Preparatory course

ESSENTIALS of CHEMISTRY

2020

WORKBOOK

CONTENTS:

OUTCOMES:

1. Essentials of calculations in chemistry
    - the ability to calculate with logarithm (pH, pK), percentage (mass concentration) and direct proportionality (dilution of solutions)
    - the ability to convert units used in an expression of concentration (basic SI units, all mass and molar units from the prefix pico- to kilo- ones)

2. Comparison of inorganic and organic compounds
    - understanding differences in an element composition, structures, properties and naming of inorganic and organic compounds
    - understanding the ability of organic compounds to form isomers due to a different order of atoms and bonds involved, including the differences only in the space arrangement
    - understanding an impact of elements and types of bonds present in organic molecules on their chemical reactivity
    - understanding differences between alicyclic and aromatic organic compounds
    - ability to distinguish different oxidative states of inorganic and organic compounds, including terms addition / elimination of hydrogen or water
    - understanding differences and similarities between inorganic and organic acids and between hydroxides and alcohols, including the process of neutralization

3. Biochemically important organic compounds I
    - ability to describe processes involved in interconversions of alcohols, aldehydes or ketones and carboxylic acids (mono- and dicarboxylic ones), including the naming and properties of these molecules
    - understanding differences between carboxylate and acyl derived from carboxylic acids
    - understanding reactions of alcohols with carboxylic acids forming esters, including the process of an ester hydrolysis and properties of esters
    - understanding mutual reactions of two acids (either both carboxylic or phoshoric and carboxylic acids) forming anhydrides, including the process of their hydrolysis and properties of anhydrides

4. Biochemically important organic compounds II
    - ability to name substitutional derivatives of carboxylic acids (hydroxy-, oxo- and amino- acids) and understanding chemical properties and reactivity of these derivatives, including their mutual interconversions
    - understanding reactions of carboxylic acids with ammonia forming amides, and their similarity with reactions of two amino acids forming a peptide
    - understanding the structure and properties of amines and their differences and similarities with amino acids and amides
    - ability to distinguish heterocyclic compounds containing nitrogen, oxygen and sulfur from other cyclic organic molecules and understanding their chemical properties
    - understanding the formation of a disulfide bond between two thiol functional groups and its importance in a structure of proteins

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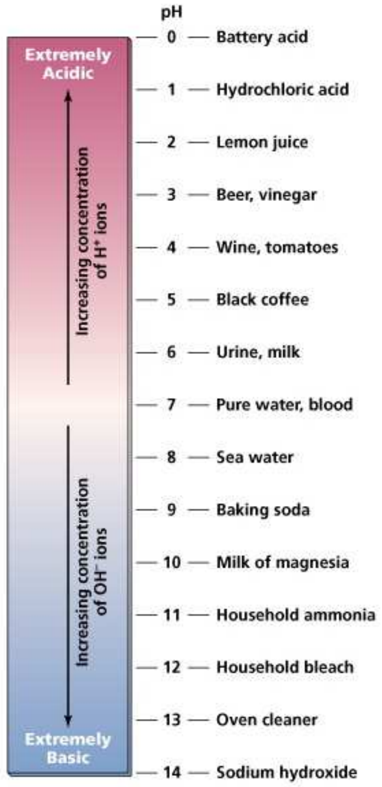
LECTURE 1 Essentials of calculations in chemistry

The human body contains approximatly 60 % of water, H_2O, by mass. It is predominantly undissociated molecule, but small amount of it exists in a form of ions: H_3O^+ and OH^- (because so called autoprotolysis of water, the acid-base reaction proceeding between two water molecules: $H_2O + H_2O \rightarrow H_3O^+ + OH^-$). The value called ionic product of water $K_w = c(H_3O^+) \times c(OH^-) = 10^{-14}$ is constant in all aqueous solutions, meaning that 10^{-7} mol/l of H_3O^+ and 10^{-7} mol/l of OH^- occur in pure water, but a different ratio of the ions occurs in various (acidic or basic) solutions. The ionic product of water is often expressed as $pK_w = -\log K_w = 14$ and the molar concentration of H_3O^+, $c(H_3O^+)$, is described by the value of $pH = -\log c(H_3O^+)$ because the concentration of it is very small ($10^{-7} = 0.0000001$ mol/l) in pure water. Thus pH of water is $-\log 10^{-7} = 7$, the value refered to as neutral pH.



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Important terms:

- percentage and percent concentration (%)
- molar concentration (molarity, mol/l)
- logarithm (common logarithm, $\log_{10}$)
- acids, bases
- dilution of solutions

percent concentration ***% = g/100g***

1% solution

⇒ 1 g of a solute is found in 100 g of the solution
(it takes one hundredth of the total mass)

0.5% solution

⇒ 0.5 g of a solute is found in 100 g of the solution

molar concentration (= molarity) ***M = mol/1000 ml***

1M solution

⇒ 1 mol of a solute is found in 1000 ml (= 1l) of the solution

0.5M solution

⇒ 0.5 mol of a solute is found in 1000 ml (= 1l) of the solution

concentration = ratio of an amount of solute / amount of solution

1 % *(read: one percentage solution) means any equivalent ratio resulting in 0.01, e.g.*

$$\frac{1\ g}{100\ g} \quad or \quad \frac{2\ g}{200\ g} \quad or \quad \frac{3\ g}{300\ g} \quad or \quad \frac{1.5\ g}{150\ g} \quad or \quad \frac{0.5\ g}{50\ g} \quad or \quad \frac{0.25\ g}{25\ g}$$

1 M *(read: one molar solution) means any equivalent ratio resulting in 0.001, e.g.*

$$\frac{1\ mol}{1000\ ml} \quad or \quad \frac{2\ mol}{2000\ ml} \quad or \quad \frac{3\ mol}{3000\ ml} \quad or \quad \frac{1.5\ mol}{1\ 500\ ml} \quad or \quad \frac{0.5\ mol}{500\ ml} \quad or \quad \frac{0.25\ mol}{250\ ml}$$

Task 1.1 How many kg of water is found in the human body, mass of which is

a) 100 kg ?
b) 60 kg ?

Task 1.2 Write the correct quantity of a solute into the table to get the given concentration:

concentration	**quantity of solute**	**quantity of solution**
10 M	**mol**	1000 ml
1 M	**mol**	1000 ml
0.1 M	**mol**	1000 ml
0.01 M	**mol**	1000 ml
0.001 M	**mol**	1000 ml
10 %	**g**	100 g
1 %	**g**	100 g
0.1 %	**g**	100 g
0.01 %	**g**	100 g
0.001 %	**g**	100 g

Task 1.3 Calculate the percent concentration of the solutions containing:

a) 5 g of NaCl in 100 g of the solution
b) 5 g of NaCl in 1000 g of the solution
c) 5 g of NaOH in 100 g of the solution
d) 5 g of NaOH in 1000 g of the solution

Task 1.4 Calculate the molar concentration of the solutions containing:

a) 58.5 g of NaCl in 1 litre of the solution
b) 117 g of NaCl in 1 litre of the solution
c) 20 g of NaOH in 1 litre of the solution
d) 40 g of NaOH in 1 litre of the solution

***m = n x MW**, m = mass in grams, n = substance amount in mol, MW = molar mass in g/mol;*
MW: NaCl 58.5 g/mol, NaOH 40 g/mol

Task 1.5 Calculate the masses of solutes needed to prepare:

a) 200 ml of 0.5 M NaOH solution, MW(NaOH) = 40 g/mol
b) 100 ml of 2 M NaCl solution, MW(NaCl) = 58.5 g/mol
c) 200 g of 0.5 % NaOH solution
d) 100 g of 2 % NaCl solution

Calculations with common logarithm ($\log_{10}$): $- \log x = y$ $x = 10^{-y}$

The term "negative logarithm" (–log) simply means the logarithm multiplied by -1. In chemistry it is used to calculate pH or pK values, because they are related to numbers lower than zero (e.g. $0.001 = 10^{-3}$), and hence resulting in negative exponent values.

common logarithm	**$- \log x = y$**	**$y = - \log_{10} x$**	**$x = 10^{-y}$**	
$- \log 0.1 =$	$- \log 10^{-1} = 1$	$pH = - \log [H^+]$	$[H^+] = 10^{-pH}$	x = concentration of protons = $[H^+]$
$- \log 0.01 =$	$- \log 10^{-2} = 2$	$pOH = - \log [OH^-]$	$[OH^-] = 10^{-pOH}$	x = concentration of OH^- = $[OH^-]$
$- \log 0.001 =$	$- \log 10^{-3} = 3$	$pK = - \log K$	$K = 10^{-pK}$	x = dissociation constant = $K = K_{dis}$
$- \log 0.0001 =$	$- \log 10^{-4} = 4$			

Autoprotolysis of water (ionisation of water)

- in aqueous solutions: $K_w = [H_3O^+] \times [OH^-] = 10^{-14}$
- using logarithm: $pK_w = pH + pOH = 14$ ($pK = - \log K$)

- $[H_3O^+] = 10^{-7}$ → $pH = - \log [H_3O^+] = - \log 10^{-7}$ → **pH = 7**
- $[OH^-] = 10^{-7}$ → $pOH = - \log [OH^-] = - \log 10^{-7}$ → **pOH = 7**

in pure water:	$[H_3O^+] = [OH^-]$	**pH = 7**
in acidic solutions:	$[H_3O^+] > [OH^-]$	**pH < 7**
in basic solutions:	$[H_3O^+] < [OH^-]$	**pH > 7**

Task 1.6 Fill in missing values of y into the table: **$y = - \log x$**

	0.1	0.01	0.001	0.0001	0.00001	0.000001	0.0000001
x	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
y							

Task 1.7 Calculate the concentration of H_3O^+ in an aqueous solution:

a) containing 0.001 mol/l of OH^-
b) containing 10^{-7} mol/l of OH^-
c) if pH of the solution is 5
d) if pH of the solution is 12

Add related values of concentrations of OH^- or pH of the solution and answer the question: which of these solutions is an acid and which one is a hydroxide?

Task 1.8

a) Calculate the pH of a 0.05 M solution of sulphuric acid.
b) What is the molar concentration of a solution of sulphuric acid with pH = 3?
c) Calculate the pH of a 0.005 M solution of $Ba(OH)_2$.
d) What is the molar concentration of a solution of $Ba(OH)_2$ with pH = 12?

Task 1.9 Fill in missing values into the table: **- log x = y x = 10^{-y}**

$[OH^-]$							
$[H^+]$							
pH	1	3	5	7	9	11	13

K							
pK	2	4	6	8	10	12	14

Dilution

- after mixing a solution of given concentration with a pure solvent (water) the concentration of the solution decreases but the substance amount (n) will remain the same
- reason: volume increases ⇒ **concentration decreases** (c = n / V)

Expression of a dilution:

- 1 part (ml or g) of solution + defined number of parts (ml or g) of solvent
  = diluted solution (sum of all parts)

- *example: 1 ml of solution + 4 ml of solvent = 5 ml of diluted solution*
- *description: 1 + 4 = 5 → it is diluted in the ratio of 1 / 5 (one part found in 5 parts of the final volume of the diluted solution)*
- *reading: 1 / 5 = 1 : 5 = five times (5x) diluted → the concentration after dilution is 5 times lower*
- *calculation: if the beginning concentration was 0.25 M, after 5x dilution the final concentration is 0.25 / 5 = 0.05 M (or 0.25 x 1/5 = 0.05 M)*

Task 1.10 Calculate the pH values of HCl and NaOH before and after dilution.
How many times were HCl and NaOH diluted?

a) 0.1 M HCl

b) 0.001 M HCl

c) 0.1 M NaOH

d) 0.001 M NaOH

Task 1.11 0.5 l of 1 M NaCl solution was diluted to 0.25 M solution:

a) How many times was the solution diluted?

b) What is the volume of the solution after the dilution?

Task 1.12

2 ml of urine sample has been diluted by 198 ml of water. Then the sample was processed to determine urea concentration, the result of which is 4.5 mmol/l. What is the urea concentration in the undiluted urine?

