

DATA BOOKLET FOR MEDICAL CHEMISTRY

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2023

Periodic Table of ELEMENTS

Relative atomic mass A_r for radioactive Isotopes with longest decaying period enclosed in square brackets [270]							2	4,003							
		III A	IV A	V A	VI A	VII A	—	⁴ He							
Symbols		5	10,81	6	12,01	7	14,01	8	16,00	9	19,00	10	20,18		
Name		Boron		Carbon		Nitrogen		Oxygen		Fluor		Neon			
Electron configuration		Aluminum		Silicon		Phosphor		Sulfur		Chlorine		Argon			
I B		II B		[He]2s ² p ¹		[He]2s ² p ²		[He]2s ² p ³		[He]2s ² p ⁴		[He]2s ² p ⁵			
29	63,55	30	65,38	31	69,72	32	72,59	33	74,92	34	78,96	35	79,90	36	83,80
1,90	Cu	1,65	Zn	1,81	Ga	2,01	Ge	2,18	As	2,55	Se	2,96	Br	—	Kr
2595	Copper	907	Zinc	2403	Gallium	2830	Germanium	280	Arsenic	685	Selenium	58,8	Bromine	-152,3	Krypton
1083	[Ar]3d ¹⁰ 4s ¹	419,6	[Ar]3d ¹⁰ 4s ²	29,8	[Ar]3d ¹⁰ 4s ² p ¹	937,4	[Ar]3d ¹⁰ 4s ² p ²	subl.	[Ar]3d ¹⁰ 4s ² p ³	217	[Ar]3d ¹⁰ 4s ² p ⁴	-7,2	[Ar]3d ¹⁰ 4s ² p ⁵	-189,2	3d ¹⁰ 4s ² p ⁶
47	107,8	48	112,4	49	114,8	50	118,7	51	121,7	52	127,6	53	126,9	54	131,29
1,93	Ag	1,90	Cd	1,98	In	2,05	Sn	2,10	Sb	2,10	Te	2,66	I	-107	Xe
2212	Silver	765	Cadmium	2080	Indium	2270	Tin	1750	Antimony	890	Tellurium	184,4	Iodine	-111,9	Xenon
962	[Kr]4d ¹⁰ 5s ¹	320,9	[Kr]4d ¹⁰ 5s ²	156,6	[Kr]4d ¹⁰ 5s ² p ¹	231,9	[Kr]4d ¹⁰ 5s ² p ²	630,7	[Kr]4d ¹⁰ 5s ² p ³	449,5	[Kr]4d ¹⁰ 5s ² p ⁴	113,5	[Kr]4d ¹⁰ 5s ² p ⁵	4d ¹⁰ 5s ² p ⁶	
79	197,0	80	200,6	81	204,4	82	207,2	83	209,0	84	208,99	85	209,99	86	222,02
2,04	Au	1,90	Hg	1,8	Tl	1,8	Pb	1,9	Bi	2,00	Po	2,20	At	-61,8	Rn
2940	Gold	356,6	Mercury	1457	Thallium	1740	Lead	1560	Bismuth	962	Polonium	302	Astatine	—	Radon
1064	[Xe]5d ¹⁰ 6s ¹	-38,9	[Xe]5d ¹⁰ 6s ²	303,5	[Xe]5d ¹⁰ 6s ² p ¹	327,5	[Xe]6s ² p ²	271,3	[Xe]6s ² p ³	252	[Xe]6s ² p ⁴	302	[Xe]6s ² p ⁵	[Xe]6s ² p ⁶	
111	[280,16]	112	[285,17]	113	[?]]	114	[289,19]			116	[293]				
—	Rg	—	Cn	—	Uut	—	Fl			—	Lv				
—	Roentgenium	—	Copernicium	—	Ununtrium	—	Flerovium			—	Livermorium				
—	[Rn]6d ¹⁰ 7s ¹	—	[Rn]6d ¹⁰ 7s ²	—	[Rn]6d ¹⁰ 7s ² p ¹	—	[Rn]d ¹⁰ 7s ² p ³			—	[Rn]d ¹⁰ 7s ² p ⁵				
64	157,2	65	158,9	66	162,5	67	164,9	68	167,3	69	168,9	70	173,0	71	175,0
1,20	Gd	1,20	Tb	1,22	Dy	1,23	Ho	1,24	Er	1,25	Tm	1,10	Yb	1,27	Lu
3233	Gadolinium	1301	Terbium	2335	Dysprosium	2720	Holmium	2510	Erbium	1727	Thulium	1193	Ytterbium	3315	Lutetium
1312	[Xe]4f ⁷ 5d ¹ 6s ²	1360	[Xe]4f ⁹ 6s ²	1409	[Xe]4f ¹¹ 6s ²	1470	[Xe]4f ¹³ 6s ²	1522	[Xe]4f ¹² 6s ²	1545	[Xe]4f ¹³ 6s ²	824	[Xe]4f ¹⁴ 6s ²	1656	[Xe]4f ¹⁴ 5d ¹ 6s ²
96	247,07	97	247,07	98	251,08	99	252,08	100	257,09	101	258,10	102	259,10	103	260,11
1,30	Cm	1,30	Bk	1,30	Cf	1,30	Es	1,30	Fm	1,30	Md	—	No	—	Lr
—	Curium	—	Berkelium	—	Californium	—	Einsteinium	—	Fermium	—	Mendelevium	—	Nobelium	—	Lawrencium
1340	[Rn]5f ⁷ 6d ¹ 7s ²	986	[Rn]5f ⁹ 7s ²	900	[Rn]5f ¹⁰ 7s ²	—	[Rn]5f ¹¹ 7s ²	—	[Rn]5f ¹² 7s ²	—	[Rn]5f ¹³ 7s ²	—	[Rn]5f ¹⁴ 7s ²	—	[Rn]5f ¹⁴ 6d ¹ 7s ²

