Chapter 4 - Water

Important points and Principles:

- Polarity and Hydrogen bonding capacity
- Ion product of Water (K_W)
- Buffers - weak acids & conjugate base
- Henderson-Hasselback equation (pH)
- Water as a reactant

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Helpful topics for review:

- Electronegativity of O,N,C & H
  - Effect on covalent and non-covalent interactions
- Structures of functional groups
  - Carbonyl, carboxyl, amino, etc.
- Condensation and hydrolysis reactions
  - H_2O participation

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Water Molecules are Unique

- Hydrogen bonding among H_2O molecules
  - (liquid, crystalline structures)
- Ionization
  - $H_2O \rightleftharpoons H^+ + OH^-$ (slight)
- Water-solute interactions
  - Ionic
  - H-bonding
- Hydrophobic interactions
  - Entropically -driven

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Hydrogen bonding gives water its unusual properties

table 4–1

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, 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.

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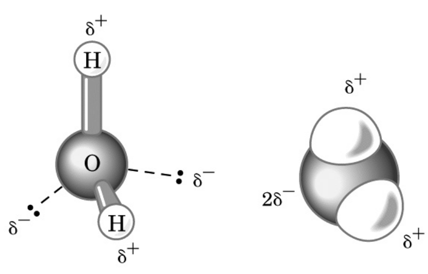
The water molecule is a tetrahedron



(a) (b)

Greater electronegativity of Oxygen atom induces a dipole

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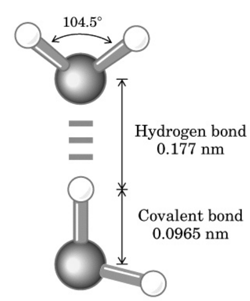
Interactions between H_2O molecules



(c)

Hydrogen bonding

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Hydrogen bonds are weaker than covalent bonds

Bond		Strength (kJ/mole)
• Covalent	(C-C)	200 - 400
• Hydrogen bond		8-20
• Ionic		
– Attraction (+/-)		42
– Repulsion (+/+)		-21
• Hydrophobic		4 - 8
• van der Waals		4

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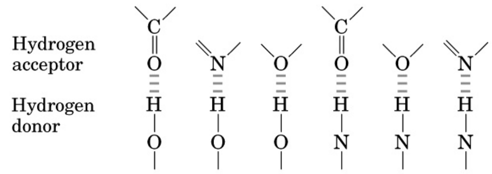
H-bonds are not unique to H_2O



H atom must be covalently bound to an electronegative atom

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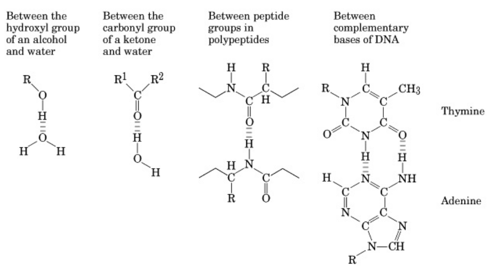
Some biologically important hydrogen bonds



Polar molecules readily dissolve in H_2O

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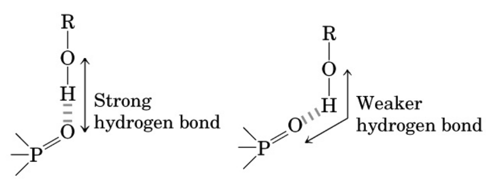
Hydrogen bonds are directional



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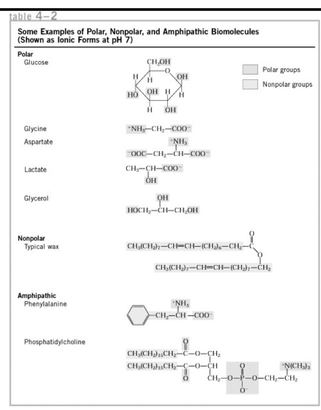
Water acts electrostatically with charged solutes

Hydrophilic - "water-loving"

