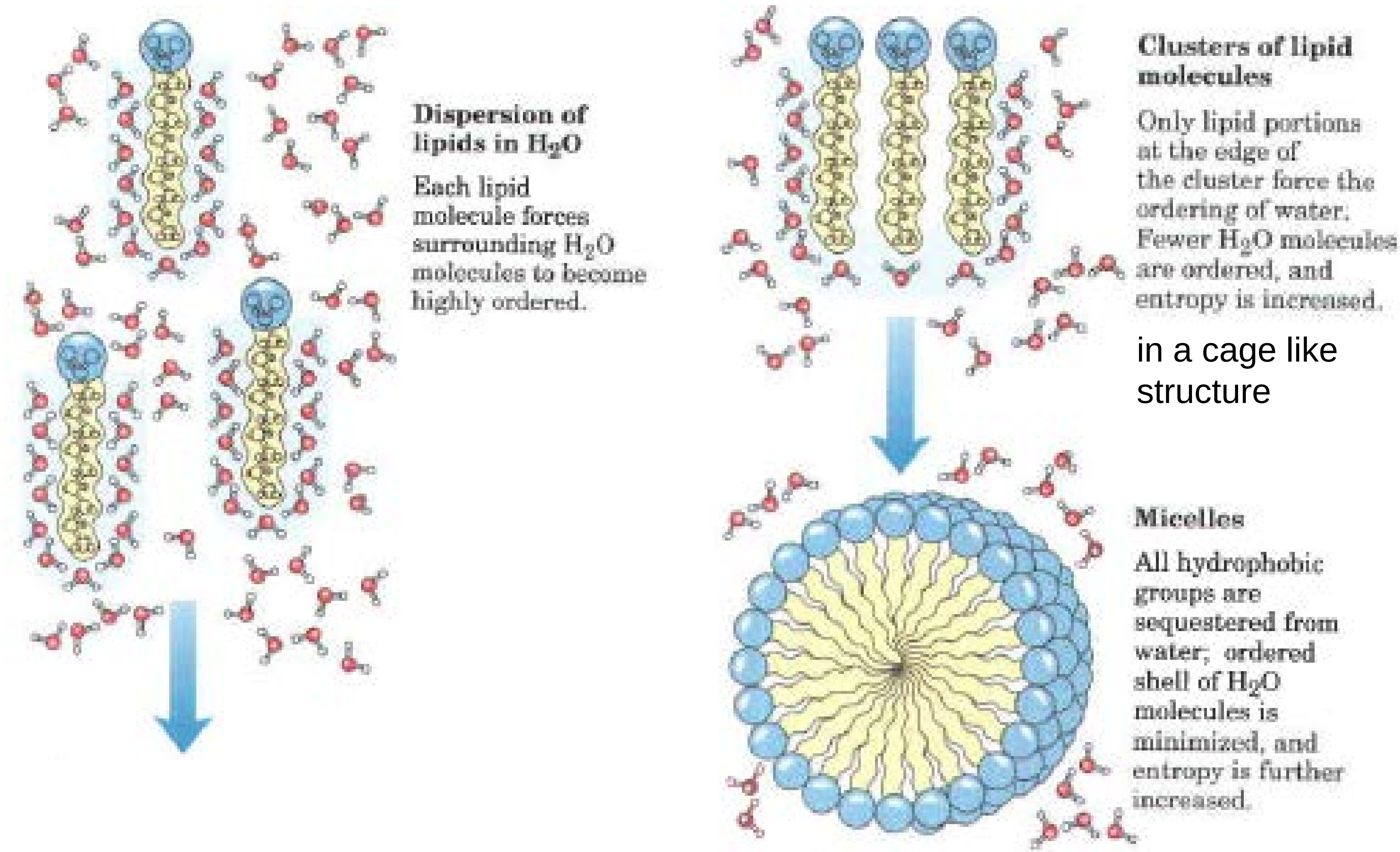
Water as a solvent



Lehninger 5th edition


I'M SORRY... WE JUST CAN'T BE TOGETHER
IS IT BECAUSE I'M FAT!?!

Hydrophobic interactions and micelle formation



in a cage like structure

Water is an excellent nucleophile

- **Nucleophiles** electron-rich molecules
- **Electrophiles** electron-poor atoms called.
- Nucleophiles and electrophiles **do not** necessarily possess a formal negative or positive charge.
- Water is a nucleophile since it has two lone pairs of electrons
- Other nucleophiles of biologic importance include
  the oxygen atoms of phosphates, alcohols, and carboxylic acids; the sulfur of thiols; the nitrogen of amines; and the imidazole ring of histidine.

-Common electrophiles include
  the carbonyl carbons in amides, esters, aldehydes, and ketones the phosphorus atoms of phosphoesters.

Water and Thermal Regulation

Water structure resists sudden and large temperature changes because:

High heat of fusion, so a large drop in temperature is needed to convert liquid water to ice.

High thermal conductivity thus, facilitates heat dissipation from high energy consumption areas into the body water pool.

High heat capacity and heat of vaporization; when liquid water (sweating) is converted to a gas and evaporates from the skin, we feel a cooling effect.