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 ₂ O	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 ₃ COO ⁻	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 ₃ COO ⁻	S	s	s	s	s	s	s	s	s

Physical Constants and Unit Conversions

	Sign	Unit	Examples
Number of moles Amount of substance	n	mol	$n(\text{H}_2\text{SO}_4) = 0.5 \text{ mol}$
Count of equivalents for reaction of compound	z	eq	Two valent acid $z(\text{H}_2\text{SO}_4) = 2$ eq
Number of equivalent moles for reaction	n^z	eq·mol	$n^z(\text{H}_2\text{SO}_4) = 1.0 \text{ eq}\cdot\text{mol}$
Mass of substance	m	g, kg, t	$m(\text{H}_2\text{SO}_4) = 49 \text{ g}$ $m = 0.049 \text{ kg}; m = 1.03 \text{ t}$
Mass of solution	m(solution)	, g	$m(\text{H}_2\text{O } 1\text{ liter}) = 1000 \text{ g}$
Volume of solution	V	L mL, m ³	$V(\text{NaCl sol.}) = 0.174 \text{ L}$ $V = 174 \text{ mL}, V = 0.000174 \text{ m}^3$
Density	ρ	g/mL kg/m ³	$\rho(\text{NaOH sol.}) = 1.04 \text{ g/mL}$ $\rho = 1.78 \text{ kg/m}^3$
Molar mass	M	g/mol	$M(\text{H}_2\text{SO}_4) = 98 \text{ g/mol}$
Mass fraction	w	Unit less no $0 < w < 1$	$w(\text{H}_2\text{SO}_4) = 0.243$
Mass fraction, %	w%	% , procentum $0\% < w\% < 100\%$	$w\%(\text{H}_2\text{SO}_4) = 24.3 \%$
parts per million	ppm	Unit less $0 < \text{ppm} < 1\ 000\ 000$	$\text{ppm}(\text{H}_2\text{SO}_4) = 243\ 000 \text{ ppm}$
Promill alcohol in blood	pml	Unit less $0 < \text{pml} < 5$	$\text{pml}(\text{H}_3\text{CCH}_2\text{OH}) = 0.1 \text{ pml}$
Molar concentration	c_M	mol/L = M olarity	$c_M(\text{H}_2\text{SO}_4) = 2.5 \text{ mol/L}$ $c_M(\text{H}_2\text{SO}_4) = 2.5 \text{ M}$ [2.5 molar solution of H ₂ SO ₄]
Normal concentration	c_N	eq·mol/L = = Normality	$c_N(\text{H}_2\text{SO}_4) = 5.0 \text{ eq}\cdot\text{mol/L}$ $c_N(\text{H}_2\text{SO}_4) = 5.0 \text{ N}$ [5.0 normal solution of H ₂ SO ₄]
temperature	t	° C , Celsius	$t = 25^\circ \text{ C}$
Absolute Temperature	T	K , Kelvin	$T = 298.15 \text{ K}$
Atomic size distance units	l	Å , angstrom	$1\text{Å} = 10^{-8} \text{ cm} = 10^{-10} \text{ m} = 0.1 \text{ nm}$

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

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

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

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

Temperature conversion from °C to K

$$T [\text{K}] = t [^\circ\text{C}] + 273.15$$

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

1 dm³ = 1 litre = $1 \times 10^{-3} \text{ m}^3 = 1 \times 10^3 \text{ cm}^3$

Table of chemical and physical values

	<i>Basic Formula</i>	<i>expression I</i>	<i>expression II</i>
<i>Substance amount n & mass m</i>	$n = \frac{m}{M}$	$m = n \cdot M$	$M = \frac{m}{n}$
<i>Density ρ of solution</i>	$\rho = \frac{m(\text{solution})}{V}$	$m(\text{solution}) = \rho \cdot V$	$V = \frac{m(\text{solution})}{\rho}$
<i>Mass fraction (from mass)</i>	$w\% = \frac{m \cdot 100\%}{m(\text{solution})}$	$m = \frac{w\% \cdot m(\text{solution})}{100\%}$ $m(\text{solution}) = \frac{m \cdot 100\%}{w\%}$	
<i>Molar concentration molarity</i>	$c_M = \frac{n}{V}$	$n = c_M \cdot V$	$V = \frac{n}{c_M}$
<i>Molar concentration molarity (from mass)</i>	$c_M = \frac{m}{M \cdot V}$	$m = c_M \cdot M \cdot V$	$M = \frac{m}{c_M \cdot V}$
<i>Normal concentration normality</i>	$c_N = c_M \cdot z$	$z = \frac{c_N}{c_M}$	$c_M = \frac{c_N}{z}$
<i>Dilution</i>	$c_{M1} \cdot V_1 = c_{M2} \cdot V_2$	$V_1 = \frac{c_{M2} \cdot V_2}{c_{M1}}$	$c_{M2} = \frac{c_{M1} \cdot V_1}{V_2}$
<i>Water addition</i> $\Delta V_{H_2O} = V_2 - V_1$	$c_{M1} \cdot V_1 = c_{M2} \cdot (V_1 + \Delta V_{H_2O})$ $V_2 = \frac{c_{M1} \cdot V_1}{c_{M2}}$		$\Delta V_{H_2O} = V_2 - V_1$

Best choice of volume is one liter that $V=1 \text{ L} \Rightarrow 1000 \text{ mL}$

