

Water

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Lecture 2
MD summer



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Life processes depend on the properties of water.

Lecture Content

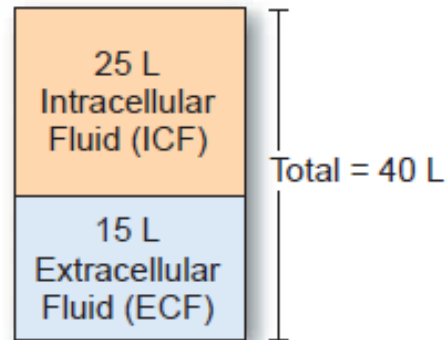
- Importance of water in biological systems
- Noncovalent interactions
- Water structure
- Water properties
- Water as a solvent
- Water movement

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 specific heat capacity.
6. A participant in many biochemical reactions.

Water distribution in body compartments

A. Total body water



B. Extracellular fluid

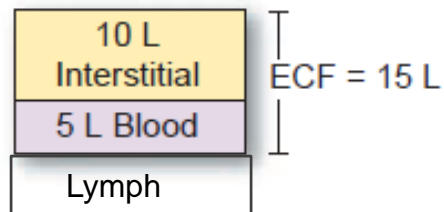


FIG. 4.2. Fluid compartments in the body based on an average 70-kg man.

