Chemical and Physical Properties of Organic Molecules

I.Elements

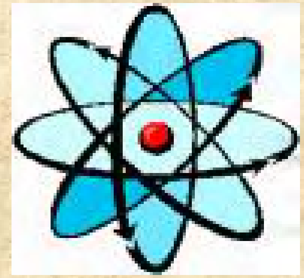
A. Chemical symbols: C H O P S N

C=carbon, H=hydrogen, O=oxygen, P=phosphorus, S=sulfur, N=nitrogen

B. Top 3

Earth's surface = O, Si, Al

Living things: C, H, O



C. Atoms: smallest particle of element

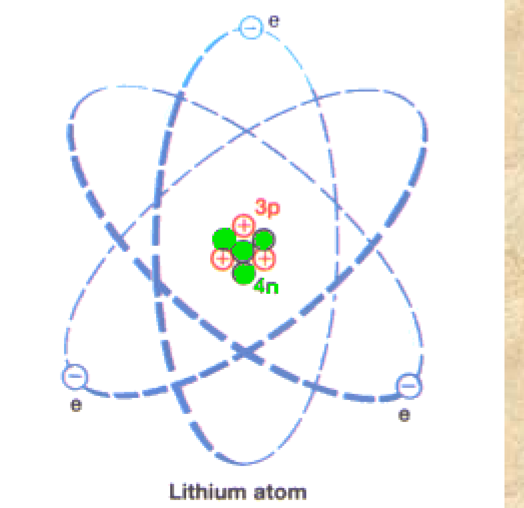
D. Parts of Atoms

1) protons (p+) = in nucleus; Atomic number; ID element

2) neutrons (n^o) = in nucleus

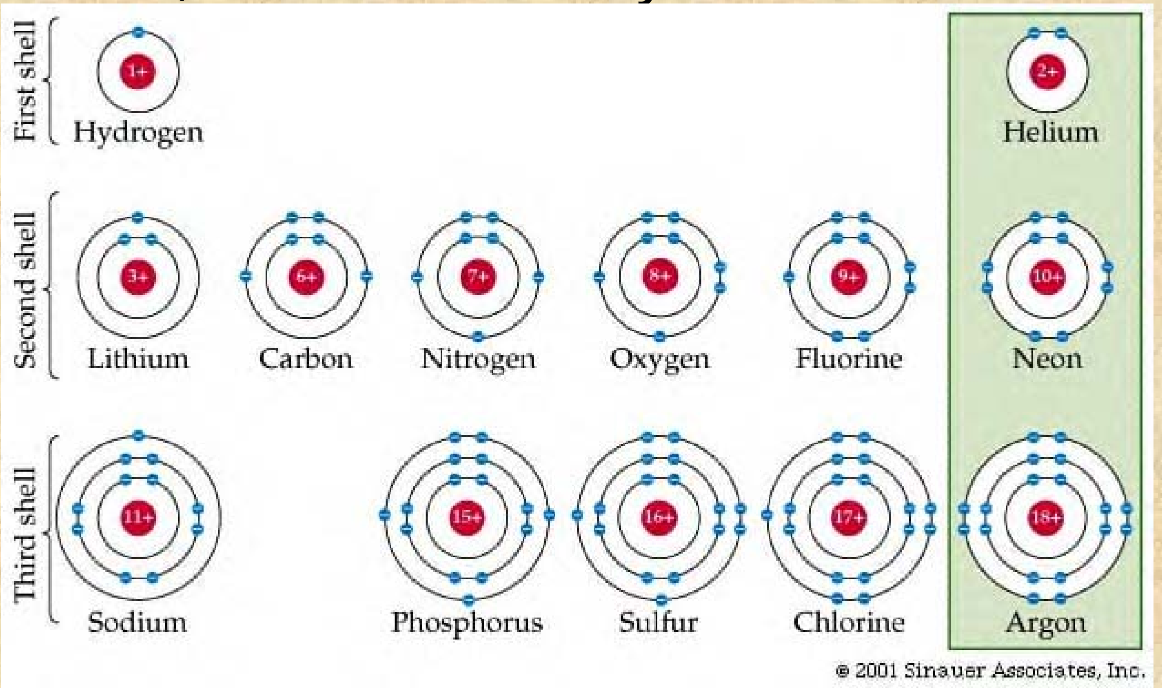
3) electrons (e^-) = orbit nucleus

*__*Neutral atoms : #p*$^+$ *= #e*$^-$__



E. Electrons

1) Travel in energy shell or levels
2) **Valence** e-: outer level; affects reactivity



3) Maximum/level: 2 = 1st 8 = 2nd 18 = 3rd

4) Ions: atom lost or gained an e^-

H *atom* (1p,0n,1e): loses 1e → H^+ *ion*

Cl *atom* gains 1e → Cl^- *ion*

Chemical symbol

Atomic number

Atomic mass (average of all isotopes)

