

Acids and Bases

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Lecture 1 MD summer

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Required material and further reading

Required:

Handout

Text books:

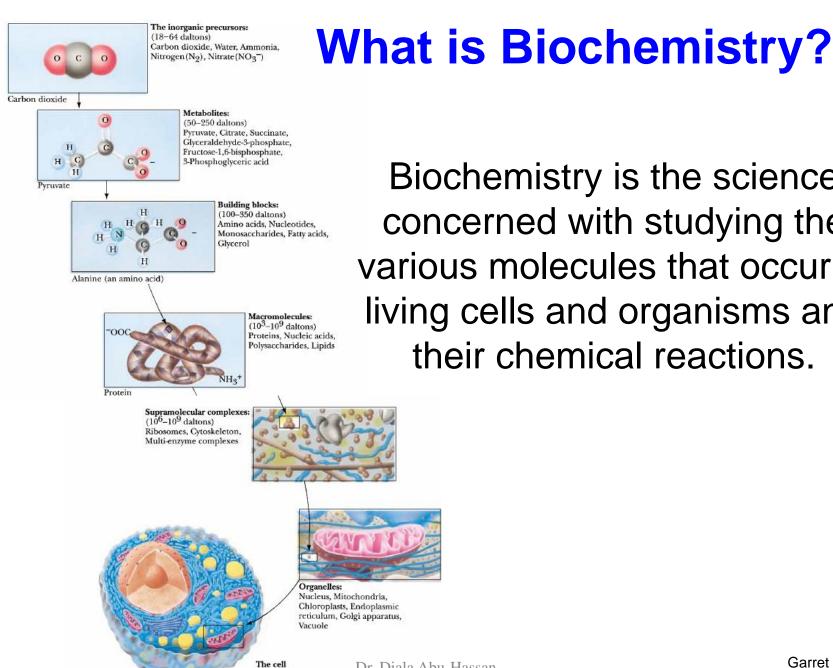
Biochemistry. Campbell Chapter 2

Fundamentals of General, Organic, and Biological Chemistry. McMurry. Chapter 10 softcopy will be sent

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Outline

- Introduction- The Science of Biochemistry
- Definitions of acids and bases
- Acid and base strength
- The dissociation constant
- Conjugate pair strength
- Water dissociation



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Biochemistry is the science concerned with studying the various molecules that occur in living cells and organisms and

Why Biochemistry is important to Human Biology?

- 1. Biochemistry is an intrinsically beautiful and fascinating body of knowledge. "Lubert Stryer"

 Because it unravels the details of the most fundamental processes in biological systems.
- 2. Biochemistry massively influences medicine and treatment development, ex. sickle-cell anemia, cystic fibrosis, hemophilia, etc.
- 3. By advances in biochemistry, researchers can tackle many questions in biology and medicine, ex. Biochemical changes in diseases, causes of diseases, lab tests..etc.

Benefits of studying biological systems at the molecular and biochemical level

When we unravel the molecular and biochemical details of biological molecules:

- 1. Molecular and biochemical basis of diseases become clear.
- 2. Manipulate the biochemical processes and simulating them in vivo and in vitro.
- 3. Molecules of life can be prepared on the bench

What makes biomolecules special?

Functional Groups	of Biochemical Importance			
Class of Compound	General Structure	Characteristic Functional Group	Name of Functional Group	Example
Alkenes	$RCH = CH_2$ RCH = CHR $R_2C = CHR$ $R_2C = CR_2$	с=с	Double bond	CH _z =CH _z
Alcohols	ROH	—он	Hydroxyl group	СН,СН,ОН
Ethers Amines	ROR RNH ₂ R ₂ NH	-0-	Ether group	CH ₅ OCH ₅
Thiols	R ₃ N RSH	−n′ −sh	Amino group Sulfhydryl group	CH ₃ NH ₂ CH ₃ SH
Aldehydes	R—C—H		Carbonyl group	СН,СН О
Ketones	R—G—R	_c_	Carbonyl group	CH,C CH,
Carboxylic acids	R—С—ОН	—с—он	Carboxyl group	CH,C OH
Esters	R—C—OR	—C—OR	Ester group	O H CH ₂ C OCH,
Amides	R—G—NR ₂	_C_N<	Amide group	∏ CH₃C N(CH₃)₂
	R—C—NHR			
	R—C—NH ₂	0		0
Phosphoric acid esters	R—O—P—OH OH	_о_р_он Он	Phosphoric ester group	СН ₃ — О — Р — ОН ОН
Phosphoric acid anhydrides	O O O P—OH OH OH	O O O O O O O O O O O O O O O O O O O	Phosphoric anhydride group	O O O HO—P—OH