↓ Temperature → ↑ H-bonds

↑ Temperature → ↓ H-bonds

Osmolality and Water Movement

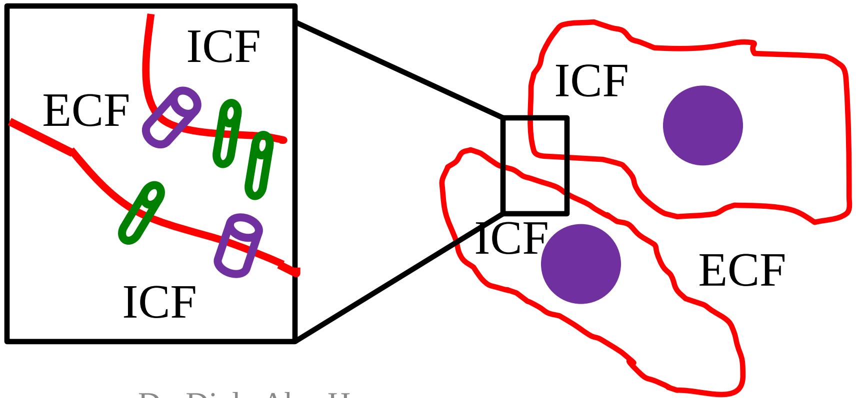
Osmolality: concentration of solutes that is expressed as milliosmoles (mOsm) per kg water.

Osmolality (fluid) α total concentration of all solutes, including ions, organic metabolites, and proteins.

Water is distributed between different fluid compartments according to the concentration of solutes in each compartment.

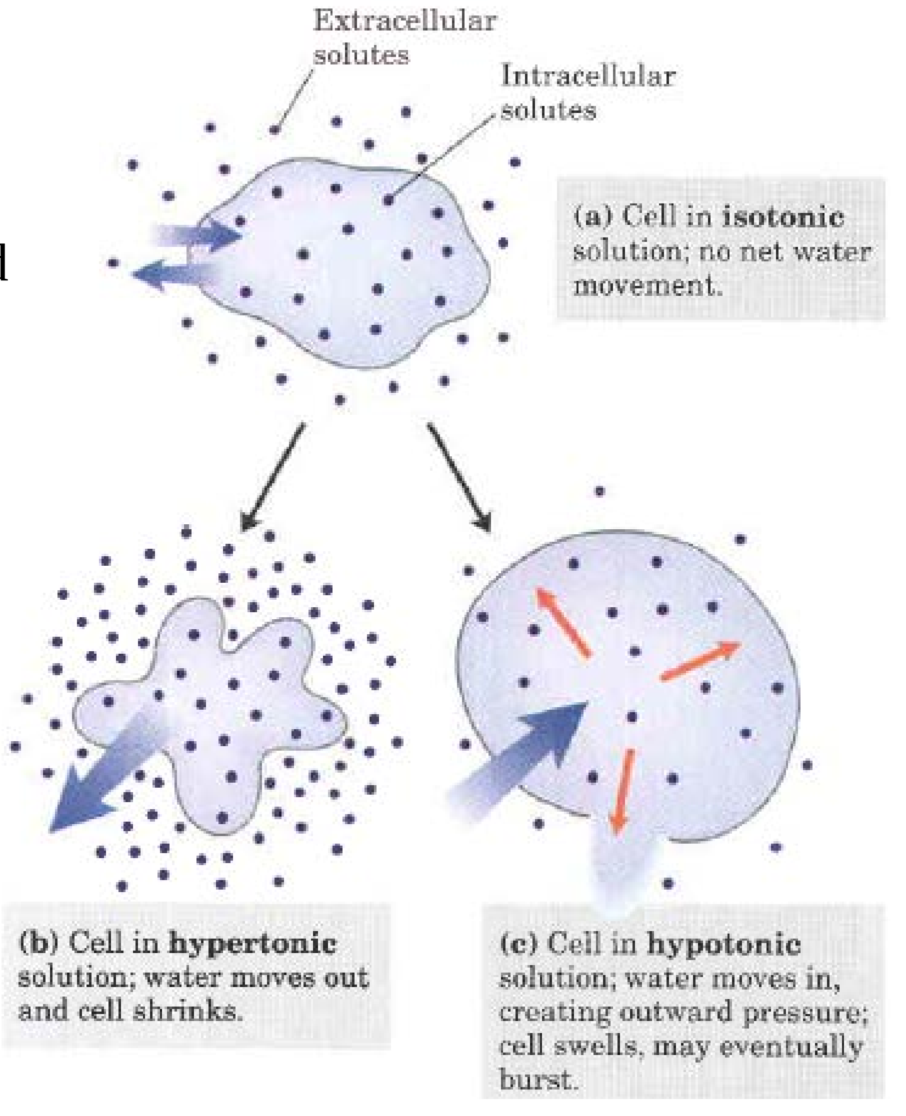
Osmotic pressure: The force it would take to keep the same amount of water on both sides of the membrane.

Water moves in and out according to solute concentration



Effect of extracellular osmolarity on water movement across a plasma membrane

As water is lost from one fluid compartment, it is replaced with water from another compartment to maintain a nearly constant osmolality.



Questions