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

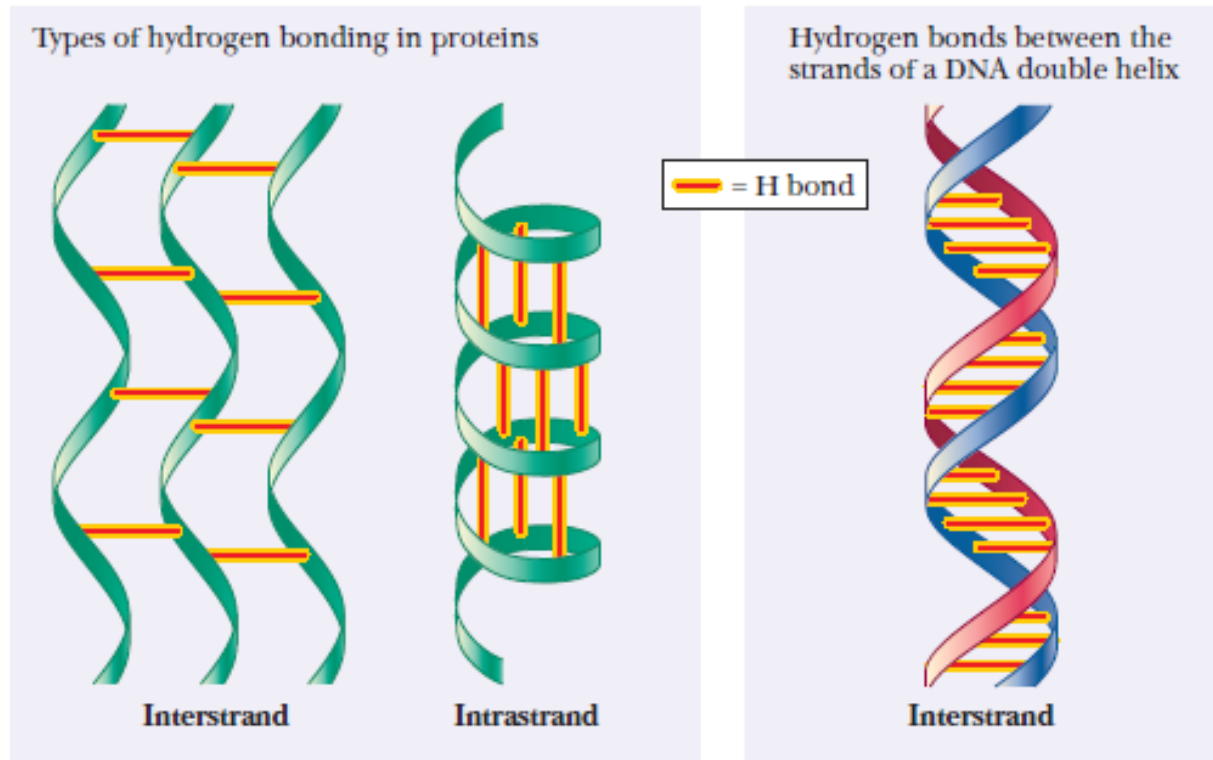
Hydrogen bonds

- 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		—NH_3	$1/r$	Longest-range force; nondirectional
(b) Charge–dipole		—NH_3	$1/r^2$	Depends on orientation of dipole
(c) Dipole–dipole			$1/r^3$	Depends on <i>mutual</i> orientation of dipoles
(d) Charge–induced dipole		—NH_3	$1/r^4$	Depends on polarizability of molecule in which dipole is induced
(e) Dipole–induced dipole			$1/r^6$	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			
	Type of Bond	Energy	
		(kJ mol ⁻¹)	(kcal mol ⁻¹)
Covalent Bonds (Strong)	O—H	460	110
	H—H	416	100
	C—H	413	105
Noncovalent Bonds (Weaker)	Hydrogen bond	20	5
	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.

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.

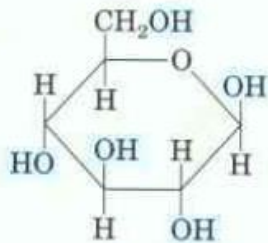
Polarity

TABLE 2-2

Some Examples of Polar, Nonpolar, and Amphipathic Biomolecules (Shown as Ionic Forms at pH 7)

