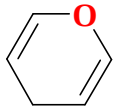
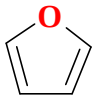
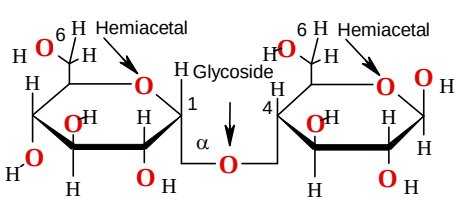
Cyclic Structure Haworth projections of Carbohydrates

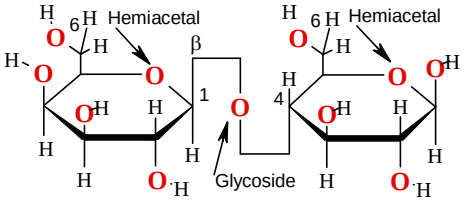
Haworth projection uses the organic molecule frames



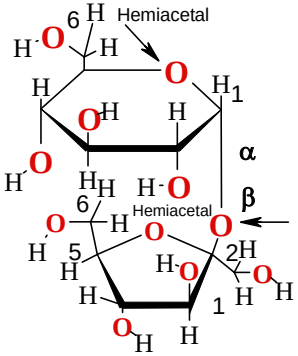
Pyranose six member cycle and *Furanose*  cycle 5 atoms

Disaccharides and polysaccharides





Maltose **Glc(α1→4)Glc-β** **Lactose** **Gal(β1→4)Glc-β**



Sucrose

α-D-Glucose unit *Pyranose six member* cycle

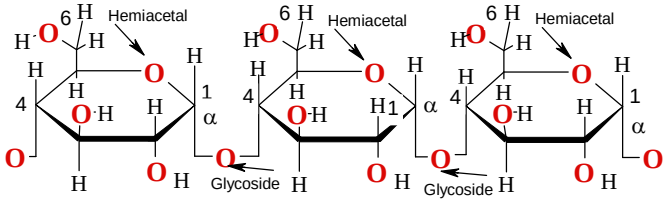
(α1→2β) **Glc(α1→2)Fruc-β**

← Glycoside bond

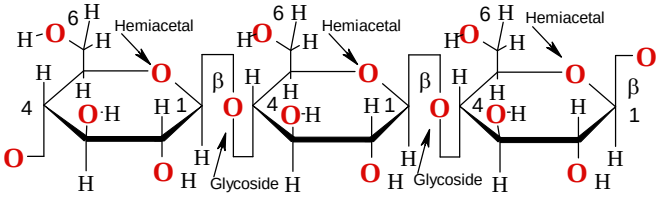
β-D-Fructose unit *Furanose* five member cycle

Starch **→4)Glc(α1→4)Glc(α1→4)Glc(α1→**

Polysaccharides



Cellulose **→4)Glc(β1→4)Glc(β1→4)Glc(β1→**



A.Kaksis, A.Brangule, M.Halitov

DATA BOOKLET FOR MEDICAL CHEMISTRY

CONTENT

RSU
2018

Periodic Table of ELEMENTS

1	IIA	IIIB	IVB	VB	VIB	VIIB	—— VIII B ——			
1 1,008 2,2 -253 -260 **H** Hydrogen $1s^1$										
3 6,941 0,98 1318 179 **Li** Lithium $[He]2s^1$	4 9,012 1,57 — 1278 **Be** Beryllium $[He]2s^2$									
11 22,99 0,93 892 97,8 **Na** Sodium $[Ne]3s^1$	12 24,30 1,31 1107 651 **Mg** Magnesium $[Ne]3s^2$									
19 39,10 0,82 774 63,7 **K** Potassium $[Ar]4s^1$	20 40,08 1,00 1487 845 **Ca** Calcium $[Ar]4s^2$	21 44,96 1,36 2832 1539 **Sc** Scandium $[Ar]3d^14s^2$	22 47,90 1,54 3260 1675 **Ti** Titanium $[Ar]3d^24s^2$	23 50,94 1,63 3380 1890 **V** Vanadium $[Ar]3d^34s^2$	24 52,00 1,66 2482 1890 **Cr** Chromium $[Ar]3d^44s^2$	25 54,94 1,55 2097 1244 **Mn** Manganese $[Ar]3d^54s^2$	26 55,85 1,83 2750 1535 **Fe** Iron $[Ar]3d^64s^2$	27 58,93 1,88 2870 1495 **Co** Cobalt $[Ar]3d^74s^2$	28 58,70 1,91 2730 1453 **Ni** Nickel $[Ar]3d^84s^2$
37 85,45 0,82 688 38,9 **Rb** Rubidium $[Kr]5s^1$	38 87,62 0,95 1384 769 **Sr** Strontium $[Kr]5s^2$	39 88,91 1,22 3337 1523 **Y** Yttrium $[Kr]4d^15s^2$	40 91,22 1,33 4377 1852 **Zr** Zirconium $[Kr]4d^25s^2$	41 92,95 1,60 4927 2468 **Nb** Niobium $[Kr]4d^45s^2$	42 95,94 2,16 5560 2610 **Mo** Molybdenum $[Kr]4d^55s^2$	43 (98) 1,9 5030 2200 **Tc** Technetium $[Kr]4d^55s^2$	44 101,1 2,20 3900 2310 **Ru** Ruthenium $[Kr]4d^65s^2$	45 102,9 2,28 3730 1966 **Rh** Rhodium $[Kr]4d^75s^2$	46 106,4 2,20 3140 1552 **Pd** Palladium $[Kr]4d^85s^2$
55 132,9 0,79 690 28,5 **Cs** Cesium $[Xe]\ 6s^1$	56 137,3 0,89 1640 725 **Ba** Barium $[Xe]\ 6s^2$	57 138,9 1,10 3454 920 **La** Lanthanum $[Xe]\ 5d^16s^2$	72 178,5 1,30 5400 2150 **Hf** Hafnium $Xe\ 4f^{14}5d^26s^2$	73 181,0 1,50 5430 2996 **Ta** Tantalum $[Xef]\ 5d^36s^2$	74 183,8 2,36 5927 3410 **W** Tungsten $[Xef]\ 5d^46s^2$	75 186,2 1,90 5630 3180 **Re** Rhenium $[Xef]\ 5d^56s^2$	76 190,2 2,20 5030 3045 **Os** Osmium $[Xef]\ 5d^66s^2$	77 192,2 2,20 4130 2410 **Ir** Iridium $[Xef]\ 5d^76s^2$	78 195,1 2,28 3830 1772 **Pt** Platinum $[Xef]\ 5d^96s^2$
87 [223,02] 0,70 — 27 **Fr** Francium $[Rn]7s^1$	88 226,03] 0,90 1140 700 **Ra** Radium $[Rn]7s^2$	89 [227,03] 1,10 — 1050 **Ac** Actinium $[Rn]\ 6d^17s^2$	104 [265,12] — — — Rutherfordium $Rn5f^{14}6d^27s^2$	105 [268,13] — — — Dubnium $[Rnf]\ 6d^37s^2$	106 [271,13] — — — Seaborgium $[Rnf]6d^47s^2$	107 [270] — — — Bohrium $[Rnf]6d^57s^2$	108 [277,15] — — — Hassium $[Rnf]6d^67s^2$	109 [276,15] — — — Meitnerium $[Rnf]6d^77s^2$	110 [281,16] — — — Darmstadtium $[Rnf]6d^87s^2$
		Lanthanoids->	58 140,1 1,12 3257 798 **Ce** Cerium $[Xe]\ 4f^26s^2$	59 140,9 1,13 3212 931 **Pr** Praseodymium $[Xe]4f^36s^2$	60 144,2 1,14 3127 1010 **Nd** Neodymium $[Xe]4f^46s^2$	61 (145) 1,13 — 1080 **Pm** Promethium $[Xe]\ 4f^56s^2$	62 150,4 1,17 1778 1072 **Sm** Samarium $[Xe]4f^66s^2$	63 151,96 1.20 1597 822 **Eu** Europium $[Xe]4f^76s^2$
		Actinoids->	90 232,0 1,30 3800 1750 **Th** Thorium $[Rn]\ 6d^27s^2$	91 231,04 1,50 — 1554 **Pa** Protactinium $[Rn]\ 5f^26d^17s^2$	92 238,0 1,38 3818 1132 **U** Uranium $[Rn]\ 5f^36d^17s^2$	93 237,05 1,36 3902 640 **Np** Neptunium $[Rn]\ 5f^46d^17s^2$	94 244,06 1,28 3327 641 **Pu** Plutonium $[Rn]\ 5f^67s^2$	95 243,06 1,30 — 1000 **Am** Americium $[Rn]\ 5f^77s^2$