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

and using density ρ for $m(\text{solution})$ calculation $V=1000 \text{ mL}$

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

Standard Electrode Potentials

El	Red. form=Oxidized form+ne ⁻	H ₂ O classic E _o	Thermodyn. H ₂ O account	Absolute -0.3982 V
H	H(Pt)+H₂O=H₃O⁺+(Pt)+e⁻	classic 0	0.10166	-0.2965
	H(Pt)+OH⁻=H₂O+(Pt)+e⁻	-0.932195	-0.93268	-1.33088
O	6H ₂ O=O ₂ (g) + 4 H ₃ O ⁺ +4e ⁻	1.2288	+1.48466	1.0865
	H ₂ O ₂ +2H ₂ O=O ₂ aq+2H ₃ O ⁺ +e ⁻	1.2764	+1.58416	1.0829
	4H ₂ O=H ₂ O ₂ +2 H ₃ O ⁺ +2e ⁻	1.776	+2.08366	1.6855
	H ₂ O ₂ aq+2H ₂ O=O ₂ aq+2H ₃ O ⁺ +2e ⁻	0.6945	0.8477	0.4495
N	NO ₂ +2OH ⁻ =NO ₃ ⁻ +H ₂ O+2e ⁻	0.01	0.0602	-0.3380
	HNO ₂ +4H ₂ O=NO ₃ ⁻ +3H ₃ O ⁺ +2e ⁻	0.94	1.2477	0.8495
	NO _{aq} +6H ₂ O=NO ₃ ⁻ +4H ₃ O ⁺ +3e ⁻	0.96	1.2677	0.8695
	NH ₄ ⁺ +13H ₂ O=NO ₃ ⁻ +10H ₃ O ⁺ +8e ⁻	0.87	1.4180	1.0198
Br	2Br ⁻ =Br ₂ (aq)+2e ⁻	1.0873	1.18896	0.79076
Bi	BiO ⁺ +6H ₂ O=BiO ₃ ⁻ +4H ₃ O ⁺ +2e ⁻	1.80	2.210645	1.812445
Mn	Mn ²⁺ +12H ₂ O=MnO ₄ ⁻ +8H ₃ O ⁺ +5e ⁻	1.51	1.8588	1.4506
	MnO ₂ +4OH ⁻ =MnO ₄ ⁻ +2H ₂ O+3e ⁻	0.603	0.6360	0.2378
	MnO ₄ ²⁻ =MnO ₄ ⁻ +e ⁻	0.558	0.6597	0.2615
Pb	Pb ²⁺ +6H ₂ O=PbO ₂ (s)+4H ₃ O ⁺ +2e ⁻	1.455	1.8656	1.4674
	Pb+H ₂ O = Pb ²⁺ +2e ⁻	-0.126	0.0272	-0.3710
S	H ₂ SO ₃ +4H ₂ O=HSO ₄ ⁻ +3H ₃ O ⁺ +2e ⁻	0.172	0.47965	0.08145
	HSO ₃ ⁻ +4H ₂ O=SO ₄ ²⁻ +3H ₃ O ⁺ +2e ⁻	0.172	0.47965	0.08145
	SO ₃ ²⁻ +2OH ⁻ =SO ₄ ²⁻ +H ₂ O+2e ⁻	-0.93	-0.87984	-1.27804
	S ²⁻ =S _{rombic} +H ₂ O + 2 e ⁻	-0.4763	-0.4261	-0.8243
	HS ⁻ +OH ⁻ =S _{rombic} +2H ₂ O+2e ⁻	-0.478	-0.4793	-0.8775
	H ₂ S _{aq} +2H ₂ O=S _{rombic} +2H ₃ O ⁺ +2e ⁻	0.142	0.3467	-0.0515
2S ₂ O ₃ ²⁻ =S ₄ O ₆ ²⁻ +2e ⁻	0.08	0.18166	-0.2165	
Fe	Fe ²⁺ =Fe ³⁺ +e ⁻	0.769	0.8717	0.4735
	Fe(s)+ H ₂ O =Fe ²⁺ +2e ⁻	-0.4402	-0.2870	-0.6852
Ag	Ag+ H ₂ O=Ag ⁺ +e ⁻	0.7994	1.0041	0.6059
	Ag(s)+Cl ⁻ =AgCl(s)+H ₂ O+e ⁻	0.2223	0.2210	-0.1772
	Ag+2NH _{3(aq)} =Ag(NH ₃) ₂ ⁺ +e ⁻	0.373	0.4747	0.0765
	2Ag+2OH ⁻ =Ag ₂ O(s)+ H ₂ O+2e ⁻	0.345	0.3952	-0.0030
I	3I ⁻ =I ₃ ⁻ +2e ⁻	0.6276	0.72926	0.33106
Cu	Cu(Hg)+H ₂ O=Cu ²⁺ +(Hg)+2e ⁻	0.3435	0.4967	0.0985
F	2F ⁻ =F ₂ (g)+2e ⁻	2.87	2.97166	2.5735
Cl	2Cl ⁻ =Cl ₂ (g)+2e ⁻	1.358	1.45966	1.06146
	Cl ₂ (g)+4H ₂ O=2HOCl+2H ₃ O ⁺ +2e ⁻	1.63	1.93765	1.53945
Cr	2Cr ³⁺ +21H ₂ O=Cr ₂ O ₇ ²⁻ +14H ₃ O ⁺ +6e ⁻	1.33	1.7921	1.3939
	Cr ³⁺ +11H ₂ O=HCrO ₄ ⁻ +7H ₃ O ⁺ +3e ⁻	1.20	1.6793	1.2811
C	H ₂ C ₂ O ₄ +2H ₂ O=2CO ₂ +2H ₃ O ⁺ +2e ⁻	-0.49	-0.28534	-0.6835
Cr	Cr+H ₂ O=Cr ³⁺ +3e ⁻	-0.744	-0.6080	-1.0062
Zr	Zn+H ₂ O=Zn ²⁺ +2e ⁻	-0.7628	-0.6096	-1.0078
Al	Al+H ₂ O=Al ³⁺ +3e ⁻	-1.662	-1.5260	-1.9242
Al	Al+4OH ⁻ = H ₂ AlO ₃ ⁻ +H ₂ O+3e ⁻	-2.33	-2.2627	-2.6609