Polar

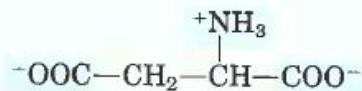
Glucose



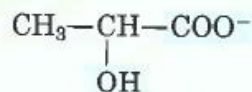
Glycine



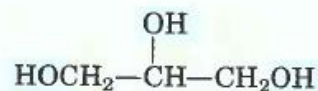
Aspartate



Lactate

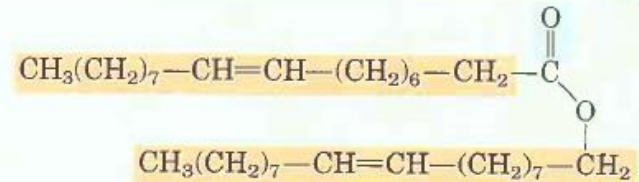


Glycerol



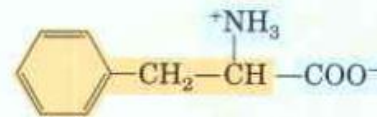
Nonpolar

Typical wax

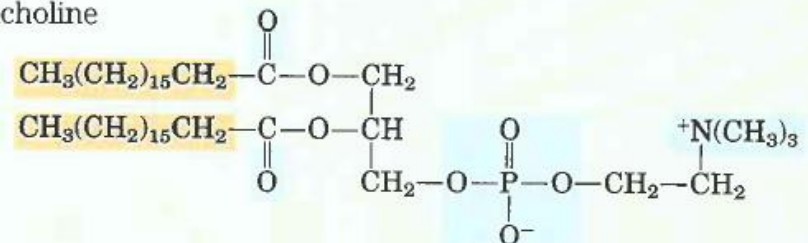


Amphipathic

Phenylalanine



Phosphatidylcholine

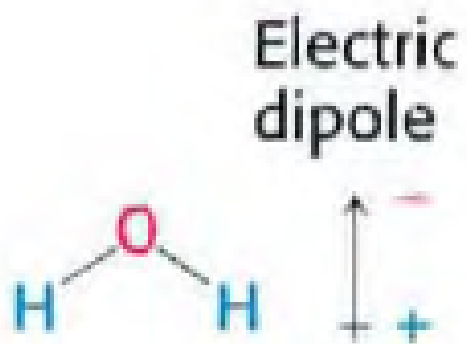


Polar groups



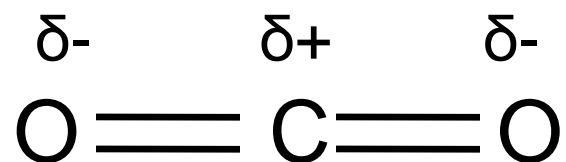
Nonpolar groups

Polarity



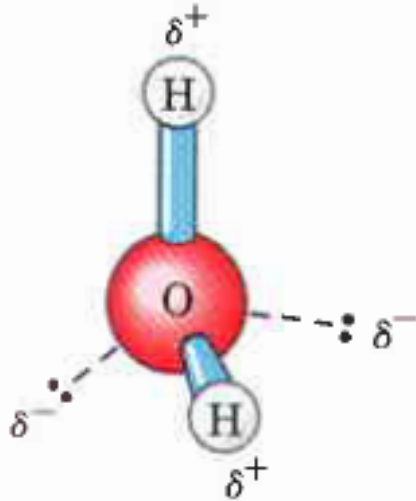
If straight?

CO₂ has polar bonds but is nonpolar



Linear- no dipole moment

Water structure

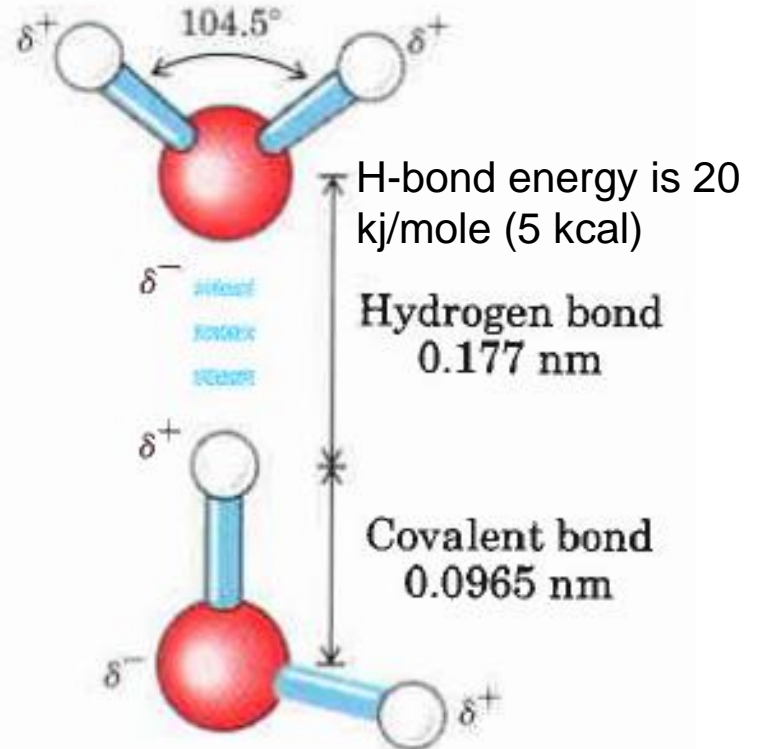


Electronegativity of O atom is 3.5

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)

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.

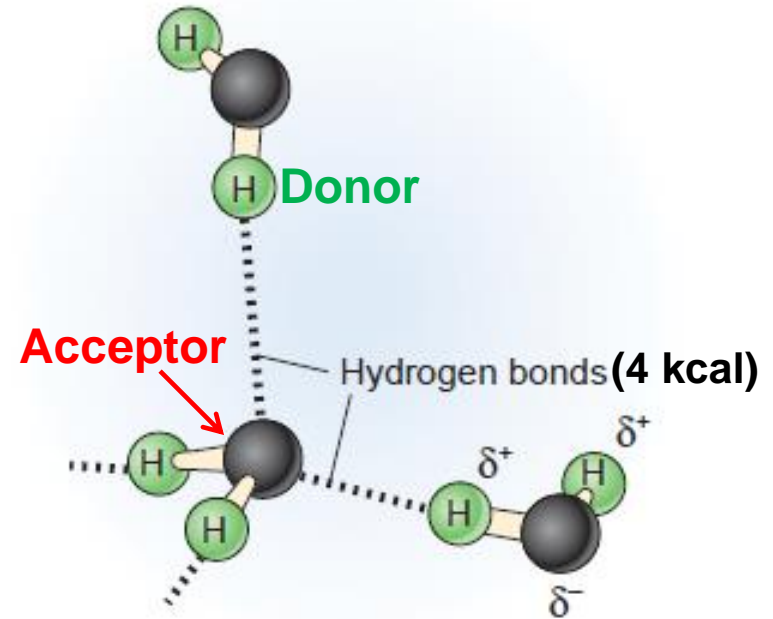


FIG. 4.3. Hydrogen bonds between water molecules. The oxygen atoms are shown in black.