Atomic number **Z** (number of Protons)
Jhon G. Gramer "Twistor" Electro negativity
Boiling point temperature
Melting point temperature
Aggregate State
Shadow letters: gas forming
Italic letters : liquid **Normal letters:** solid
Outline letters : all in nature radio active isotopes

25 54,94 1,55 2097 1244 **Mn** Manganese $[Ar]3d^54s^2$

Riga (**RSU**)

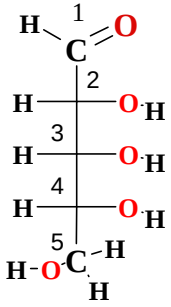
Stradin's University

Human Physiology and Biochemistry department

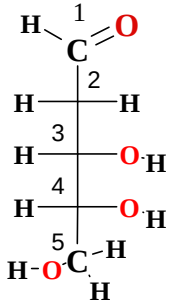
Asist.prof. A. Kaksis 2013. g.

Structural Formulas of Carbohydrates The Fischer tree projections for open chain structures

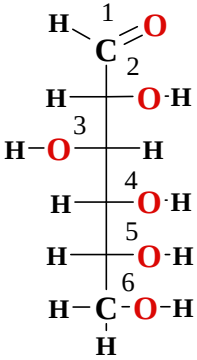
Pentoses–Aldoses: **Hexoses – Aldohexoses:**



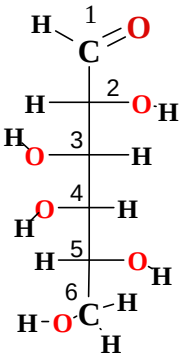
D-Ribose



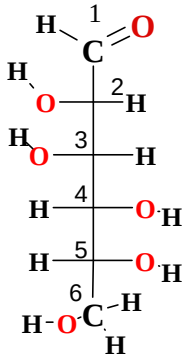
D-2-deoxy-ribose



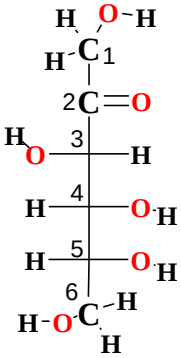
D-Glucose



D-Galactose



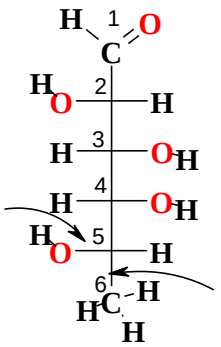
D-Mannose



D-Fructose

Haworth projection

Fisher projection

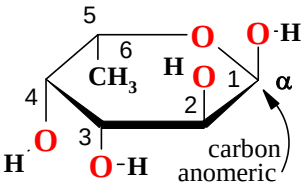


L-monosaccharide because **HO**- on carbon 5 is on the left

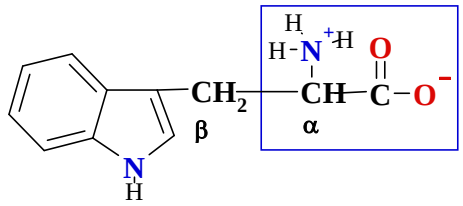
and is down carbon 6 6methyl –**CH_3**

Cyclic α-L-Fucose

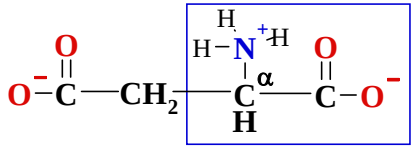
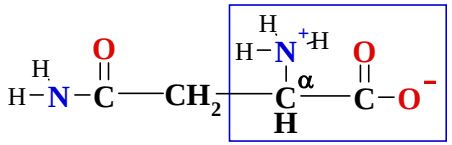
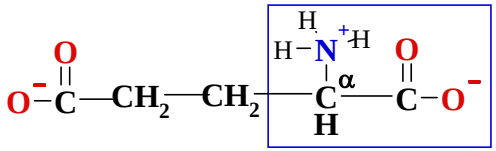
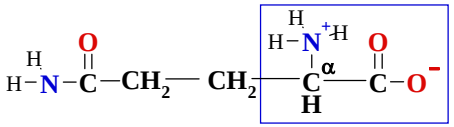
Hemi acetal ↓ oxygen



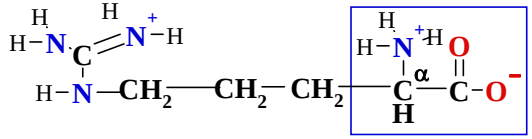
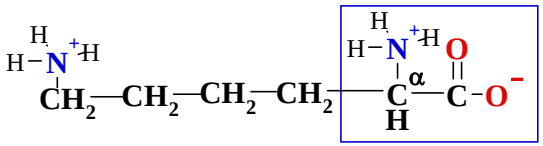
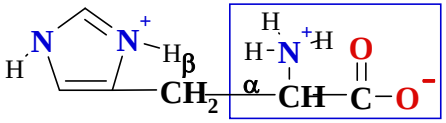
Carbon 6 is –**CH_3** rather than –**CH_2-OH**