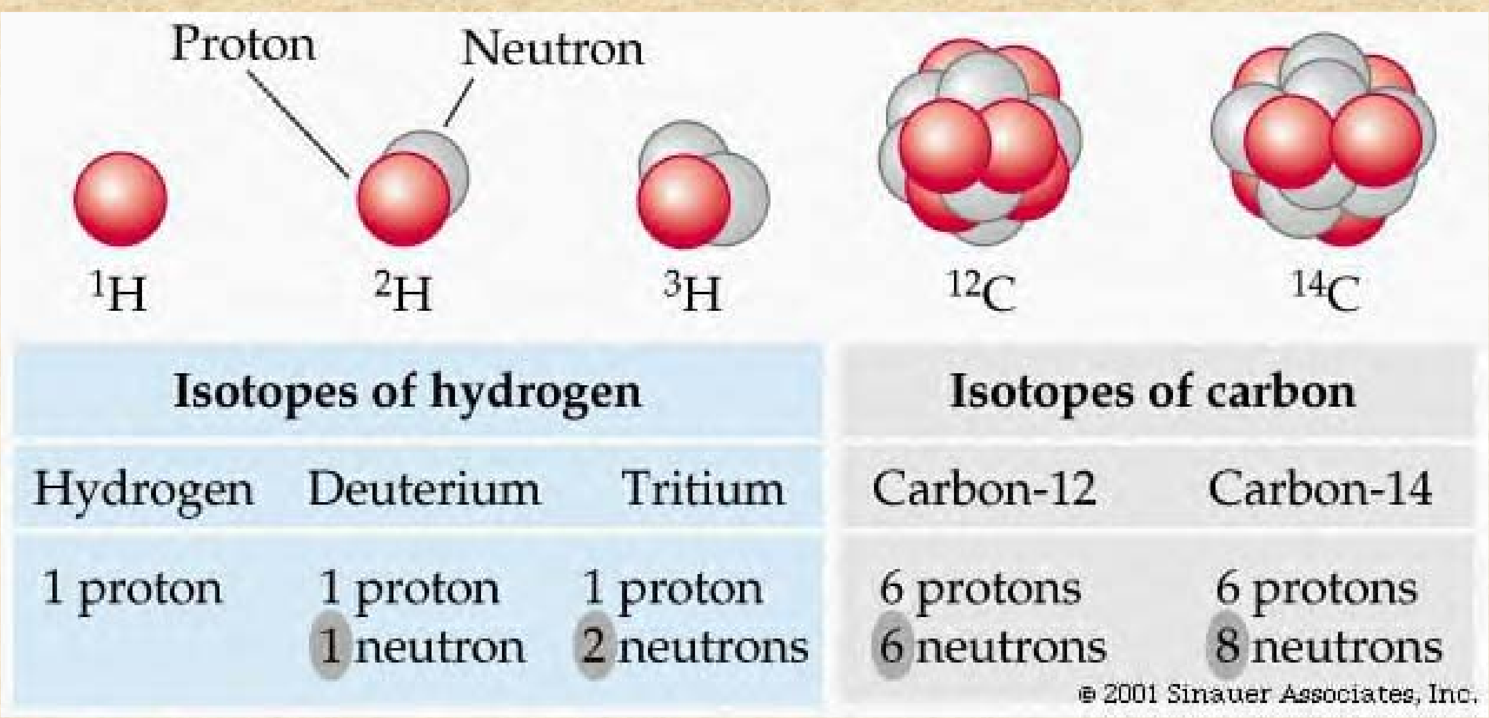
1 H 1.0079																	2 He 4.003
3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.179
11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.06	17 Cl 35.453	18 Ar 39.948
19 K 39.098	20 Ca 40.08	21 Sc 44.956	22 Ti 47.88	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.847	27 Co 58.933	28 Ni 58.69	29 Cu 63.546	30 Zn 65.38	31 Ga 69.72	32 Ge 72.59	33 As 74.922	34 Se 78.96	35 Br 79.909	36 Kr 83.80
37 Rb 85.4778	38 Sr 87.62	39 Y 88.906	40 Zr 91.22	41 Nb 92.906	42 Mo 95.94	43 Tc (99)	44 Ru 101.07	45 Rh 102.906	46 Pd 106.4	47 Ag 107.870	48 Cd 112.41	49 In 114.82	50 Sn 118.69	51 Sb 121.75	52 Te 127.60	53 I 126.904	54 Xe 131.30
55 Cs 132.905	56 Ba 137.34	71 Lu 174.97	72 Hf 178.49	73 Ta 180.948	74 W 183.85	75 Re 186.207	76 Os 190.2	77 Ir 192.2	78 Pt 195.08	79 Au 196.967	80 Hg 200.59	81 Tl 204.37	82 Pb 207.19	83 Bi 208.980	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra 226.025	103 Lr (260)	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (269)	109 Mt (268)	110 (269)	111 (272)	112 (277)	113	114 (285)	115 (289)	116	117	118 (293)

Lanthanide series	57 La 138.906	58 Ce 140.12	59 Pr 140.9077	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.924	66 Dy 162.50	67 Ho 164.930	68 Er 167.26	69 Tm 168.934	70 Yb 173.04
Actinide series	89 Ac 227.028	90 Th 232.038	91 Pa 231.0359	92 U 238.02	93 Np 237.0482	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)