-The cellular apparatus of living organisms is made up of carbon compounds.

Different Definitions of Acids and Bases

- Arrhenius
- Bronsted-Lowry
- Lewis

Arrhenius Definition of Acids and Bases and Their Reactions

Arrhenius Acids and Bases Acids are

- Acids in H₂O are H⁺ donors
- Bases in H₂O are OH⁻ donors

Neutralization of acids and bases produces salt and water.

NaOH
$$\xrightarrow{H_2O}$$
 Na⁺ + OH⁻
HCL $\xrightarrow{H_2O}$ Cl⁻ + H⁺
H⁺ + H- Ö: \longrightarrow H₃O⁺
H



Arrhenius 1903 Nobel Prize

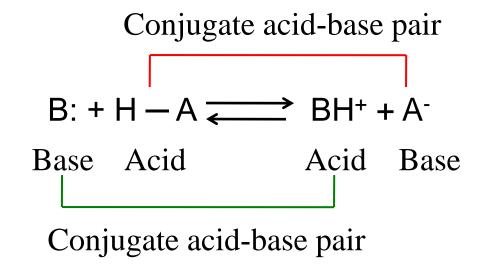
Drawbacks:

- 1. Reactions has to happen in aqueous solutions
- 2. H₃O⁺ is released but not H⁺

Bronsted-Lowry Definition of Acids and Bases and Their Reactions

Bronsted-Lowry Acids and Bases (1923)

- Acids donate H⁺
- Bases accept H⁺ (non-bonding pairs)



Lewis Definition of Acids and Bases and Their Reactions

- Acids accept electrons
- Bases donate electrons (non-bonding pairs)

$$BF_3 + :NH_3 \longrightarrow F_3B^{\dots}:NH_3$$
Acid base

Common Acids

- HCI- hydrochloric- stomach acid
- H₂SO₄- sulfuric acid car batteries
- HNO₃ nitric acid explosives
- HC₂H₃O₂- acetic acid vinegar
- H₂CO₃-carbonic acid sodas
- H₃PO₄- phosphoric acid -flavorings











Common Bases

- NaOH- sodium hydroxide (LYE) soaps, drain cleaner
- Mg (OH)₂ magnesium hydroxide-antacids
- Al(OH)₃-aluminum hydroxide-antacids, deodorants
- NH₄OH-ammonium hydroxide- "ammonia"







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Water as both an acid and a base

$$CH_3COO^- + H_2O \longrightarrow CH_3COOH + OH-$$
base acid base

 $H_2O + HCI \longrightarrow H_3O^+ + CI-$
base acid base

 $HA + H_2O \longrightarrow H_3O^+ + A^-$
(strong acid) (weak base)

 $HA + H_2O \longrightarrow H_3O^+ + A^-$
(strong base)

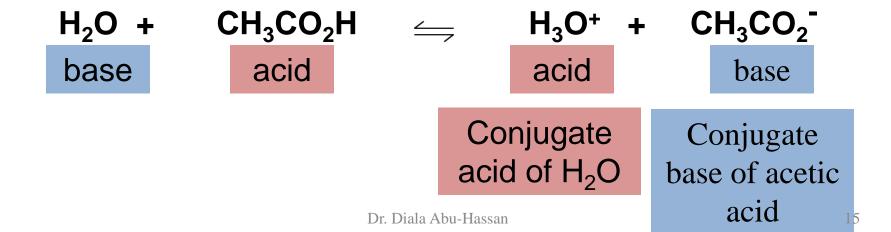
Strong acid + strong base \longrightarrow weak base + weak acid

