Slide#7 solution

Molecular weight of HOCl = 52.46 g/mole

Unit conversion - mg/L to molarity:

$$\frac{15\ mg\ HOCl}{1\ L\ water} \times \frac{1}{52.46\ g\ HOCl/mole\ HOCl} \times 10^{-3}\ g/mg = 2.86 \times 10^{-4}\ M$$

$HOCl = H^{+} + OCl^{-}$, $pK_a = 7.54$

weak acid → only a fraction dissociates

$$K_a = 10^{-7.54} = \frac{[H^+][OCl^-]}{[HOCl]} = \frac{10^{-7} \cdot [OCl^-]}{[HOCl]}$$

$$[HOCl] = 3.47[OCl^-]$$

$$[HOCl] + [OCl^-] = 4.47[OCl^-] = 2.86 \times 10^{-4}\ M$$

$[OCl^-] = 0.64 \times 10^{-4}\ M$

$[HOCl] = 2.22 \times 10^{-4}\ M$

Basic Biology Concepts

Basic biology concepts

- Chemical composition of life
- Cell, cell contents, and cellular functions
- Energy and metabolism
- How biological principles are applied to environmental engineering

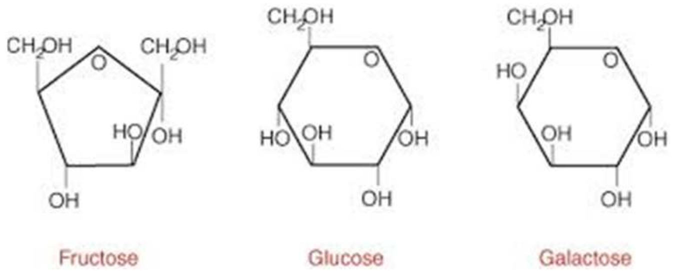
Chemical composition of life

- Major elements: C, H, O, N, S, P
  - Liebig's law of the minimum

- Major classes of [macro]molecules:
  - Carbohydrates
  - Lipids
  - Protein
  - Nucleic acids

Carbohydrates

- Energy source, building materials for cells
- Monomers, dimers, polymers
  - Monosaccharides: building blocks