Nr.	Name	Three, one	Structural formula **pH=7.36**
19.	Tryptophan	Trp, W	

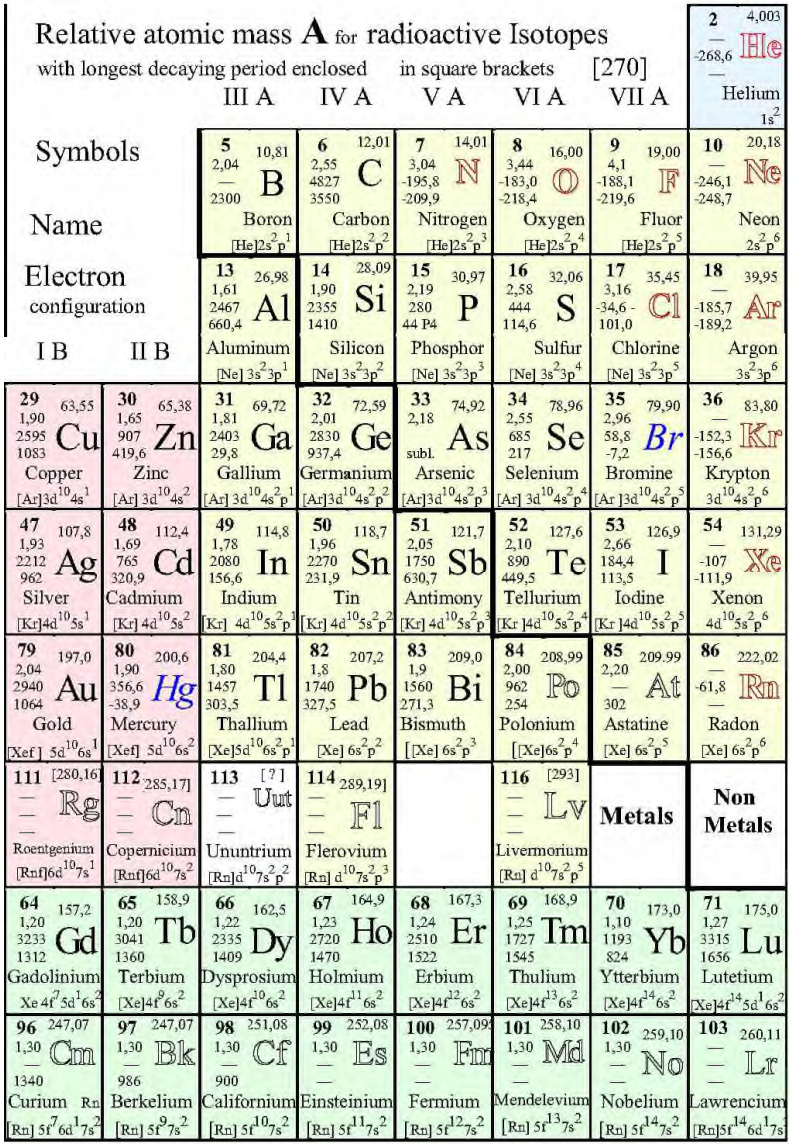
Acidic α-amino acids **red colors of oxygen O**

Nr.	Name	Three, one	Structural formula
10.	Aspartate Aspartic acid salt	Asp, D	
11.	Asparagine	Asn, N	
12.	Glutamate Glutamic acid salt	Glu, E	
13.	Glutamine	Gln, Q	

Basic α-amino acids **blue colors of nitrogen N** **pH=7.36**

Nr.	Name	Three, one	Structural formula
14.	Arginine	Arg, R	
15.	Lysine	Lys, K	
16.	Histidine	His, H	

Periodic Table of ELEMENTS



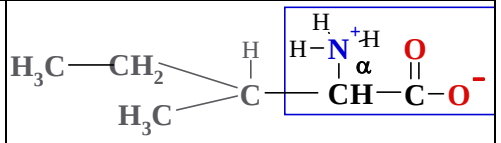
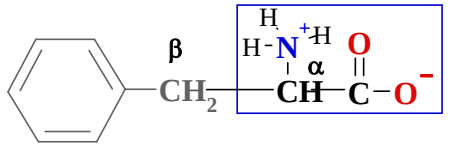
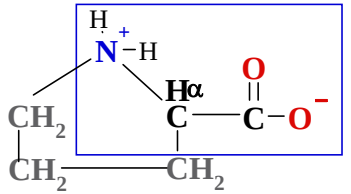
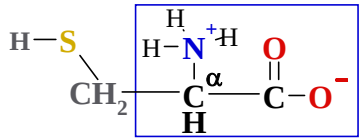
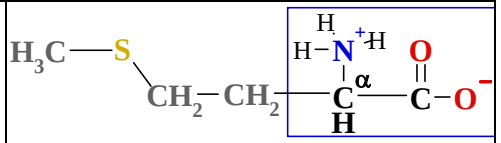
Solubility Table

SOLUBILITY OF ACIDS, BASES AND SALTS IN WATER

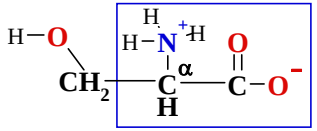
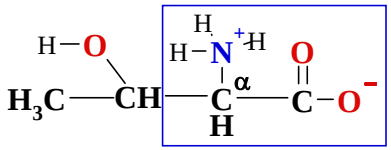
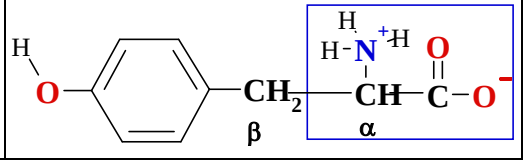
	H^+	NH_4^+	K^+	Na^+	Li^+	Ba^{2+}	Sr^{2+}	Ca^{2+}	Mg^{2+}	Al^{3+}
OH^-	H_2O	**s**	**s**	**s**	**s**	**s**	**m**	**m**	**n**	**n**
F^-	**s**	**s**	**s**	**s**	**n**	**m**	**n**	**n**	**m**	**m**
Cl^-	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**
Br^-	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**
I^-	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**
S^{2-}	s	**s**	**s**	**s**	**s**	**s**	**s**	+	**n**	+
SO_3^{2-}	s↑	**s**	**s**	**s**	**s**	**n**	**n**	**n**	**m**	+
SO_4^{2-}	∞	**s**	**s**	**s**	**s**	**n**	**n**	**m**	**s**	**s**
PO_4^{3-}	**s**	**s**	**s**	**s**	**m**	**n**	**n**	**n**	**n**	**n**
CO_3^{2-}	s↑	**s**	**s**	**s**	**s**	**n**	**n**	**n**	**n**	+
SiO_3^{2-}	**n**	-	**s**	**s**	**s**	**n**	**n**	**n**	**n**	**n**
NO_3^-	∞	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**
CH_3COO^-	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**

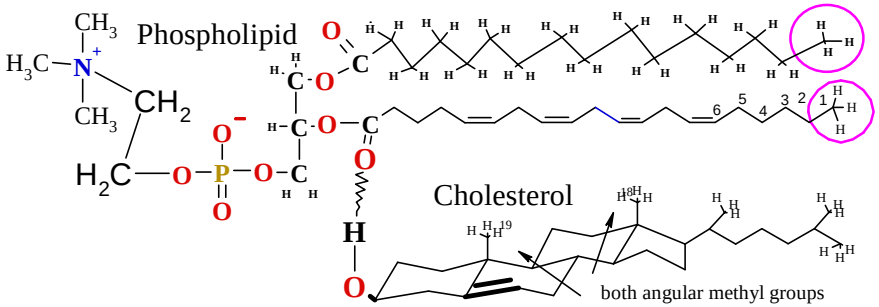
s – soluble; **m** – slightly soluble; n – **insoluble**; ∞-unlimited solubility;
s↑ - decomposes in water with gas emission; + - reacts with water;
– - substance does not exist