Hydrogen Bonds (H-bonds)

H-bond is stronger if

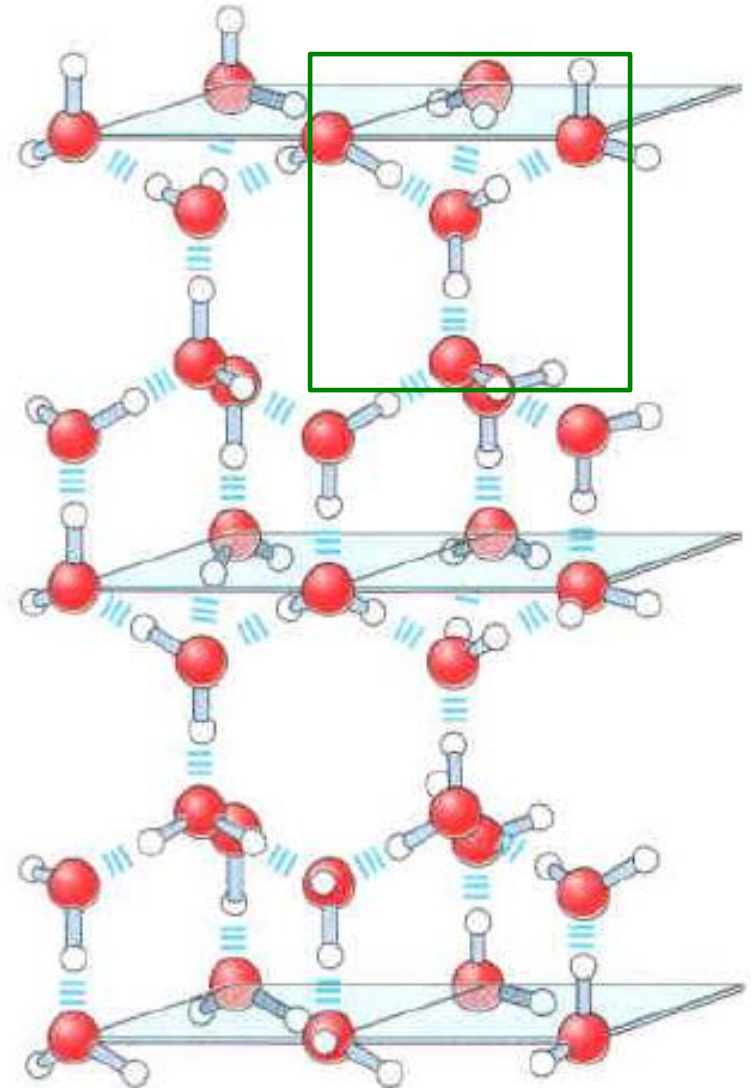
$X-H \cdots A$

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



H-bonding gives water its unusual properties

Higher melting and boiling points

Heat of vaporization

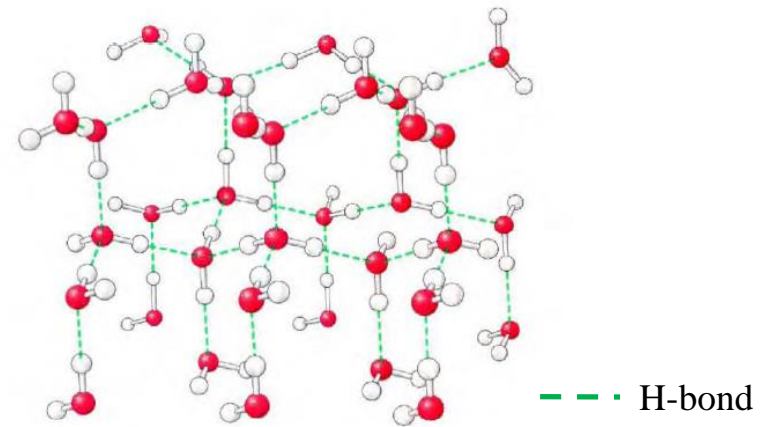
Higher freezing point

Surface tension

H-bond has:

A bond energy of 20 kJ/mole

Life time 1×10^{-9} second



Highly cohesive (ice)

Physical properties of water

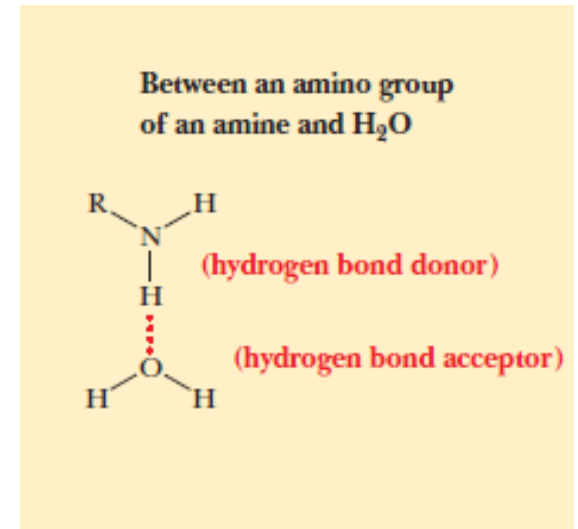
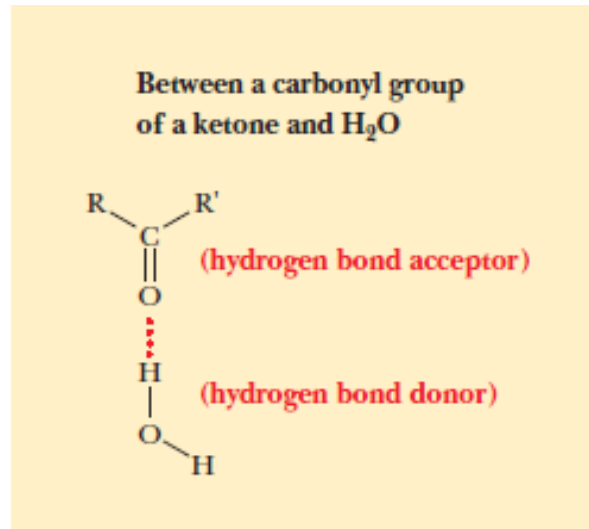
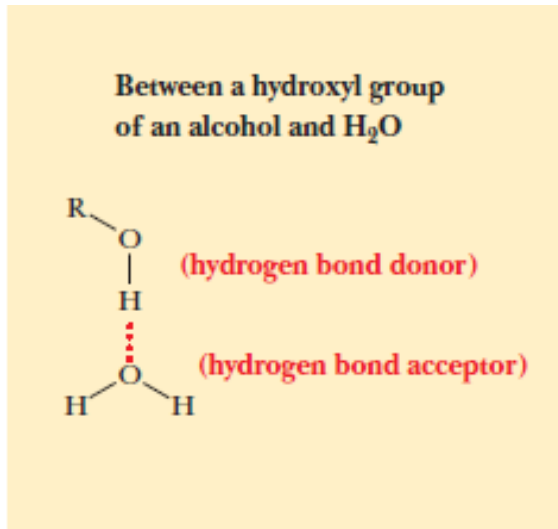
TABLE 2-1

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 ₃ OH)	-98	65	1,100
Ethanol (CH ₃ CH ₂ OH)	-117	78	854
Propanol (CH ₃ CH ₂ CH ₂ OH)	-127	97	687
Butanol (CH ₃ (CH ₂) ₂ CH ₂ OH)	-90	117	590
Acetone (CH ₃ COCH ₃)	-95	56	523
Hexane (CH ₃ (CH ₂) ₄ CH ₃)	-98	69	423
Benzene (C ₆ H ₆)	6	80	394
Butane (CH ₃ (CH ₂) ₂ CH ₃)	-135	-0.5	381
Chloroform (CHCl ₃)	-63	61	247