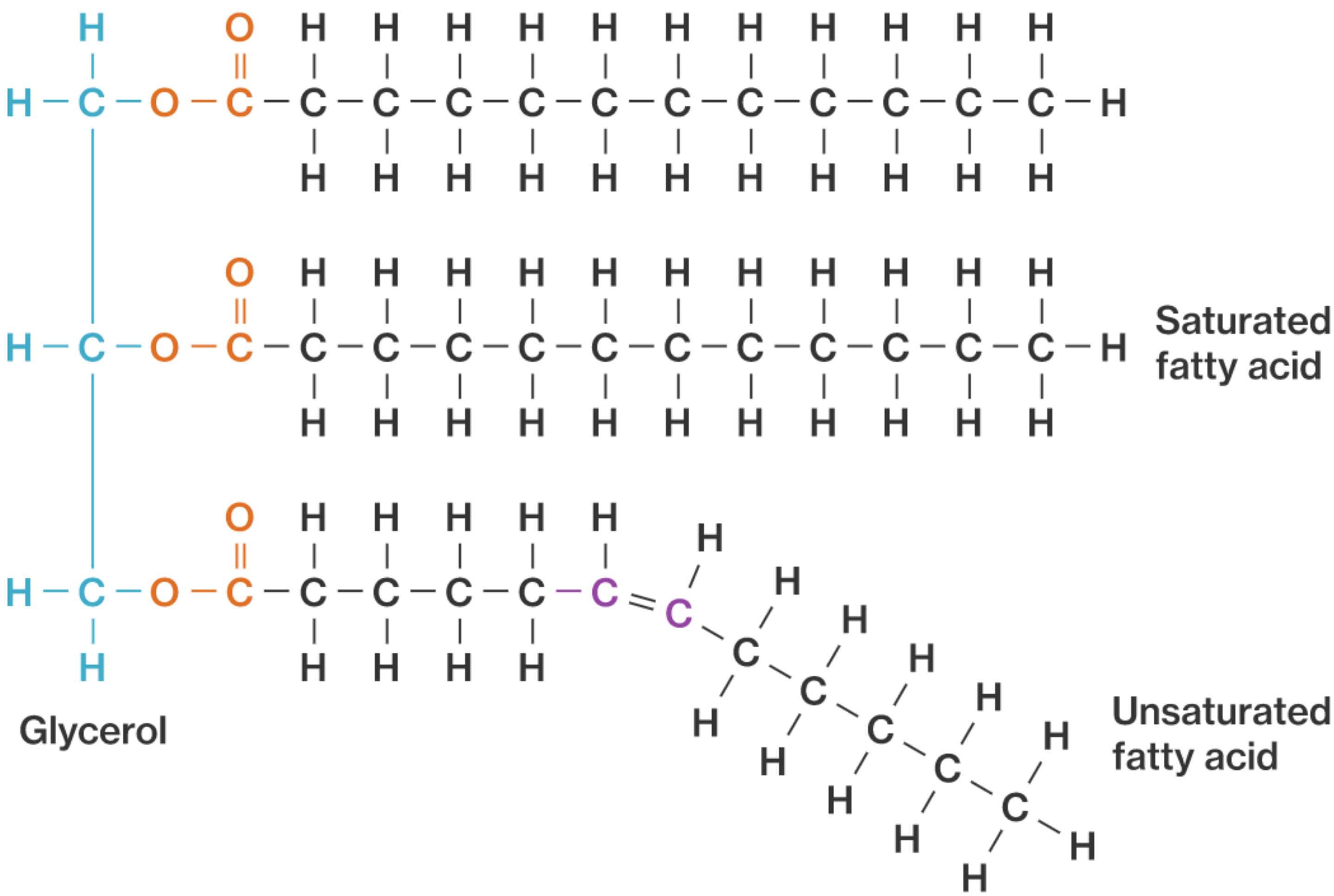


  - Disaccharides: sucrose, lactose, maltose
  - Polysaccharides: 100s – 1000s of monosaccharides

Lipids

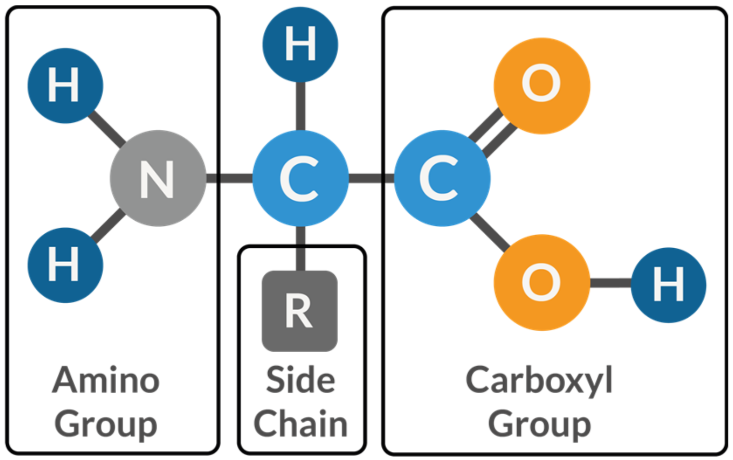
- Not polymeric (no monomers, dimers, polymers)
- Various structures
- Common characteristic: hydrophobic (repulsion of water)
- Fats, phospholipids, and steroids
  - fats: store energy
  - phospholipids: major component of cell membranes
  - steroids: signaling (ex: steroid hormones)