Hydrophobic - "water-fearing"



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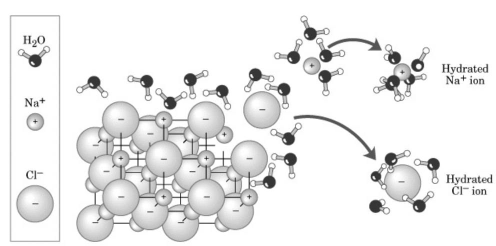
Water replaces solute-solute interactions with solute-water interactions



High H_2O dielectric constant favors dissolution of ions

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Nonpolar gases are poorly soluble in H_2O

table 4–3

Solubilities of Some Gases in Water

Gas	Structure*	Polarity	Solubility in water (g/L)†
Nitrogen	N≡N	Nonpolar	0.018 (40 °C)
Oxygen	O=O	Nonpolar	0.035 (50 °C)
Carbon dioxide	O=C=O (δ⁻ ← → δ⁻)	Nonpolar	0.97 (45 °C)
Ammonia	NH_3 (H, H, H on N; arrow δ⁻)	Polar	900 (10 °C)
Hydrogen sulfide	H_2S (H, H on S; arrow δ⁻)	Polar	1,860 (40 °C)

*The arrows represent electric dipoles; there is a partial negative charge (δ^-) at the head of the arrow, a partial positive charge (δ^+; not shown here) at the tail.

†Note that polar molecules dissolve far better even at low temperatures than do nonpolar molecules at relatively high temperatures.

Many organisms have water-soluble carrier proteins (Hb, Mb) that facilitate transport of gases

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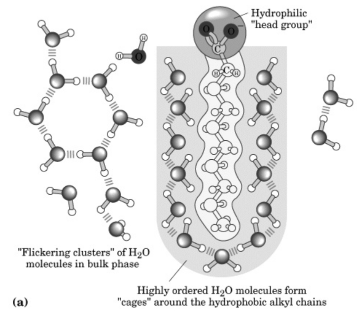
Nonpolar compounds are hydrophobic



They force energetically <u>unfavorable</u> changes in the structure of H_2O

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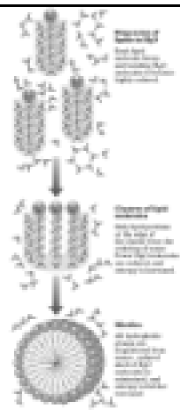
Amphipathic compounds contain polar and nonpolar regions

Nonpolar regions cluster together in micelles to minimize contact with water



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<u>Hydrophobic interactions</u> arise by minimizing contact with H_2O - energetically more favorable

Amphipathic biological molecules:

- Fatty acids (energy)
- Phospholipids (membranes)
- Proteins (interior vs. exterior)
- Vitamins (A, D, E)
- Sterols (cholesterol, testosterone)

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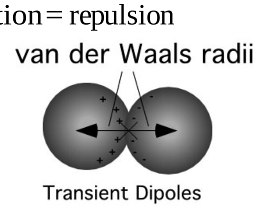
<u>van der Waals Interactions</u>

- Weak attractions
- Formed from transient dipoles
- Dependent on proximity of atoms
- Van der Waals radii
  - Attraction = repulsion



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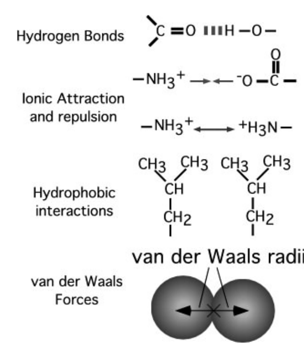
Weak interactions are crucial to macromolecular structure and function



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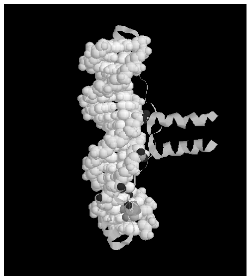
Weak, transient nature of non-covalent interactions allows for flexibility in proteins, DNA, and RNA