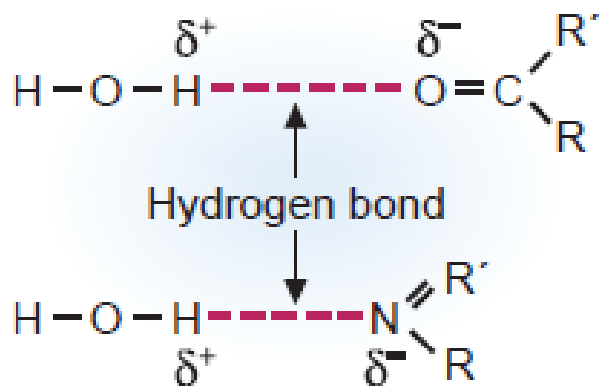
*The heat energy required to convert 1.0 g of a liquid at its boiling point and at atmospheric pressure into its gaseous state at the same temperature. It is a direct measure of the energy required to overcome attractive forces between molecules in the liquid phase.

Water forms H-bonds with other polar molecules

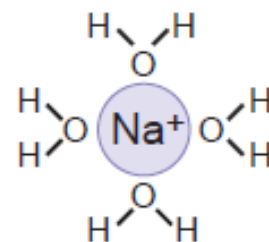


- H-bonds are not unique only for water
- H atoms bonded to O, N or any electronegative atom can form H-bond
- H atoms bound to carbon atoms, which are not electronegative, do not form H-bonds

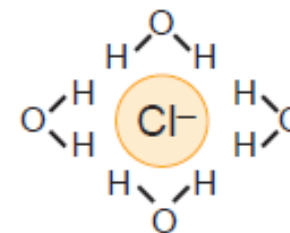
Water as a solvent



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



Hydration shells surrounding anions and cations.



where water is

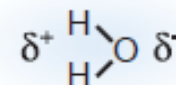


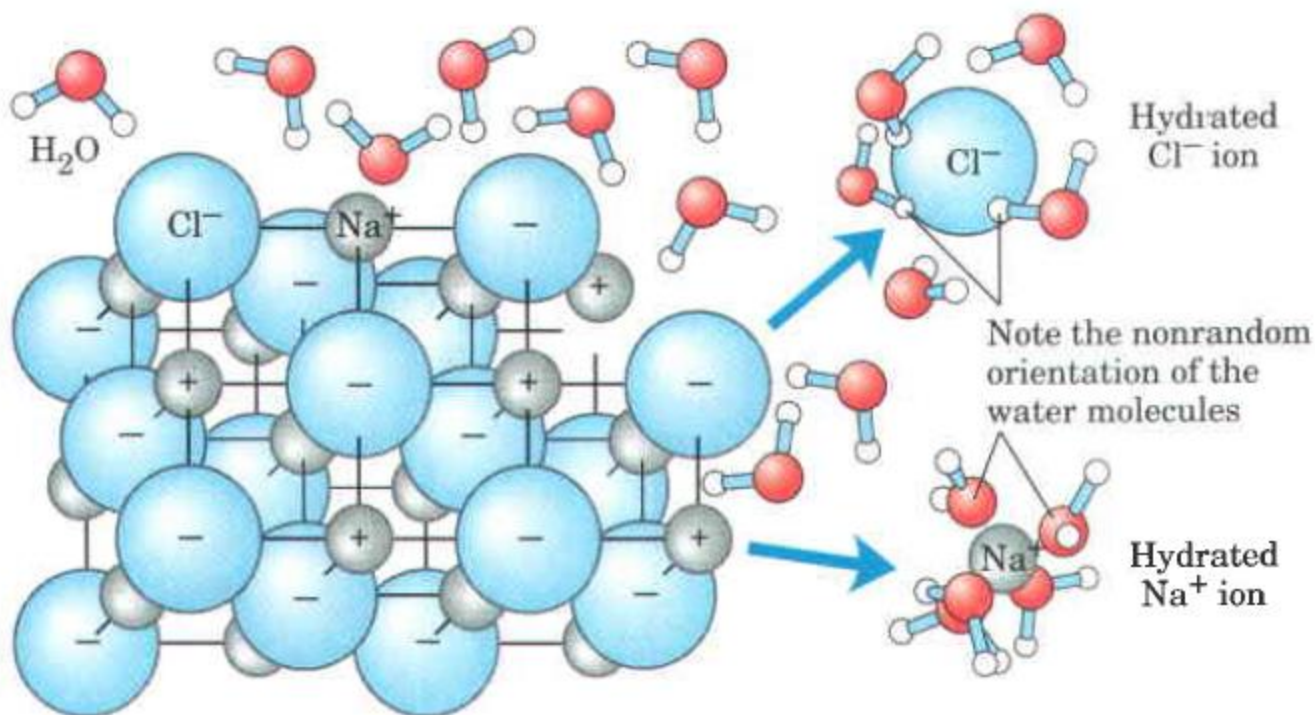
Table 4.1 Distribution of Ions in Body Fluids