- Fat = fatty acid + glycerol
- Saturated fat vs. Unsaturated fat



Proteins

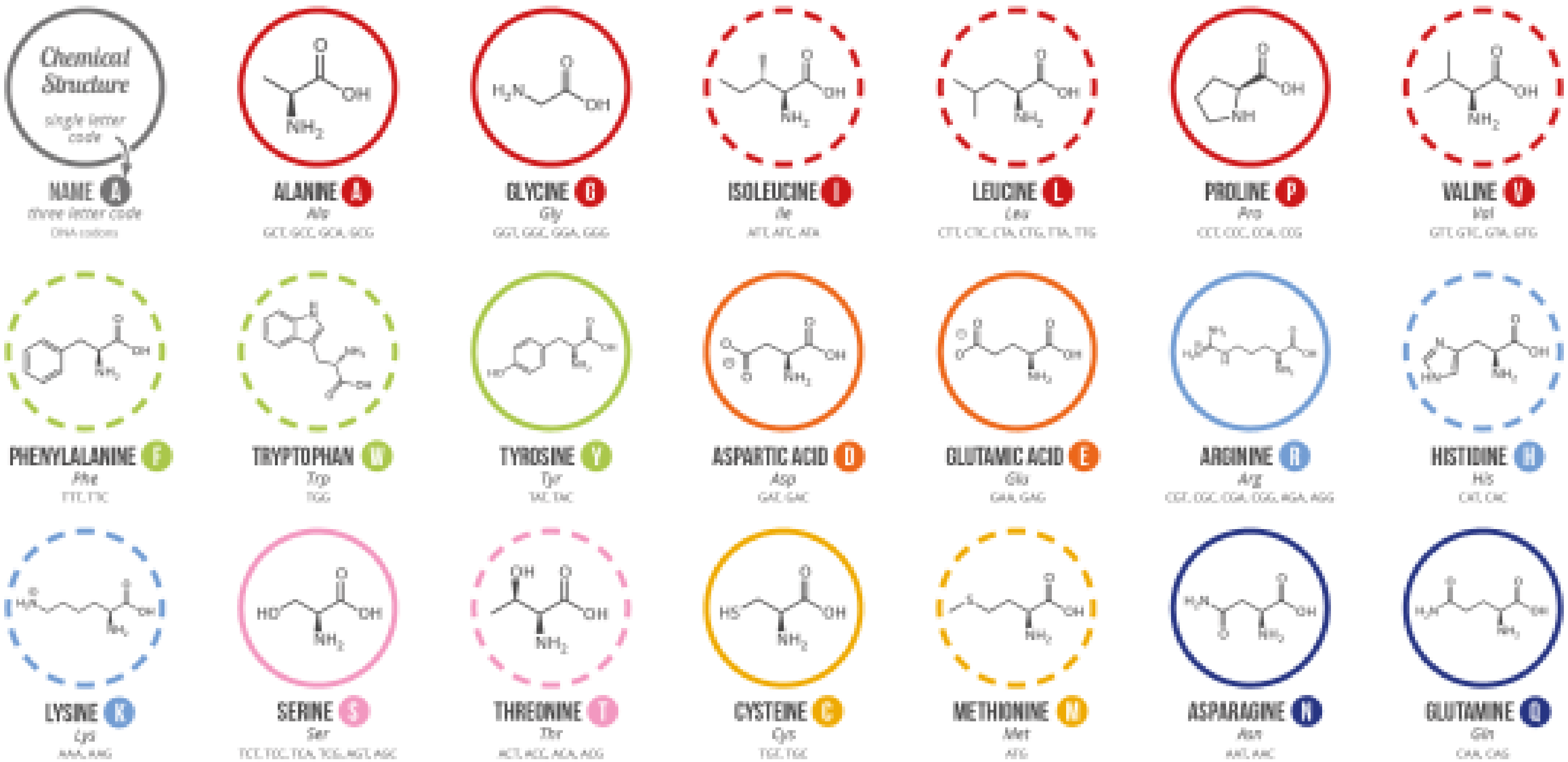
- Affect almost all cellular functions (enzymes, immunoglobulins, hemoglobins, etc.)
- Structural support of organisms
- Monomers: amino acids (20) / polymers: polypeptides



