WATER & PH

- Simple and abundant
- Extraordinary physical, chemical and biological properties
- Vital to all forms of life
  70% to 85% the wt. of typical cell

Biological Roles of Water

- Biological Solvent

- Water serves as an essential buffer to regulate Temp. and pH.
  High specific heat capacity

- Water is a participant in many biochemical reactions
  - Hydrolysis
  - photosynthesis

$$6CO_2 + 6H_2O \xrightarrow{h\nu} C_6H_{12}O_6 + 6O_2$$

  - Respiration - aerobic metabolism
  - others

Noncovalent Interactions in Biomolecules

- Ionic bonds
  between oppositely charged atoms or group
  Energy 20-30 kJ/mole

- Hydrogen bonds
  between H atom linked to electronegative atom (O, N or F) and electronegative atom
  10 – 30 kJ/mole

- van der Waals Interactions
  1-5 kJ/mole

- Hydrophobic interactions
  5-30 kJ/mole

Characteristics of Non Covalent Interactions:-

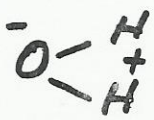
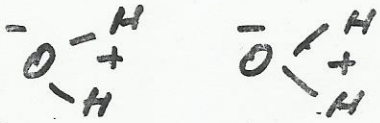
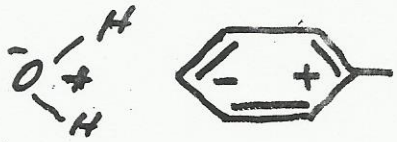
- relatively weak
  1-30 kJ/mole as compared to 350 kJ/mole in C-C

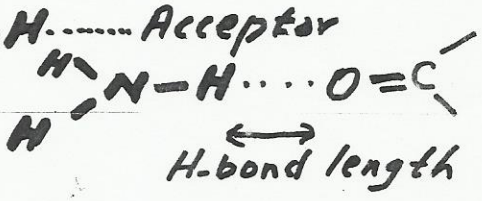
- Reversible

- Binding between molecules is specific

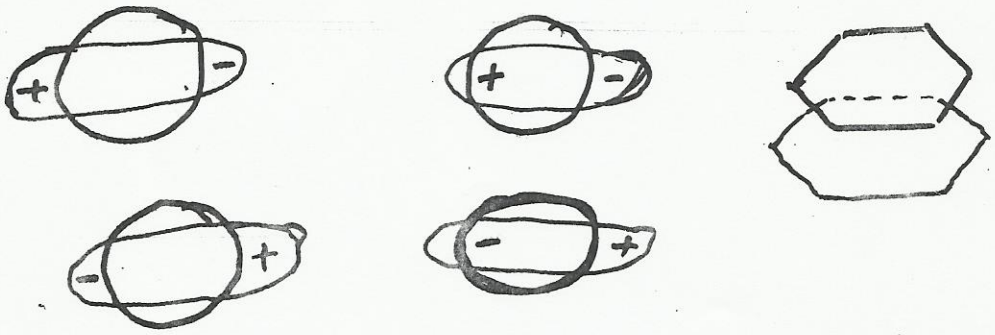
Weak Interactions in an Aqueous Environment

The nature of non-covalent interactions
(Essentially Electrostatics)

- Charge-Charge $-NH_3^+$ 
- Charge-dipole $-NH_3^+$ 
- Dipole-dipole 
- Charge-induced dipole $-NH_3^+$ 
- Dipole-induced dipole 
- Dispersion
- Hydrogen bond Doner—H.....Acceptor