Ist type **Electrode potential E**

Red(Me) \leftrightarrow Ox(Meⁿ⁺) + ne⁻, n=3, E_{oCr}=-1.3939 V (classic E_o=-0,744 V)
Cr+H₂O=Cr³⁺+3e⁻; n = 3; **CrCl₃** salt is conc. of ion [**Cr³⁺**]=0.03 M

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

Red-Ox **Electrode potential E** ; E=E_{oH₂O}+0.0591/n•lg([Ox]/[Red]);

$$E = E_{\text{oH}_2\text{O}} + 0.0591/5 \log([\text{MnO}_4^{2-}][\text{H}_3\text{O}^+]^8/[\text{Mn}^{2+}][\text{H}_2\text{O}]^{12});$$

Mn²⁺+12H₂O=MnO₄²⁻+8H₃O⁺+5e⁻; E_{oH₂O}=1,4506 V (classic E_o+1,51 V)

| —Ox form — | \leftrightarrow | —Red form— | if ([MnO₄²⁻][H₃O⁺]⁸=[Mn²⁺][H₂O]¹²;

$$E = E_{\text{oH}_2\text{O}} = 1.86 + \log(1) = 1.86 + 0 = 1.86 \text{ V}$$

Ostwald's dilution law

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

For weak acid $\alpha = \frac{\sqrt{K_{\text{dis.}}}}{\sqrt{c_M}}$;

$$K_a = 1.75 \cdot 10^{-5} ; c_M = 0,01 \text{ M} ; \text{pH} = 3.3785$$

$$\alpha = \frac{\sqrt{1.75 \cdot 10^{-5}}}{\sqrt{0.01 \text{ M}}} = 0.0418 = 4.18\%$$

$$C = \frac{[H^+]^2}{K_a} = \frac{10^{-\text{pH} \cdot 2}}{K_a}$$

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

For strong electrolytes

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

$$\alpha = \frac{[H^+]}{z \cdot C} = \frac{10^{-\text{pH}}}{z \cdot C}$$

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

Isotonic coefficient

$$i = 1 + \alpha \cdot (m - 1) ; 0 < \alpha < 1$$

for total osmolarity Δc_{osm}

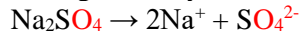
is $i \cdot c_M$ total osmolar

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

Glucose as non electrolyte $\alpha = 0$

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

Na₂SO₄ strong electrolyte $0.3 < \alpha < 0.999$



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

Osmotic pressure kPa on membrane is energy

At temperature 25 C or 298.15 K

Joules in cell volume liter

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

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

0.2M glucose non-electrolyte, $\alpha = 0$; $i = 1$ sol.

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

0.2M Na₂SO₄ strong electrolyte, $\alpha = 1$; $i = 3$ sol.

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

Ionic strength I or μ

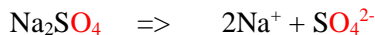
$$I = \frac{1}{2} \sum \alpha \cdot c_i \cdot z_i^2$$

is total concentration of ions

$$I = 1/2 (2 \cdot 0.2 \text{ M} \cdot (+1)^2 + 0.2 \text{ M} \cdot (-2)^2),$$

0.2M Na₂SO₄ solution $\alpha = 1$

salt \Rightarrow sodium and sulfate ions



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

Hess law and Prigogine Thermodynamics

Hess Enthalpy of reaction: $\Delta H_{\text{Hess}} = \sum \Delta H^{\circ}_{\text{products}} - \sum \Delta H^{\circ}_{\text{reactants}}$.

Dispersed (lost) heat in surrounding : $\Delta S_{\text{heat_dispersed}} = - \Delta H_{\text{Hess}} / T$

Hess Entropy of reaction: $\Delta S_{\text{Hess}} = \sum \Delta S^{\circ}_{\text{products}} - \sum \Delta S^{\circ}_{\text{reactants}}$.

Hess Gibbs free energy of reaction $\Delta G_{\text{Hess}} = \Delta H_{\text{Hess}} - T \bullet \Delta S_{\text{Hess}}$

Negative ΔG means that the process (reaction) is **spontaneous** ($\Delta G < 0$)

Positive ΔG means that the process is forbidden, **non-spontaneous** ($\Delta G > 0$)

Prigogine attractor the Gibbs free energy change minimum ΔG_{min} :

$$|\Delta G_{\text{Hess}}| > |\Delta G_{\text{min}}| = |\Delta G_{\text{equilibrium}}|; \Delta G_{\text{eq}} = -R \bullet T \bullet \ln(K_{\text{eq}})$$

$$\Delta G_{\text{homeostasis}} = \Delta G_{\text{eq}} + R \bullet T \bullet \ln(K_{\text{homeostasis}})$$

Total energy dispersion entropy $\Delta S_{\text{total}} = \Delta S_{\text{Hess}} + \Delta S_{\text{heat_dispersed}}$

Total entropy negative $T \bullet \Delta S_{\text{total}} < 0$ tandem accumulate energy in products $\Delta G > 0$,

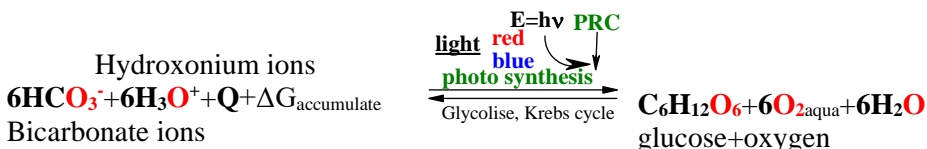
Total entropy positive $T \bullet \Delta S_{\text{total}} > 0$ spontaneous dispersed energy $\Delta G < 0$.