SI base units in chemistry

The International System of Units (SI) defines seven units of measure as a basic set from which all other SI units can be derived. The SI base units and their physical quantities are the metre (m) for measurement of length, the **kilogram (kg) for mass**, the **second (s) for time**, the ampere (A) for electric current, the kelvin (K) for temperature, the candela (cd) for luminous intensity, and the **mole (mol) for amount of substance**. Several other units, such as the litre (l), are formally not part of the SI, but are accepted for use with SI.

Prefixes of units**:**

prefix	atto-	femto-	pico-	nano-	micro-	mili-	centi-	deci-	kilo-	mega-	giga-	tera-
symbol	**a**	**f**	**p**	**n**	**µ**	**m**	**c**	**d**	**k**	**M**	**G**	**T**
multiple	10^{-18}	10^{-15}	10^{-12}	10^{-9}	10^{-6}	10^{-3}	10^{-2}	10^{-1}	10^{3}	10^{6}	10^{9}	10^{12}

Common prefixes in medical chemistry:

- *concentration*:
  a) molar concentration: pmol/l, nmol/l, **µmol/l, mmol/l**, mol/l
  b) mass concentration: pg/l, ng/l, **µg/l, mg/l, g/l**
- *volume*: **µl, ml, dl, l** **1 ml = 1 cm^3 1 l = 1 dm^3**
- *density*: g/cm^3 = g/ml, kg/dm^3 = kg/l
- *pressure*: Pa, kPa **1 atm = 101 325 Pa = 760 Torr (= mmHg)**
- *energy content*: J, kJ or cal, kcal **1 cal = 4,2 J**
- *substance amount:* pmol, nmol, **µmol, mmol,** mol **1 mol = 6.022 x 10^{23} particles**

Task 1.13 Fill in missing values into the table:

substance amount	**whole number**	**exponential number**
1 mol	x	x
= ? mmol		
= ? µmol		
= ? nmol		
= ? pmol		
1 mmol	x	x
= ? mol		
1 µmol	x	x
= ? mol		

example: ***1 kg*** *= 1 000 g* *= 10^3 g*

Task 1.14
Air contains: 78% N_2 / 21% O_2 / 1% water / 0.04% CO_2 / inert gases.
Calculate the partial pressure (in Pa) of oxygen and the partial pressure of carbon dioxide in the atmosphere if the total atmospheric pressure is approximately 100 kPa.

pressure = the force acting normally on unit area of a surface (units: pascals, Pa)   1 kPa = 10^3 Pa
partial pressure = pressure of one gas present in a mixture of gases
Dalton´s law = the total pressure of a mixture of gasses or vapours is equal to the sum of the partial pressures of its components

Task 1.15
Convert the concentration of cholesterol 200 mg/dl to mmol/l (MW of cholesterol = 386.7 g/mol)

Task 1.16
The mass of a lump of sugar (= sucrose, $C_{12}H_{22}O_{11}$) is 10.0 g. How many molecules of sucrose are found in the lump, if it contains 96 % of the sucrose? The Avogadro´s number (N_A) = 6.022×10^{23}, atomic mass unit (amu) = 1.661×10^{-27} kg.

Task 1.17
The amount of plasma in a human body (adult man, 75 kg) is about 3.5 l. The plasmatic sodium cation concentration is 140 mmol/l. What is the total mass (in grams) of sodium in plasma?

Task 1.18
Convert values of concentrations of the metabolites occuring in blood plasma to the given units:

a) urea 36.4 mg/100 ml = ... mmol/l MW = 60.0 g/mol
b) creatinine 1.5 mg/100 ml = ... µmol/l MW = 113.0 g/mol
c) glucose 90.0 mg/100 ml = ... mmol/l MW = 180.0 g/mol

Task 1.19
Blood plasma contains around 40 g/l of albumin. What is the molar concentration of albumin? Molar mass (MW) of albumin = 66 300 g/mol.

Task 1.20
Urine daily sample (1 800 ml /24 hours) was analyzed in the laboratory: 0.204 grams of calcium were found in the sample. Calculate the molar concentration of calcium in the urine sample. Use the simplification: 1 ml = 1 g of urine. Molar mass of calcium = 40.8 g/mol.

Task 1.21
A treatment of diarrhea includes correction of body hydration by drinking a solution containing:
3.5 g of NaCl, 20 g of glucose, 2.5 g of $NaHCO_3$ and 1.5 g of KCl in 1 litre of water. Calculate

a) percent concentration of each of the components (in g/100 ml)
b) molar concentration of each of the components
c) molar concentrations of individual **ions** found in the solution

Task 1.22
1 litre of blood plasma contains around 140 mmol of Na^+, 100 mmol of Cl^-, 4.5 mmol of K^+, 24 mmol of HCO_3^- and 5 mmol of glucose. Calculate the percent concentration (in g/100 ml) of the ions and glucose. *Relative atomic masses (A_r): Na = 23, Cl = 35.5, H = 1, O = 16, C = 12, K = 39*

Task 1.23
Order the solutes present, among others, in blood plasma of an adult women from the highest to the lowest concentration: estradiol 210 pmol/l, testosterone 1.5 nmol/l, glucose 4.5 mmol/l, iron 20 µmol/l

LECTURE 2 Comparison of organic and inorganic compounds

As discussed in the first lecture, the human body consists predominantly of water, the inorganic solvent present in cells and also extracellularly. However the human body is built up of proteins, organic macromolecules, they are the most abundand organic molecules by mass present in the body. In fact cells, extracellular matrix and fluids contain a lot of other inorganic and organic low and high molecular weight compounds. So in the medicine you will meet both types of substances – inorganic and organic ones. In chemistry, these compounds are named by different ways, because their chemical composition, properties and reactivity differ. This is why it is useful to understand differences in these two classes of chemicals. Many of them are involved in patological processes, so it is useful to understand them thoroughly.

Important terms:

- structure of compounds and its effect on their properties
- structure of compounds and its effect on their chemical reactivity
- structure of compounds and its effect on their chemical naming
- differences and similarities of inorganic and organic chemical reactions

Task 2.1 Have a look at the molecular formulas listed in the table below and compare the **element composition** of inorganic and organic compounds:

common name	**inorganic** (molecular formula)	**common name**	**organic** (molecular formula)
salt	NaCl	*sugar*	$C_{12}H_{22}O_{11}$
water	H_2O	*cholesterol*	$C_{27}H_{46}O$
baking soda	$NaHCO_3$	*fat*	$C_{51}H_{98}O_6$
hypermangan	$KMnO_4$	*vinegar*	$C_2H_4O_2$
calomel	Hg_2Cl_2	*alcohol*	C_2H_6O
quartz	SiO_2	*urea*	CH_4N_2O
limestone (chalk)	$CaCO_3$	*beta-carotene*	$C_{40}H_{56}$
ammonia	NH_3	*benzene*	C_6H_6

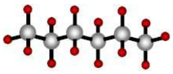
DO NOT MEMORIZE MOLECULAR FORMULAS OF ORGANIC COMPOUNDS !!!

In **organic compounds** carbon (C) and hydrogen (H) are always present. These compounds are called **HYDROCARBONS**.
Some other elements can be also involved, the most common are oxygen (O) and nitrogen (N).
If these or other elements are present the compounds are called **HYDROCARBON DERIVATIVES**.

Task 2.2 Carbon atom occurs also in some inorganic compounds: write formulas of the following one-carbon-containing **inorganic** compounds:

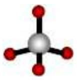
carbon monoxide *carbon dioxide* *hydrocyanic acid* *cyanic acid* *carbonic acid* *bicarbonate*

A unique features of **CARBON** present in organic compounds:



1) ability to bind to other carbon atoms to *give chains and rings* of various lengths
2) tetravalence (covalence of four: it has four valence-shell electrons) makes possible the *branching of chains* and the *fusion of several rings*
3) formation of quite stable *single, double and triple bonds*
4) formation of strong covalent bonds with many other atoms → *existence of many different compounds*

The list of **organic** one-carbon containing compounds includes the smallest hydrocarbon and its derivatives:

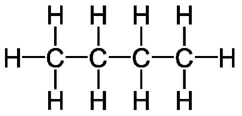


rational structural formula	**systematic name** *(substitutional principle)*	**systematic name** *(radical-functional principle)*	**common name** *(= trivial name)*
CH_4	meth**ane**	x	x
CH_3OH	methan**ol**	meth**yl** alcohol	x
HCHO	methan**al**	x	formaldehyde
HCOOH	methan**oic acid**	x	formic acid
CH_3NH_2	methan**amine**	meth**yl** amine	x

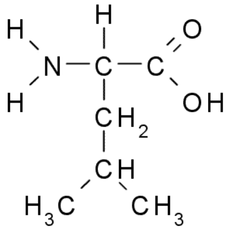
In **systematic names** the number of carbons of an organic molecule is expressed by a *prefix*
(1C = meth-),
whereas the type of hydrocarbon or hydrocarbon derivative is determined by its *suffix*
(-ane, -ol / -al / -oic acid / -amine).
In **common names** the number of carbons, or the type of chemical, is not mostly expressed
(these names resemble „nicknames“).

Task 2.3 Most of organic compounds contains two or more carbons attached together, forming a **carbon skeleton** that can be linear (A), branched (B,D) or cyclic (C). All elements are bound to each other by **covalent bonds**.

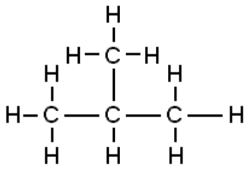
(A)



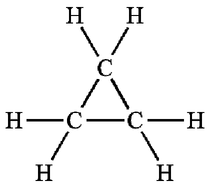
D)



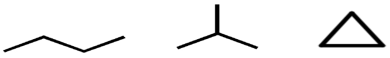
(B)



(C)



abbreviated (scientific) formulas of A, B, C: only carbon skeletons



a) Use a colored pencil and mark the carbon skeleton of the pictured hydrocarbon derivative (D)

b) Count the number of each element in this molecule and write its molecular formula *(see the introduction table in the Task 2.1)*:

c) Redraw the structural formula of the derivative with all bonds expressed *(for example C-H instead of CH)*

d) Count the number of valence electrons of each of the element involved in the covalent bonds:
carbon: hydrogen: oxygen: nitrogen:

e) Electronegativities of involved elements are: 2.5 (C), 2.2 (H), 3.5 (O), 3.1 (N). Using values of the electronegativity difference of bonded atoms state which bonds in the hydrocarbon derivative are called „nonpolar covalent“ and which are „polar covalent“. Use different colors and mark these different types of bonds.

HINT** – ranges of the electronegativity difference: **0.0-0.4 / 0.5-1.7 / 1.8 and more
it is used in classification: 0 - 0.4 for nonpolar covalent bond, 0.5 - 1.7 for polar covalent bond, 1.8 and more for ionic bond;
ionic bond is not common in organic compounds but occurs in inorganic ones

Carbon skeleton of organic compounds can be linear, branched or cyclic.

The number of bonds in which an element is always involved in organic compounds is called **valency**:
C is tetravalent (C-4), N is trivalent (N-3), O and S are divalent (O-2, S-2), H is monovalent (H-1)

Hydrocarbons contain only nonpolar covalent bonds (C-C and C-H), hence they **are nonpolar** (= hydrophobic = lipophilic) compounds that are insoluble in water (polar solvent), but they are soluble in organic (nonpolar) solvents.

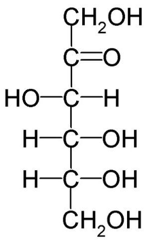
Hydrocarbon derivatives contain some polar covalent bonds that are polarized (partial charges are formed on bonded atoms, e.g. $O^{-}— H^{+}$), hence they are **more water soluble** in comparison to hydrocarbons; but the atoms are still bound, only some of them form free ions in aqueous solutions.