	Zn^{2+}	Fe^{2+}	Fe^{3+}	Mn^{2+}	Pb^{2+}	Cu^{2+}	Hg^{2+}	Ag^+	Cr^{3+}
OH^-	**n**	**n**	**n**	**n**	**n**	**n**	-	-	**n**
F^-	**m**	**m**	**n**	**s**	**m**	**s**	+	**s**	**m**
Cl^-	**s**	**s**	**s**	**s**	**m**	**s**	**s**	**n**	**s**
Br^-	**s**	**s**	**s**	**s**	**m**	**s**	**m**	**n**	**s**
I^-	**s**	**s**	-	**s**	**n**	-	**n**	**n**	**s**
S^{2-}	**n**	**n**	+	**n**	**n**	**n**	**n**	**n**	-
SO_3^{2-}	**n**	**n**	+	**n**	**n**	-	-	**n**	-
SO_4^{2-}	**s**	**s**	**s**	**s**	**n**	**s**	+	**m**	**s**
PO_4^{3-}	**n**	**n**	**n**	**n**	**n**	**n**	**n**	**n**	**n**
CO_3^{2-}	**n**	**n**	+	**n**	**n**	-	-	**n**	-
SiO_3^{2-}	**n**	**n**	**n**	**n**	**n**	**n**	-	-	-
NO_3^-	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**
CH_3COO^-	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**	**s**

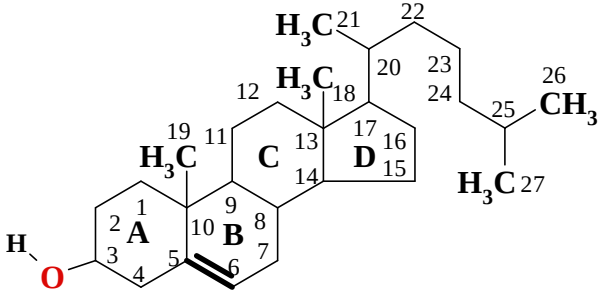
Nr.	Name	Three, one	Structural formula **pH=7.36**
5.	Isoleucine	Ile, I	
17.	Phenylalanine	Phe, F	
20.	Proline	Pro, P	
8.	Cysteine **S sulfur** non-polar	Cys, C	
9.	Methionine **S sulfur** non-polar	Met, M	

Polar R groups pink colors due to oxygen **O** bluish colors of nitrogen **N**

6.	Serine	Ser, S	
7.	Threonine	Thr, T	
18.	Tyrosine	Tyr, Y	

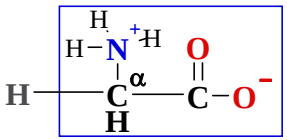
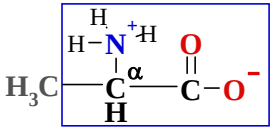
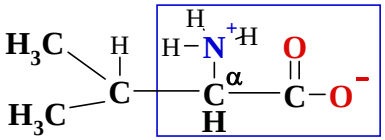
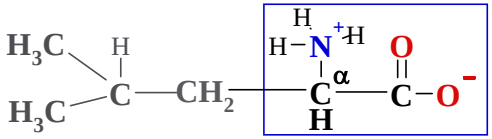


Phosphatidyl **Choline**/**Cholesterol** complex in cell **membranes**



Cholesterol Steroid Lipid Rings are labeled **A**, **B**, **C** and **D**. Double bond between 5 and 6 >**C=C**< and alcohol **HO-** at carbon 3. Angular methyl groups **–CH_3** labeled 18, 19 or splinter 21, 26, 27 clutch fixing molecules in membrane stabile.

Lα-Amino Acids Non-polar, aliphatic, aromatic R groups left C**α**

Nr.	Name	Three, one	Structural formula **pH=7.36**
1.	Glycine	Gly, G	
2.	Alanine	Ala, A	
3.	Valine	Val, V	
4.	Leucine	Leu, L	

Physical Constants and Unit Conversions

	Sign	Unit	Examples
Number of moles Amount of substance	**n**	mol	*$n(H_2SO_4)$ = 0.5 mol*
Count of equivalents for reaction of compound	**z**	eq	*Two valent acid $z(H_2SO_4)$ = 2 eq*
Number of equivalent moles for reaction	**n^z**	eq·mol	*$n^z(H_2SO_4)$ = 1.0 eq·mol*
Mass of substance	**m**	g, kg, t	*$m(H_2SO_4)$ = 49 g* *m = 0.049 kg; m = 1.03 t*
Mass of solution	**m(solution)**	, g	*$m(H_2O$ 1liter) = 1000 g*
Volume of solution	**V**	L mL, m^3	*V (NaCl sol.) = 0.174 L* *V = 174 mL, V =0.000174 m^3*
Density	**ρ**	g/mL kg/ m^3	*ρ(NaOH sol.) = 1.04 g/mL* *ρ = 1.78 kg/m^3*
Molar mass	**M**	g/mol	*$M(H_2SO_4)$ = 98 g/mol*
Mass fraction	**w**	Unit less no 0 < w < 1	*$w(H_2SO_4)$ = 0.243*
Mass fraction,%	**w%**	% , ***procentum*** 0%< w% <100%	*w%(H_2SO_4) = 24.3 %*
parts per million	**ppm**	Unit less 0<ppm<1 000 000	*ppm(H_2SO_4) = 243 000 ppm*
Promill alcohol in blood	**pml**	Unit less 0<pml<5	*pml(H_3CCH_2OH) = 0.1 pml*
Molar concentration	**c_M**	mol/L = M olarity	*$c_M(H_2SO_4)$ = 2.5 mol/L* *$c_M(H_2SO_4)$ = 2.5 M* *[2.5 molar solution of H_2SO_4]*
Normal concentration	**c_N**	eq·mol/L = = N ormality	*$c_N(H_2SO_4)$ = 5.0* eq·mol/L *$c_N(H_2SO_4)$ = 5.0 N* *[5.0 normal solution of H_2SO_4]*
temperature	**t**	**° C , Celsius**	*t = 25° C*
Absolute Temperature	**T**	**K , Kelvin**	*T = 298.15 K*
Atomic size distance units	**l**	**Å , angstrem**	*1Å = 10^{-8} cm= 10^{-10} m= 0.1 nm*

Universal gas constant *R* = 8.3144 $J \cdot K^{-1} \cdot mol^{-1}$

Molar volume V_o of an ideal gas at 273 K and $1.01 \cdot 10^5$ Pa $V_o = 2.24 \times 10^{-2}$ $m^3 \cdot mol^{-1}$ **(V_o=22.4 L·mol^{-1})**

Specific heat capacity C_p of water = 4.18 $kJ \cdot kg^{-1} \cdot K^{-1}$ (= 4.18 $J \cdot g^{-1} \cdot K^{-1}$)