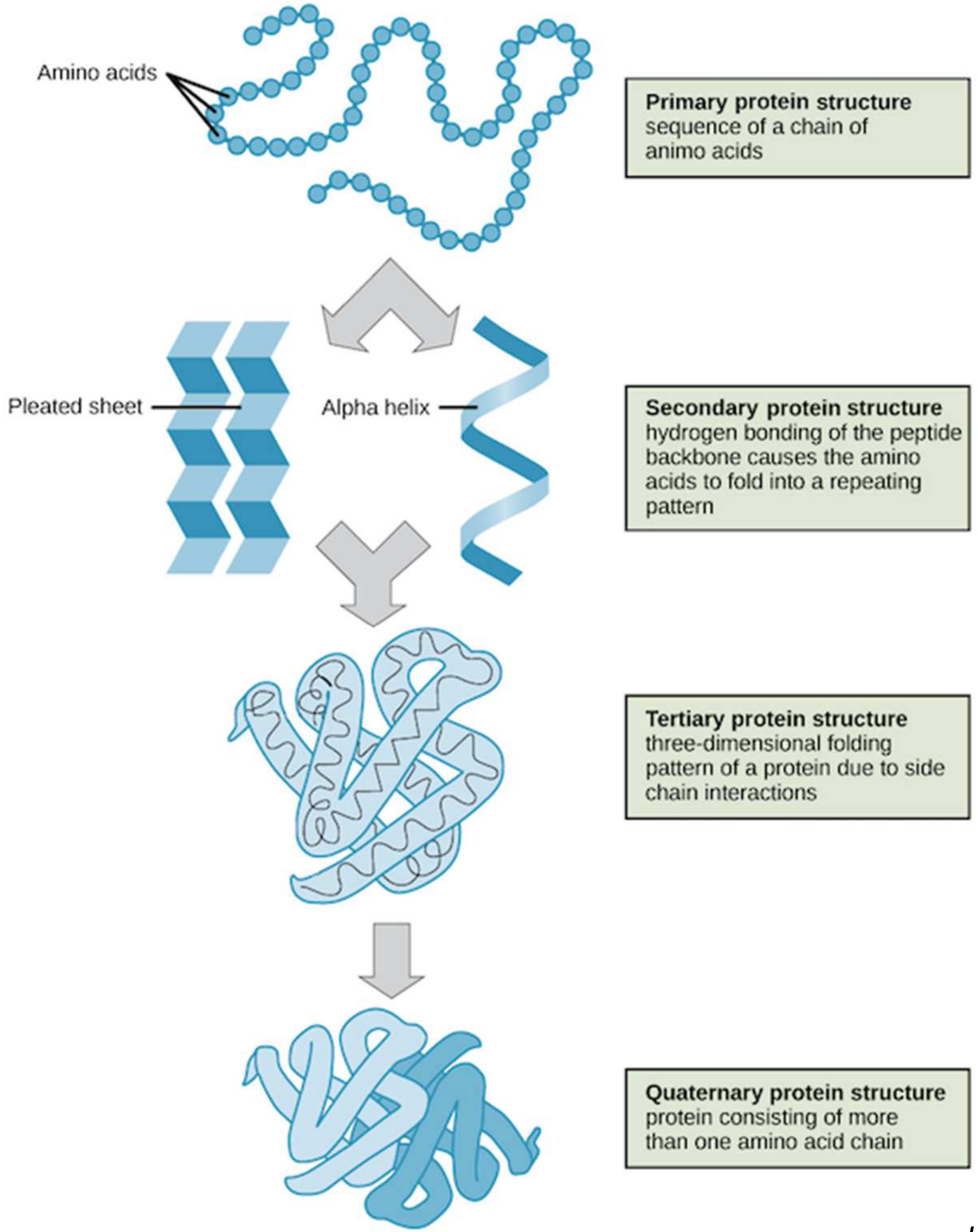
A GUIDE TO THE TWENTY COMMON AMINO ACIDS

AMINO ACIDS ARE THE BUILDING BLOCKS OF PROTEINS IN LIVING ORGANISMS. THERE ARE OVER 500 AMINO ACIDS FOUND IN NATURE - HOWEVER, THE HUMAN GENETIC CODE ONLY DIRECTLY ENCODES 20. 'ESSENTIAL' AMINO ACIDS MUST BE OBTAINED FROM THE DIET, WHILST NON-ESSENTIAL AMINO ACIDS CAN BE SYNTHESISED IN THE BODY.

Chart Key: ALIPHATIC · AROMATIC · ACIDIC · BASIC · HYDROXYLIC · SULFUR-CONTAINING · AMIDIC · NON-ESSENTIAL · ESSENTIAL



Note: This chart only shows those amino acids for which the human genetic code directly codes for. Selenocysteine is often referred to as the 21st amino acid, but is encoded in a special manner. In some cases, distinguishing between asparagine/aspartic acid and glutamine/glutamic acid is difficult. In these cases, the codes asx (B) and glx (Z) are respectively used.