Task 2.4 Draw all possible organic structures (linear, branched or cyclic) that can be described by the following molecular formulas. Use only single bonds connecting carbons (C-C) and add the proper number of hydrogens to each carbon:

C_6H_{14}

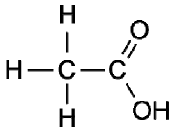
C_6H_{12}

Task 2.5 Following structures of organic compounds are examples of chemicals affecting human sensory perception, they all are hydrocarbon derivatives:



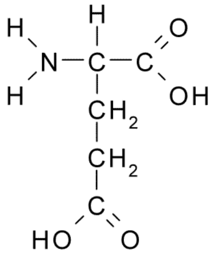
FRUCTOSE

= fruit sugar, the sweetest naturally occuring monosaccharide



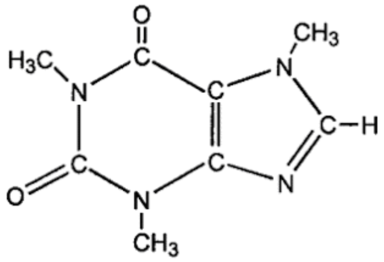
ACETIC ACID

= organic acid, its aqueous solution has acidic taste - you know it as vinegar



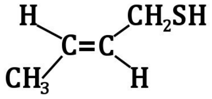
GLUTAMIC ACID

= one of amino acids found in proteins, its taste is called „meet taste“ (umami taste)



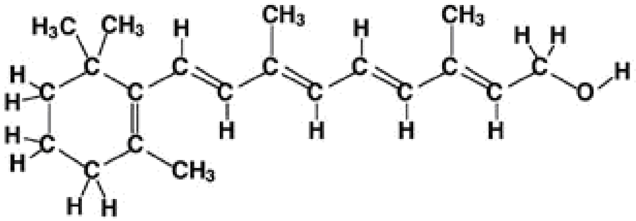
CAFFEINE

= an alkaloid of coffee beans having bitter taste



SKUNK SPRAY (but-2-ene-1-thiol)

= occuring in a skunk secret, its foul odor protects skunks from predators



VITAMIN A

= chemical essential in a diet, it is necessary for eyesight

Have a look at the structural formulas of the above mentioned organic compounds and then answer questions below:

1. Organic compounds found around us often contain a single covalent bond between carbons (C-C), but some molecules include one or more double bonds (C=C): use a colored pencil and mark all these double bonds in the structures above

2. Find and compare two compounds containing a ring in their structures: the ring can be built up of carbons only or it can include some other element - in this case it is reffered to as a „heterocyclic compound".

3. It is common that one-carbon containing -CH_3 group (called **methyl group**) forms a „branch" of a linear parent molecule (the longest chain - called „parent chain" or „carbon skeleton") or it is bound to a cyclic structure: use a colored pencil and mark all these methyl groups;

   ***ATTENTION**: -CH_3 group also occurs at the end(s) of the linear parent chain - in this case it is not a „branch", but it is its component, often marked as the firs or last carbon of the carbon skeleton*

4. Oxygen often occurs as a part of so called „functional groups" from which three are included in the above structural formulas: =O (**keto = oxo group**), -OH (**hydroxyl group**), -COOH (**carboxylic acid group**, which is a combination of both the keto and the hydroxyl group that are bound to the same carbon); use a colored pencil and mark all these functional groups.

5. Find compounds containing nitrogen: it can be either incorporated in a cyclic structure of a molecule (heterocyclic structure) or it forms the functional group -NH_2 (**amino group**).

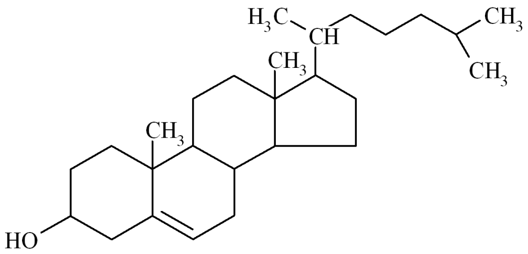
6. One of the compounds contains sulfur as a component of the functional group -SH (**thiol group**); low molecular weight molecules with the thiol group often have a strong unpleasant odor but other can smell well, for example like grapefruit.

7. Please **keep in mind the names of the above mentioned functional groups**.

So called **heteroatoms** (O, S, N) occur in organic compounds either arranged in a form of **functional groups** (often the most reactive parts of molecules, because of their properties) or incorporated in a ring structure of cyclic molecules called **heterocyclic compounds**.

If all carbons of a carbon skeleton are connected by simple C-C bonds, the molecule is refered to as a **SATURATED** hydrocarbon (or its derivative), whereas if one or more carbons are connected by the double C=C bond it is an **UNSATURATED** hydrocarbon (or its derivative). Double bonds are shorter and more reactive than single bonds.

Task 2.6. Look at the structure of cholesterol (below) and mark all its important structural parts:



a) the only polar functional group, name it
b) all saturated rings (cyclic structures)
c) unsaturated ring (cyclic structure)
d) methyl branches
e) branched hydrocarbon chain,
   count the number of its carbons
f) write its molecular formula

Task 2.7 Which of the following **systematic (IUPAC) names** of chemicals do name organic compounds?

sodium hydrogencarbonate, ethanoic acid, propyl amine, silicon dioxide, ferrous hydroxide, cyclohexane, nitric acid, methyl ethanoate, potassium butanoate, sodium ethanoate, potassium permanganate, methane, ethyne, hydrogen peroxide, nitrogen monoxide, hexanol, octadecanoic acid, hydrocyanic acid

Systematic (IUPAC) **names of inorganic compounds** are composed of *a name of cation and a name of anion* present in the molecule, *multiple prefixes* are used if necessary.

Systematic (IUPAC) **names of organic compounds** are always composed of *a prefix* expressing the number of carbons and *a suffix* specific to the type of the hydrocarbon or its derivative.

Task 2.8 Using the list of *prefixes* expressing the **number of carbons** *(which is useful to be memorized)* write the full structural formulas (all bonds) of given hydrocarbons in all their forms (linear and all possible branched structures); add their **molecular formulas**

HINT *– apply your knowledge of valency of atoms found in organic compounds*

meth-	**eth-**	**prop-**	**but-**	**pent-**	**hex-**	**hept-**	**oct-**	**non-**	**dec-**
1	2	3	4	5	6	7	8	9	10

propane: pentane:

Molecules having the same molecular formula but different structure are called **isomers** (iso- means „the same"). They need to be distinguished by different names because they *differ in chemical properties and reactivity.*

Isomers can differ either in their **constitution** (= order of atoms and bonds) or in their **configuration** (= arrangement in space)

Task 2.9 Which of the following pairs of hydrocarbon derivatives are isomers?

a) CH_3-CH_2-OH and CH_3-O-CH_3 b) CH_3-OH and HCHO c) CH_3-CO-CH_3 and CH_3-CH_2-CHO

Task 2.10 Write full structural formulas (all bonds expressed) of these functional groups:
***(**apply your knowledge of valency of atoms found in organic compounds)*

carboxylic acid group / **-COOH**
(found in most of organic acids)

sulfonic acid group / **-SO_3H**
(found in rare organic acids)

aldehyde group / **-CHO**
(found in aldehydes and most of saccharides)

keto group / **>C=O**
(found in ketones and in some saccharides)

hydroxyl group / **-OH**
(found in alcohols and in all saccharides)

thiol group / **-SH**
(rare, important in proteins)

amino group / **-NH_2**
(found in amines and in amino acids)

a) mark the **heteroatom** having the highest electronegativity in the above full structural formulas

b) describe its **interaction with water molecules** in aqueous solutions (the formation of hydrogen bonds) – it is the cause of the ability of hydrocarbon derivatives to dissolve in water

c) nitrogen atom (occuring in the 5th group of periodic table) has five valence electrons but only three of them commonly form covalent bonds in organic compounds: the last two electrons are often free, unbound electrons, or they can bind H^+ (proton) - draw the functional group produced by this reaction: it is called organic **ammonium cation**, and is positively charged

In case of presence of **only one functional group** in a hydrocarbon derivative, its presence is expressed in the name by a *suffix* and is used for the *classification of the derivative*
(carboxylic acid, sulfonic acid, aldehyde, ketone, alcohol, thiol, amine).

If a hydrocarbon derivative contains **two or more functional groups**, the principal one is expressed by a suffix in the name *(that one which is written more on the left in the above list)*, presence of other functional groups is expressed in the name by *prefixes*.

*example: CH_3-CH_2-OH is ethan**ol** (= alcohol), CH_3-CH_2-NH_2 is ethan**amine** (= amine),*
*whereas H_2N-CH_2-CH_2-OH is 2-aminoethan**ol** (= alcohol)*

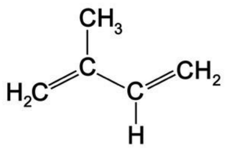
Task 2.11
The table below sumarizes **prefixes** used to express the number of carbons found in organic compounds, examples of suffixes are also included. Fill in missing names into the table:

number of CARBONS	**prefix-**	**alkane** *(saturated, only single bonds)*	**alkene** *(unsaturated, one double bond)*	**alkyne** *(unsaturated, one triple bond)*	**cycloalkane** *(saturated, cyclic, only single bonds)*	**alcohol** *(example of saturated alcohols)*
1	**meth-**	**meth**ane	X	X	X	**meth**anol
2	**eth-**	**eth**ane	**eth**ene	**eth**yne	X	**eth**anol
3	**prop-**		**prop**ene	**prop**yne	cyclo**prop**ane	**prop**anol
4	**but-**	**but**ane	**but**ene		cyclo**but**ane	**but**anol
5	**pent-**	**pent**ane	**pent**ene	**pent**yne	cyclo**pent**ane	
6	**hex-**	**hex**ane		**hex**yne	cyclo**hex**ane	**hex**anol
7	**hept-**	**hept**ane	**hept**ene	**hept**yne		**hept**anol
8	**oct-**		**oct**ene	**oct**yne	cyclo**oct**ane	**oct**anol
9	**non-**	**non**ane	**non**ene		cyclo**non**ane	**non**anol
10	**dec-**	**dec**ane	**dec**ene	**dec**yne	cyclo**dec**ane	
11	**undec-**	**undec**ane	**undec**ene	**undec**yne	X	**undec**anol
12	**dodec-**	**dodec**ane		**dodec**yne	X	**dodec**anol
13	**tridec-**	**tridec**ane	**tridec**ene	**tridec**yne	X	**tridec**anol
14	**tetradec-**		**tetradec**ene	**tetradec**yne	X	**tetradec**anol

Prefixes used to express the number of multiple bonds, branches and heteroatoms or functional groups found in an organic compound *(they are also used in naming inorganic compounds):*

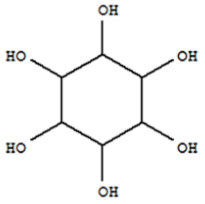
	1	2	3	4	5	6	7	8	9	10	11	12
multiple prefix	mono	di	tri	tetra	penta	hexa	hepta	octa	nona	deca	un deca	do deca

The multiple prefix is inserted into the name directly before the structure to which it is related:



2-methyl**but**a-1,3-<u>di</u>ene *(common name: isoprene)*

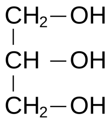
- one methyl group binds to the 2nd carbon (prefix mono is not used)
- <u>two</u> double bonds (-ene) rise from the 1st and the 3rd carbons



cyclo**hex**ane-1,2,3,4,5,6-**hex**ol

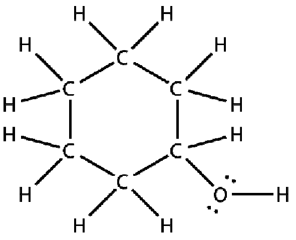
<u>Task 2.12</u> Using systematic (IUPAC) organic nomenclature, name the following compounds:

a)

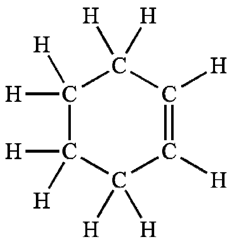


$$\begin{array}{l} CH_2-OH \\ | \\ CH\ -OH \\ | \\ CH_2-OH \end{array}$$

b)



c)



Some *derivatives of hydrocarbons* are named by **names created by radical-functional principle**. In chemistry the term radical refers to a substance having free unpaired electron(s). So the structure formed by a loss of H from a hydrocarbon, <u>which electron still remains in the hydrocarbon</u>, is called **hydrocarbon radical** *(or hydrocarbon rest or alkyl)*. The name of the hydrocarbon rest (commonly abbreviated R–) can be included in names of organic molecules in which these structures are present.