F. **Isotopes**: atoms of same element that differ by # of neutrons

ex: C-14 or ^{14}C; *mass # = #p^+ + #n^o*

$\underline{^{12}C}$	$\underline{^{14}C}$
$p^+ = 6$	$p^+ = 6$
$e^- = 6$	$e^- = 6$
$n^o = 6$	$n^o = 8$



II. Chemical Bond: 2 or more atoms joined together

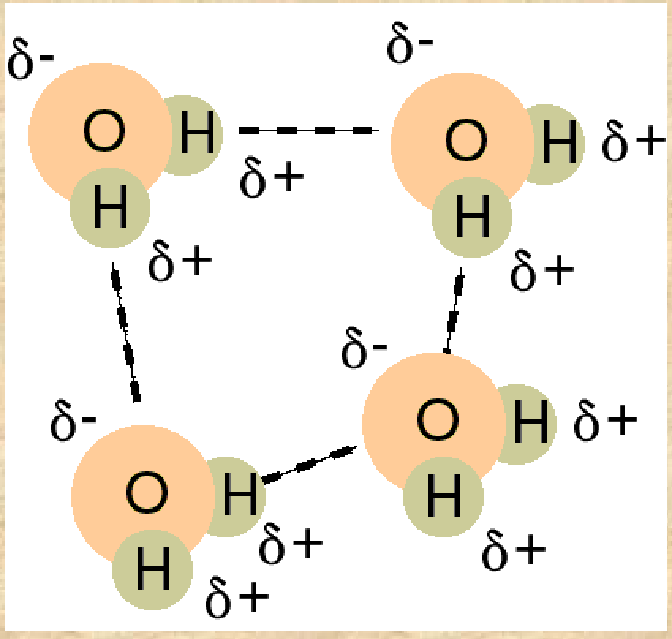
A. **Covalent**: sharing e- between elements