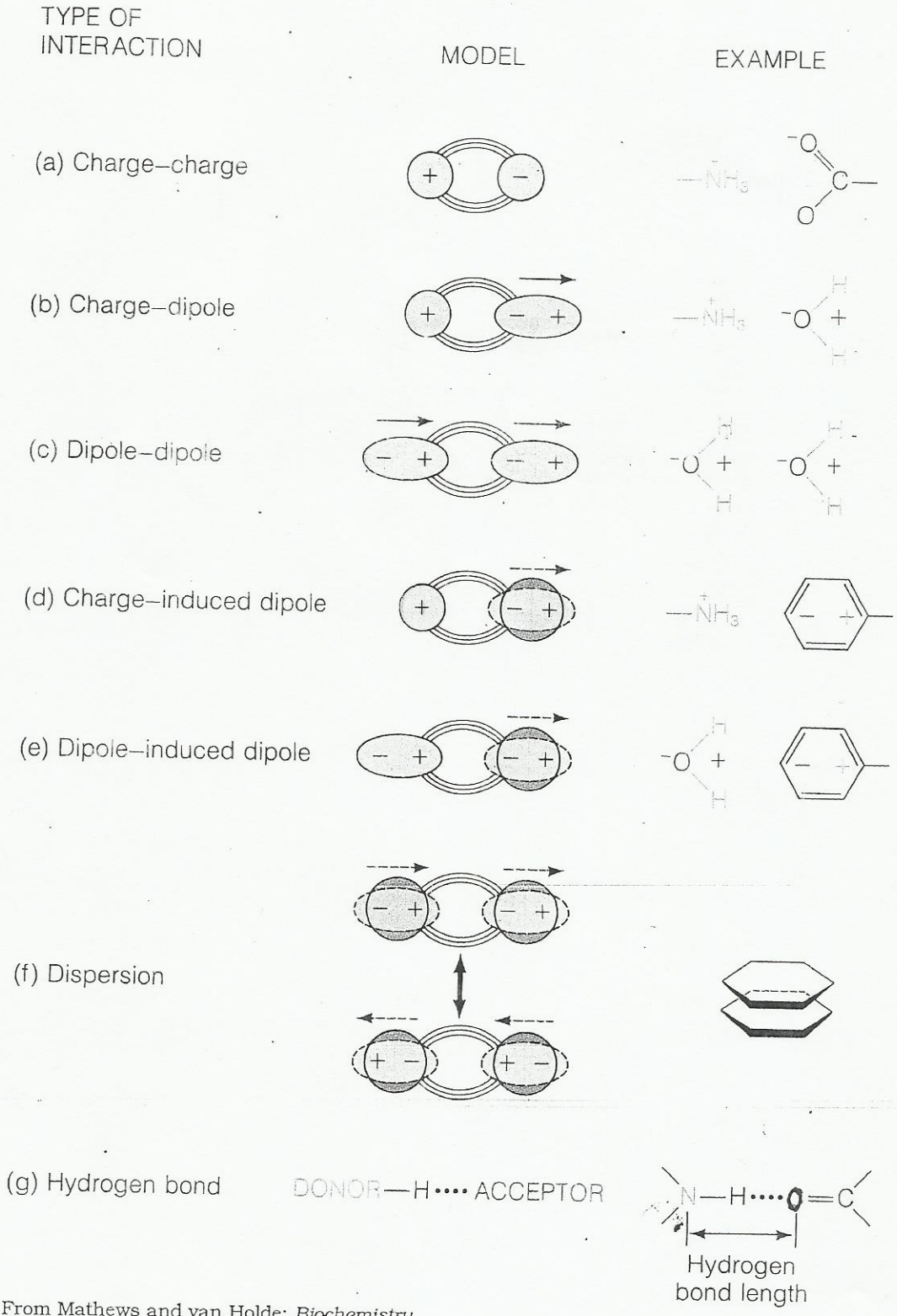


- Dispersion



Types of noncovalent interactions

Figure 2.1



Structure of Water

· electronegativity of O atom is 3.5
" H " " 2.1

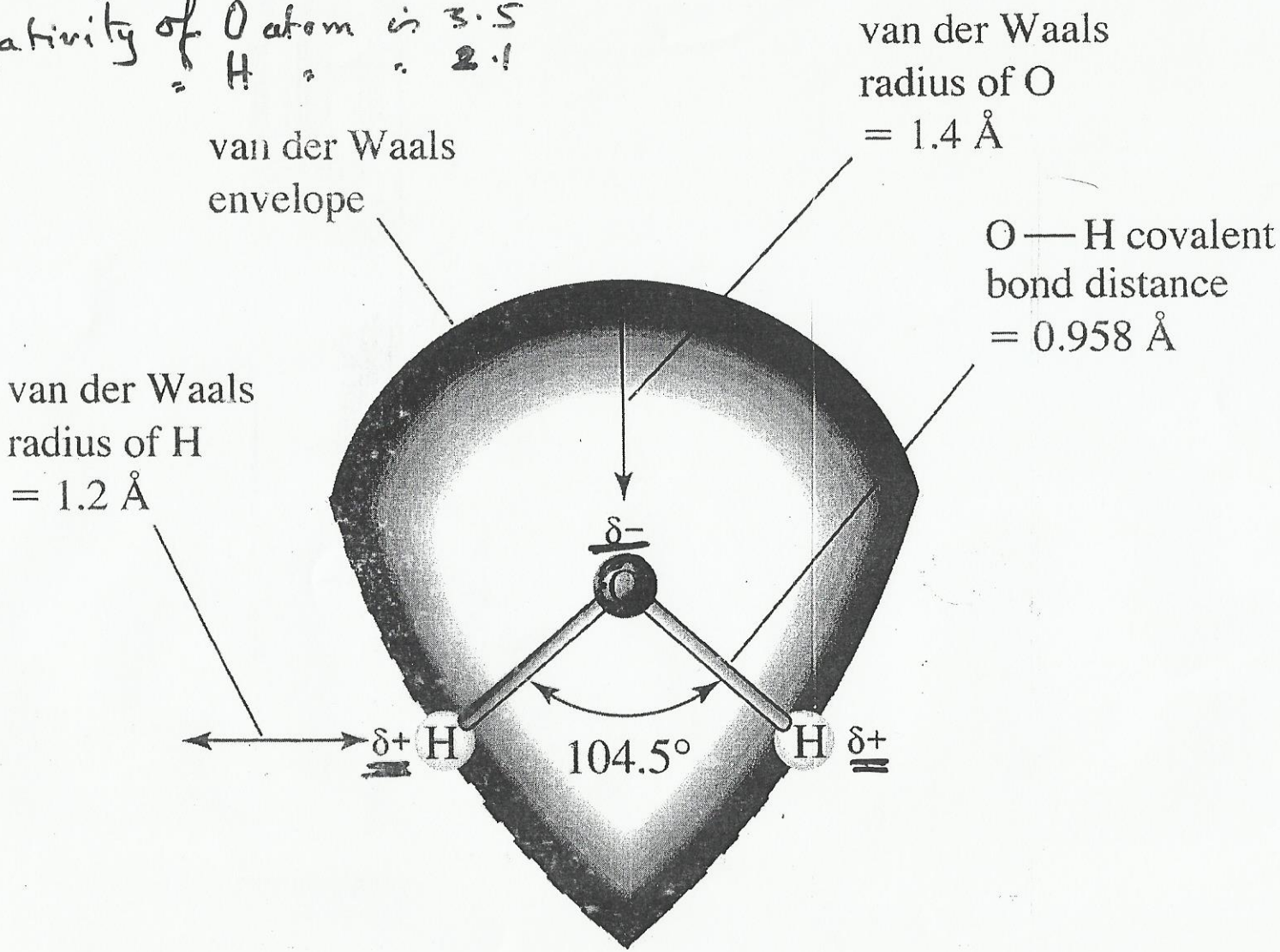


Figure 2-1a Concepts in Biochemistry, 3/e

Water is electrically neutral (no net charge) but has relatively large dipole moment because of its bent geometry