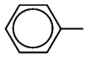
Names of hydrocarbon rests are suffixed by **–yl**

<u>example</u>: *CH_3- is called **methyl**, because it is formed from **meth**ane CH_4,*
*hence methanol CH_3-OH is also called <u>**methyl** alcohol</u>*

Recall that the names of hydrocarbon rests are also used in a naming branched hydrocarbons.

CH_4 **methane**	→	**CH_3-** **methyl**	→	**-CH_2-** **methylene**
CH_3-CH_3 **ethane**	→	**CH_3-CH_2-** **ethyl**	→	**-CH_2-CH_2-** **ethylene**
CH_2=CH_2 **ethene** *(common name: „ethylene“)*	→	**CH_2=CH-** **ethenyl or <u>vinyl</u>**	→	**-CH=CH-** **vinylene**

Task 2.13 Fill in missing formulas and names into the table:

hydrocarbon name	structural formula	hydrocarbon rest name	structural formula
methane	CH_4	**meth**yl	CH_3-
ethane		**eth**yl	
propane			$CH_3CH_2CH_2$-
butane	$CH_3CH_2CH_2CH_3$		
pentane			
hexane			
heptane		**hept**yl	
octane			$CH_3(CH_2)_6CH_2$-
nonane			
decane	$CH_3(CH_2)_8CH_3$		
benzene		**phenyl** *(NOT benzyl!)*	

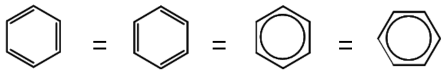
Task 2.14
Draw structural formulas of the following compounds and keep in mind their **common** = trivial **names** (they are common in naming these compounds in practice).

a) 2-methylbuta-1,3-diene = **ISOPRENE**

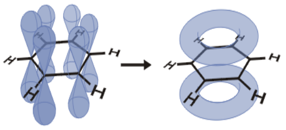
b) vinyl benzene = **STYRENE**

Both the molecules form polymers = long chains in which the molecule a) or b) is a repetitive unit (x) (monomer): x-x-x-x-x-x-x-x-x-x-x-x-........... Thus, for example, styrene forms plastic polystyrene (PS).

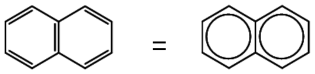
There is one kind of cyclic organic molecules that strongly differs from others by properties, reactivity, and also by naming: these molecules form **planar cycles** with **alternating double and single bonds** (so called conjugated double bonds). The group of compounds is refered to as **arenes** or „aromatic compounds“, in which all carbon atoms are equivalent and lay in one plane. Electrons of their double bonds are delocalized above and under the plane of their rings. The simplest arene is called **benzene**, other examples (below) are called polyaromatic hydrocarbons (PAH) – all are toxic.



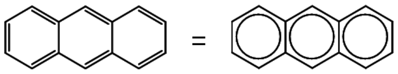
benzene



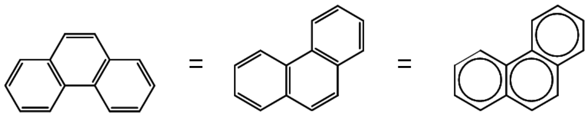
delocalized electrons



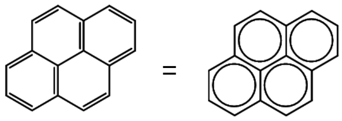
naphtalene



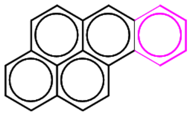
anthracene



phenanthrene



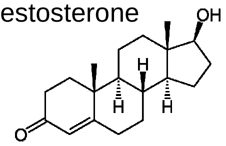
pyrene



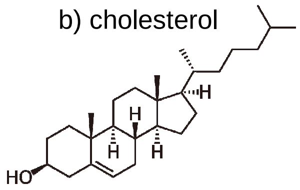
benzo(a)pyrene

Task 2.15 From the biologically important molecules below choose those containing an aromatic ring:

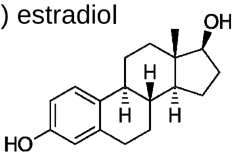
a) testosterone



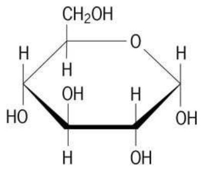
b) cholesterol



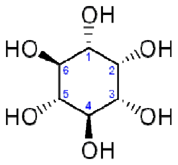
c) estradiol



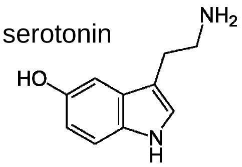
d) glucose



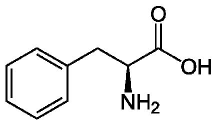
e) inositol



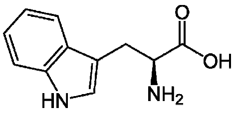
f) serotonin



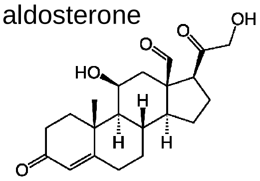
g) phenylalanine



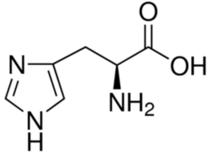
h) tryptophan



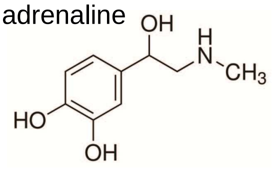
i) aldosterone



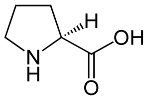
j) histidine



k) adrenaline



l) proline



Task 2.16 Add missing names or formulas of the hydrocarbon derivatives into the table:

hydrocarbon derivative	example	structural formula	name
carboxylic acid	CH_3-CH_2-COOH propanoic acid		ethanoic acid
sulfonic acid	CH_3-CH_2-CH_2-SO_3H propane-1-sulfonic acid	CH_3-SO_3H	
aldehyde	CH_3-CH_2-CHO propanal		butanal
ketone	CH_3-CO-CH_3 propanone *or dimethyl ketone*	CH_3-CH_2-CO-CH_2	or ?
alcohol	CH_3-CH_2-CH_2-OH propan-1-ol *or propyl alcohol*		methanol or ?
thiol	CH_3-CH_2-CH_2-SH propane-1-thiol	CH_3-CH_2-CH_2-CH_2-CH_2-SH	
amine	CH_3-CH_2-CH_2-NH_2 propan-1-amine *or propyl amine*		hexan-1-amine or ?
ether	CH_3-CH_2-O-CH_3 ethyl methyl ether	CH_3-CH_2-O-CH_2-CH_3	
sulfide	CH_3-CH_2-S-CH_3 ethyl methyl sulfide		dimethyl sulfide
halogen derivative	CH_3-CH_2-CH_2-Cl 1-chloropropane	CH_3-CHCl-CH_2-CH_3	
nitro derivative	CH_3-CH_2-CH_2-NO_2 1-nitropropane		2-nitropropane

HINT

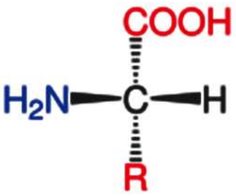
the functional group always gets the lowest locant as possible

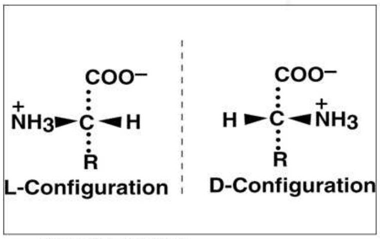
(e.g. propan-1-amine, NOT propan-3-amine)

If any carbon in an organic molecule binds **four different** „partners“ (called substituents, because they have substituted hydrogens of methane, the simplest hydrocarbon), it has special properties: it is called „**chiral**“ or „**assymetrical**“ carbon, and it is able to interact with linearly polarized light – it causes its rotation (sometimes the term „optical active“ carbon or molecule is used). This kind of molecule forms two isomers, called **enantiomers**, in biochemistry distinguished by letters L- and D- before the name. They differ in a spatial arrangement and look like mirror images of each other, that are non-superposable (not identical), as one's left and right hands. Thus amino acids found in proteins are only L-amino acids whereas monosaccharides are mostly D-monosaccharides. The enantiomers have different biological acivity, one is efficient and the other can be toxic to the human body.

<u>general formula of an amino acid</u>:

- *carbon binds hydrogen, amino group, carboxylic acid group and something else (R = side chain, various structures)*
- *dotted bonds direct under the plane of paper, wedge-type bonds go above the plane of it (toward you)*





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Task 2.17 Which of the molecules from the above table (see Task 2.16) forms two enantiomers?

Organic compounds form two main classes: hydrocarbons and hydrocarbon derivatives. *The molecular formula of an organic compound can describe more than one structure***,** these molecules are called *isomers*, and they have different properties and chemical reactivity.

Inorganic compounds form many classes, e.g. oxides, hydroxides, peroxides, acids and other. *Molecular formulas of inorganic compounds are common in use*, because they do not form isomers.

In organic chemistry and biochemistry **it is useful to work with structural formulas** of compounds for better understading their properties and chemical reactivity.

Task 2.18

Write formulas of the following inorganic compounds and put them in order from the lowest to the highest oxidation state of chlorine:

perchloric acid, chlorous acid, chloric acid, hydrochloric acid, chlorine, hypochlorous acid

HINT

In inorganic compounds the oxidation state is given by an oxidation number – ***it is not determined in organic compounds****, but the number of oxygen atoms and hydrogens in a molecule can help ;)*

Oxidation in organic chemistry is not described by a simple loss of electrons, as it does in inorganic chemistry. There are no oxidation numbers specified in organic compounds.
Organic molecule is oxidized if the number of hydrogen atoms decreases and / or the number of oxygen atoms increases in its molecule.

Reduction of organic compounds is also seen from their element composition: **the number of oxygen atoms in the molecule decreases and /or the number of hydrogen atoms increases if the organic molecule is reduced.**

<u>The most reduced form</u> of an organic compound (its carbon skeleton) is a saturated hydrocarbon – it is absolutely SATURATED BY HYDROGENS.

<u>Task 2.19</u>
Decide which process (A or B) describes an oxidation and which one is a reduction. Fill in correct names next to each of the partial reactions of the processes, you can choose any from these names:

hydrogenation (= addition of hydrogen) / dehydrogenation (elimination of hydrogen)
hydration (= addition of water) / dehydration (= elimination of water)

(A) $\mathbf{CH_3\text{-}CH_3 \rightarrow CH_2{=}CH_2 \rightarrow CH_3\text{-}CH_2\text{-}OH \rightarrow CH_3\text{-}CHO \rightarrow CH_3\text{-}COOH}$

a) $CH_3\text{-}CH_3 \rightarrow CH_2{=}CH_2 + H_2$

b) $CH_2{=}CH_2 + H_2O \rightarrow CH_3\text{-}CH_2\text{-}OH$

c) $CH_3\text{-}CH_2\text{-}OH \rightarrow CH_3\text{-}CHO + H_2$

d) $CH_3\text{-}CHO + H_2O \rightarrow CH_3\text{-}COOH + H_2$

(B) $\mathbf{CH_3\text{-}COOH \rightarrow CH_3\text{-}CHO \rightarrow CH_3\text{-}CH_2\text{-}OH \rightarrow CH_2{=}CH_2 \rightarrow CH_3\text{-}CH_3}$

a) $CH_3\text{-}COOH + H_2 \rightarrow CH_3\text{-}CHO + H_2O$

b) $CH_3\text{-}CHO + H_2 \rightarrow CH_3\text{-}CH_2\text{-}OH$

c) $CH_3\text{-}CH_2\text{-}OH \rightarrow CH_2{=}CH_2 + H_2O$

d) $CH_2{=}CH_2 + H_2 \rightarrow CH_3\text{-}CH_3$

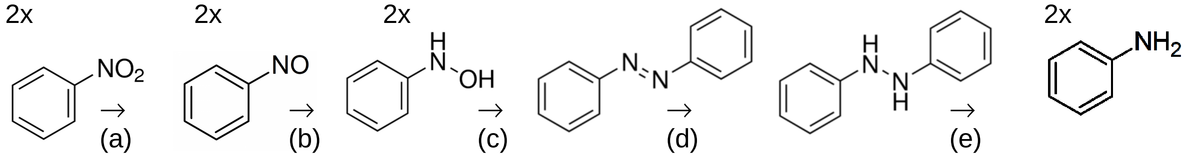
HINT
*max. number of **hydrogens** → max. number of **oxygens***
<u>the most reduced molecule</u> <u>the most oxidized molecule</u>

<u>Task 2.20</u> Name all organic molecules from the Task 2.19.