Opposite singe with identical value ΔG for bound energy $\Delta G_{\text{dispersed}} = T \bullet \Delta S_{\text{total}}$

Combustion heat of reaction for food containing energy amount evaluation:

$$\Delta H_{\text{Hess}} = \sum \Delta H_{\text{reactants}}^{\text{combustions}} - \sum \Delta H_{\text{products}}^{\text{combustions}}$$

Photo Synthesis assimilate light **blue red** photon energy $E = h\nu$



$$\Delta H_{\text{Hess}} = (\Delta H^{\circ}_{\text{C}_6\text{H}_{12}\text{O}_6} + 6\Delta H^{\circ}_{\text{O}_2}) - (6\Delta H^{\circ}_{\text{H}_2\text{O}} + 6\Delta H^{\circ}_{\text{CO}_2})$$

$$\Delta S_{\text{Hess}} = (\Delta S^{\circ}_{\text{C}_6\text{H}_{12}\text{O}_6} + 6\Delta S^{\circ}_{\text{O}_2}) - (6\Delta S^{\circ}_{\text{H}_2\text{O}} + 6\Delta S^{\circ}_{\text{CO}_2})$$

$$\Delta G_{\text{Hess}} = \Delta H_{\text{Hess}} - T \bullet \Delta S_{\text{Hess}}$$

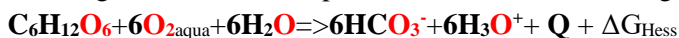
$$\Delta S_{\text{heat_dispersed}} = - \Delta H_{\text{Hess}} / T$$

$$\Delta S_{\text{total}} = \Delta S_{\text{Hess}} + \Delta S_{\text{heat_dispersed}}$$

accumulate energy in products $\text{C}_6\text{H}_{12}\text{O}_6 + 6 \text{O}_{2\text{aqua}} + 6\text{H}_2\text{O}$

organisms by oxidation produce heat, energy, concentration gradients

for osmosis against and for transport down the concentration gradient:



Thermodynamic of equilibrium and homeostasis

Thermodynamic equilibrium constant K_{eq} is expressed as $K_{eq} = e^{-\frac{\Delta G_{eq}}{RT}}$, where depends on: $R = 8.3144$ **Universal gas constant** & $e = 2.7$ natural number,
 1) $\Delta G_{equilibrium}$ free energy change and on
 2) temperature T

Equilibrium constant K not depends but **Homeostasis constant** depends on concentrations X_A, X_B, X_C, X_D for mixture of compounds A, B, C, D

which ratio products over reactants for constant expression $K = \frac{X_C^c \cdot X_D^d}{X_A^a \cdot X_B^b}$

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

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

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

Concentration decreases time and temperature influence on time

$t = \frac{\ln \frac{C^\circ}{C}}{k}$ time in which concentration decreases from $C^\circ > t_0 > C$.

Half life time or half reactant time $\tau_{1/2} = \frac{\ln 2}{k}$,

In which concentration decreases per half $C^\circ / C = 2$

$$t_{T2} = \frac{t_{T1}}{\gamma^{10}} \qquad t_{150^\circ\text{C}} = \frac{t_{140^\circ\text{C}}}{3^{10}}$$

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

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

Strong Acid, Base protolytic dissociation $\text{pH}+\text{pOH}=14$

Formula	Example
$\text{pH} = -\log [\text{H}^+] = -\log(\alpha \cdot z \cdot c_M)$	What is the pH of 0.0850 M HNO_3 if $\alpha = 1$ $z = 1$? $\text{pH} = -\lg(0.085) = 1.07$
$\text{pOH} = -\log [\text{OH}^-] = -\log(\alpha \cdot z \cdot c_M)$	What is the pH of 0.00765 KOH if $\alpha = 1$ $z = 1$ $[\text{KOH}] = [\text{OH}^-]$
$\text{pH} + \text{pOH} = 14$	$\text{pOH} = 2.12$; $\text{pH} = 14 - \text{pOH}$ and $\text{pH} = 11.88$
$[\text{H}^+] = 10^{-\text{pH}}$	$\text{pH} = 1$; $[\text{H}^+] = 10^{-1} = 0.1$
$[\text{OH}^-] = 10^{-\text{pOH}}$	$\text{pOH} = 1$; $[\text{OH}^-] = 10^{-1} = 0.1$