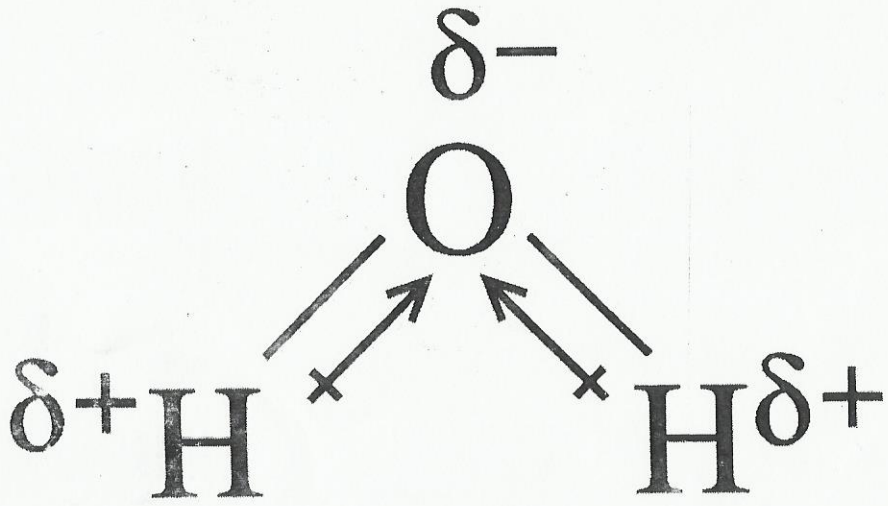


Figure 2-1b Concepts in Biochemistry, 3/e

CO_2 has polar bonds caused by electronegativity between C and O atoms but no dipole moment because it is linear

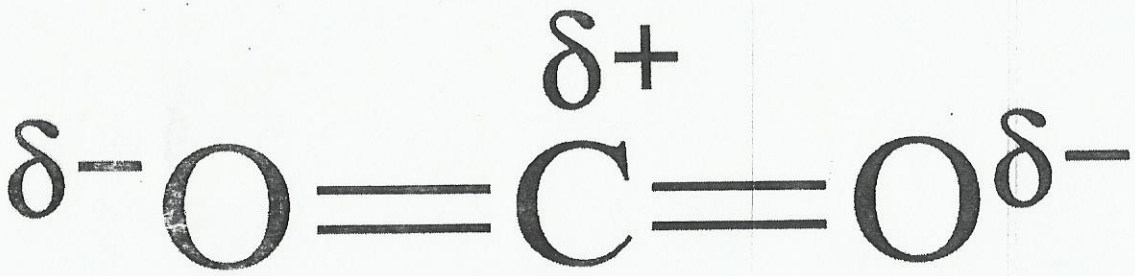


Figure 2-2 Concepts in Biochemistry, 3/e

Hydrogen bond between two water molecules

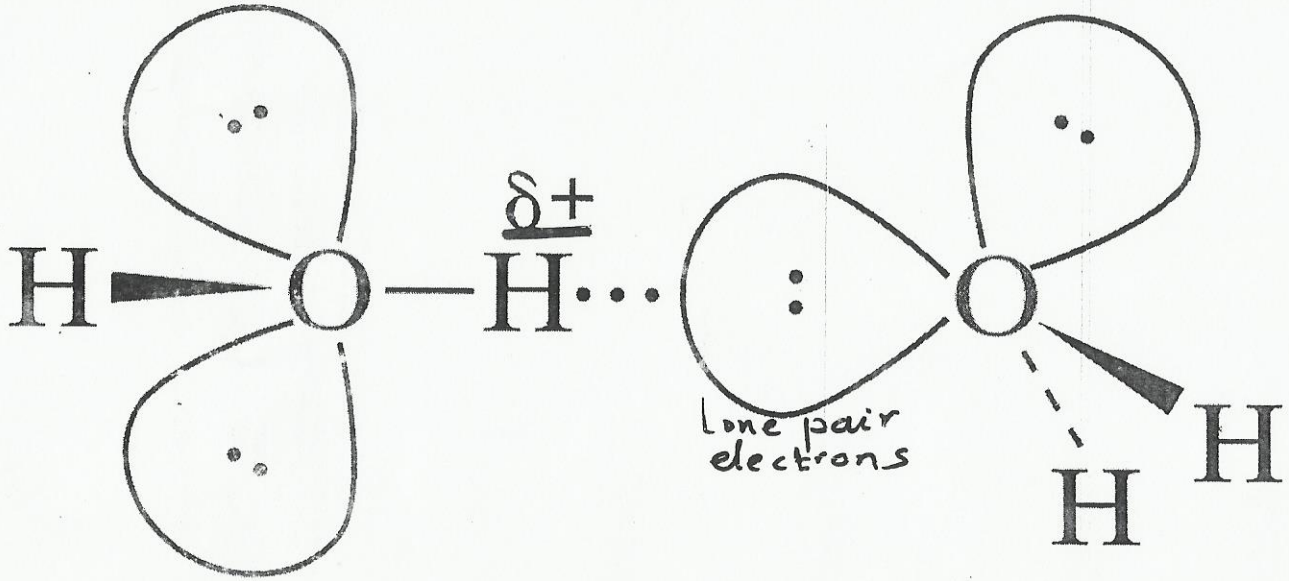
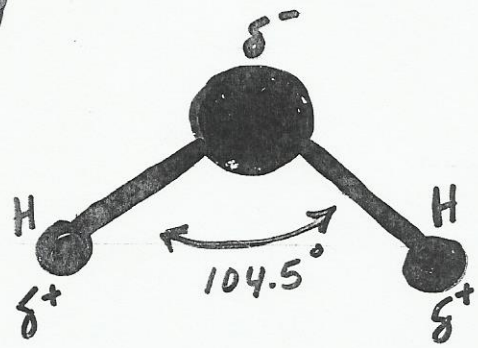