Task 2.21
Is the reaction below an oxidation or reduction? Explain. Name all the molecules.

$CH_3\text{-}SH + CH_3\text{-}SH \rightarrow CH_3\text{-}S\text{-}S\text{-}CH_3 + H_2$

Task 2.22
The following sequence of reactions describes the step-by-step conversion of nitrobenzene to benzenamine. Is it oxidation or reduction? Explain.



Which of the above partial reactions can be described as hydrogenation or dehydration ?

Task 2.23
Compare each pair of molecules below, name them and state which one is more oxidized:

A) $CH_3\text{-}SO_3H$ $CH_3\text{-}SH$

B) $CH_3\text{-}OH$ HCHO

C) HCOOH HCHO

D) $CH_3\text{-}CH_3$ $CH_2\text{=}CH_2$

E) $CH_3\text{-}NH_2$ $CH_3\text{-}NO_2$

Task 2.24

For each of the following acids write the chemical reaction of its dissociation in water (use formulas). State the chemical nature of each of the acids (inorganic / organic) and its strenght (strong / week).

a) carbonic acid

b) acetic acid

c) hydrochloric acid

d) butanoic acid

e) sulfuric acid

f) propanedioic acid

Both **inorganic and organic acids** are defined as molecules able to donate proton(s) (H^+), both can be monoprotic or polyprotic – the ability to donate the second or other proton is lower than the first one, their strenght is described by dissociation constants (K_a).

Most of organic acids are week, their dissociation constant $K_a = 10^{-2}$ or lower (which means: $pK_a = 2$ or higher).

Acids can react either with hydroxides (bases) in the reaction called **neutralization** or with alcohols in the process caled **esterification.** Whereas the neutralization proceeds spontaneously, similarly as a dissociation of acids in water, esterification needs to be catalyzed.

Task 2.25

Name all the molecules and then compare the reaction processes. What is similar in all these reactions? Choose the terms: *neutralization / esterification* and put them correctly to the reactions.

a) $CH_3COOH + NaOH \rightarrow CH_3\text{-}COONa + H_2O$

b) $HNO_3 + NaOH \rightarrow NaNO_3 + H_2O$

c) $CH_3COOH + CH_3OH \rightarrow CH_3\text{-}CO\text{-}OCH_3 + H_2O$

d) $HNO_3 + CH_3OH \rightarrow CH_3\text{-}O\text{-}NO_2 + H_2O$

LECTURE 3 Biochemically important organic compounds I

There are many types of organic compounds in the human body, but carboxylic acids are the most common in the human metabolism. They originate from all nutrients: proteins are composed of amino acids, fat contains fatty acids, and saccharides - by chemical structure polyhydroxyderivatives of aldehydes or ketones - are oxidized to carboxylic acids as well. The central metabolic pathway, Krebs cycle, is a process of an interconversion of various carboxylic acids and their derivatives. In aqueous solutions, that is almost everywhere in the body, week carboxylic acids always occur in two forms: undissociated molecules and their anions, called carboxylates. Their naming is often simplified to names of anions only. If nutrients are oxidized, anhydrides - important derivatives of acids – are often produced. They are highly unstable in aqueous solutions, and this property is used in a conversion of energy in the course of cellular metabolism. Other important metabolic acid derivatives are esters.

Important terms:

- interrelationships of alcohols, aldehydes, and carboxylic acids
- mono- and dicarboxylic acid derivatives: anions, acyls, esters, anhydrides

oxidation of primary alcohol → aldehyde → carboxylic acid

$$\mathbf{R\text{-}CH_2\text{-}OH \rightarrow R\text{-}CHO \rightarrow R\text{-}COOH}$$

oxidation of secondary alcohol → ketone → not oxidized to carbox. acids

$$\mathbf{R_1\text{-}CH(OH)\text{-}R_2 \rightarrow R_1\text{-}CO\text{-}R_2}$$

Primary alcohols = hydroxyl group is bound to the end of their hydrocarbon skeleton.
Secondary alcohols = hydroxyl group is attached whithin their unbranched hydrocarbon chain.

Task 3.1

Use the general rule on oxidation of *carbonyl compounds* (= aldehyde and ketones, because both contain the *carbonyl functional group, >C=O*), and fill in gaps in the table below: add missing names.

alcohol	aldehyde	ketone	carboxylic acid
CH_3-OH methanol or methyl alcohol	HCHO methanal or ***formaldehyde***	x	HCOOH methanoic acid or ***formic acid***
CH_3-CH_2-OH ? or ?	CH_3-CHO ? or ***acetaldehyde***	x	CH_3-COOH ? or ***acetic acid***
CH_3-CH_2-CH_2-OH propan-1-ol or propyl alcohol	CH_3-CH_2-CHO propanal or ***propionaldehyde***	x	CH_3-CH_2-COOH propanoic acid or ***propionic acid***
CH_3-CH(OH)-CH_3 propan-2-ol or isopropyl alcohol	x	CH_3-CO-CH_3 propanone or ***acetone*** or dimethyl ketone	x
CH_3-CH_2-CH_2-CH_2-OH butan-1-ol or butyl alcohol	CH_3-CH_2-CH_2-CHO ? or ***butyraldehyde***	x	CH_3-CH_2-CH_2-COOH ? or ***butyric acid***
CH_3-CH_2-CH(OH)-CH_3 butan-2-ol or *secondary* butyl alcohol	x	CH_3-CH_2-CO-CH_3 butan-2-one or ethyl methyl ketone	x

in bold: ***common names*** ***common name*** ***common names***

Task 3.2

Reduction is the reverse reaction to oxidation. Thus carboxylic acids can be, in two steps, reduced to primary alcohols: fill in proper names into the table below.

number of carbons	carboxylic acid	aldehyde	alcohol
5	pentanoic acid	pentanal	pentan-1-ol
6	hexanoic acid	hexanal	
8	octanoic acid		octan-1-ol
10	decanoic acid	decanal	
12	dodecanoic acid ***= lauric acid***	dodecanal	dodecan-1-ol
14	? ***= myristic acid***	tetradecanal	
16	? ***= palmitic acid***	hexadecanal	
18	? ***= stearic acid***	octadecanal	
20	eicosanoic acid		
22	docosanoic acid		

in bold: common names

HINT

*Even-carbons containing monocarboxylic acids (from 4 carbons) occur in fat - they are called „fatty acids“ and in biochemistry we used to call them by **common names**.*

Hydroxyl and aldehyde groups are polar, they can form hydrogen bonds with water molecules, so **low molecular weight alcohols and aldehydes are water soluble**.

Carboxylic acid functional group can dissociate in aqueous solutions resulting in a negative charge, so acids are even more water soluble. Ions are easily surrounded by water molecules, and thus dissoved in water.

Nevertheless: <u>as the hydrocarbon chain elongates</u>, the nonpolar character of the molecule predominates, and <u>solubility in water decreases</u>.
This is why long-chain fatty acids (from C12) are very little soluble in water, hence their name.

Task 3.3
Name the following compounds and choose these which are alcohols:

a) $HO\text{-}CH_2\text{-}CH_2\text{-}NH_2$

b) $HO\text{-}CH_2\text{-}CHO$

c) $HO\text{-}CH_2\text{-}CH_2\text{-}OH$

d) $CH_3\text{-}CO\text{-}OH$

Task 3.4
Draw hydrogen bonds between

a) two water molecules

b) two molecules of ethanol

c) water and ethanol

d) water and hexanol

Task 3.5
Draw all possible difunctional alcohols (= containing two hydroxyl groups) derived from benzene and name them. How many isomers do exist?

Alcohol derived from benzene with only one hydroxyl group is called **phenol**. This is the simplest phenol, because all aromatic alcohols with one or more *hydroxyl groups directly attached to the aromatic ring* are refered to as „phenols“ (they have individual common names). Properties of phenols differ from properties of other alcohols due to their aromatic ring to which -OH group is attached.

Alcohol derived from toluene, hydroxyl group of which is not directly attached to the benzene ring, *is not phenol*. Toluene is methyl benzene, so the hydroxyl group can be attached to its methyl group (one H of which is replaced by -OH). This alcohol is called **benzyl alcohol**, and it can be oxidized to carboxylic acid as other primary alcohols.

Task 3.6
Write the two-step oxidation of *benzyl alcohol (→ benzaldehyde → benzoic acid)*:

Task 3.7
Draw structures of all possible methyl derivatives of phenol (containing one methyl group). How many isomers do exist? They are called **cresols**, and their aqueous solution has germicide effect (it can be used as a desinfection).

Task 3.8
Write the reaction describing the oxidation of propane-1,2,3-triol (= **glycerol**), if

a) only one primary alcohol (hydroxyl) group is oxidized; state both oxidation steps:

b) only its secondary alcohol group is oxidized:

Name all the above products formed by oxidation of glycerol (use systematic names).

Multifunctional alcohols (containing two or more hydroxyl groups) **are sweet** molecules, this is why ethane-1,2-diol is called *glycol* and propane-1,2,3-triol is known as *glycerol (from Greek word glykys = sweet)*.

Saccharides are polyhydroxyderivatives of aldehydes or ketones, hence their sweet taste. The simplest – three carbons containing saccharides are derived from glycerol, their common names are **glyceraldehyde** and **glycerone** (= dihydroxyacetone), see Task 3.8.

Task 3.9

Use given boiling point values of the fatty acids to order the acids according to their solubility in water **from the most to the least water soluble** *(HINT: boiling point depends on the molecular weight)*

myristic acid (326 °C) stearic acid (361 °C) butyric acid (164 °C) caproic acid (206 °C)

lauric acid (298 °C) caprylic acid (240 °C) palmitic acid (351 °C) capric acid (269°C)

Task 3.10

Common dicarboxylic acids have the general formula: $HOOC\text{-}(CH_2)_n\text{-}COOH$ in which n = 0,1,2,3,...
In biochemistry we are used to draw them vertically, so the smallest dicarboxylic acid (ethanedioic acid) is:

C2 C3 C4 C5 C6

COOH
I
COOH

Draw the rational structural formulas of other most common dicarboxylic acids (above) and name them by systematic names. Their carboxylic groups are always at both ends of the molecule.

Task 3.11

Dissociation of dicarboxylic acids, as well as of monocarboxylic acids, depends on the surrounding pH. Carboxylic acids are often only partially dissociated in aqueous solutions (= only some % of their molecules exists as ions), but both –COOH groups of dicarboxylic acids are ionized.
Draw anions of the above dicarboxylic acids:

C2 C3 C4 C5 C6

COO^-
I
COO^-

Task 3.12

Names of anions of carboxylic acids (= carboxylates) are often derived from the cammon names of related acids using the suffix **-ate** instead of the suffix **-ic acid** (acetic acid → acetate).