1) most common type

2) distribution

a) **nonpolar**: equal sharing of charge

b) **polar**: unequal sharing; ex: H_2O



B. **Hydrogen**: occurs between **H** in one atom and (**O or N**) in another

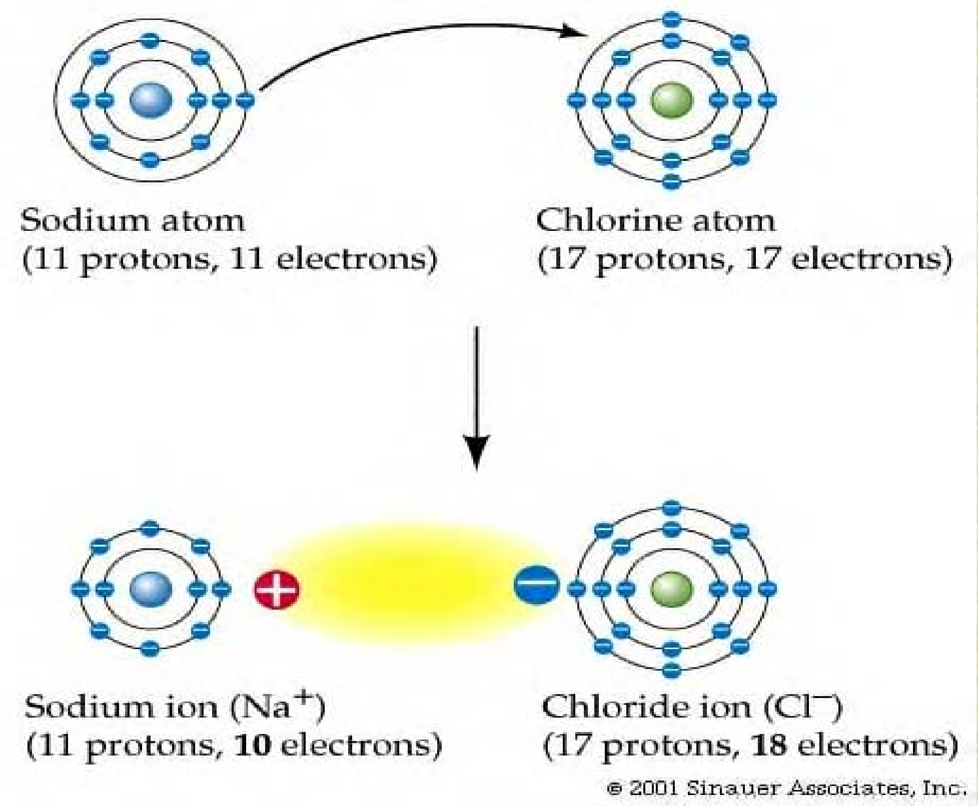
* More easily broken than covalent

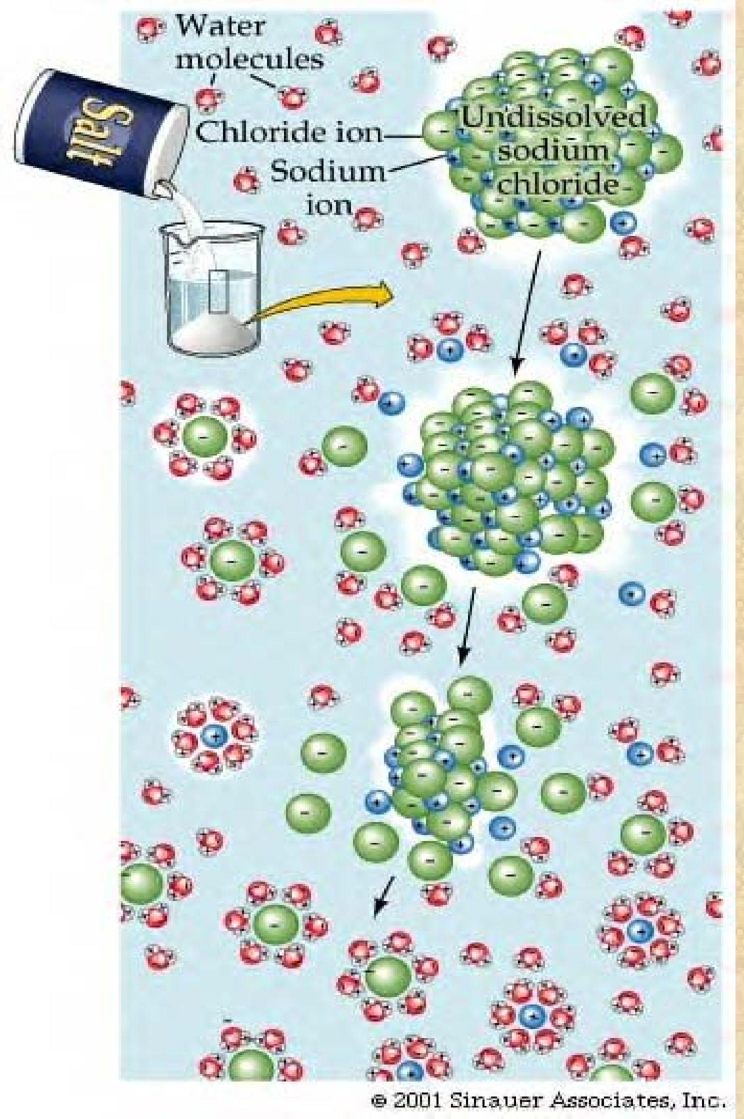
1) between 2 water molecules

2) between N-bases in DNA

II. C. Ionic: transfer of electrons

1) Table salt: NaCl
2) Occurs between ions
3) Usually dissolve in water

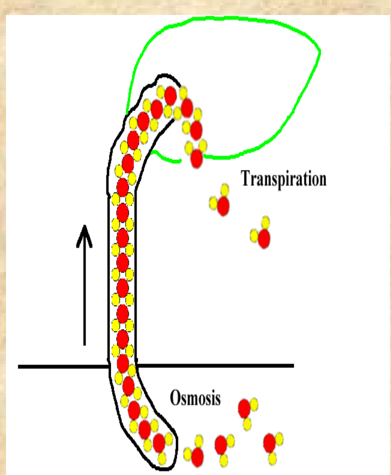


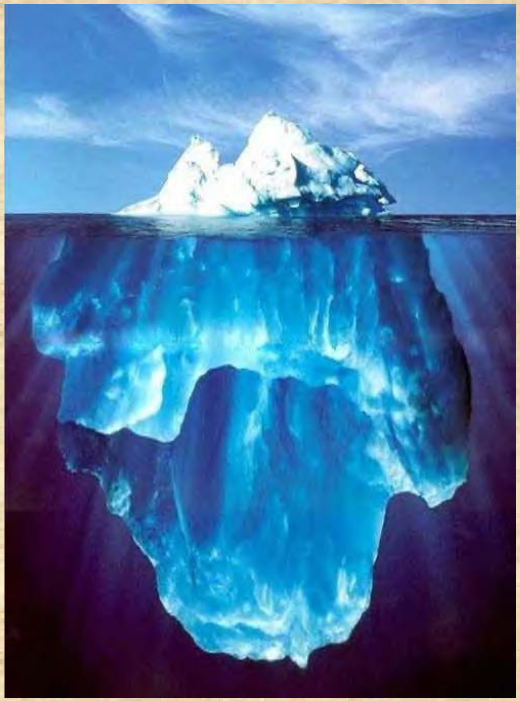


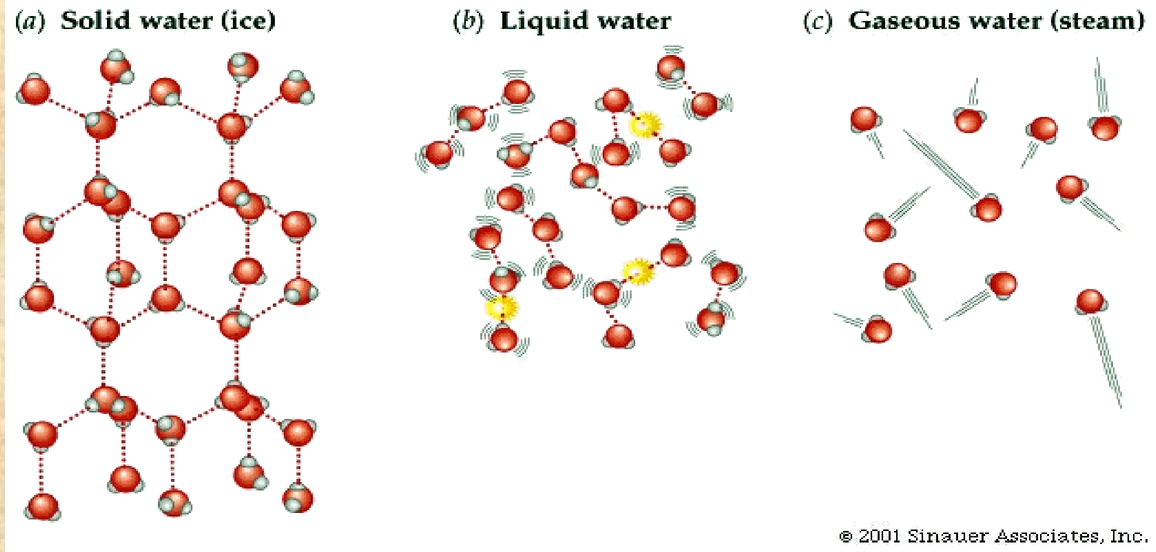
III. Water

A. Properties