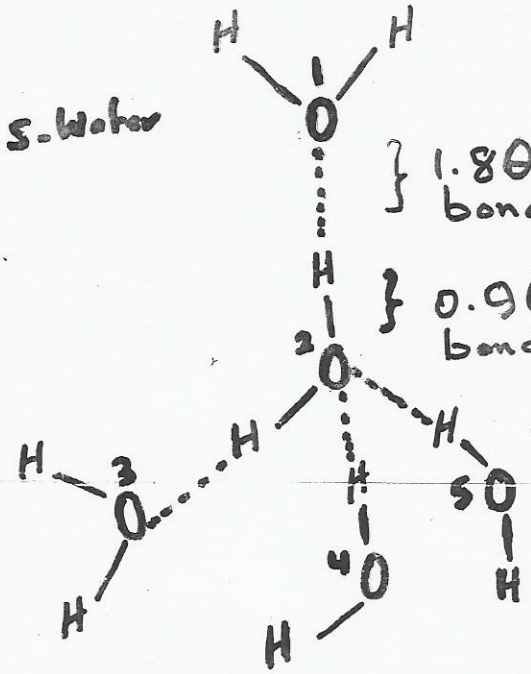
Figure 2-3 Concepts in Biochemistry, 3/e

Hydrogen Bonds Between Water Molecules:-

The H–O–H bond angel



Tetrahedral H-bonding of s-water molecules



} 1.80 Å = 0.18 nm
bond energy = 20 kJ/mole (5 kcal/mol)

} 0.96 Å
bond energy 460 kJ/mole (110 kcal...)

Hydrogen bond is strongest when the three atoms X—H- - - A

A can be oxygen, nitrogen or fluorine

X can be oxygen, nitrogen or fluorine

- Many biomolecules have atoms that can hydrogen bond with: Water, themselves & other molecules

Functional groups that participate in H-bonding include:

- -OH gr in alcohols, org. acids & carbohydrate
- Carbonyl groups in aldehydes, Ketones, acids, amides & esters
- N-H groups in Amines & amides