Name the anions from the Task 3.11 using the **common** names of the dicarboxylic acids:

C2 ethanedioic acid = **oxalic** acid

C3 propanedioic acid = **malonic** acid

C4 butanedioic acid = **succinic** acid

C5 pentanedioic acid = **glutaric** acid

C6 hexanedioic acid = **adipic** acid

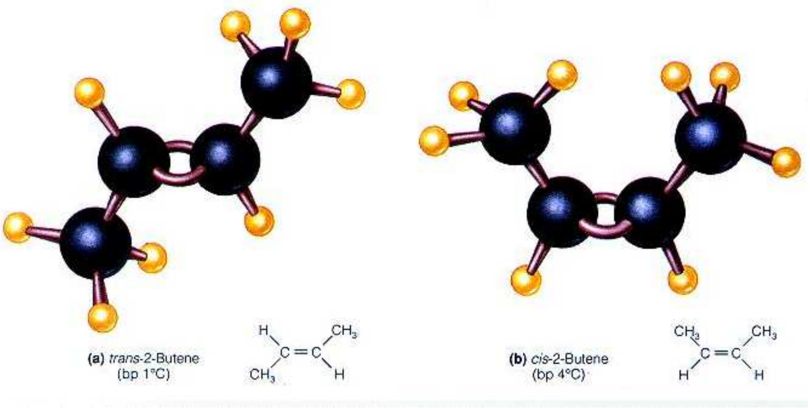
Anions of carboxylic acids, **R-COO$^-$**, are formed by a release of H^+ from the carboxylic functional group. After removing OH from the -COOH functional group we get the „rest" af a carboxylic acid, generaly called **acyl**: **R-CO-** *(compare with rests of hydrocarbons, e.g. methyl CH_3-)*. Acyls do not exist separately, they are structural parts of some other (bigger) structures. Names of acyls are often derived from common names of acids by substitution of the suffix –ic acid by the **suffix –yl** *(e.g. acetic acid → acetyl, the root of the name stays the same)*

Task 3.13

Fill in missing names into the table:

number of carbons	IUPAC name	common name	anion name	acyl name
	monocarboxylic acids:			
C1	methanoic acid	**formic acid**	**form**ate	**form**yl
C2		**acetic acid**		
C3		**propionic acid**		
C4		**butyric acid**		
C5		**valeric acid**		
C6		**caproic acid**		
C8		**caprylic acid**		
C10		**capric acid**		
C12		**lauric acid**		
C14		**myristic acid**		
C16		**palmitic acid**		
C18		**stearic acid**		
	dicarboxylic acids:			
C2	ethanedioic acid	**oxalic acid**	**oxal**ate	**oxal**yl
C3		**malonic acid**		
C4		**succinic acid**		
C5		**glutaric acid**		
C6		**adipic acid**		

Similarly as hydracarbons can be saturated or unsaturated, carboxylic acids contain either **saturated or unsaturated hydrocarbon chain**. Unsaturated hydrocarbon chain forms two types of spatial isomers (different in the space arrangement): you can imagine the double bond laying in one plane and hydrogens attached to the unsaturated carbons can be bound either from the opposite sides (***trans* isomer**) or the same side (***cis* isomer**). The two isomers differ in physico-chemical properties.



Task 3.14

Draw the most common **unsaturated** fatty acids containing *cis* double bonds (their positions are counted from the carboxylic functional group)

number of carbons : number of double bonds ; position of double bond(s)

a) **18:1; 9** = octadec-9-enoic acid = **oleic acid**

b) **18:2; 9,12** = octadeca-9,12-dienoic acid = **linoleic acid**

c) **18:3; 9,12,15** = octadeca-9,12,15-trienoic acid = **α-linolenic acid**

d) **20:4; 5,8,11,14** = eicosa-5,8,11,14-tetraenoic acid = **arachidonic acid**

Task 3.15

Using the common names of the above unsaturated fatty acids (see on the right in bold) add names of their anions and acyls.

Task 3.16

Name the following fatty acids (use systematic = IUPAC names) and describe them by the common labeling: number of carbons : number of double bonds ; positions of double bonds (example: 18:2; 9,12)

(use the prefixes: C20 = eicosa-, C22 = docosa)

Task 3.17

Draw two isomers of but-2-endioic acid and distinguish them by their full names (add *cis* or *trans* prefix). The common name of the cis isomer is **maleic acid** and the name of the trans isomer is **fumaric acid**: write names of their anions and acyls.

Task 3.18

Write structural formulas of these rests of carboxylic acids (= acyls):

a) butyryl

b) formyl

c) acetyl

d) succinyl

e) malonyl

f) stearoyl

g) propionyl

h) glutaryl

Task 3.19
Write formulas of reactants and formulas and names of products of the reactions:

1. oxidation of methanol (two steps)
2. reduction of acetone
3. dehydration of butan-1-ol
4. hydration of ethene
5. dissociation of acetic acid

Task 3.20
Write common names of acyls and anions derived from these carboxylic acids

- CH_3COOH
- $HCOOH$
- CH_3CH_2COOH
- $CH_3(CH_2)_{16}COOH$
- $HOOC\text{-}CH_2\text{-}CH_2\text{-}COOH$
- $(COOH)_2$
- $CH_3(CH_2)_{14}COOH$

Task 3.21
Write names of the smallest

a) monocarboxylic acid b) dicarboxylic acid c) fatty acid

In chemistry the term **condensation** describes a reaction in which two molecules are coupled together with simultaneous release of water as the second product. For example the production of esters or anhydrides of carboxylic acids can be described as condensation of their functional groups:

A) carboxylic acid + alcohol → ester + water

$R_1\text{-CO-}\mathbf{OH} + \mathbf{H}\text{O-}R_2 \rightarrow R_1\text{-CO-O-}R_2 + \mathbf{H_2O}$

B) carboxylic acid + carboxylic acid → anhydride + water

$R_1\text{-CO-}\mathbf{OH} + \mathbf{H}\text{O-CO-}R_2 \rightarrow R_1\text{-CO-O-CO-}R_2 + \mathbf{H_2O}$

Similarly, a carboxylic acid can condense with an inorganic acid (e.g. H_3PO_4), or two inorganic acids can condense together as well, resulting also in a formation of an anhydride:

C) carboxylic acid + phosphoric acid → anhydride + water

$R_1\text{-CO-}\mathbf{OH} + \mathbf{H}\text{O-PO-(OH)}_2 \rightarrow R_1\text{-CO-O-PO-(OH)}_2 + \mathbf{H_2O}$

D) phosphoric acid + phosphoric acid → anhydride + water

$\text{(HO)}_2\text{-PO-}\mathbf{OH} + \mathbf{H}\text{O-PO-(OH)}_2 \rightarrow \text{(HO)}_2\text{-PO-O-PO-(OH)}_2 + \mathbf{H_2O}$

HINT - *phosphorus has five valence electrons;* H_3PO_4 *or* $O{=}P(OH)_3$

The reverse reaction to the condensation is called **hydrolysis**, or hydrolytical cleavage, because water is needed to restore the original molecules (carboxylic acid and alcohol in ester hydrolysis, or two acids in hydrolysis of anhydrides).

Task 3.22

Write structural formulas and names of products of the hydrolytical cleavage of the following esters (= ester hydrolysis):

a) $CH_3\text{-}CH_2\text{-}CH_2\text{-CO-O-}CH_3$ →
(ester: methyl butyrate)

b) $CH_3\text{-}CH_2\text{-}CH_2\text{-CO-O-}(CH_2)_4\text{-}CH_3$ →
(ester: pentyl butyrate)

c) $CH_3\text{-CO-O-}(CH_2)_4\text{-}CH_3$ →
(ester: pentyl acetate)

d) $CH_3\text{-}CH_2\text{-}CH_2\text{-CO-O-}CH_2\text{-}CH_3$ →
(ester: ethyl butyrate)

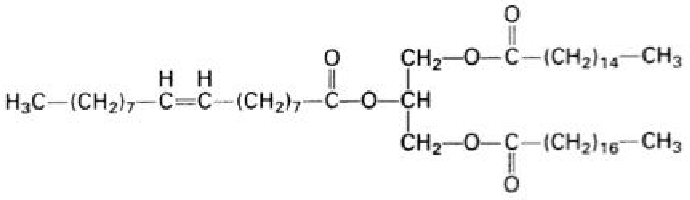
e) $H\text{-CO-O-}CH_2\text{-}CH_3$ →
(ester: ethyl formate)

Most of these esters occur in various fruits, they are volatile compounds (easily evaporating) having fruit smell.

Task 3.23

The structure below describes an example of triacylglycerol (TAG) molecule that is an ester of glycerol (= propan-1,2,3-triol) with three fatty acids. In biochemistry we call this kind of ester „body fat“, because it is stored in the adipose tissue as an energy reserve.

Mark all three ester functional groups (-CO-O-) of the TAG and name fatty acids produced by its hydrolysis:



Task 3.24

Write the structural formula of the ester produced by the condensation of the following molecules. Its common name is acetylcholine, and it is a signalling molecule used as a neurotransmitter in the human body. Why is the nitrogen atom of the second molecule (= choline) positively charged?

CH_3-COOH + HO-CH_2-CH_2-$^+N(CH_3)_3$ →

Task 3.25

Name the following molecules and for each state what type of organic compound it is:

a) CH_3-CH_2-CH_2-CO-O-CH_3

b) CH_3-CH_2-O-CH_3

c) CH_3-$(CH_2)_{14}$-COOH

d) CH_3-CH_2-CH_2-COONa

e) $(CH_3$-CH_2-$COO)_2Ca$

f) CH_3-CH_2-O-CO-H

Task 3.26

Draw structural formulas of anhydrides produced by condensation of the acids below and mark all the anhydride functional groups (-CO-O-CO- or -CO-O-PO-):

a) CH_3-COOH + HOOC-CH_3 →

b) HCOOH + HOOCH →

c) CH_3-COOH + HOOCH →

d) CH_3-CH_2-COOH + HO-PO-$(OH)_2$ →

e) HOOC-CH_2-CH_2-COOH →
(it forms cyclic anhydride)

Task 3.27

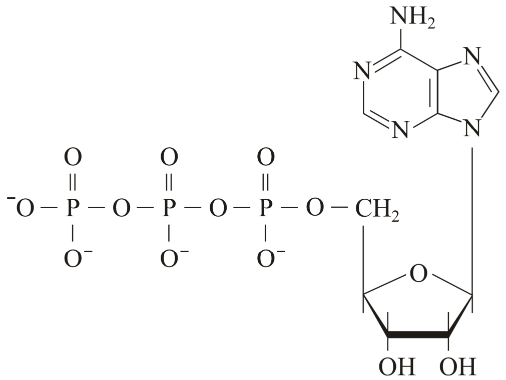
The structure below describes the molecule of ATP, a donor of energy for many energy-consuming processes in cells. Its energy is released by a hydrolytical cleavage of its anhydride bonds.

a) Mark the anhydride bonds and draw and name acids released by their hydrolysis.

b) Find and mark the ester bond (functional group) of ATP molecule.

c) Mark and name all functional groups present after the hydrolysis of the ester bond.

d) Which of the heterocycles is aromatic – the oxygen-containing or the four-nitrogens-containing?



LECTURE 4 Biochemically important organic compounds II

Most of organic acids involved in a human metabolism are in fact derivatives of carboxylic acids. Some of them still contain the carboxylic acid functional group, with its ability to be ionized in aqueous solutions, so they still have an acidic character. But there are also derivatives of carboxylic acids, carboxylic group of which has been changed, so they are not more „acids“. In addition to anions of acids, carboxylic group of which is also „changed“, you know two of this kind of derivatives from the previous lecture: esters and anhydrides. Other types of the derivatives will be discussed in this lecture. Even proteins belong into this class of carboxylic acid derivatives. Many of the previously mentioned organic chemistry topics will again appear in the chemistry of proteins: amino group, hydroxyl group, thiol group, aromatic and heterocyclic structures as well. And because proteins build up our body, each of these functional groups and structures is essential for life, each needs to be understood thoroughly also on the level of its chemical properties and reactivity.

Important terms:

- substitutional derivatives of carboxylic acids and their chemical reactions
- differences between amines and amides
- covalent bonds involved in structures of proteins
- common names and properties of heterocyclic compounds

If a carboxylic acid contains one or more other functional group(s), in addition to its carboxylic acid group, it is called **substitutional derivative** of the acid.

The most common substitutional derivatives are hydroxy acids, oxo (= keto) acids and amino acids. All of them are interconvertable: **hydroxy acid** can be oxidized to **oxo acid**, which can be converted to **amino acid** – all having the same carbon skeleton, only differing in the functional group. All the reactions are reversible.

This is why it is useful to learn them together, in groups.

Task 4.1

Write structural formulas of molecules formed by the oxidation of hydroxyl groups of the following hydroxy acids. Name all the substitutional derivatives, including reactants, by systematic names.

a) CH_3-CH(OH)-COOH →

b) CH_3-CH(OH)-CH_2-COOH →

c) HOOC-CH_2-CH(OH)-COOH →

d) HOOC-CH_2-CH_2-CH(OH)-COOH →

Task 4.2

Write structural formulas of molecules formed by the reduction of oxo groups of the following oxo acids. Name all the substitutional derivatives, including reactants, by systematic names.

a) CH_3-CO-COOH →

b) CH_3-CO-CH_2-COOH →

c) HOOC-CH_2-CO-COOH →

d) HOOC-CH_2-CH_2-CO-COOH →

Task 4.3

Write structural formulas of molecules formed by the transamination of the following oxo acids. Name all the products by systematic names.