Weak acid protolytic equilibria buffer solution

Protolysis-dissociation weak acid deprotonation equilibrium: $\text{CH}_3\text{COOH} \rightleftharpoons \text{CH}_3\text{COO}^- + \text{H}^+$	$\text{CH}_3\text{COOH} + \text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{CH}_3\text{COO}^-$; $K_a = \frac{[\text{H}^+] \cdot [\text{CH}_3\text{COO}^-]}{[\text{CH}_3\text{COOH}]_{\text{nedis}}} = 10^{-\text{p}K_a} = 10^{-4,76}$
$\text{p}K_a = -\lg [K_a]$	$K_a = 1.745 \cdot 10^{-5}$; $\text{p}K_a = -\lg(1.745 \cdot 10^{-5}) = 4.76$
$K_a = 10^{-\text{p}K_a}$	$\text{p}K_a = 9,25$; $K_a = 10^{-9,25} = 5,618 \cdot 10^{-10}$
$\text{NH}_4^+ + \text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{NH}_3_{\text{aqua}}$	$K_a = \frac{[\text{H}^+] \cdot [\text{NH}_3]_{\text{aqua}}}{[\text{NH}_4^+]} = 10^{-\text{p}K_a} = 10^{-9,25}$
Weak acid protolysis deprotonation equilibrium buffer solution $\text{pH} = \text{p}K_a + \lg\left(\frac{n_{\text{base}}}{n_{\text{acid}}}\right)$ $\text{pH} = \text{p}K_a + \lg\left(\frac{c_{\text{base}} \cdot v_{\text{base}}}{c_{\text{acid}} \cdot v_{\text{acid}}}\right)$	Calculate pH of a formiate buffer ($\text{HCOOH}/\text{HCOONa}$), $\text{HCOOH} + \text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{HCOO}^-$; if the buffer is composed from 300 mL of 0.15 M HCOOH and 200 mL of 0.09 M HCOONa solutions, $K_a = 2 \cdot 10^{-4}$ $\text{pH} = \text{p}K_a + \lg \frac{c_{\text{base}} \cdot v_{\text{base}}}{c_{\text{acid}} \cdot v_{\text{acid}}} = -\lg 2 \cdot 10^{-4} + \lg \frac{200 \times 0.09}{300 \times 0.15} =$ $= 3.7 + \lg \frac{18}{45} = 3.7 + \lg 0.4 = 3.7 - 0.398 = 3.3$
Weak acid protolysis $\text{NH}_4^+ + \text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{NH}_3_{\text{aqua}}$ ammonium NH_4^+ deprotonation equilibrium buffer solution $\text{pH} = \text{p}K_a + \lg \frac{n_{\text{NH}_3}}{n_{\text{NH}_4^+}}$ $\text{pH} = \text{p}K_a + \lg \frac{c_{\text{NH}_3} \cdot v_{\text{NH}_3}}{c_{\text{NH}_4^+} \cdot v_{\text{NH}_4^+}}$	$\text{NH}_4^+ + \text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{NH}_3_{\text{aqua}}$; Calculate buffer solution pH , that formed of 80 mL 0.1 M ammonia $\text{NH}_3_{\text{aqua}}$ and 120 mL 0.17 M NH_4Cl solution, $K_a = 5,618 \cdot 10^{-10}$. $\text{pH} = \text{p}K_a + \lg \frac{c_{\text{NH}_3} \cdot v_{\text{NH}_3}}{c_{\text{NH}_4^+} \cdot v_{\text{NH}_4^+}} = -\lg 5,62 \cdot 10^{-10} + \lg \frac{80 \times 0.1}{120 \times 0.17} =$ $= 9,25 + \lg \frac{8}{20.4} = 9,25 + \lg 0,392 = 9,25 - 0,4065 = 8.844$

Weak acid protolytic equilibria buffer solution

Calculate, how many milliliters of 0,1 M HCOOH and 0,2 M HCOONa have to be taken to obtain a buffer, having $\text{pH}=3,0$ and total volume 1 liter. $K_a=2 \cdot 10^{-4}$

$$\text{pH} = \text{p}K_a + \log \left(\frac{c_{\text{base}} \cdot V_{\text{base}}}{c_{\text{acid}} \cdot V_{\text{acid}}} \right)$$

$$V_{\text{salt}} = x; \quad V_{\text{acid}} = 1000 - x$$

$$3,0 = -\log(2 \cdot 10^{-4}) + \log \left(\frac{0,2x}{0,1 \cdot (1000 - x)} \right)$$

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

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

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

$$0,199 = \left(\frac{0,2x}{0,1 \cdot (1000 - x)} \right)$$

$$0,199 \cdot (1000 - 0,1x) = 0,2x$$

$$x = 90,6 \text{ mL}$$

$$V_{\text{salt}} = 90,6 \text{ mL}; \quad V_{\text{acid}} = 1000 - 90,6 \text{ mL} = 909,5 \text{ mL}$$

Weak acid protolytic equilibria buffer solution

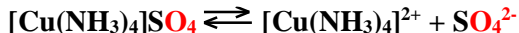
1. Buffer solution to be composed of a weak acid and deprotonated weak acid salt as base form,
2. Buffer formed of protonated NH_4^+ and deprotonated NH_3 ammonia,
3. Buffer solution can be composed of a weak acid and strong base in limited supply,
4. Buffer formed of deprotonated base and strong acid 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.
7. Proteins Buffers in human organism are long amino acid polypeptide chains with four type protolytic weak acid groups (see 14th page)

Complex compounds and light absorption

Charges and coordination numbers of some central ions.

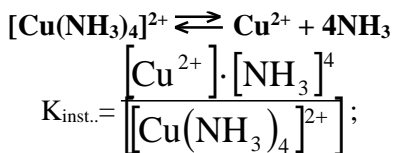
Charge of central ion	Coord. number by empiric rule	examples	Other possible coord. numbers	examples
+1	2	Ag ⁺ , Cu ⁺ , Au ⁺	4	Li ⁺
+2	4	Cu ²⁺ , Hg ²⁺ , Pt ²⁺ , Ni ²⁺ , Zn ²⁺ , Cd ²⁺ , Co ²⁺ , Pb ²⁺ ,	6	Fe ²⁺
+3	6	Fe ³⁺ , Al ³⁺ , Cr ³⁺ , Co ³⁺	4	Au ³⁺

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

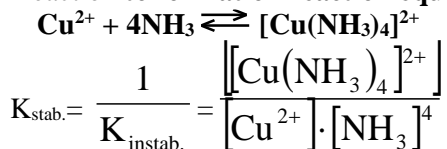


Instability constant $K_{\text{inst.}}$ of complex compound $[\text{Cu}(\text{NH}_3)_4]^{2+}$ destruction

in *secondary dissociation* complex compound $[\text{Cu}(\text{NH}_3)_4]^{2+}$ equilibrium :