<u>Amphoterism</u> - an ion or molecule can act as an acid or base depending upon the reaction conditions

Water in NH₃ serves as an acid

$$H_2O + NH_3 \rightleftharpoons NH_4^+ + OH^-$$
 acid base base

Water in acetic acid serves as a base



Measuring concentrations

Molarity: the number of moles in a liter of solution

Unit: Mole/Liter = M

 $mM = 10^{-3} M$, $uM = 10^{-6} M$

Symbol: [X]

Concentration = Amount of solute
Amount of solvent

Dissolve 2 moles of glucose in 5 liters of H₂0. what is the concentration?

[Glucose] = 2/5 = 0.4 M

Acid and Base Strength

- Some acids can cause burns if come in contact with skin, other acids are safe. why?
- How easy can the acid produce proton
 - Strong acid: gives up H+ easily (100% dissociated in water)

$$HCI \longrightarrow H^+ + CI^-$$

Weak acid: gives up H⁺ with difficulty (less than 100% dissociated)

Acid dissociation constant, K_a

– The general ionization of an acid is as follows:

$$HA + H_2O \longleftrightarrow H_3O^+ + A^-$$

So the acid dissociation constant is as follows:

$$K_a = \frac{[H_3O^+][A^-]}{[HA][H_2O]}$$

 $[H_2O] = 55.5$ M and is constant in all equations

$$K_a = \frac{[H_3O^+][A^-]}{[HA]}$$

Acid dissociation constant

– The general ionization of an acid is as follows:

$$HA \longleftrightarrow H^+ + A^-$$

So the acid dissociation constant is as follows:

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

There are many orders of magnitude spanned by K_a values, so pK_a is used instead:

$$pK_a = log 1/K_a = -log_{10} K_a$$

The larger the value of the pK_a, the smaller the extent of dissociation.

The equilibrium constant, Ka

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

Larger K_a means:
More dissociation
Smaller pK_a
Stronger acid

TABLE 8-2	Acidit	y Constants in W	/ater at 25°C	3
Acid	Formula	Conjugate Base	K _a	pK _a
Hydriodic	НІ	I-	$\approx 10^{11}$	≈ -11
Hydrobromic	HBr	Br^{-}	$\approx 10^9$	≈ -9
Perchloric	HClO ₄	ClO ₄	$\approx 10^7$	≈ -7
Hydrochloric	HC1	Cl ⁻	$\approx 10^7$	≈ -7
Chloric	HClO ₃	ClO ₃	$\approx 10^3$	≈ -3
Sulfuric (1)	H ₂ SO ₄	HSO_4^-	$\approx 10^2$	≈ -2
Nitric	HNO ₃	NO_3^-	≈ 20	≈ -1.3
Hydronium ion	H_3O^+	H_2O	1	0.0
Urea acidium ion	(NH ₂)CONH ₃ ⁺	(NH ₂) ₂ CO (urea)	6.6×10^{-1}	0.18
Iodic	HIO ₃	IO_3^-	1.6×10^{-1}	0.80
Oxalic (1)	$H_2C_2O_4$	$HC_2O_4^-$	5.9×10^{-2}	1.23
Sulfurous (1)	H_2SO_3	HSO_3^-	1.5×10^{-2}	1.82
Sulfuric (2)	HSO ₄	SO_4^{2-}	1.2×10^{-2}	1.92
Chlorous	HClO ₂	ClO_2^-	1.1×10^{-2}	1.96
Phosphoric (1)	H_3PO_4	$H_2PO_4^-$	7.5×10^{-3}	2.12
Arsenic (1)	H ₃ AsO ₄	$H_2AsO_4^-$	5.0×10^{-3}	2.30
Chloroacetic	CICH ₂ COOH	CICH ₂ COO ⁻	1.4×10^{-3}	2.85
Hydrofluoric	HF	F^-	6.6×10^{-4}	3.18
Nitrous	HNO ₂	NO_2^-	4.6×10^{-4}	3.34
Formic	НСООН	HCOO ⁻	1.8×10^{-4}	3.74