Ionic product constant for water $K_w = 1.00 \cdot 10^{-14}$ at 298 K

Temperature conversation from °C to K T [K] = t [°C] + 273.15

1 atm = $1.013 \cdot 10^5$ Pa = 760 mm Hg

1 dm^3 = 1 litre = 1×10^{-3} m^3 = 1×10^3 cm^3

Table of chemical and physical values

	Basic Formula	expression I	expression II
Substance amount n & *mass* m	$n = \frac{m}{M}$	$m = n \cdot M$	$M = \frac{m}{n}$
Density ρ *of solution*	$\rho = \frac{m(solution)}{V}$	$m(solution) = \rho \cdot V$	$V = \frac{m(solution)}{\rho}$
Mass fraction (from mass) $w_{\%} = \frac{m \bullet 100\%}{m(solution)}$		$m = \frac{w\% \bullet m(solution)}{100\%}$ $m(solution) = \frac{m \bullet 100\%}{w\%}$	
Molar concentration molarity	$c_M = \frac{n}{V}$	$n = c_M \cdot V$	$V = \frac{n}{c_M}$
Molar concentration molarity (from mass)	$c_M = \frac{m}{M \bullet V}$	$m = c_M \cdot M \cdot V$	$M = \frac{m}{c_M \bullet V}$
Normal concentration normality	$c_N = c_M \cdot z$	$z = \frac{c_N}{c_M}$	$c_M = \frac{c_N}{z}$
Dilution	$c_{M1} \cdot V_1 = c_{M2} \cdot V_2$	$V_1 = \frac{c_{M2} \bullet V_2}{c_{M1}}$	$c_{M2} = \frac{c_{M1} \bullet V_1}{V_2}$
Water addition $\Delta V_{H2O} = V_2 - V_1$	$c_{M1} \cdot V_1 = c_{M2} \cdot (V_1 + \Delta V_{H2O})$ $V_2 = \frac{c_{M1} \bullet V_1}{c_{M2}}$		$\Delta V_{H2O} = V_2 - V_1$

Best choice of volume is one liter that V=1 L =>1000 mL

$$c_M = \frac{m}{M \bullet V} \; ; \; c_M = \frac{m}{M \bullet 1\text{Liter}} = \frac{m}{M}$$

and using density ρ for m(solution) calculation V=1000 mL

$m(solution) = \rho \cdot V = \rho \cdot 1000$ mL (units of m(solution) is in grams)

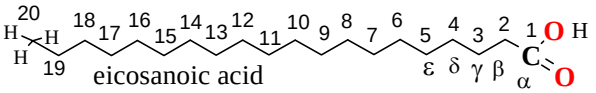
FATTY ACIDS

Saturated **name**	**C**	*Unsaturated* **Common name**	**Name of salt**	**C:Double bonds ? :**	**ω ?**
Caproic acid					
Caprylic acid	8:0	Myristoleic acid	Myristoleate	14:1	**ω-5**
Capric acid	10:0	Palmitoleic acid	Palmitoleate	16:1	**ω-7**
Lauric acid	12:0	Sapienic acid	Sapienoate	16:1	**ω10**
Myristic acid	14:0	Oleic acid	Oleate	18:1	**ω-9**
Palmitic acid	16:0	Elaidic acid	Elaidinoate	18:1	trans
Stearic acid	18:0	Vaccenic acid	Vacceniate	18:1	trans
Arachidic acid	20:0	Linoleic acid	Linoleate	18:2	**ω-6**
Behenic acid	22:0	Linoelaidic acid	Linoelaidiate	18:2	trans
Lignoceric acid	24:0	α-Linolenic acid	α-Linolenate	18:3	**ω-3**
Cerotic acid	26:0	Arachidonic acid	Arachidonate	20:4	**ω-6**
		Eicosapentaenoic acid	Eicosapentaenoate	20:5	**ω-3**
		Erucic acid	Eruciate	22:1	**ω-8**
		Docosahexaenoic acid	Docosahexaenoate	22:6	**ω-3**

Saturated fatty acids

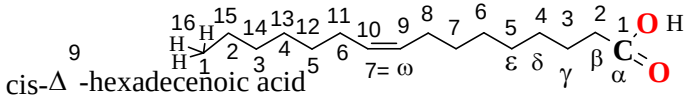
$CH_3(CH_2)_{14}CO_2H$ - hexadecanoic acid — palmitic acid **C16**

$CH_3(CH_2)_{16}CO_2H$-octadecanoic acid — stearic acid **C18**

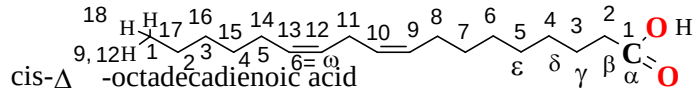


arachidic acid **C20:0**

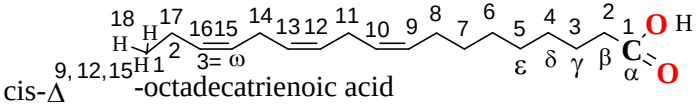
Unsaturated fatty acids



palmitoleic acid **C16:1** ; ω-7



linoleic acid **C18:2** ; ω-6

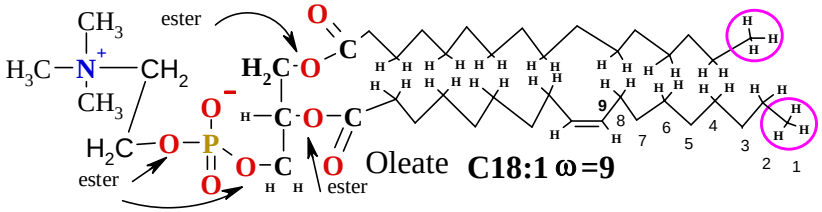


Essential ω-6,-3

α-linolenic acid **C18:3** ; ω-3

Phosphatidyl **Choline** **Membrane** building molecular components

Phosphate ester of glycerol C3 **Palmitate** ester of glycerol C1



Choline **Glycerol** All atoms colored **CPK** labels

Amino Acid	pKa-COOH	pKa-NH3+	pKa R group
Isoleucine	2.36	9.68	
Valine	2.32	9.62	
Leucine	2.36	9.60	
Phenylalanine	1.83	9.13	
Cysteine	1.96	10.28	8.18
Methionine	2.28	9.21	
Alanine	2.34	9.69	
Proline	1.99	10.96	
Glycine	2.34	9.60	
Threonine	2.11	9.62	
Serine	2.21	9.15	
Tryptophan	2.38	9.39	
Tyrosine	2.20	9.11	10.07
Histidine	1.82	9.17	6.00
Aspartate	1.88	9.60	3.65
Glutamate	2.19	9.67	4.25
Asparagine	2.02	8.80	
Glutamine	2.17	9.13	
Lysine	2.18	8.95	10.53
Arginine	2.17	9.04	12.48

Protein constitute amino acids protolytic equilibria average calculation expression for

protolytic constant as well isoelectric point pK_a=IEP value

with number of NpK_a summed constants pK_a in each molecule given in table includes the sum of: side groups $\Sigma pKa_{R\ group}$, N-terminus $pKa_{Nterminus}NH_3^+$ and C-terminus $pKa_{CterminusCOO^-}$. In *Ostwald's dilution law* pH calculation is used pK_a by concentration C logarithm

$$pH=\frac{pK_a-\log C}{2}=.....$$

$$pK_a=IEP=(\Sigma pK_{aR\ side\ residue}+pK_{aNterminus}+pK_{aCterminus})/NpK_a$$

Amino acid or protein molecules have four type acidic functional groups: **-COOH** neutral, **-NH_3^+** positive charged, phenol **-OH** neutral, **-SH** neutral. At physiologic pH 7.36 groups exist prevailing: negative charged **R-COO^-**, positive charged amino groups **R-NH_3^+** , neutral group of Tyrosine phenol-**OH** and Cysteine sulfo hydrogen **R--SH**.