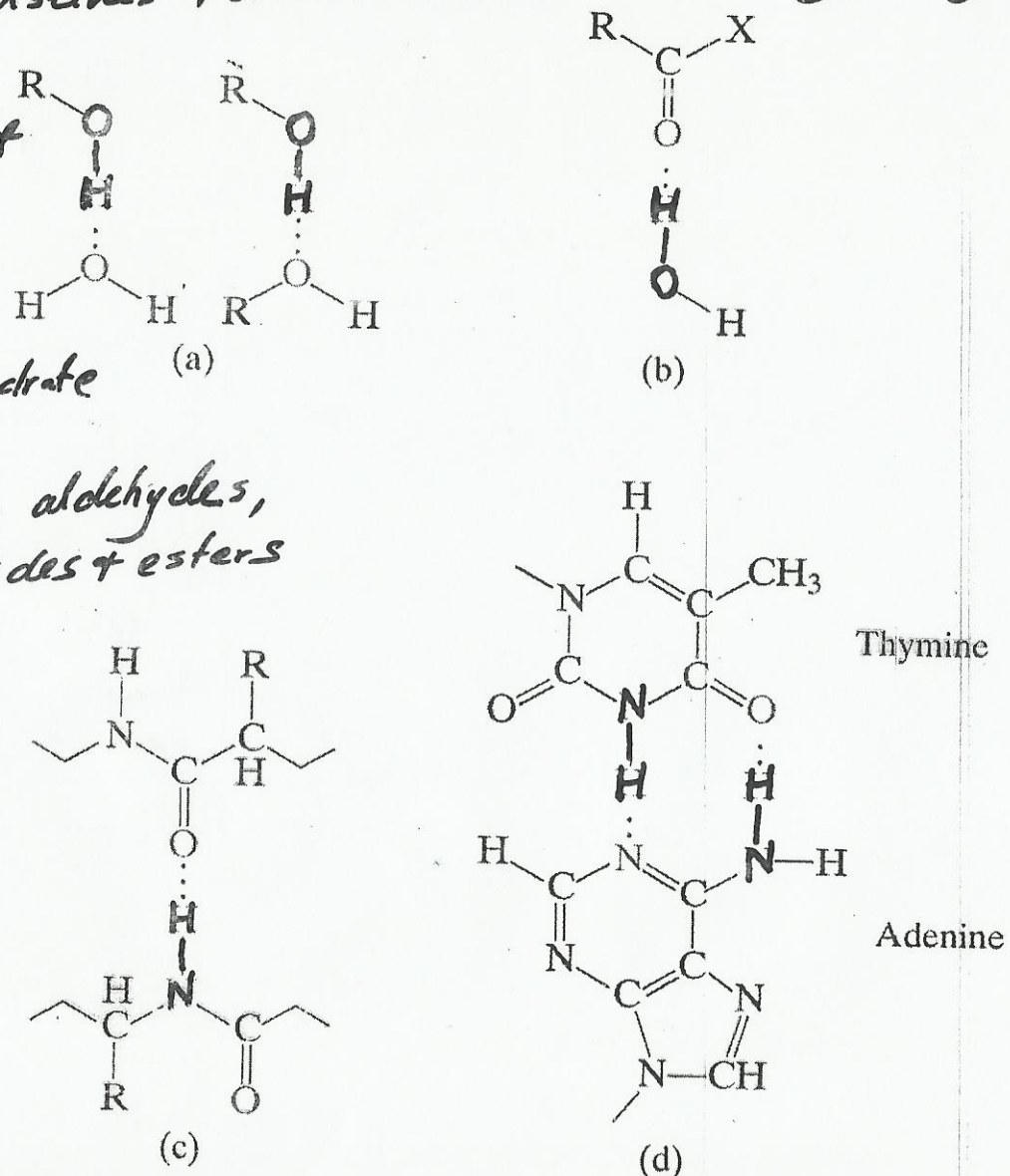


Figure 2-4 Concepts in Biochemistry, 3/e

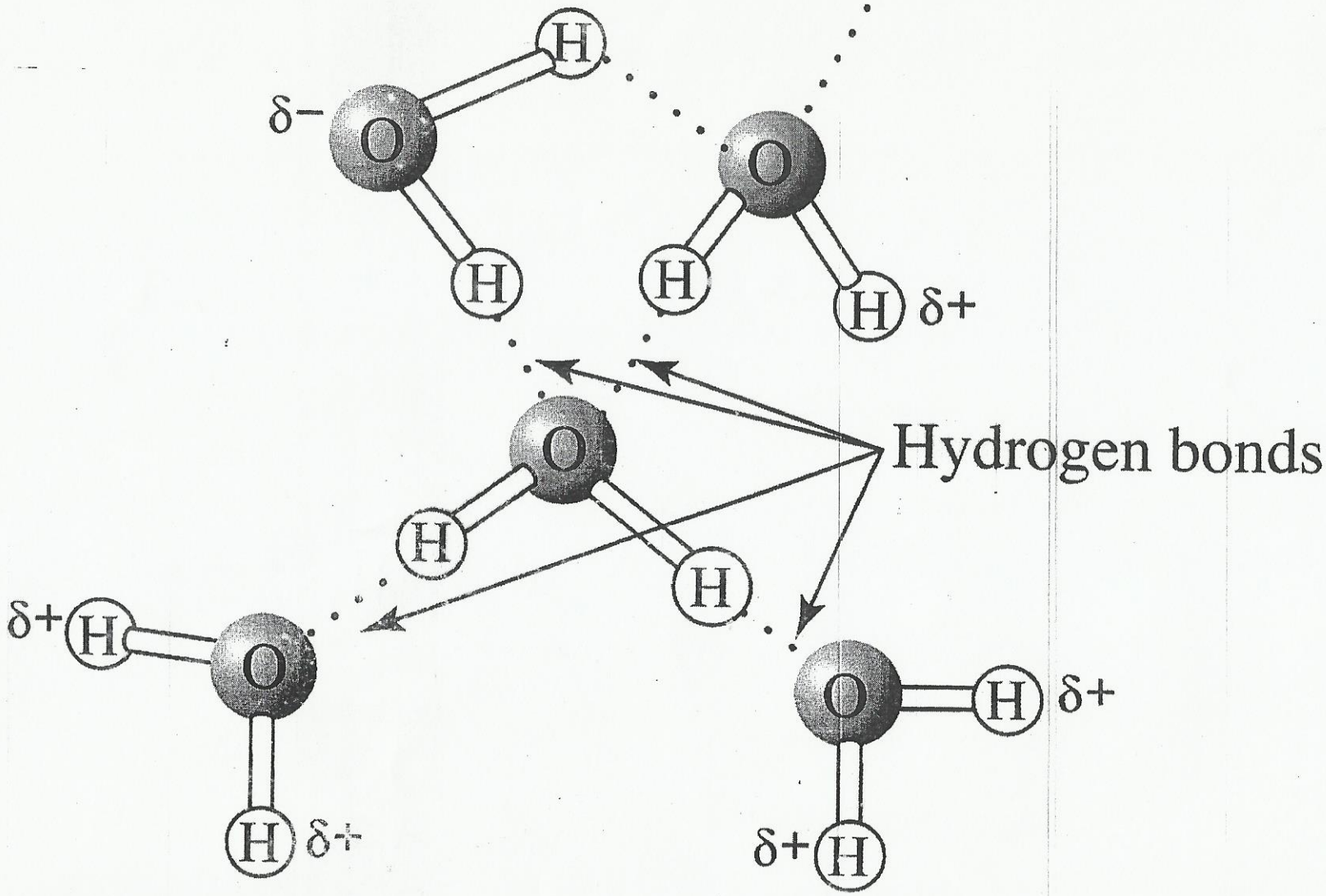
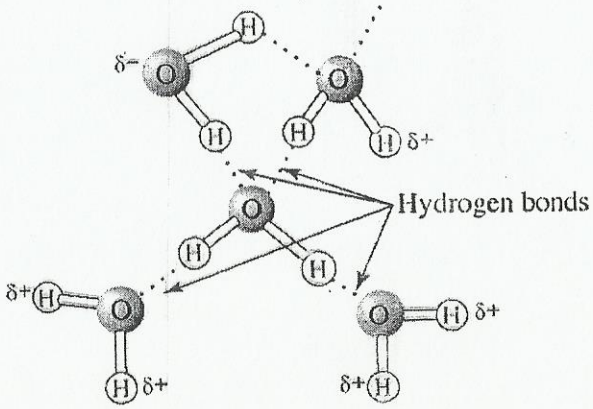