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Acid dissociation constant

Acid Dissociation Constants and pK_a Values for Some Weak Electrolytes (at 25°C)

Acid	$K_a(M)$	pK_a
HCOOH (formic acid)	1.78×10^{-4}	3.75
CH ₃ COOH (acetic acid)	1.74×10^{-5}	4.76
CH ₃ CH ₂ COOH (propionic acid)	1.35×10^{-5}	4.87
CH₃CHOHCOOH (lactic acid)	1.38×10^{-4}	3.86
$HOOCCH_2CH_2COOH$ (succinic acid) pK_1^*	6.16×10^{-5}	4.21
HOOCCH ₂ CH ₂ COO ⁻ (succinic acid) pK ₂	2.34×10^{-6}	5.63
H_3PO_4 (phosphoric acid) pK_1	7.08×10^{-3}	2.15
$H_2PO_4^-$ (phosphoric acid) p K_2	6.31×10^{-8}	7.20
HPO_4^{2-} (phosphoric acid) p K_3	3.98×10^{-13}	12.40
$C_3N_2H_5^+$ (imidazole)	1.02×10^{-7}	6.99
$C_6O_2N_3H_{11}^+$ (histidine–imidazole group) pK_R^\dagger	9.12×10^{-7}	6.04
H_2CO_3 (carbonic acid) pK_1	1.70×10^{-4}	3.77
HCO_3^- (bicarbonate) p K_2	5.75×10^{-11}	10.24
(HOCH ₂) ₃ CNH ₃ ⁺ (tris-hydroxymethyl aminomethane)	8.32×10^{-9}	8.07
NH ₄ ⁺ (ammonium)	5.62×10^{-10}	9.25
CH ₃ NH ₃ ⁺ (methylammonium)	2.46×10^{-11}	10.62

^{*}These pK values listed as pK_1 , pK_2 , or pK_3 are in actuality pK_a values for the respective dissociations. This simplification in notation is used throughout this book.

Data from CRC Handbook of Biochemistry, The Chemical Rubber Co., 1968.

 $^{{}^{\}dagger}pK_R$ refers to the imidazole ionization of histidine.

Base dissociation constant

$$B + H_2O \iff BH^+ + OH^-$$

$$K_b = \frac{[BH+][OH^-]}{[B]}$$

Reverse the reaction:

$$K_a = \frac{[B][H^+]}{[BH^+]}$$

Weak Bases

		Conjugate	$K_{ m b}$	
Name	Formula	Acid		
Ammonia	NH ₃	NH ₄ ⁺	1.8×10^{-5}	
Methylamine	CH ₃ NH ₂	CH ₃ NH ₃ ⁺	4.38×10^{-4}	
Ethylamine	$C_2H_5NH_2$	$C_2H_5NH_3^+$	5.6×10^{-4}	
Aniline	$C_6H_5NH_2$	$C_6H_5NH_3^+$	3.8×10^{-10}	
Pyridine	C_5H_5N	$C_5H_5NH^+$	1.7×10^{-9}	

Strong Acids

- Dissociate readily
- Ka is very large
- Examples: Hydrochloric, Nitric; Sulfuric

Ex.
$$HCI \rightarrow H^+ + CI^-$$

$$Ka = [H^+][Cl^-]$$

[HCl]

$$[H^+] = [acid]$$

Ex.1 M solution of HCl has a [H+] of 1 M

1 mM HCl solution has a [H+] of 1 mM

0.1 M H₂SO₄ solution has a [H+] of 0.2 M

Weak Acids

- Dissociate slightly
- Ka is smaller than strong acids
- Examples: Acetic, Boric, Nitrous, Phosphoric, Sulfurous