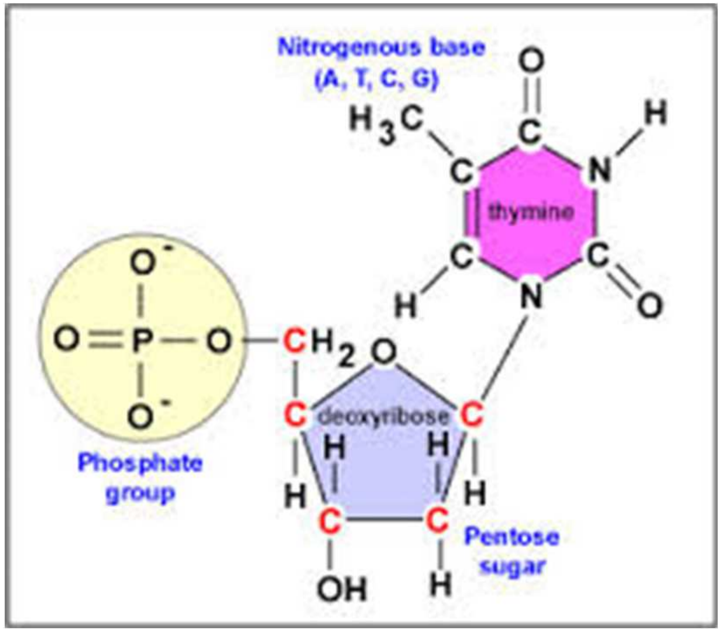


- Protein structure
  - Primary
  - Secondary
  - Tertiary
  - Quaternary

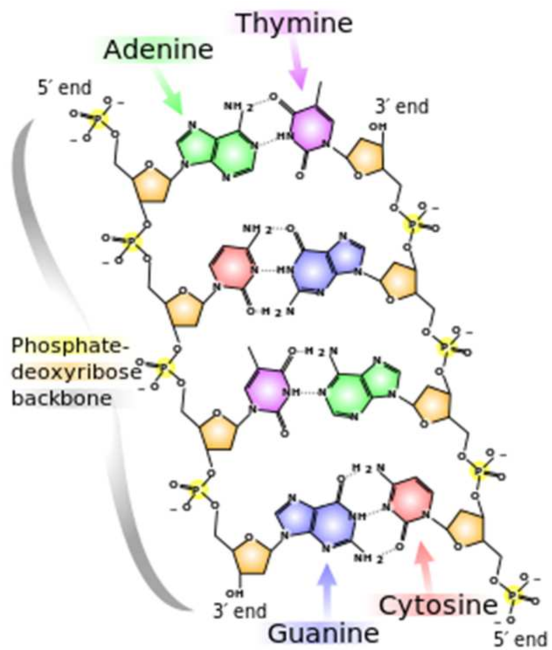
http:.//khanacademy.org

Nucleic acids

- Store and transmit hereditary information
- Monomers: nucleotides / polymers: DNA & RNA