HINT

Transamination is a process catalyzed by enzymes.
They use an amino acid as a donor of the amino group and transfer it into the molecule of an oxo acid.
Oxo group of the oxo acid is thus replaced by the amino group.
Result:
oxo acid is changed by the reaction into an amino acid, its carbon chain remains the same

a) CH_3-CO-COOH →

b) HOOC-CH_2-CO-COOH →

c) HOOC-CH_2-CH_2-CO-COOH →

Task 4.4

Write formulas of fully ionized amino acids produced by the reactions of the Task 4.3
What is the net charge difference between the first and the other two ionized amino acids?

Task 4.5

Complete the table: add numbers of carbons, anion and acyl names

number of carbons	**IUPAC name**	**common name**	**anion name**	**acyl name**
-OH	**hydroxy acids:**			
	2-hydroxypropanoic acid	**lactic acid**		
	3-hydroxybutanoic acid	**β-hydroxybutyric acid**		
	2-hydroxybutanedioic acid	**malic acid**		
6	2-hydroxypropane-1,2,3-tricarboxylic acid	**citric acid**		
	2-hydroxybenzoic acid	**salicylic acid**		
=O	**oxo acids:**			
	2-oxopropanoic acid	**pyruvic acid**		
	3-oxobutanoic acid	**acetoacetic acid**		
	2-oxobutanedioic acid	**oxaloacetic acid**		
	2-oxopentanedioic acid	**α-ketoglutaric acid**		
$-NH_2$	**amino acids:**			
	2-aminoethanoic acid	**glycine**	**x**	
	2-aminopropanoic acid	**alanine**	**x**	
	3-aminopropanoic acid	**β-alanine**	**x**	
	2-amino-3-phenylpropanoic acid	**phenylalanine**	**x**	
	2-aminobutanedioic acid	**aspartic acid**		
	2-aminopentanedioic acid	**glutamic acid**		

HINT

Create your flesh cards for better memorizing:
structural formula on one side / common name on the other side

Task 4.6

Draw structural formulas of **prop**anoic acid derivatives (**C3-group**) containing given functional group on its α-carbon (= 2^{nd} carbon) and write their systematic and common names.

hydroxyl group	oxo group	amino group

Task 4.7

Draw **but**anedioic acid (vertically) and its hydroxy-, oxo- and amino-derivatives (**C4-group**); name the derivatives by systematic and common names:

Task 4.8

Draw **pent**anedioic acid (vertically) and its alpha oxo- and alpha amino-derivatives (alpha, α, carbon is the second carbon of a carboxylic acid); name the derivatives (**C5-group**) by systematic and common names:

Task 4.9

Draw the amino acids from the Tasks 4.7 and 4.8 in their fully ionized forms. What is their net charge?
(do not forget that the amino group can also be charged)

Task 4.10
Name the following compounds by all possible names:

a) $H_2N-CH_2-CH_2-CH_2-COOH$

b) $CH_3-CO-CH_2-COOH$

c) $CH_3-CH(OH)-CH_2-COOH$

d) $CH_3-CH_2-CO-O-CH_2-CH_3$

e) $CH_3-CO-COOH$

f) $CH_3-CH_2-O-CH_2-CH_3$

g) $CH_3-CO-CH_2-CH_3$

h) $CH_3-(CH_2)_{16}-COOH$

i) $CH_3-CH_2-CH_2-COOK$

j) $(CH_3-COO)_2Mg$

k) $CH_3-O-CO-H$

Task 4.11
Write names of <u>reactants</u> and formulas and names of <u>products</u> of the reactions:

a) oxidation of $CH_3-CH(OH)-COOH \rightarrow$

b) $HCOOH + CH_3-CH_2-OH \rightarrow$

c) $HOOC-COOH + Ca(OH)_2 \rightarrow$

d) $HOOC-CH=CH-COOH + H_2O \rightarrow$

Task 4.12

Look at the following molecules and put the correct classification to each of them. Choose from the classes of compounds: *ammonia / amine / amino acid / amide / substituted amide*

a) $NH_3 + H^+ \rightarrow NH_4^+$

b) $CH_3\text{-}CH_2\text{-}NH_2 + H^+ \rightarrow CH_3\text{-}CH_2\text{-}NH_3^+$

c) $H_2N\text{-}CH_2\text{-}COOH + H^+ \rightarrow H_3N^+\text{-}CH_2\text{-}COOH$

d) $CH_3\text{-}CH_2\text{-}CO\text{-}NH_2 + H^+ \rightarrow$ no reaction

e) $H_2N\text{-}CH_2\text{-}CO\text{-}NH\text{-}CH(CH_3)\text{-}COOH + H^+ \rightarrow H_3N^+\text{-}CH_2\text{-}CO\text{-}NH\text{-}CH(CH_3)\text{-}COOH$

All amino derivatives are structuraly derived from **ammonia** (a), inorganic basic gas. Its nitrogen has two unpaired electrons, that can accept H^+ resulting in a formation of **ammonium** cation (NH_4^+).

Amines (b) are molecules in which one H of ammonia has been substituted by a hydrocarbon rest. They still have basic property of ammonia, can accept H^+ resulting in an organic ammonium cation (in this case: ethyl ammonium).

Amino acids (c) contain other (principal) carboxylic functional group, this is why they are not called amines. They are substitutional amino derivatives of carboxylic acids, still able to accept H^+.

Amides (d) are refered to as „functional derivatives of carboxylic acids“, their carboxylic group has been changed by the replacement of $-OH$ by $-NH_2$ resulting in the *amide group*: **-CO-NH₂** which is stable and does not accept H^+. It means that **amide group is NOT charged**.

Simple substituted amides are formed by a substitution (replacement) of one or both hydrogens of the amide group by some other structure. **Peptides** (e) and proteins are special kind of substituted amides, that are formed by the reaction of a carboxylic group of one amino acid with an amino group of other amino acid. In this case the structure **-CO-NH-** is called „*peptide bond*“.

Amides can be hydrolyzed to carboxylic acid and ammonia or amine (in case of substituted amides), because they has been formed by **condensation** of the molecules.

Task 4.13

Write the reaction describing an ionization of ammonia in water (use the structural formula of ammonia), name the reaction product:

Task 4.14

Name the compounds below by systematic (IUPAC) names using the radical-functional principle. All the molecules are amines:

a) $CH_3\text{-}NH_2$

b) $CH_3\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$

c) $CH_3\text{-}CH_2\text{-}N(CH_3)\text{-}CH_2\text{-}CH_2\text{-}CH_3$

d) $H_2N\text{-}(CH_2)_4\text{-}NH_2$

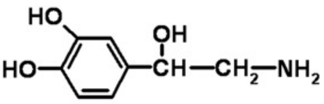
Amino group **–NH_2** occurs only in **primary amines**. If one or both hydrogens of the amino group has been replaced by a hydrocarbon rest, these amines are called **secondary** or **tertiary** amines, respectively (see molecules (b) and (c) in the Task 4.14)

In case that the free electron pair of nitrogen binds the fourth hydrocarbon rest resulting in a positively charged amine, it is called **quarternary** ammonium cation (amine).

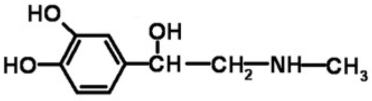
Task 4.15

The following substances are signalling molecules present in the human body (norepinephrine, epinephrine, and acetylcholine, respectively). Identify all functional groups in their molecules, and in case of the amino group specify its type.

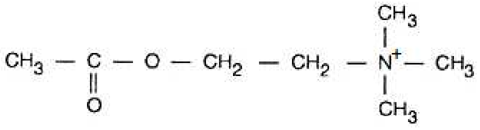
a)



b)



c)



$$CH_3-\underset{\underset{O}{\|}}{C}-O-CH_2-CH_2-\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{N^+}}-CH_3$$

Task 4.16

Mark the molecules that are NOT amines. In case of amines note their type: primary, secondary or tertiary. Finally name the compounds (in the radical-functional naming the hydrocarbon rests must be ordered alphabetically, e.g. **e**thyl **m**ethyl **p**ropyl ....).

a) CH_3-CH_2-NH_2

b) CH_3-$CH(NH_2)$-CH_3

c) CH_3-CH_2-$N(CH_3)$-CH_2-CH_2-CH_3

d) CH_3-$CH(NH_2)$-CH_2-CH_3

e) CH_3-$CH(NH_2)$-CH_2-OH

f) H_2N-$(CH_2)_3$-NH_2

g) CH_3-CH_2-$CH(NH_2)$-COOH

h) $(CH_3)_2NH$

i) CH_3-CH_2-CH_2-$N(CH_3)$-CH_2-CH_3

Task 4.17

Amides can be formed by condensation of carboxylic acids with ammonia. Write and name products of the following reactions.

Names of amides are derived from the common names of acids: root of the name + the suffix –amide.

a) $HCOOH$ (formic acid) + NH_3 $\rightarrow$ formamide:

b) $CH_3\text{-}COOH$ + NH_3 $\rightarrow$

c) $CH_3\text{-}CH_2\text{-}COOH$ + NH_3 $\rightarrow$

d) $CH_3\text{-}CH_2\text{-}CH_2\text{-}COOH$ + NH_3 $\rightarrow$

e) $\mathbf{HOOC}\text{-}CH_2\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$ + $\mathbf{NH_3}$ $\rightarrow$

(use the carboxylic group written in bold for the last reaction)

*this molecule is called **glutamine**, it is one of amino acids found in proteins*

Task 4.18

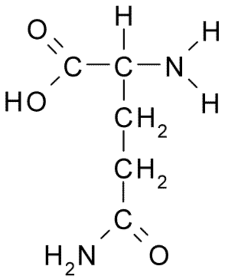
Draw the peptide formed by the condensation of the following amino acids. It is always the carboxylic group of the first amino acid that condenses with the amino group of the second amino acid. Resulting peptide bond connects the two amino acids in a peptide called dipeptide (= composed of two amino acids).

alanine (= 2-aminopropanoic acid) **+ glycine** (2-aminoethanoic acid) → **alanyl-glycine** (= dipeptide)

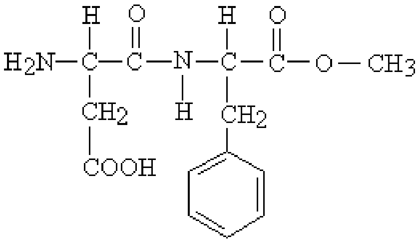
Task 4.19

Draw and name the tripeptide formed by the condensation of glycine + alanine + glycine, respectively.

Task 4.20
Mark and name individual functional groups found in the following compound and draw and name products of its hydrolysis *(only one of the functional groups can be hydrolyzed ;)*



Task 4.21
The formula below describes the structure of an artificial sweetener Aspartame: mark the following structures in its molecule



a) amino group
b) carboxylic group
c) ester group (ester bond)
d) substituted amide group (peptide bond)

and draw and name products of its hydrolysis (three molecules):

Task 4.22
Name reactants and products of the reactions describing a protonation of N-containing compounds:

a) ionization in water (aqueous solution)

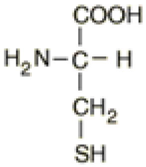
$NH_3 + H_2O \leftrightarrow NH_4^+ + OH^-$ $CH_3NH_2 + H_2O \leftrightarrow CH_3NH_3^+ + OH^-$

b) reaction with a strong acid

$NH_3 + HCl \leftrightarrow NH_4^+ + Cl^-$ $CH_3NH_2 + HCl \leftrightarrow CH_3NH_3^+ + Cl^-$

Task 4.23
Amino acids in proteins are connected by the peptide bonds. But proteins often contain another covalent bond important for their spatial arrangement. This bond is called „disulfide bond“ and is *formed by oxidation* of a thiol functional group found in the structure of amino acid **cysteine**.