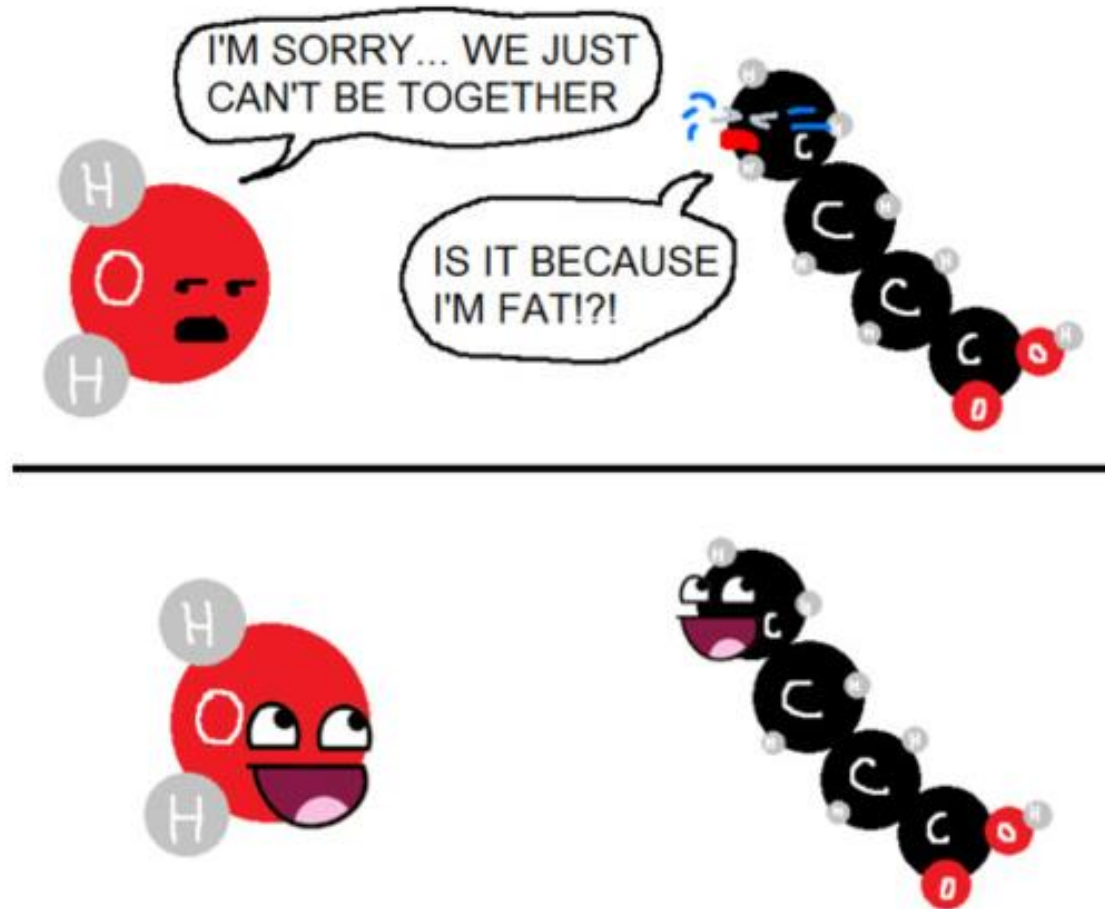
	ECF ^a (mmol/L)	ICF (mmol/L)
Cations		
Na ⁺	145	12
K ⁺	4	150
Anions		
Cl ⁻	105	5
HCO ₃ ⁻	25	12
Inorganic phosphate	2	100

ECF, extracellular fluid; ICF, intracellular fluid.