Flip over reaction to formation reaction equilibrium



Light absorption $A = \log(I_0/I) = a \cdot c_M \cdot l$

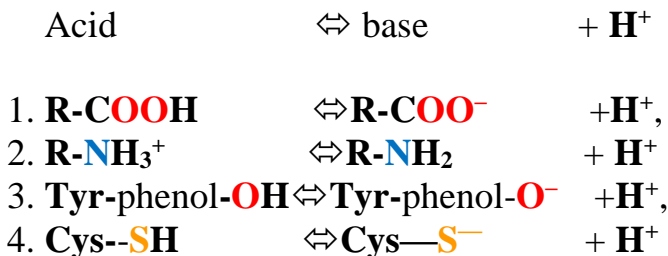
Amino Acid	pKa-COOH	pKa-NH3+	pKa R group
Isoleucine	2.36	9.68	
Valine	2.32	9.62	
Leucine	2.36	9.60	
Phenylalanine	1.83	9.13	
Cysteine	1.96	10.28	8.18
Methionine	2.28	9.21	
Alanine	2.34	9.69	
Proline	1.99	10.96	
Glycine	2.34	9.60	
Threonine	2.11	9.62	
Serine	2.21	9.15	
Tryptophan	2.38	9.39	
Tyrosine	2.20	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_mean} =IEP value with total of NpK_a sum constants pK_a for molecule given in table includes the sum of: side groups $\sum pK_{aR_group}$, N-terminus $pK_{aNterminus}NH_3^+$ and C-terminus $pK_{aCterminus}COO^-$. In *Ostwald's dilution law* pH calculation is used pK_{a_mean} by concentration C logarithm
$$pH = \frac{pK_{a_mean} - \log C}{2} = \dots$$

$$pK_{a_mean} = IEP = (\sum pK_{aRside_residue} + pK_{aNterminus} + pK_{aCterminus}) / NpK_a$$

Amino acid or protein molecules have four type acidic functional groups: **-COOH** neutral, **-NH3+** positive charged, phenol **-OH** neutral, **-SH** neutral. At physiologic pH 7.36 groups exist prevailing: negative charged **R-COO-**, positive charged amino groups **R-NH3+**, neutral group of Tyrosine phenol-**OH** and Cysteine sulfo hydrogen **R-SH**.

Four parallel protolytic equilibria:



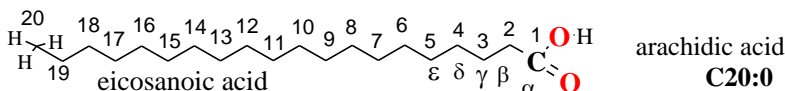
FATTY ACIDS

<i>Saturated</i> name C		<i>Unsaturated</i>		C:Double bonds	
Caproic acid		Common name	Name of salt	C :	ω ?
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	ω 10
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	Vacceniato	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

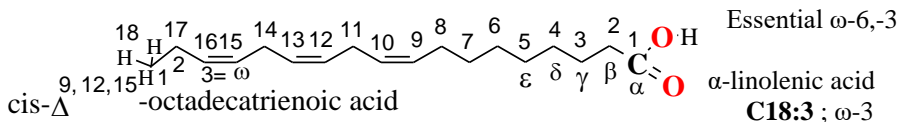
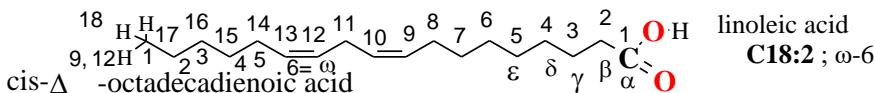
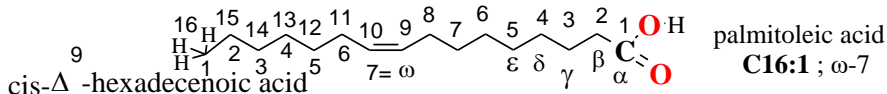
Saturated fatty acids

$\text{CH}_3(\text{CH}_2)_{14}\text{CO}_2\text{H}$ - hexadecanoic acid palmitic acid **C16**

$\text{CH}_3(\text{CH}_2)_{16}\text{CO}_2\text{H}$ -octadecanoic acid stearic acid **C18**

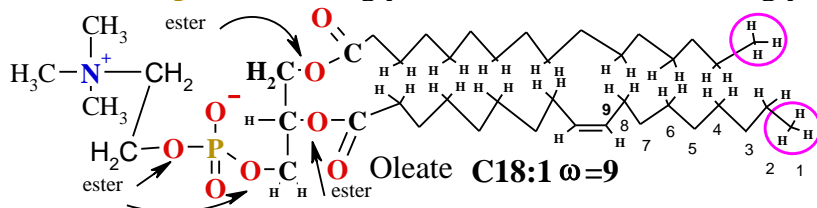


Unsaturated fatty acids



Phosphatidyl Choline Membrane building molecular components

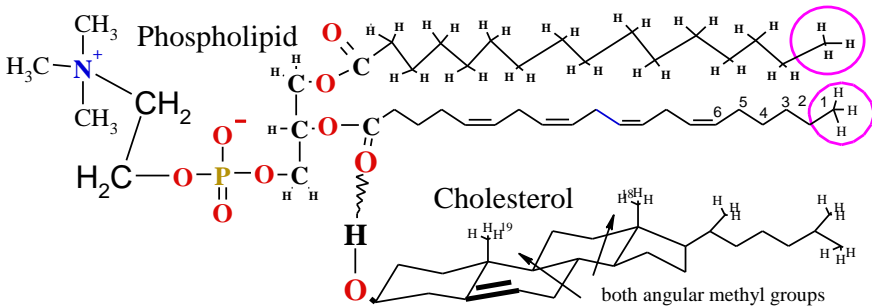
Phosphate ester of glycerol C3 **Palmitate** ester of glycerol C1



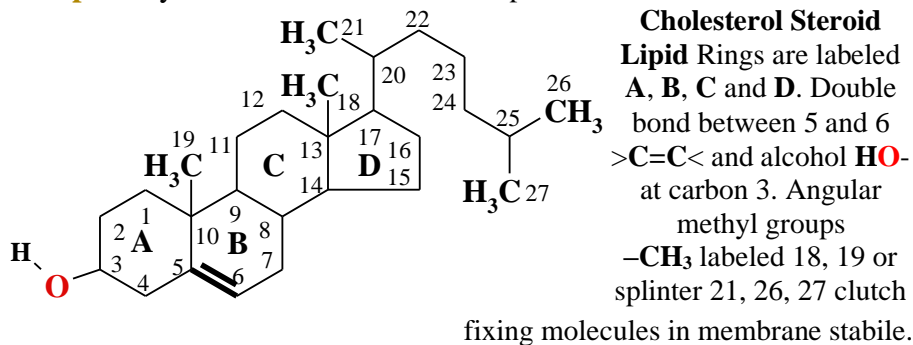
Choline

Glycerol

All atoms colored CPK labels



Phosphatidyl Choline/Cholesterol complex in cell membranes



α-Amino Acids Non-polar, aliphatic, aromatic R groups left Cα

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	
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	