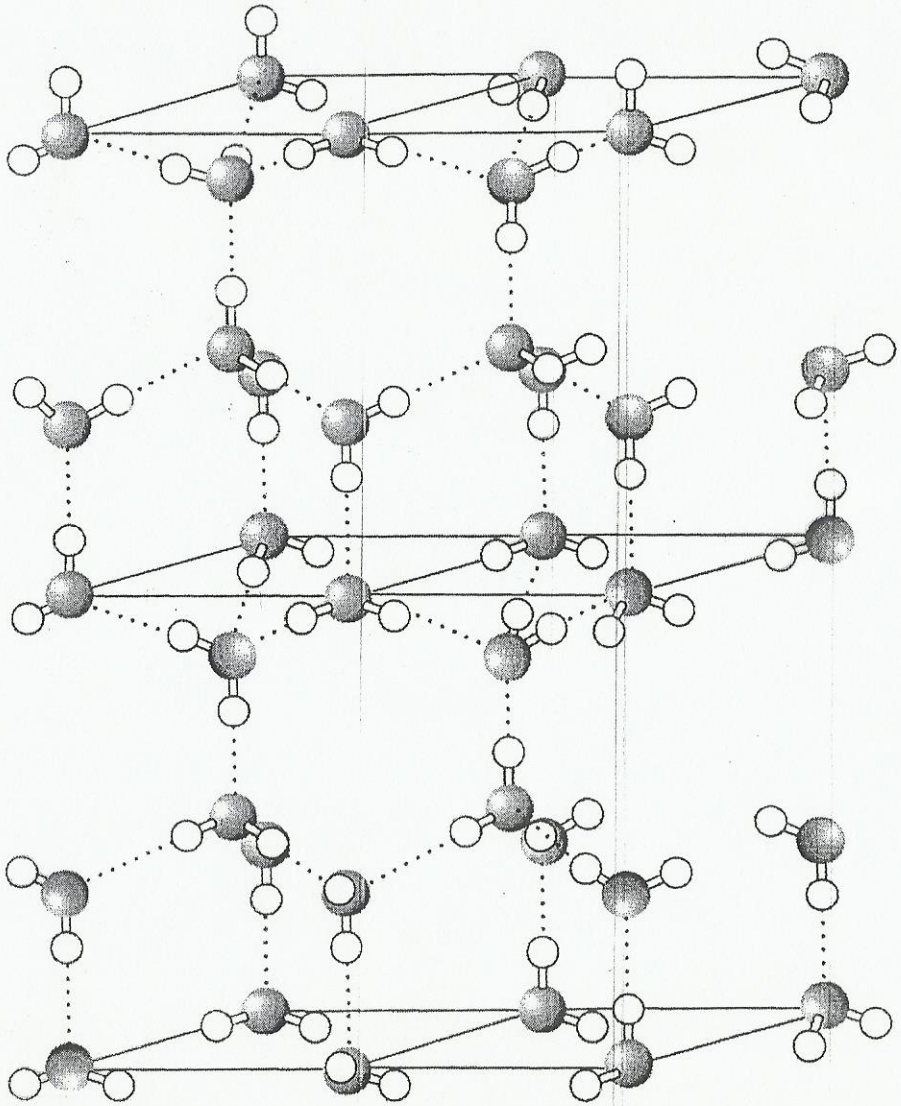
Figure 2-5a Concepts in Biochemistry, 3/e

The network of Potential H-bonds in water

- Average number of H-bonds to each molecule in liquid water at 10°C is ~ 3.0
- Number of H-bonds decrease with increasing temp.
- In crystalline ice, the number approaches four



(a)



(b)

Figure 2-5 Concepts in Biochemistry, 3/e

Table 2.3
A comparison of some physical properties of water with hydrides of other nonmetallic elements: N, C, and S

Property	H_2O	NH_3	CH_4	H_2S
Molecular weight	18	17	16	34
Boiling point (°C)	100	−33	−161	−60.7
Freezing point (°C)	0	−78	−183	−85.5
Viscosity[a]	1.01	0.25	0.10	0.15

[a] Units are centipoise.

Physical Properties of Water:

- Hydrogen bonding Gives Water its unusual Properties
  - higher m.P. ; B.P. ; heat of vaporization, higher freezing , surface tension

H-O-H bond angle is 104.5°

Bond energy of H-bond is 20 kj/mole

life-time 1×10^{-9} s O-H 460 kj/mole bond energy

in liquid state each water molecule hydrogen bond with another 3.4 H_2O molecules

In ice — $\underbrace{4\ H_2O}_{\text{Larger vol. + less dense the ice-lattice}}$ molecules

- Water forms Hydrogen bonds with solutes

H-bonds are not unique only to Water

- Hydrogen atoms covalently bonded to carbon atoms, which are not electronegative, do not participate in H-bonding

— O - H --- O = C <
— O - H --- N ≡
— O - H --- O <
> N - H --- O = C <
> N - H --- O <
> N - H --- N ≡

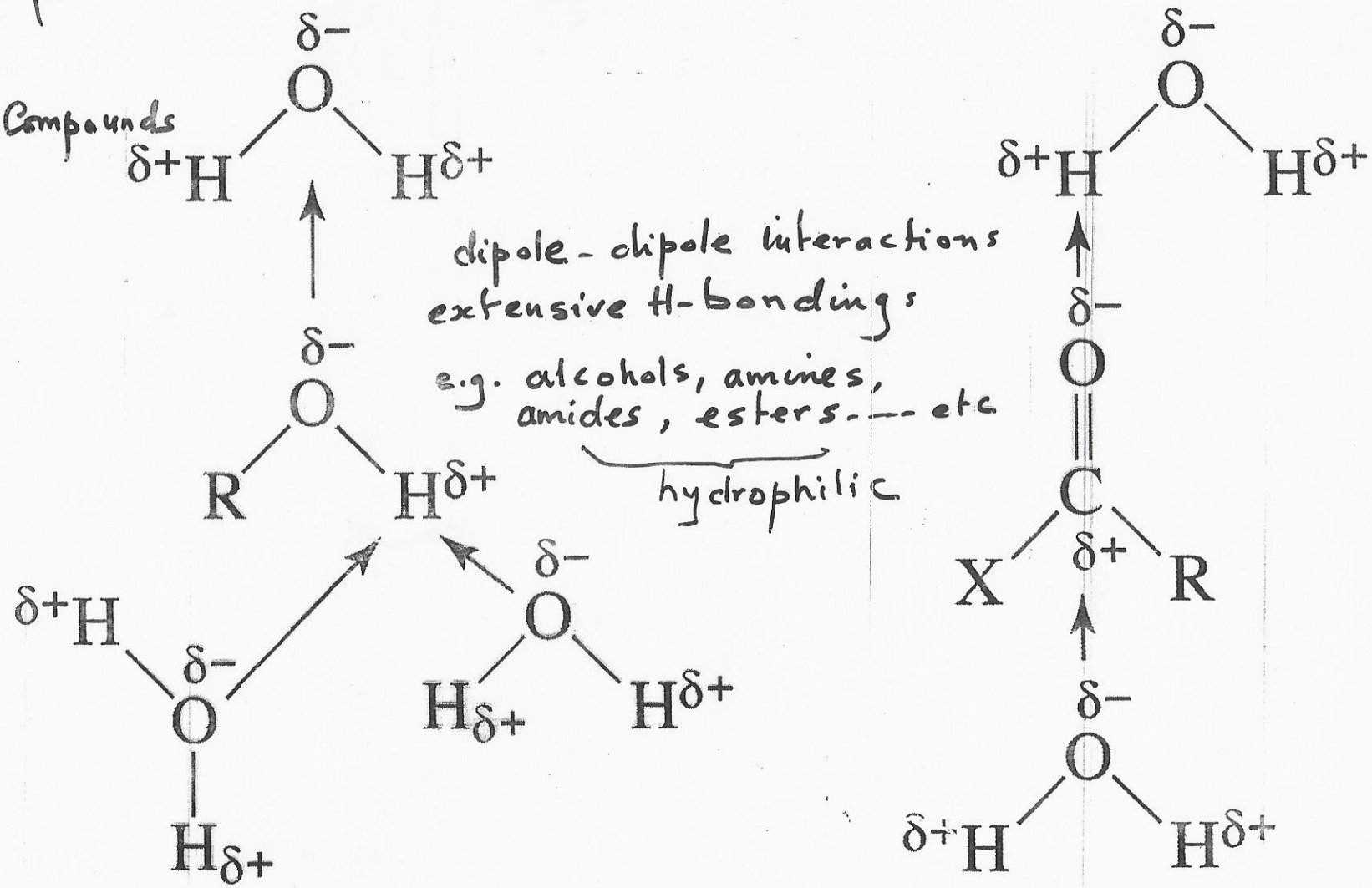
e.g.