Four parallel protolytic equilibria:

Acid ⇔ base + H^+

1. **R-COOH** ⇔ **R-COO^-** + H^+,
2. **R-NH_3^+** ⇔ **R-NH_2** + H^+
3. **Tyr**-phenol-**OH** ⇔ **Tyr**-phenol-**O^-** + H^+,
4. **Cys--SH** ⇔ **Cys—S^-** + H^+

Standard Electrode Potentials

Element	Oxidized form	Number of electrons e^-	Reduced form	Standard potential E^o, V
N	$NO_3^-+2H^+$	1	$NO_{2\,(g)}+H_2O$	+0,80
	$NO_3^-+H_2O$	2	$NO_2^-+2OH^-$	+0,01
	$NO_3^-+2H^+$	2	$NO_2^-+H_2O$	+0,94
	$NO_3^-+4H^+$	3	$NO_{(g)}+2H_2O$	+0,96
	$NO_3^-+7H_2O$	8	$NH_4OH+9OH^-$	–0,12
	$NO_{2(g)}$	1	NO_2^-	+0,88
	$NO_2^-+2H^+$	1	$NO_{(g)}+H_2O$	+0,99
Br	Br_2	2	$2Br^-$	+0,96
Bi	$BiO_3^-+6H^+$	2	$Bi^{3+}+3H_2O$	+1,80
H	**$2H^+$**	**2**	**H_2**	**+0,00**
O	$O_{2\ aqua}+4H^+$	4	$2H_2O$	+1,22
	$H_2O_2+2H^+$	2	$2H_2O$	+1,78
	$O_{2\,(g)}+2H^+$	2	H_2O_2	+0,68
Mn (H^+)	$MnO_4^-+8H^+$	5	$Mn^{2+}+4H_2O$	+1,51
(H_2O)	$MnO_4^-+2H_2O$	3	$MnO_2\downarrow+4OH^-$	+0,60
(OH^-)	MnO_4^-	1	MnO_4^{2-}	+0,56
Pb	$PbO_2\downarrow+4H^+$	2	$Pb^{2+}+2H_2O$	+1,80
S	$SO_4^{2-}+2H^+$	2	$SO_3^{2-}+H_2O$	+0,20
	$SO_4^{2-}+H_2O$	2	$SO_3^{2-}+2OH^-$	–0,93
	$S\downarrow$	2	S^{2-}	–0,48
	$S\downarrow+2H^+$	2	H_2S	+0,17
	$S_4O_6^{2-}$	2	$2S_2O_3^{2-}$	+0,10
Fe	Fe^{3+}	1	Fe^{2+}	+0,77
Ag	**Ag^+**	1	**Ag**	+0,799
I	I_2	2	$2I^-$	+0,54
Cu	**Cu^{2+}**	2	**Cu**	+0,337
F	F_2	2	$2F^-$	+2,87
Cl	**Cl_2**	2	**$2Cl^-$**	+1,36
hypochlorite	OCl^-+2H^+	2	H_2O+Cl^-	+1,49
Cr	$Cr_2O_7^{2-}+14H^+$	6	$2Cr^{3+}+7H_2O$	+1,33
	$CrO_4^{2-}+4H_2O$	3	$Cr(OH)_3\downarrow+5OH^-$	–0,13
C	$2CO_2+2H^+$	2	$H_2C_2O_4$	–0,49
Cr	**Cr^{3+}**	3	**Cr**	–0,744
Zn	**Zn^{2+}**	2	**Zn**	–0,763
Al	$AlO_2^-+2H_2O$	3	$Al+4OH^-$	–2,35

Ist type **Electrode potential E**

Red(Me)↔ Ox(Me^{n+}) + ne^-,n=3, E_o= -0.744V

Cr ⇌ Cr^{3+} + $3e^-$; n = 3; $CrCl_3$ salt is conc. of ion [Cr^{3+}]= 0.03 M

$E = E^o + 0.0591/n \cdot \lg[Me^{n+}]$; $E = E_o + 0.0591/n \cdot \log([Cr^{3+}]/[Cr])$

Red-Ox **Electrode potential E** ; $E = E^o + 0.0591/n \cdot \lg([Ox]/[Red])$;

$E = E_o + 0.0591/n \cdot \log([MnO_4^{2-}] \cdot [H^+]^8/[Mn^{2+}])$; concentration $[H^+]^8 = 10^{-pH \cdot 8}$

$MnO_4^- + 8H^+ + 5e^- \rightleftharpoons Mn^{2+} + 4H_2O$; E_o=+1,51 V

|——Ox form —| ↔|—Red form—| if [MnO_4^{2-}]=[Mn^{2+}] & pH=7;

$E = 1.51 + 0.0591/5 \cdot \log(10^{-8 \cdot pH}) = 1.51 - 8 \cdot 7 \cdot 0.01182 = 1.51 - 0.01182 \cdot 56 = 1.51 - 0.662 = 0.848$

Ostwald's dilution law

$$K_{dis.} = \frac{\alpha^2 \cdot c_M}{1-\alpha}$$

For weak electrolytes

$K_{a.} = 1.75 \cdot 10^{-5}$; c_M = 0,01 M ; pH = 3.3785

$\alpha = \sqrt{\frac{K_{dis.}}{c_M}}$; $C_b = \frac{[OH^-]^{-2}}{K_b} = \frac{10^{-pOH \bullet 2}}{K_b}$; $\alpha = \sqrt{\frac{1.75 \cdot 10^{-5}}{0.01\,M}} = 0.0418 = 4.18\%$

$C = \frac{[H^+]^2}{K_a} = \frac{10^{-pH \bullet 2}}{K_a}$ $K_a = \frac{[H^+]^{-pH \bullet 2}}{1 \cdot 0.01\,M} = \frac{10^{-3.3785 \bullet 2}}{0.01} = \frac{10^{-6.757}}{0.01} = 1.75 \cdot 10^{-5}$

For strong electrolytes

HCl strong acid pH = 2.4 ; c_M = 0,01 M

$\alpha = \frac{[H^+]}{z \cdot C} = \frac{10^{-pH}}{z \cdot C}$ $\alpha = \frac{[H^+]}{1 \cdot 0.01\,M} = \frac{10^{-2.4}}{0.01} = 0.3981 = 39.81\%$

Isotonic coefficient

i=1+α·(m-1); 0 < α < 1

for total osmolarity Δc_{osm} is $i \cdot c_M$ total osmolar concentration $\Delta c_{osm} = i \cdot c_M$

Glucose as non electrolyte α=0

i=1+0·(1-1)=1 , $\Delta c_{osm} = 1 \cdot c_M$

Na_2SO_4 strong electrolyte 0.3<α< 0.999

$Na_2SO_4 \rightarrow 2Na^+ + SO_4^{2-}$

i=1+0,999·(3-1) = 2.998 , $\Delta c_{osm} = 2.998 \cdot c_M$

Osmotic pressure kPa on membrane is energy Jouls in cell volume liter

$\pi = \Delta c_{osm} \cdot R \cdot T$; $kPa = \frac{J}{L}$

$\Delta c_{osm} = i \cdot c_M$

At temperature 25 C or 298.15 K

0.2M glucose non-electrolyte, α=0; i = 1 sol.