1) Capillary action: transport process drawing water up into plants
2) H-bonds in water makes ice float
3) Our bodies 60% water
4) Dissolves things
   a) solvent: dissolves other molecules
   b) solutes: substance being dissolved; lesser amount
   *salt water: water is solvent, salt solute
5) Hydrophilic: water loving; sugar & salt
6) Hydrophobic: water-fearing; does not dissolve in wate







III. B. Acids-Bases

1) **pH scale**: 0 – 14

   a) **Acid** = below 7 (more H^+); *vinegar, lemon juice, stomach acid (HCl)*

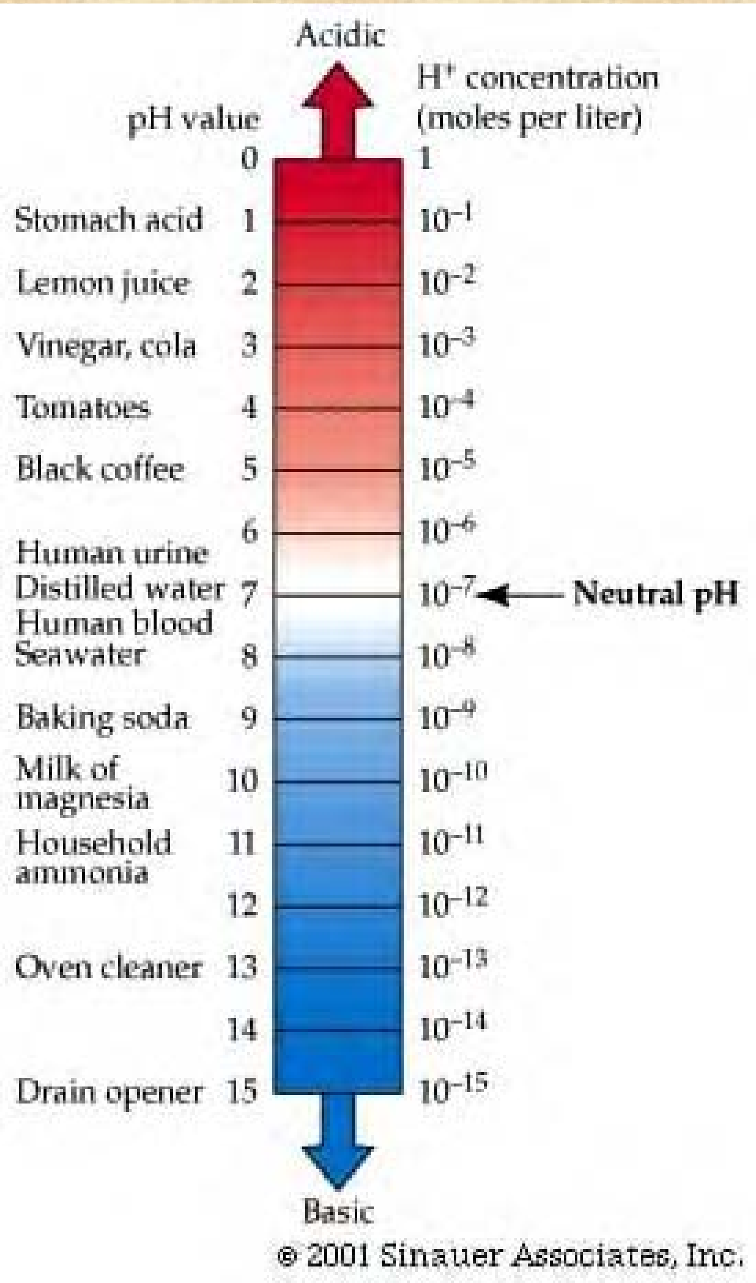
   b) **Neutral** = 7

   c) **Base (alkaline)** = above 7 (more OH^-); *ammonia, soap*

2) $H_2O \rightarrow H^+ + OH^-$ (hydroxide ion)