- B.P. for butanol = 117 °C
  $CH_3 . CH_2 . CH_2 . CH_2 . OH$
- B.P for butane = -0.5 °C
  $CH_3 . CH_2 . CH_2 . CH_3$

Water as a Solvent

Important solvent and transporter

1. Polar Compounds



dipole - dipole interactions
extensive H-bondings

e.g. alcohols, amines, amides, esters --- etc

hydrophilic

Figure 2-6a Concepts in Biochemistry, 3/e

2- Ionic Compounds

Individual ions are hydrated (solvated) by polar water molecules

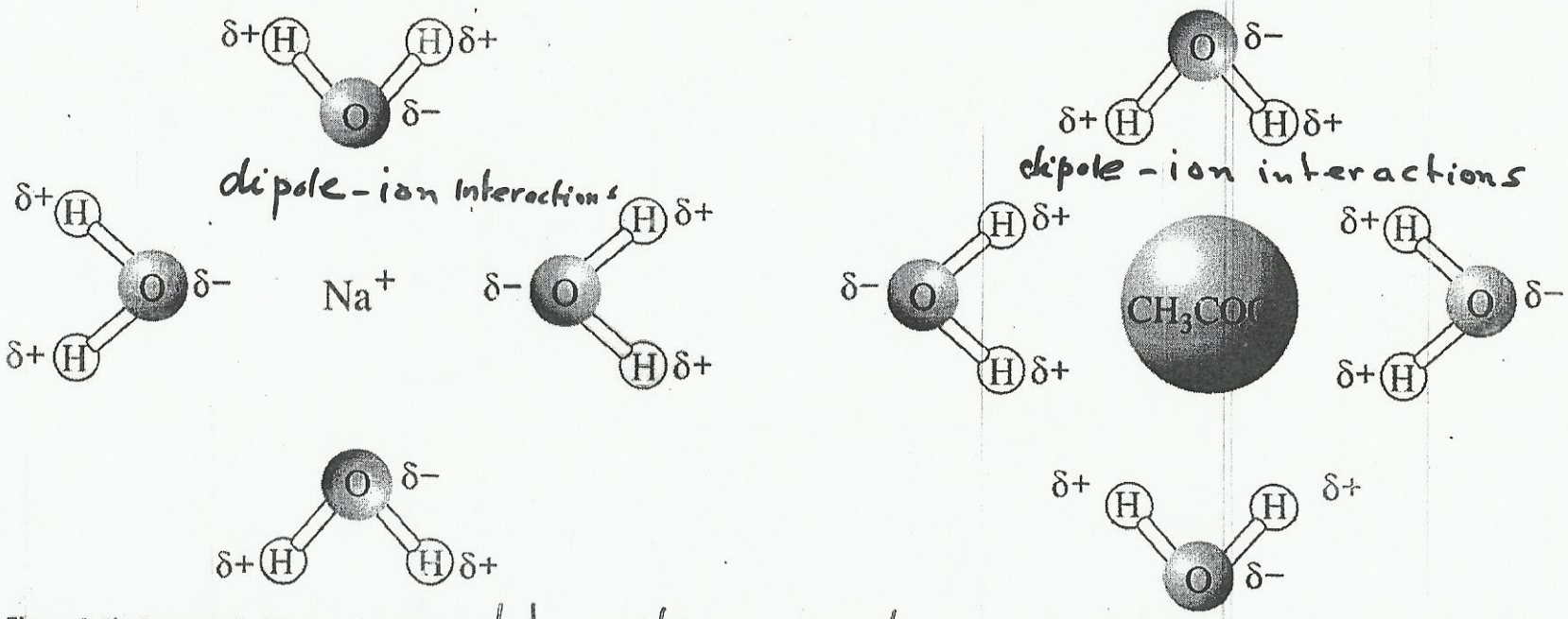


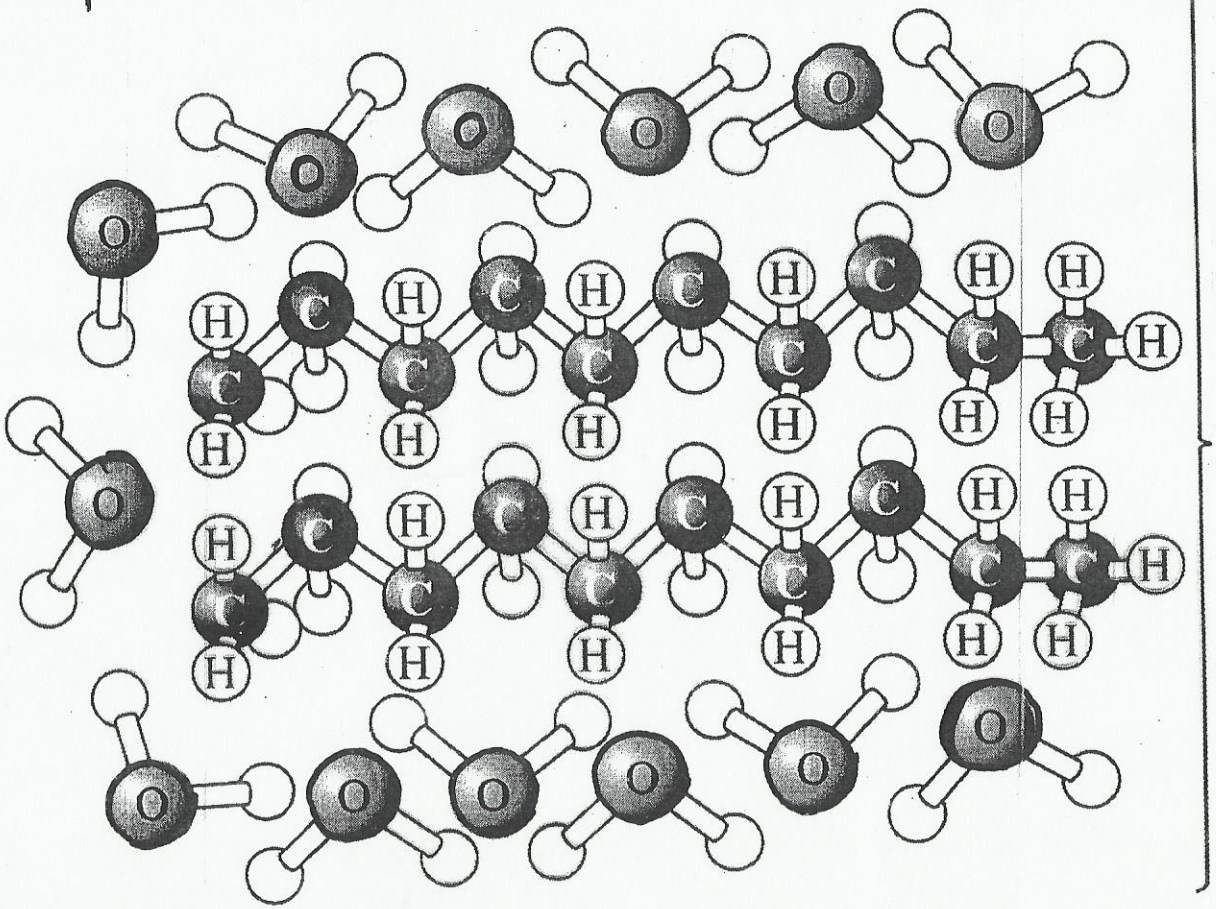
Figure 2-6b Concepts in Biochemistry, 3/e

Interactions are strong enough to overcome the tendency of anions and cations to recombine.

3- Nonpolar Compounds :- e.g. decane, benzene - - etc

. They do <u>not</u> contain ions or polar functional groups - Hydrophobic.