$\pi = 1 \cdot 0.2M \cdot 8.3144 \frac{J}{K \cdot mol} \cdot 298.15K = 495.79$ kPa

0.2M Na_2SO_4 strong electrolyte, α=1; i = 3 sol.

$\pi = 3 \cdot 0.2M \cdot 8.3144 \frac{J}{K \cdot mol} \cdot 298.15K = 1487.38$ kPa

Ionic strength I or μ

$I = \frac{1}{2} \sum \alpha \cdot c_i \cdot z_i^2$

is total concentration of ions

$I = 1/2\ (2 \cdot 0.2M \cdot (+1)^2 + 0.2M \cdot (-2)^2$

0.2M Na_2SO_4solution

salt => sodium and sulfate ions

Na_2SO_4 => $2Na^+ + SO_4^{2-}$

$= \frac{1}{2}(2 \cdot 0.2M \cdot 1 + 0.2M \cdot 4) = \frac{1}{2}(0.4 + 0.8) = 0.6$

Complex compounds and light absorption

Charges and coordination numbers of some central ions.

Charge of central ion	*Coord. number by empiric rule*	*examples*	*Other possible coord. numbers*	*examples*
+1	2	Ag^+, Cu^+, Au^+	4	Li^+
+2	4	Cu^{2+}, Hg^{2+}, Pt^{2+}, Ni^{2+}, Zn^{2+} Cd^{2+}, Co^{2+}, Pb^{2+},	6	Fe^{2+}
+3	6	Fe^{3+}, Al^{3+}, Cr^{3+}, Co^{3+}	4	Au^{3+}

Outer sphere dissociation as strong electrolyte
because complex compounds always are water soluble
strong electrolytes like as salts, strong acids and strong bases:

$$[Cu(NH_3)_4]SO_4 \rightleftharpoons [Cu(NH_3)_4]^{2+} + SO_4^{2-}$$

Instability constant $K_{inst.}$ ***of complex compound*** $[Cu(NH_3)_4]^{2+}$ **destruction**

in secondary *dissociation* *complex compound* $[Cu(NH_3)_4]^{2+}$ **equilibrium :**

$$[Cu(NH_3)_4]^{2+} \rightleftharpoons Cu^{2+} + 4NH_3$$

$$K_{inst.} = \frac{[Cu^{2+}] \cdot [NH_3]^4}{[Cu(NH_3)_4]^{2+}};$$

Flip over reaction **to formation reaction equilibrium**

$$Cu^{2+} + 4NH_3 \rightleftharpoons [Cu(NH_3)_4]^{2+}$$

$$K_{stab.} = \frac{1}{K_{instab.}} = \frac{[Cu(NH_3)_4]^{2+}}{[Cu^{2+}] \cdot [NH_3]^4}$$

Light absorption **A=log(Io/I)=a•c_M•l**

Acid-Base Calculations. Buffer Solutions

Calculate, how many milliliters of 0,1 M HCOOH and 0,2 M HCOONa have t taken
to obtain a buffer, having pH=3,0 and total volume 1 liter. Ka=$2\cdot10^{-4}$

$$\mathbf{pH = pK_a + \log\left(\frac{c_{salt}\cdot v_{salt}}{c_{acid}\cdot v_{acid}}\right)}$$

V_{salt}= x; V_{acid} = 1000 – x

$$3,0 = -\log(2\cdot10^{-4)} + \log\left(\frac{0,2x}{0,1\cdot(1000-x)}\right)$$

$$3,0 = 3,7 + \log\left(\frac{0,2x}{0,1\cdot(1000-x)}\right)$$

$$-0,7 = \log\left(\frac{0,2x}{0,1\cdot(1000-x)}\right)$$

$$10^{-0,7} = \left(\frac{0,2x}{0,1\cdot(1000-x)}\right)$$

$$0.199 = \left(\frac{0,2x}{0,1\cdot(1000-x)}\right)$$

0,199 · (100 – 0,1x) = 0,2x
x = 90,6 mL
V_{salt}= 90,6 mL; V_{acid} = 1000 – 90,6 mL=909,5 mL

1. *Buffer system can be composed of a weak acid and its salt with a strong base,*
2. *Buffer system can be composed of a weak base and its salt with a strong acid,*
3. *Buffer system can be composed of a weak acid and strong base in limited supply,*
4. *Buffer system can be composed of a weak base and strong acid in limited supply,*
5. *Buffer system can be composed of a weak bivalent acid and its acidic salt,*
6. *Buffer system can be composed of two salts of the same polyvalent acid, differing in **1** hydrogen ion*, where the salt containing greater number of hydrogen ions plays the role of acid and the salt, containing lower number of hydrogen ions plays the role of the base.

Thermodynamic Calculations

Enthalpy of reaction: $\Delta H_{reaction} = \sum\Delta H^o_{products} - \sum\Delta H^o_{initial\ comp.}$

Dispersed (lost) heat in surrounding : $\Delta S_{dispersed} = -\Delta H_{reaction} / T$

Entropy of reaction: $\Delta S_{reaction} = \sum\Delta S^o_{products} - \sum\Delta S^o_{initial\ comp.}$

Gibbs free energy of reaction $\Delta G^o_{reaction} = \Delta H^o_{reaction} - T\bullet\Delta S^o_{reaction}$

Negative **ΔG** means that the process (reaction) is **spontaneous** (**ΔG<0)**
Positive **ΔG** means that the process is **non-spontaneous** (**ΔG>0)**
ΔG = 0 means that the process is at an equilibrium

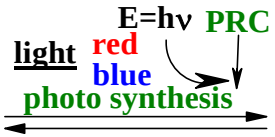
For total account of energy dispersion $\Delta S_{total} = \Delta S_{reaction} + \Delta S_{heat\_dispersed}$
If ΔS_{total} negative energy accumulates $\Delta G_{accumulate} = T\bullet\Delta S_{total} > 0$ in products and if ΔS_{total} positive energy dispersed, lost is $\Delta G_{dispersed} = T\bullet\Delta S_{total} < 0$.
$\Delta G^o_{reaction}$ is opposite singe with identical value $\Delta G^o_{reaction} = |T\bullet\Delta S_{total}|$