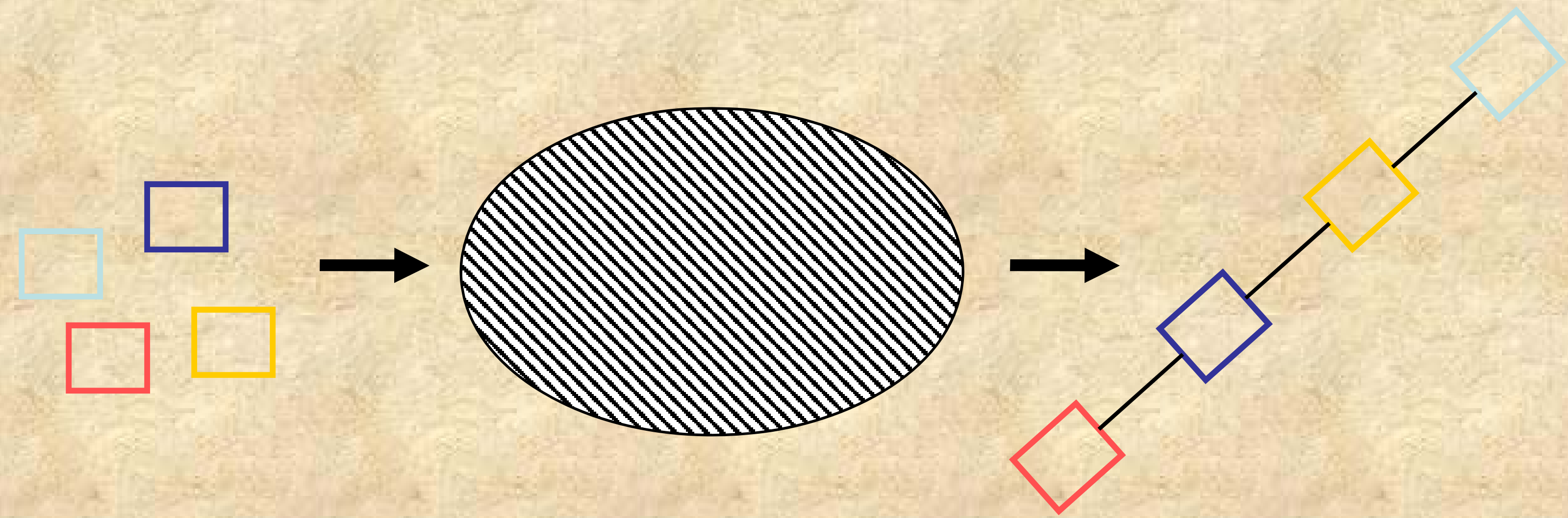
3) Blood: pH = 7.4

4) Buffer: chemicals that control pH, keep it close to 7

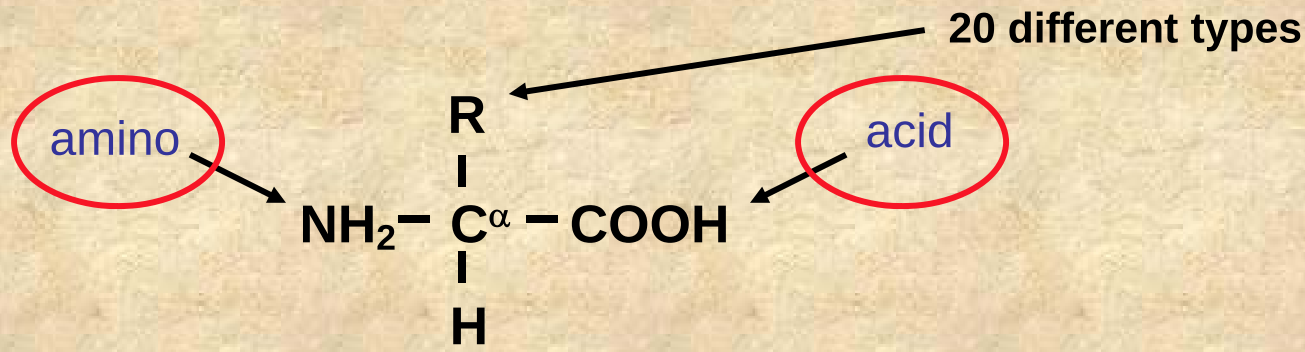


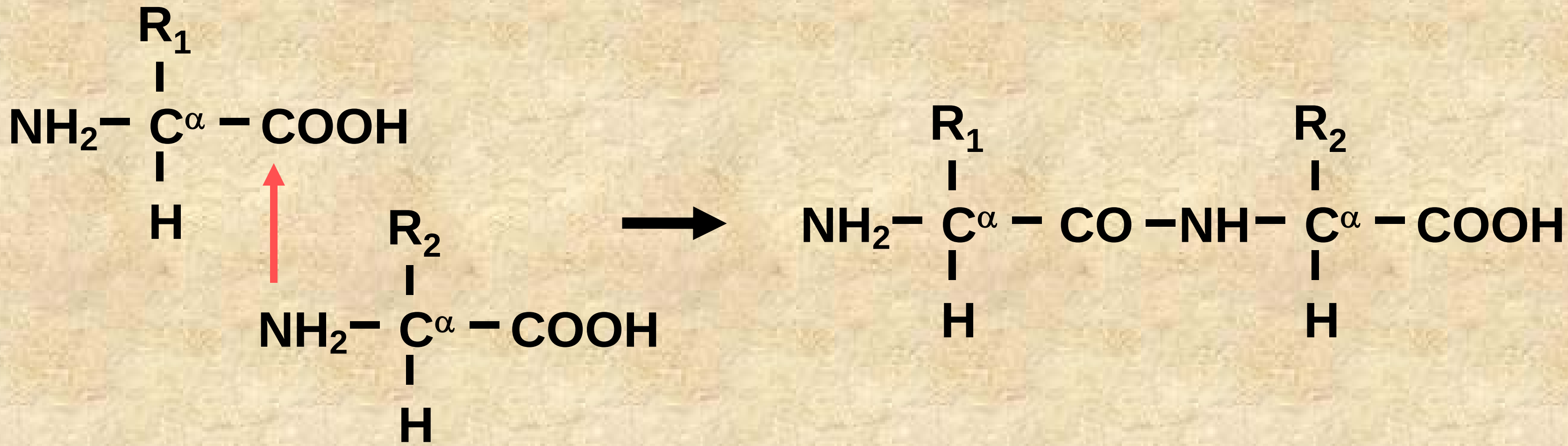
Proteins are amino acid polymers

- **20 different amino acids: many combinations**
- **Proteins are made in the *RIBOSOME***



Amino Acid Chemistry





Amino acid ⟷ **Polypeptide** ⟷ **Protein**

Water, pH and pKa's

The following sections are taken from a website created by Dr. Michael W. King at Indiana University School of Medicine

http://www.indstate.edu/thcme/mwking/home.html

K_{eq}, K_w and pH

As H_2O is the medium of biological systems one must consider the role of this molecule in the dissociation of ions from biological molecules. Water is essentially a neutral molecule but will ionize to a small degree. This can be described by a simple equilibrium equation:

H_2O <-------> $H^+ + OH^-$ Eqn. 1

The equilibrium constant can be calculated as for any reaction:

$K_{eq} = [H^+][OH^-]/[H_2O]$ Eqn. 2

Since the concentration of H_2O is very high (55.5M) relative to that of the $[H^+]$ and $[OH^-]$, consideration of it is generally removed from the equation by multiplying both sides by 55.5 yielding a new term, K_w:

$K_w = [H^+][OH^-]$ Eqn. 3

K_{eq}, K_w and pH (cont.)

This term is referred to as the ion product. In pure water, to which no acids or bases have been added:

$K_w = 1 \times 10^{-14}\ M^2$ Eqn. 4

As K_w is constant, if one considers the case of pure water to which no acids or bases have been added:

$[H^+] = [OH^-] = 1 \times 10^{-7}\ M$ Eqn. 5

This term can be reduced to reflect the hydrogen ion concentration of any solution. This is termed the pH, where:

$pH = -\log[H^+]$ Eqn. 6

pKa

Acids and bases can be classified as proton donors (A-H $\rightarrow$ A^- + H^+) and proton acceptors (B + H^+ $\rightarrow$ BH^+). In biology, various weak acids and bases are encountered, e.g. the acidic and basic amino acids, nucleotides, phospholipids etc.

Weak acids and bases in solution do not fully dissociate and, therefore, there is an equilibrium between the acid (HA) and its conjugate base (A^-).

HA <-----> A^- + H^+ Eqn. 7

This equilibrium can be calculated and is expressed in terms of the association constant K_a.

$K_a = [H^+][A^-]/[HA]$ Eqn. 8

The equilibrium is also sometimes expressed as the dissociation constant $K_d = 1/K_a$.

pKa

As in the case of the equilibrium of H^+ and OH^- in water, the equilibrium constant K_a can be expressed as a pK_a:

$$pK_a = -\log K_a$$ **Eqn. 9**

Therefore, in obtaining the -log of both sides of the equation describing the association of a weak acid, we arrive at the following equation:

$$-\log K_a = -\log[H^+][A^-]/[HA]$$ **Eqn. 10**

Since as indicated above $-\log K_a = pK_a$ and taking into account the laws of logarithms:

$$pK_a = -\log[H^+] - \log[A^-]/[HA]$$ **Eqn. 11**

$$pK_a = pH - \log[A^-]/[HA]$$ **Eqn. 12**

The Henderson-Hasselbalch Equation

By rearranging the above equation we arrive at the Henderson-Hasselbach equation:

$$pH = pK_a + \log[A^-]/[HA] \quad \text{Eqn. 13}$$

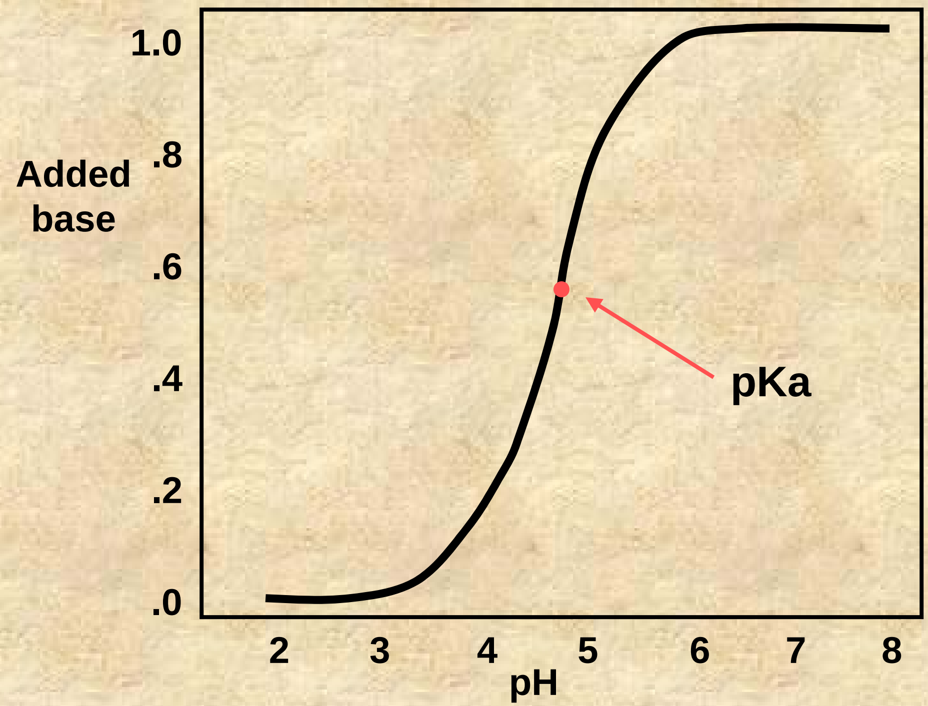
The pH of a solution of any acid can be calculated knowing the concentration of the acid, [HA], and its conjugate base $[A^-]$. At the point of the dissociation where the concentration of the conjugate base $[A^-]$ = to that of the acid [HA]:

$$pH = pK_a + \log[1] \quad \text{Eqn. 14}$$

The log of 1 = 0. Thus, at the mid-point of a titration of a weak acid:

$$pK_a = pH \quad \text{Eqn. 15}$$

The term pK_a is that pH at which an equivalent distribution of acid and conjugate base (or base and conjugate acid) exists in solution.



Buffering

It should be noted that around the pK_a the pH of a solution does not change appreciably even when large amounts of acid or base are added. This phenomenon is known as buffering. In most biochemical studies it is important to perform experiments, that will consume H^+ or OH^- equivalents, in a solution of a buffering agent that has a pK_a near the pH optimum for the experiment.

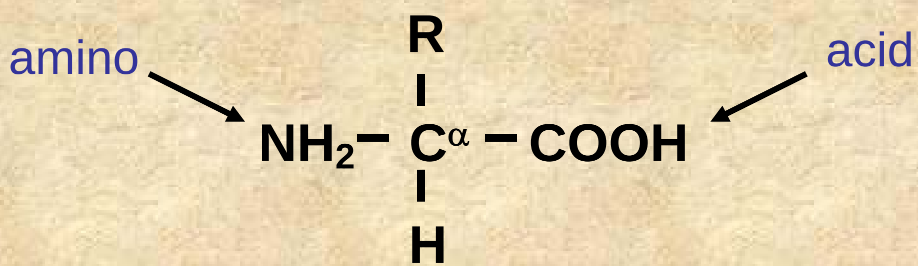
Thinking beyond the lecture

- Clinical significance of blood buffering
- Role of kidneys in acid-base balance

See Dr. King's website:

http://www.indstate.edu/thcme/mwking/ionic-equilibrium.html

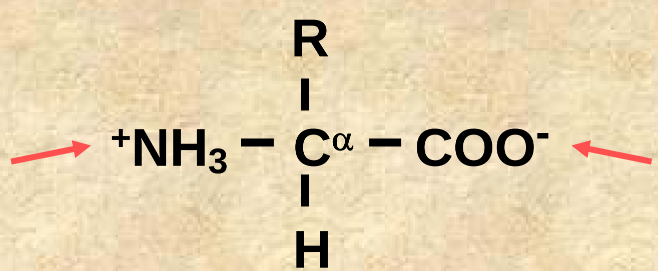
Amino Acid Chemistry



The free amino and carboxylic acid groups have pKa's

$NH_3^+ \longleftarrow NH_2$ $\qquad$ $COOH \longrightarrow COO^-$

pKa ~ 9.4 $\qquad$ **pKa ~ 2.2**



At physiological pH, amino acids are zwitterions

Amino Acid Chemistry