Ex.
$$CH_3COOH + H_2O \longleftrightarrow CH_3COO^- + H_3O^+$$

$$Ka = [H+] [CH3COO-]$$
[CH₃COOH]

What is the H+ of a 0.1 M solution of acetic acid? Ka= 1.74 X 10⁻⁵

$$1.74 \times 10^{-5} = x^2/0.1$$

$$x^2 = 1.74 \times 10^{-6}$$
, or $x = 1.32 \times 10^{-3} M$

Conjugate pair strength

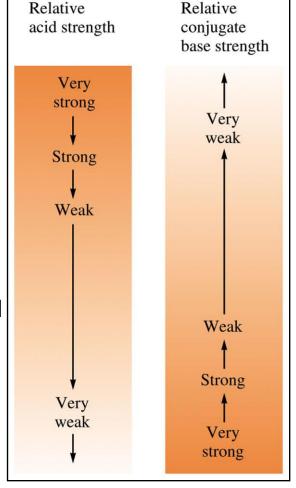
$$HA + H_2O \longrightarrow H_3O^+ + A^-$$

$$HA + H_2O \longrightarrow H_3O^+ + A^-$$

$$CH_3COOH + H_2O \longrightarrow CH_3COO^- + H_3O^+$$

Weak acid weak base strong base strong acid

$$CH_3COOH + OH^- \longrightarrow CH_3COO^- + H_2O$$
Stronger acid strong base weak base weak acid



Equilibrium constant and the pH of water

H₂O dissociates to a slight extent to form hydrogen (H⁺) and hydroxyl (OH⁻) ions.

$$H_2O \rightleftharpoons H^+ + OH^ K_{eq} = \frac{[H^+][OH^-]}{[H_2O]}$$
 $K_{eq} = \frac{(10^{-7})(10^{-7})}{55.5} = 1.8 \times 10^{-16}$

Because the concentration of H_2O in pure water is essentially constant, a new constant, K_w , the ion product of water, can be written as

$$K_{\rm w} = 55.5 \ K_{\rm eq} = 10^{-14} = [{\rm H}^+][{\rm OH}^-]$$

[H+] of pure water is only 0.0000001 M

Dissociation of water

• $K_w = [H^+][OH^-] = 10^{-14}$

Example: A solution has an [OH-] = 10-9 M

$$[H_3O^+] = 10^{-5} M$$

Problem solving

Example:

What is the [H⁺] of a 0.01 M NaOH solution?

$$Kw = [H^+] \times [OH^-] = [H^+] \times 10^{-2} = 10^{-14}$$

$$[H^+] = 10^{-12} M$$

Example:

What is the [OH-] of a 0.01 M HCl solution?

$$Kw = [H^+] \times [OH^-] = 10^{-2} \times [OH^-] = 10^{-14}$$

$$[OH^{-}] = 10^{-12} M$$

Example:

Find the K_a of a 0.04 M weak acid HA whose [H⁺] is 1 x 10⁻⁴?

$$HA \longrightarrow H^+ + A^-$$

$$K_a = [A^-][H^+]/[HA] = [H^+]^2/[HA] = 10^{-4} \times 10^{-4}/0.04 = 2.5 \times 10^{-7}$$

Example 2:

What is the $[H^+]$ of a 0.05 M Ba $(OH)_2$?

$$Ba(OH)_2 \longrightarrow Ba + 2OH^-$$

$$[OH^{-}] = 2x \ 0.05 = 0.10 \ M = 1 \ x \ 10^{-1}$$

$$[H^+] = 1x \ 10^{-13}$$

Example 4:

The [H⁺] of a 0.03 M weak base solution is 1 x 10⁻¹⁰ M. Calculate pKb?

$$B + H_2O \longrightarrow BH^+ + OH^-$$

$$[OH^{-}] = 10^{-4}$$

$$K_b = (10^{-4} \times 10^{-4}) / 0.03 = 3.33 \times 10^{-7} M$$

$$pK_b = -log K_b = 6.48$$