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

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

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**

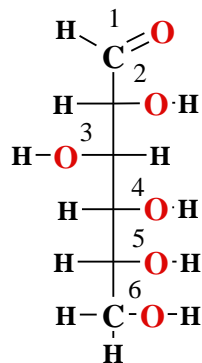
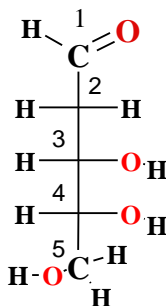
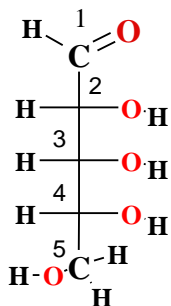
14.	Arginine	Arg, R	
15.	Lysine	Lys, K	
16.	Histidine	His, H	

Structural Formulas of Carbohydrates The Fischer tree projections

for open chain structures

Pentoses–Aldoses:

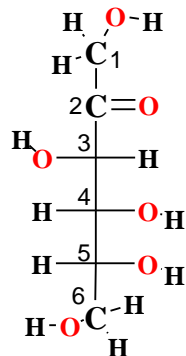
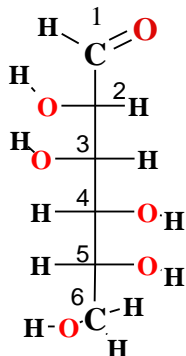
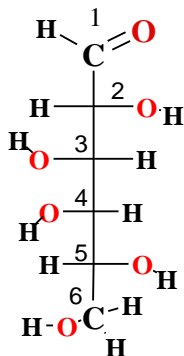
Hexoses – Aldohexoses:



D-Ribose

D-2-deoxy-ribose

D-Glucose



D-Galactose

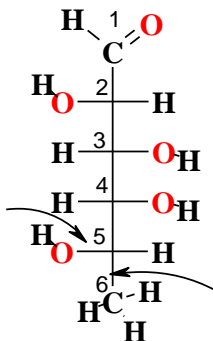
D-Mannose

D-Fructose

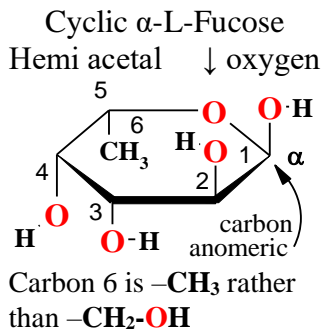
Fisher projection

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

and is down carbon 6
6methyl -CH₃

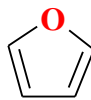
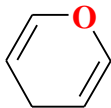


Haworth projection



Cyclic Structure Haworth projections of Carbohydrates

Haworth projection uses the organic molecule frames

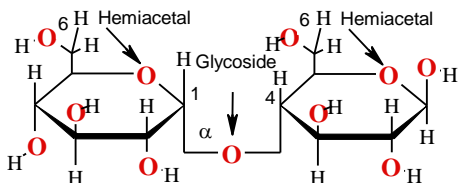


Pyranose six member cycle

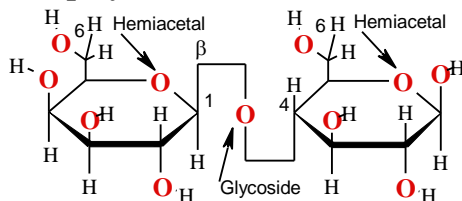
and Furanose

cycle 5 atoms

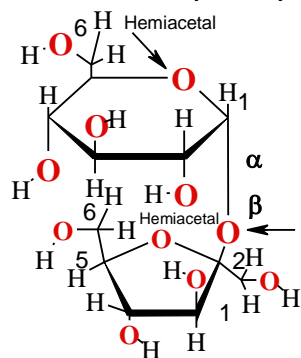
Disaccharides and polysaccharides



Maltose $\text{Glc}(\alpha 1 \rightarrow 4)\text{Glc}-\beta$



Lactose $\text{Gal}(\beta 1 \rightarrow 4)\text{Glc}-\beta$



Sucrose

Pyranose six member cycle

α -D-Glucose unit

$(\alpha 1 \rightarrow 2\beta)$

$\text{Glc}(\alpha 1 \rightarrow 2)\text{Fruc}-\beta$

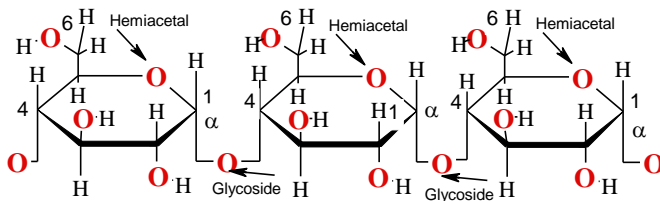
← Glycoside bond

β -D-Fructose unit

Furanose five member cycle

Starch $\rightarrow 4)\text{Glc}(\alpha 1 \rightarrow 4)\text{Glc}(\alpha 1 \rightarrow 4)\text{Glc}(\alpha 1 \rightarrow$

Polysaccharides



Cellulose $\rightarrow 4)\text{Glc}(\beta 1 \rightarrow 4)\text{Glc}(\beta 1 \rightarrow 4)\text{Glc}(\beta 1 \rightarrow$