. Amphiphilic e.g. sodium stearate



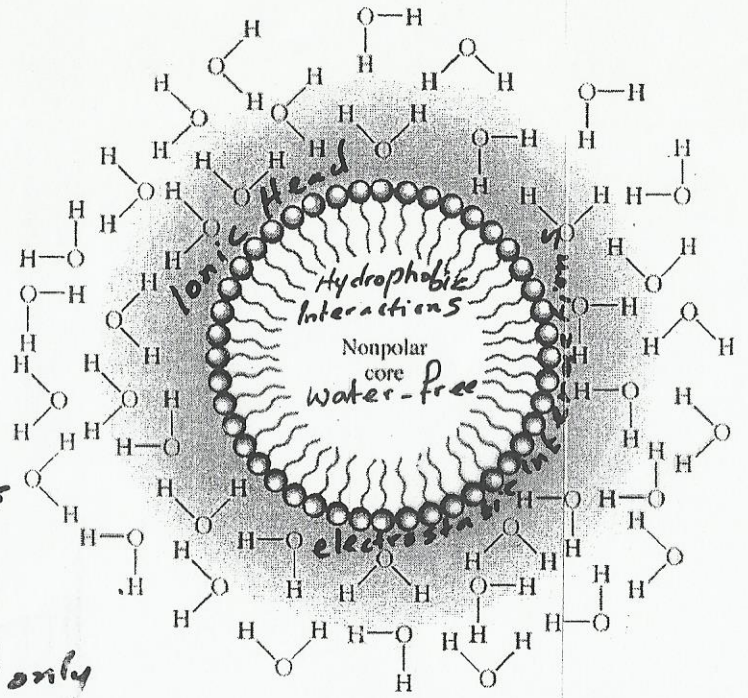
Water molecules in cage around hydrocarbon chain

Formation of this highly ordered cage of water requires much energy, which comes from hydrophobic interactions

Figure 2-7 Concepts in Biochemistry, 3/e

Amphiphilic Molecules

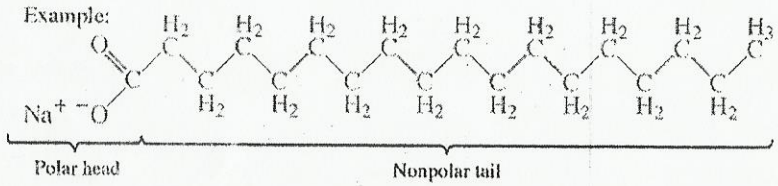
- Soap action
- Changes in water structure by solutes
- Changes in solutes structure by water
- Nucleic acids, proteins and some lipids are amphiphilic
- Ordered arrangement only are often associated with biological activity



Sodium Stearate Micelle

Key: Polar head of sodium stearate

Nonpolar tail of sodium stearate



Amphiphilic Compound

Figure 2-8 Concepts in Biochemistry, 3/e