Nucleotide for DNA



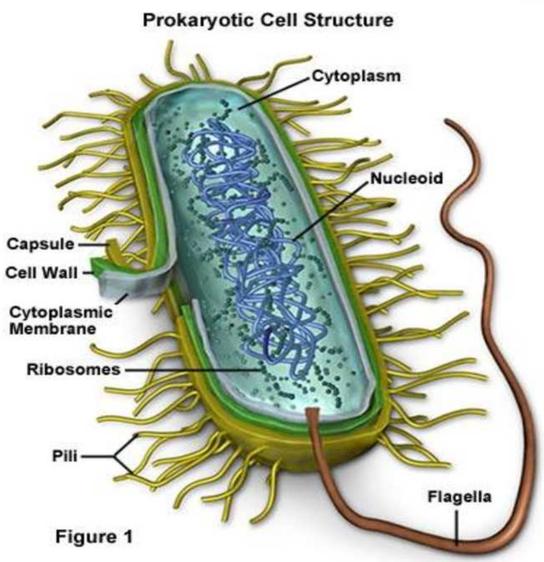
Structure of a DNA

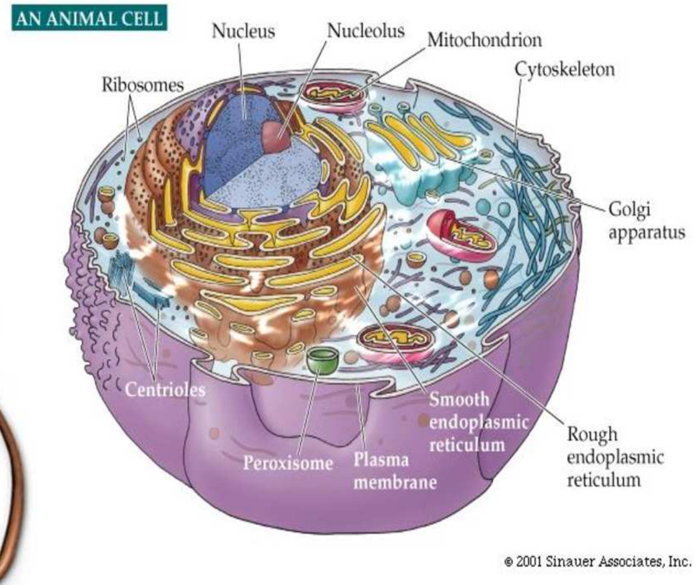
DNA vs. RNA

	DNA (deoxyribonucleic acid)	RNA (ribonucleic acid)
Sugar	deoxyribose	ribose
Strand	double-stranded	single-stranded
Base	adenine (A), thymine (T), guanine (G), cytosine (C)	adenine (A), uracil (U), guanine (G), cytosine (C)
Function	long-term storage of genetic information; transfer genetic information to other cells and new organisms	transfer the genetic code from the DNA to ribosomes to make proteins

The cells

- Prokaryotes vs. Eukaryotes: absence/presence of a nucleus





Davis & Masten (2014)

Composition of a cell

- Cell membrane
  - separates the interior of the cells from outside
  - exhibit selective permeability to control material movement in & out of a cell
- Nucleus: contains chromosomes (eukaryotic cells)
- Ribosomes: synthesize proteins
- Mitochondria: produce ATP
- Cell wall: give rigidity to a cell (prokaryotes/plant cells)

Energy and metabolism

- Photosynthesis: convert energy from sunlight into chemical energy

$$6CO_2 + 6H_2O + \text{sunlight} \xrightarrow{\text{chlorophyll}} \underset{\text{glucose}}{C_6H_{12}O_6} + 6O_2$$

Energy and metabolism

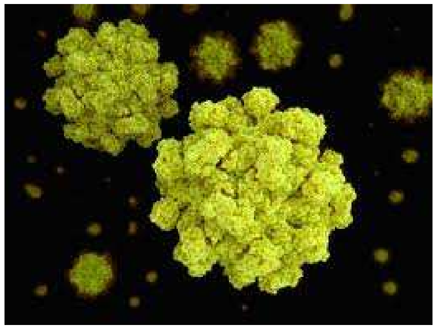
- Metabolism: life-sustaining chemical transformations within cells of living organisms
  - catabolism: process to break down molecules into smaller units to generate energy (ATP)
  - anabolism: process to construct macromolecules from smaller molecules (consumes ATP)

Biology and environmental engineering

- Quality of natural water (rivers, lakes, oceans..)
  - self-purification of natural water environments: microorganisms in water degrade contaminants
  - oxygen depletion: if organic contaminants are present in excess, microorganisms deplete dissolved oxygen in water → fish kills!
  - pathogen risk: limit recreation (fishing, swimming, …) and impact the ecosystem
  - algae problems (algal bloom – excessive algal growth)

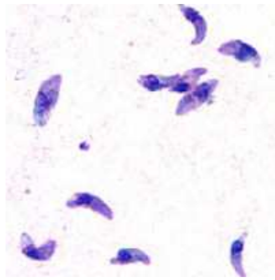
Biology & EE: Water treatment

- Drinking water should be treated to prevent spreading of water-related diseases
  - Pathogens involved can be bacteria, protozoa, virus, helminth
- Primary removal processes in drinking water treatment plants: filtration & disinfection



Norovirus

Vibrio cholerae



Toxoplasma gondii

Biology & EE: Wastewater treatment

- Biological wastewater treatment
  - Use abilities of microorganisms to degrade/transform organic substances
  - Main player: bacteria
  - Let them work not in a river but in a reactor!
  - Has been the most successful & economic way to treat wastewater for ~100 yrs

Biology & EE: Hazardous waste treatment

- Bioremediation of sites impacted by hazardous wastes
  - Use microorganisms to degrade hazardous chemicals in soils, sediments, and groundwater into non-toxic chemicals
  - Microorganisms' ability to deal with complex chemical structures & newly developed chemicals
    - Microorganisms in the environment exist as consortium (a group of millions of different species working together)
    - Microorganisms have excellent ability to evolve – may develop capability to degrade new chemicals within a short time period (<years)