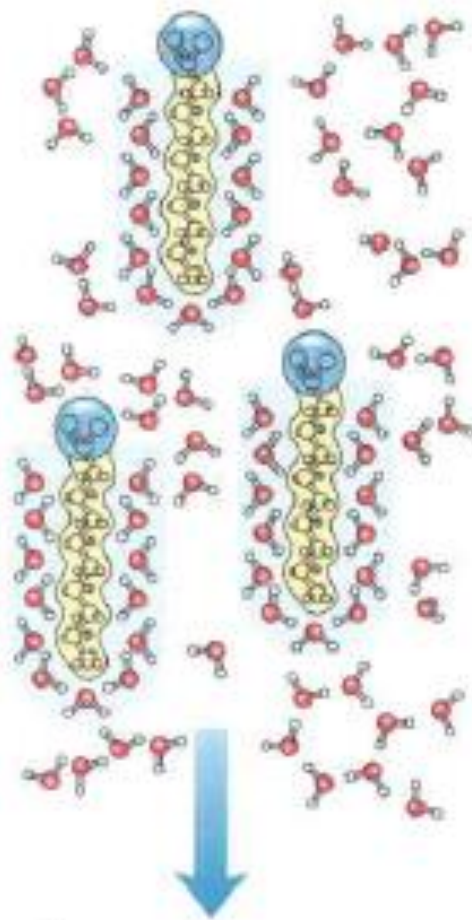
^aThe content of inorganic ions is very similar in plasma and interstitial fluid, the two components of the ECF.

Water as a solvent



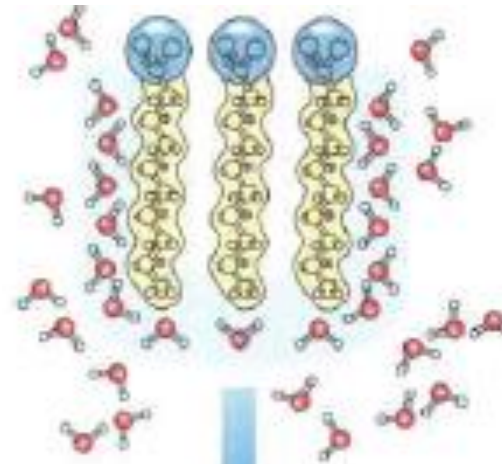


Hydrophobic interactions and micelle formation



Dispersion of lipids in H₂O

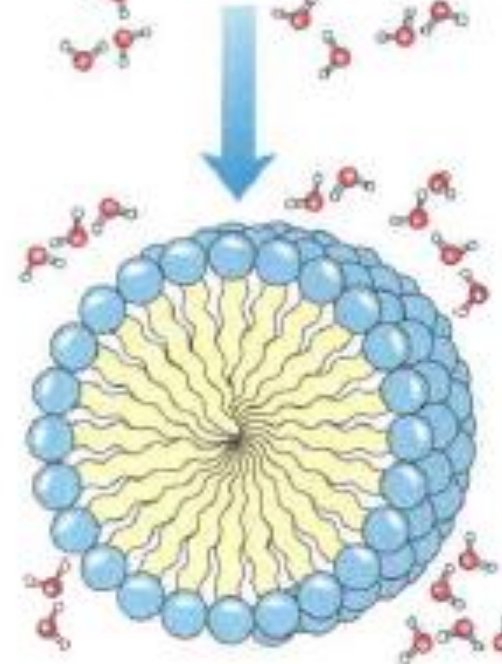
Each lipid molecule forces surrounding H₂O molecules to become highly ordered.



Clusters of lipid molecules

Only lipid portions at the edge of the cluster force the ordering of water; Fewer H₂O molecules are ordered, and entropy is increased.

in a cage like structure



Micelles

All hydrophobic groups are sequestered from water; ordered shell of H₂O molecules is minimized, and entropy is further increased.

Water and Thermal Regulation

Water structure resists sudden and large temperature changes because:

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

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

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.