Gibbs free energy for equilibrium: $\Delta G_{reaction} = \sum\Delta G^o_{product} - \sum\Delta G^o_{initialcomp.}$

Combustion heat of reaction for food containing energy amount evaluation:

$$\Delta H^{combustion}_{reaction} = \sum\Delta H^{combustion}_{initial\_comp.} - \sum\Delta H^{combustion}_{products}$$

Photo Synthesis PRC light **blue red** photon energy **E=hν**



6 CO_{2aqua} + 6 H_2O + Q → **$C_6H_{12}O_6$ + 6 O_{2aqua}**
Carbon dioxide water glucose oxygen

$$\Delta H_{reaction} = (\Delta H^\circ_{C6H12O} + 6\Delta H^\circ_{O2}) - (6\Delta H^\circ_{H2O} + 6\Delta H^\circ_{CO2})$$

$$\Delta S_{reaction} = (\Delta S^\circ_{C6H12O} + 6\Delta S^\circ_{O2}) - (6\Delta S^\circ_{H2O} + 6\Delta S^\circ_{CO2})$$

$$\Delta G^o_{reaction} = \Delta H^o_{reaction} - T\bullet\Delta S^o_{reaction}$$

$$\Delta S_{dispersed} = -\Delta H_{reaction} / T$$

$$\Delta S_{total} = \Delta S_r + \Delta S_{dispersed}$$

acumulate energy $\Delta G_{accumulate} = T\bullet\Delta S_{total}$ in products **$C_6H_{12}O_6$ + 6 O_{2aqua}**

$\Delta G_{accumulate} = -\Delta G^o_{reaction}$ organisms use in Krebs cycle producing :
$C_6H_{12}O_6$ + 6 O_{2aqua} => **6 $CO_{2\ aqua}$ + 6 H_2O + Q** heat and energy for life

Thermodynamic Calculations for reactions

Equilibrium constant K is expressed as $K = e^{-\frac{\Delta G}{RT}}$, where

depends on: R = 8.3144 **Universal gas constant** & **e**=2.7…natural number,

1) $\Delta G_{reaction}$ free energy change and on

2) temperature T

Equilibrium $aA + bB \underset{revers}{\overset{direct}{\rightleftarrows}} cC + dD$ **constant** K not depends on:

concentrations X_A, X_B, X_C, X_D for mixture of compounds A, B, C, D

being in the state of **Equilibrium** $K = \frac{X_C^c \cdot X_D^d}{X_A^a \cdot X_B^b}$

Reaction velocity temperature coefficient γ is average from range 2÷4

$\gamma = \frac{k_{T+10}}{k_T} = 2 \div 4$ times greater velocity constant k_{T+10} as for k_T,

for experimentally example: $\gamma = \frac{k_{150^\circ}}{k_{140^\circ}} = 3$ times greater at T=150ºC

Reaction time at different temperatures

$$t_{T_2} = \frac{t_{T_1}}{\gamma^{\frac{T_2 - T_1}{10}}} \qquad t_{150^\circ C} = \frac{t_{140^oC}}{3^{\frac{150^oC - 140^oC}{10}}}$$

If $t_{140^\circ C} = 900$ s and $\gamma = \frac{k_{150^oC}}{k_{140^oC}} = 3$

$$t_{150^\circ C} = \frac{900\ s}{3^{\frac{150^oC - 140^oC}{10}}} = \frac{900\ s}{3^{\frac{10}{10}}} = \frac{900\ s}{3^1} = \frac{900\ s}{3}\ s = 300s$$

Acid-Base Calculations. Buffer Solutions

Formula	Example
pH= -log [H$^+$]= -log(α·z·c$_M$)	What is the pH of 0.0850 M HNO_3 if **α** =1 **z** =1? pH = - lg (0.085) = 1.07
pOH= -log [OH$^-$]=-log(α·z·c$_M$)	What is the pH of 0.00765 KOH if **α** =1 **z** =1? [KOH] = [OH$^-$]
pH + pOH = 14	pOH = 2.12 and pH = 11.88 pH = 14 - pOH
pK$_a$ = - lg [K$_a$] **pK$_b$ = - lg [K$_b$]**	$K_a = 1.74 \cdot 10^{-5}$ $pK_a = -\lg(1.74 \cdot 10^{-5}) = 4.75$
[H$^+$] = 10 $^{-pH}$	pH=1; [H$^+$] =10^{-1} = 0.1
[OH$^-$] = 10 $^{-pOH}$	pOH=1; [OH$^-$] =10^{-1} = 0.1
K=10 $^{-pK}$	pKa = 4.75 ; Ka= $10^{-4.75}$ =$1.74 \cdot 10^{-5}$
	pKb = 4.74 ; Kb= $10^{-4.74}$ =$1.79 \cdot 10^{-5}$
Dissociation constant, weak acid **K$_a$** = $\frac{[H^+]\cdot[A^-]}{[HA]}$	$CH_3COOH \rightleftarrows CH_3COO^- + H^+$ $K_a = \frac{[CH_3COO^-]\cdot[H^+]}{[CH_3COOH]}$
Dissociation constant, weak base: **K$_b$**= $\frac{[OH^-]\cdot[B^+]}{[BOH]}$	$NH_4OH \rightleftarrows NH_4^+ + OH^-$ **K$_b$** = $\frac{[OH^-]\cdot[NH_4^+]}{[NH_4OH]}$
Buffer solution (weak acid/salt of weak acid) **pH = pK$_a$ + lg**$\left(\frac{n_{salt}}{n_{acid}}\right)$ **pH = pK$_a$ + log**$\left(\frac{c_{salt}\cdot v_{salt}}{c_{acid}\cdot v_{acid}}\right)$	Calculate **pH** of a formiate buffer **(HCOOH/HCOONa)**, if the buffer is composed from **300** mL of **0.15** M **HCOOH** and **200** mL of **0.09** M **HCOONa** solutions, **K$_a$**=**2·10^{-4}** **pH=pK$_a$+log** $\frac{c_{salt}\cdot v_{salt}}{c_{acid}\cdot v_{acid}}$ **= -log2·10^{-4}+log** $\frac{200\times0.09}{300\times0.15}$ = **= 3.7+log** $\frac{18}{45}$ **= 3.7+log** 0.4= 3.7-0.398=3.3
Buffer solution (weak base/salt of weak base) **pOH = pK$_b$ + log**$\left(\frac{n_{salt}}{n_{base}}\right)$ **pOH = pK$_b$ + log**$\left(\frac{c_{salt}\cdot v_{salt}}{c_{base}\cdot v_{base}}\right)$	Calculate **pH** of a buffer, composed from **80** mL **0.1** M **NH$_4$OH** and **120** mL of **0.17** M **NH$_4$Cl** solutions, **K$_b$**=**1.8·10^{-5}**. **pOH=pK$_b$+log** $\frac{c_{salt}\cdot v_{salt}}{c_{base}\cdot v_{base}}$ **= -log1.8·10^{-5}+log** $\frac{120\times0.17}{80\times0.1}$ = **= 4.74+log** $\frac{20.4}{8}$ **= 4.74+log** 2.55= 4.744+0.406=5.15