Suggested readings

[ENG] pp. 97 – 121, 139 – 143

[KOR] pp. 91 – 117, 136 – 142

Next class

Mass balance & Reactors I

- Mass balance – principles, applications & related concepts
- State of "mixing"
- Reactor analysis using mass balance

Basic Chemistry Concepts II

Basic chemistry concepts II

- Equilibrium chemistry (continued)
  - Acid-base equilibria
  - Gas dissolution
- Reaction kinetics
- Carbonate system
- Alkalinity

Chemical equilibrium: acid-base equilibria

- Ionization of water: $H_2O + H_2O = H_3O^+ + OH^-$

$$K = \frac{\{H_3O^+\}\{OH^-\}}{\{H_2O\}^2}$$

$$\{H_2O\} = \gamma_{H_2O} \cdot [H_2O], \quad \gamma_{H_2O} \approx 1, \quad [H_2O] = 55.6\ M$$

- Dissociation constant of water, K_w

$$K_w = K \cdot \{H_2O\}^2 = \{H_3O^+\}\{OH^-\}$$

Chemical equilibrium: acid-base equilibria

$K_w = \{H_3O^+\}\{OH^-\}$ or $K_w = \{H^+\}\{OH^-\}$

$pK_w = 14$ (at 25˚C)

$pH < 7 \longrightarrow \{H^+\} > \{OH^-\}$ acidic

$pH > 7 \longrightarrow \{H^+\} < \{OH^-\}$ basic

Acid dissociation constant

$$HA = H^+ + A^-$$

- Acid dissociation constant, K_a

$$K_a = \frac{\{H^+\}\{A^-\}}{\{HA\}} = \frac{\gamma_{H^+}[H^+]\gamma_{A^=}[A^-]}{\gamma_{HA}[HA]} \approx \frac{[H^+][A^-]}{[HA]}$$

in dilute solutions (<5% error if I < 10^{-3} M)

- Strong acid = strong tendency to dissociate = high K_a = low pK_a
- Weak acid = only a small fraction dissociates = low K_a = high pK_a

Dissociation constants of some acids

Acid	**Reaction**	**pK_a**
Hydrochloric acid	$HCl = H^+ + Cl^-$	≈-3
Nitric acid	$HNO_3 = H^+ + NO_3^-$	-1
Sulfuric acid	$H_2SO_4 = H^+ + HSO_4^-$	≈-3
Bisulfate	$HSO_4^- = H^+ + SO_4^{2-}$	1.9
Acetic acid	$CH_3COOH = H^+ + CH_3COO^-$	4.75
Carbonic acid	$H_2CO_3^* = H^+ + HCO_3^-$ $HCO_3^- = H^+ + CO_3^{2-}$	6.35 10.33
Phosphoric acid	$H_3PO_4 = H^+ + H_2PO_4^-$ $H_2PO_4^-\ \ H^+ + HPO_4^{2-}$ $HPO_4^{2-} = H^+ + PO_4^{3-}$	2.12 7.20 12.32

Strong (Hydrochloric acid – Bisulfate)

Weak (Acetic acid – Phosphoric acid)

Acid dissociation constant

Q: A solution of HOCl is prepared in water by adding 15 mg HOCl to a volumetric flask, and adding water to the 1.0 L mark. The final pH is measured to be 7.0. What are the concentrations of HOCl and OCl^-?

(T = 25˚C)

Chemical equilibrium: gas dissolution

- Henry's Law: partial pressure of a chemical in the gas phase is linearly proportional to the concentration of the chemical in the aqueous phase

$$P_{gas} = kC^*$$

where P_{gas} = partial pressure in the gas phase

C^* = concentration in the water

k = constant

Caveat!