Most stable structure when weak bonding possibilities are maximized

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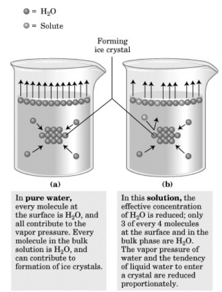
Colligative Properties: VP, BP, FP, Osmotic Pressure



Solutes reduce the concentration of H_2O in solution

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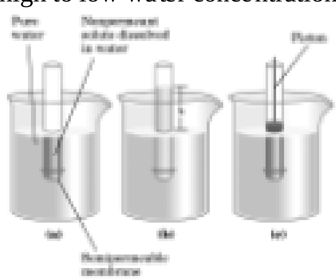
H_2O molecules tend to move from areas of high to low water concentration



Osmotic pressure = pressure required to <u>halt</u> movement of water from high to low concentration

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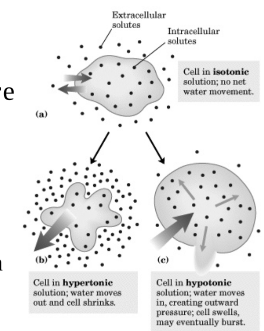
Osmosis - movement of water across semi-permeable membranes. Driven by osmotic pressure



Isotonic
- equal osmolarity solution

Hypertonic
- higher osmolarity solution

Hypotonic
- lower osmolarity solution

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<u>Ionization of Water, Weak Acids and Weak Bases</u>

$$H_2O \rightleftharpoons H^+ + OH^-$$

$$(2\ H_2O \rightleftharpoons H_3O^+ + OH^-)$$

H_2O molecules have a slight tendency to undergo reversible ionization

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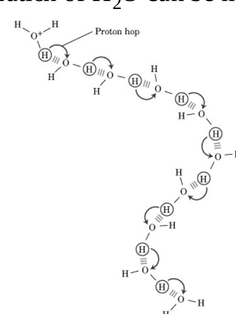
Ionization of H_2O can be measured



Acid-Base reactions in H_2O are exceptionally fast

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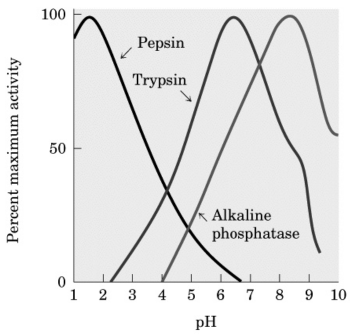
pH affects structure and activity of biomolecules



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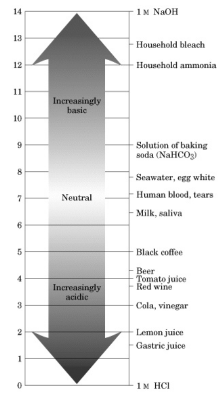
pH of various fluids

pH of blood and urine is one method used in medical diagnosis



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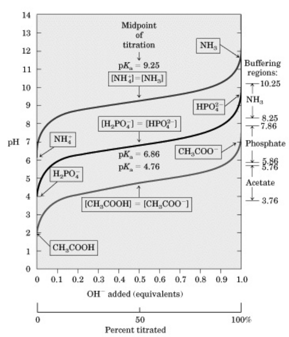
Weak acids and their buffering ranges



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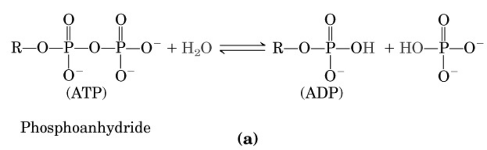
Participation of H_2O in biological reactions



Hydrolysis

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The ionization of H_2O is expressed by an equilibrium constant

$$A + B \quad C + D$$

$$K_{eq} = \frac{(C)(D)}{(A)(B)}$$

$$K_{eq} = \frac{(H^+)(OH^-)}{(H_2O)}$$

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