- The equilibrium/solubility product constants do not tell anything about the reaction rate!
- Differentiate equilibrium and kinetics

Reaction kinetics

- Reaction kinetics: study of the speed at which reactions proceed

$$aA + bB \rightarrow cC$$

$$r_A = \frac{d[A]}{dt} = -k[A]^{\alpha}[B]^{\beta}$$

r_A = reaction rate with respect to chemical A [conc./time]

k = reaction rate constant

$\alpha + \beta$ = overall reaction order

Reaction orders and half life

Overall Reaction order	**Rate expression**	**Units on *k***
Zero	$r_A = -k$	$(conc.)(time)^{-1}$
First	$r_A = -k[A]$	$(time)^{-1}$
Second	$r_A = -k[A]^2$	$(conc.)^{-1}(time)^{-1}$
Second	$r_A = -k[A][B]$	$(conc.)^{-1}(time)^{-1}$

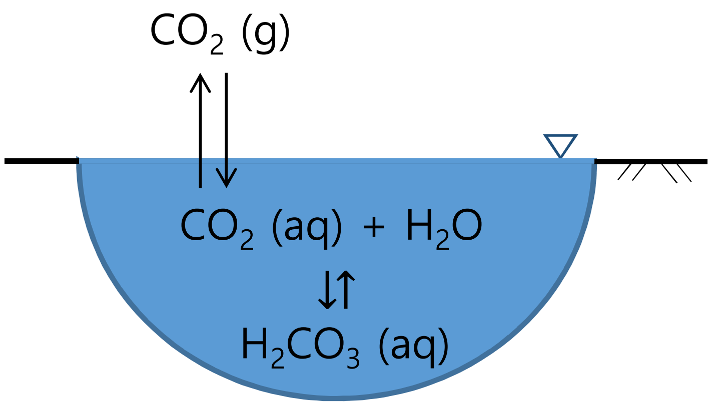
- Half-life ($t_{1/2}$): time required for the concentration to reach ½ of its initial conc.
  - Defined for 1^{st} order reactions only

Carbonate system – a natural buffer system

- Atmospheric CO_2 dissolves in water to produce a weak acid, which provides the potential to act as a natural pH buffer:

$$CO_2\ (g) + H_2O = H_2CO_3{}^{*} = H^{+} + HCO_3{}^{-} = 2H^{+} + CO_3{}^{2-}$$

H_2CO_3* = sum of true H_2CO_3(aq) and $CO_2(aq)$



What's a pH buffer?

- A solution that resists large changes in pH
- A solution containing a weak acid and its conjugate base (or a weak base and its conjugate acid)

ex) CH_3COOH (pK_a=4.75, weak acid)

+ CH_3COONa (to provide conjugate base (CH_3COO^-)]

Carbonic acid dissociation

$$H_2CO_3{}^* = H^+ + HCO_3{}^- \,, \quad K_{a1} = 10^{-6.35} \quad \text{(at 25°C)}$$

$$HCO_3{}^- = H^+ + CO_3{}^{2-} \,, \quad K_{a2} = 10^{-10.33} \quad \text{(at 25°C)}$$

* A buffer works at a pH range close to the pK_a of the weak acid component (check slide#6)

Alkalinity

- Measure of the resistance of water to the addition of strong acid

- Sum of all titratable bases to a pH of approximately 4.5

$$Alkalinity = [HCO_3^{\,-}] + 2[CO_3^{\,2-}] + \cdots + [OH^-] - [H^+]$$

Include $B(OH)_4^-$, PO_4^{3-}, HPO_4^{2-}, $SiO(OH)_3^-$, etc. if significant

Alkalinity

- HCO_3^- & CO_3^{2-} are major alkalinity contributors in natural waters

$$Carbonate\ alkalinity = [HCO_3{}^-] + 2[CO_3{}^{2-}]$$

- For ordinary water with neutral pH,

  Alkalinity ≈ Carbonate alkalinity ≈ $[HCO_3{}^-]$

  (why??)

Unit of alkalinity

- Using molarity for each species, we get "eq/L"
- "eq": equivalent, moles of H^+ ion in an acid-base solution or electrons in a redox reaction
- More common unit is "mg/L as $CaCO_3$"
- 100 g $CaCO_3$ contains 1 mole CO_3^{2-} ($CaCO_3$ molecular weight = 100) → produces 2 eq alkalinity
- Unit conversion: 1 meq/L = 10^{-3} eq/L = 50 mg/L as $CaCO_3$

$$(1\ meq\ Alk/L) \times \left(\frac{100\ mg\ CaCO_3}{2\ meq\ Alk}\right) = 50\ mg/L\ as\ CaCO_3$$

Suggested readings

[ENG] pp. 56 – 64, 74 – 80

[KOR] pp. 51 – 60, 71 – 77

Next class

Basic biology concepts

- Chemical composition of life
- Cell, cell contents, cellular functions
- Energy and metabolism
- How biological principles are applied to environmental engineering