Mark the thiol functional group in the structure of cysteine below and draw two cysteines connected by the disulfide bond:



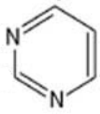
$H_2N-CH(COOH)-CH_2-SH$

Task 4.24
Sulfur is less common in hydrocarbon derivatives than oxygen or nitrogen, but all these three heteroatoms can occur in heterocyclic compounds. The most important nitrogen-containing heterocycles are:

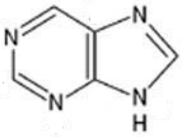
a) five-membered, one nitrogen-containing ring called **pyrrole**
b) six-membered, one nitrogen-containing ring called **pyridine**
c) six-membered, two nitrogen-containing ring called **pyrimidine**
d) five-membered, two nitrogen-containing ring called **imidazole**
e) two condensed rings: pyrimidine and imidazole called **purine**
f) two condensed rings: benzene and pyrole called **indol**

Identify the above-mentioned heterocycles (all are aromatic compounds):

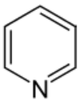
1)



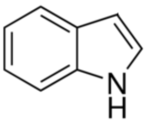
2)



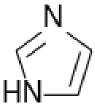
3)



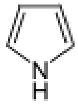
4)



5)

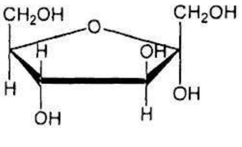


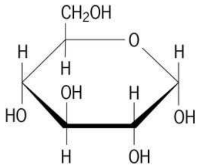
6)



Task 4.25
The most important oxygen-containing heterocycles occur in structures of saccharides.
It is five-membered ring called tetrahydro**furan** and six-membered ring called tetrahydro**pyran**.

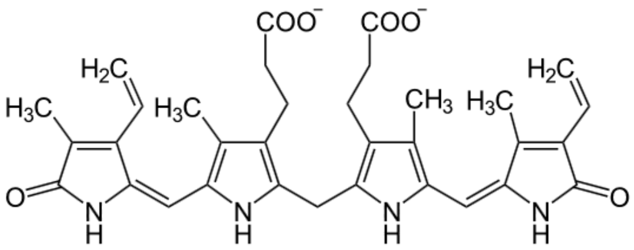
Mark the rings in structures of fructose and glucose, respectively:



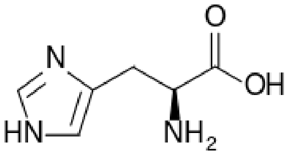


Task 4.26
Use a colored pencil and mark and name all heterocycles you recognise in the following compounds; name also all substituents attached to the heterocycles and functional groups found in the molecules:

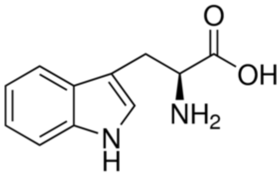
bilirubin *(bile pigment)*



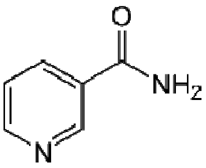
histidine *(amino acid found in proteins)*



tryptophan *(amino acid found in proteins)*

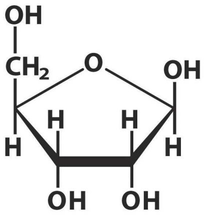


nicotinamide *(vitamine B3)*



adenine *(base found in nucleic acids)*

ribose *(monosaccharide found in RNA)*



Appendix 1

Chemical calculations

Important terms

- **solute** = a substance dissolved in a solvent in forming a solution
- **solvent** = a liquid that dissolves another substance or substances to form a solution
- **solution** = a homogeneous mixture of a liquid (the solvent) with a gas or solid (the solute)
- **concentration** = the quantity of dissolved substance per unit quantity of solution or solvent (concentration = solute / solution)
- **density** (ρ) = the mass of a substance per unit of volume ($kg.m^{-3}$ or $g.cm^{-3}$)
  ρ = m/V *(cm^{-3} = ml)*
- **mass** (in grams) **m = n x MW**
- **amount of substance** (n) **=** a measure of the number of entities present in a substance (in moles)
  Avogadro constant (NA) = the number of entities in one mole of a substance
  ($N_A = 6.022 \times 10^{23}$)
- **molar weight** (MW) = molar mass = mass of one mole of a substance in grams (unit: g/mol)
- **relative atomic mass** (A_r) = mass of an atom expressed in atomic mass unit (atomic mass unit (u) = 1/12 of the mass of ^{12}C atom; the atomic mass unit is also called **dalton**: Da)
- **relative molecular mass** (M_r) = sum of relative atomic masses (A_r) of all atoms that comprise a molecule; MW (g/mol) = Mr (no units) = their numerical values are the same
  (the mass expressed in Da is the same as in g/mol)
- **dilution** = process of preparing less concentrated solutions from a solution of greater concentration
- pH = negative logarithm of activity (or concentration) of hydroxonium cations H_3O^+ in a solution; pH scale is a logarithmic scale for expressing the acidity or alkalinity of a solution

Important formulas

$pH = -\log c(H_3O^+) = -\log c(H^+)$	**ACIDS**	**BASES**
$pH + pOH = 14$	strong: $pH = -\log c_a$	strong: $pOH = -\log c_b$
	weak: $pH = \frac{1}{2} pK_a - \frac{1}{2} \log c_a$	weak: $pOH = \frac{1}{2} pK_b - \frac{1}{2} \log c_b$
$pK = -\log K$		$pH = 14 - pOH$
$K = 10^{-pK}$	weak acid: $pK_a > 2$ or $K < 10^{-2}$	weak base: $pK_b > 2$ or $K_b < 10^{-2}$

Logarithm *is the inverse function to exponentiation. That means the logarithm of a given number x is the exponent to which another fixed number, the base b, must be raised, to produce that number x.*

In the simplest case the logarithm counts repeated multiplication of the same factor, e.g. ten: since $10 \times 10 \times 10 = 1000 = 10^3$. *The "logarithm to base 10" of 1000 is 3, where b = 10, x = 1000 and the exponent y = 3: the logarithm of x to base b is denoted as* $\log_b x = y$ *(in this case:* $\log_{10} 1000 = 3$ *because* $10^3 = 1000$*). More generally, exponentiation allows any positive real number to be raised to any real power, always producing a positive result, so the logarithm for any two positive real numbers b and x where b is not equal to 1, is always a unique real number y.*

The logarithm to base 10 (that is b = 10) is called the ***common logarithm*** *and has many applications in science. It is often simplified:* $\log_b x = y$ *in this case* $\log_{10} x = y$ *is written as* $\log x = y$*)*

Appendix 2

Nomenclature of inorganic compounds

Memorize:

1) classification of elements, see Periodic table
2) symbols and English names of elements
3) Latin names of elements
4) names of common cations and anions
5) common names of selected compounds

Symbol	**Latin name**	**English name**
Na	**Natrium**	sodium
K	**Kalium**	potassium
Sn	**S**ta**n**num	tin
Pb	**P**lum**b**um	lead
Sb	**S**ti**b**ium	antimony
W	**W**olframium	tungsten
Fe	**Fe**rrum	iron
Cu	**Cu**prum	copper
Ag	**A**r**g**entum	silver
Au	**Au**rum	gold
Hg	**H**ydrar**g**yrum	mercury

Keep in mind the rules:

1. names of compounds are derived from the names of cations, anions and polyatomic ions: *cation anion (NaCl = sodium chloride)*
2. total charge of molecule is ZERO
3. all binary compounds end in **–ide** *(compounds composed of two different elements)*
   CaO, H_2O_2, $NaCl$, $HF(g)$, ZnS
   (calcium oxide, hydrogen peroxide, sodium chloride, hydrogen fluoride, zink sulfide)
4. binary compounds composed of **two nonmetals**: *Greek prefixes* are used
   SO_2, N_2O_5, CO
   (sulfur dioxide, dinitrogen pentoxide, carbon monoxide)
5. binary compounds composed of a **metal** ion with fixed or variable oxidation numbers and nonmetal ion: *no Greek prefixes*

   a) -ous / -ic suffix system, e.g. FeO = ferrous oxide, Fe_2O_3 = ferric oxide

   b) Stock system (prefered), *e.g. iron(II) oxide / iron(III) oxide*
6. ternary compounds (examples: H_2SO_4 or Na_2SO_4 or $NaOH$) *(composed of three different elements)*
   - hydrogen cation H^+ (= acid)
   - or metal cation (= salt or hydroxide) / fixed or variable oxidation number
   - and a polyatomic anion (e.g. SO_4^{2-} or OH^{1-})

Names of CATIONS

1) cations found only in one oxidation state
name of the cation = name of the element

H, Li, Na, K, Ag	**+I**
Be, Mg, Ca, Sr, Ba, Zn	**+II**
B, Al	**+III**

see position of the elements in the Periodic table

2) cations found in two oxidation states
root of the Latin name + two suffixes:

lower oxidation state: ***-ous***
higher oxidation state: ***-ic***

Cu, Hg	**+I / +II**
Fe, Co	**+II / +III**
Sn, Pb	**+II / +IV**

Names of ANIONS

1) one oxidation state
a) root of Latin name + suffix: *-ide*

halogen	**→ halide**	**F, Cl, Br, I**		**-I**
hydrogen	**→ hydride**	**H**		**-I**
oxygen	**→ oxide**	**O**	**-II**	
sulfur	**→ sulfide**	**S**	**-II**	
hydroxide		**OH**	**-1**	
cyanide		**CN**	**-1**	

one oxidation state of a central atom
b) root of Latin name + suffix: *-ate*

carbonate	CO_3^{-2}	C^{IV}
silicate	SiO_3^{-2}	Si^{IV}
chromate	CrO_4^{-2}	Cr^{VI}
borate	BO_3^{-3}	B^{III}

oxidation state of oxygen in anions is always –II
(exception: in peroxides = -I)

oxidation states are in Roman numerals
charges of polyatomic ions in Arabic numerals

2) two oxidation states of a central atom
root of Latin name + two suffixes:

lower oxidative state: ***-ite***
higher oxidative state: ***-ate***

nitrite / nitrate	NO_2^- / NO_3^-	$N^{+III}/^{+V}$
phosphite/phosphate	PO_3^{-3} / PO_4^{-3}	$P^{+III}/^{+V}$
sulfite / sulfate	SO_3^{-2} / SO_4^{-2}	$S^{+IV}/^{+VI}$
selenite / selenate	SeO_3^{-2} / SeO_4^{-2}	$Se^{+IV}/^{+VI}$

3) more oxidative states of a central atom
root of Latin name + prefixes and suffixes:

the lovest oxidative state:	***hypo-***	***-ite***
lower oxidative state:		***-ite***
higher oxidative state:		***-ate***
the highest oxidative state:	***(hy)per-***	***-ate***

- **Cl, Br, I, Mn**

(hypochlorite,	chlorite,	chlorate,	perchlorate)
ClO^-	ClO_2^-	ClO_3^-	ClO_4^-

Compounds called by their common names

H_2O	water	H_3O^+	hydroxonium
NH_3	ammonia	NH_4^+	ammonium
NO	nitric oxide		
NaCl	salt		
HCO_3^-	bicarbonate		

Types of compounds
ionic compounds are composed of:

cation and anion
- cation is positively charged
- anion is negatively charged

molecule: *its total charge is ZERO*
- naming the compounds:
  cation name + anion name

Oxides **anion: O^{-II}**

- *acid-forming*: **nonmetal / oxygen**
  use multiple prefixes (mono, di, tri,...)
- *base-forming*: **metal / oxygen**
  use sufixes –ous / -ic or (*oxidation state*)
- amphoteric

Peroxides **anion: O_2^{-2} ⇒ O^{-I}**

- s^1 elements (H and alkali metals): M_2O_2
- s^2 elements (alkali earth metals): MO_2

Hydroxides anion: $(OH)^{-1}$ -hydroxide

- basic properties (pH > 7)
- strong or weak hydroxides

- metal / hydroxide anion
  for metal use sufixes –ous / -ic
  or (*oxidation state*)

- ammonium / hydroxide anion

Oxygen-free Acids cation: H^+ (pH < 7)

hydro-..................-ic acid

HF, HCl, HBr, HI, H_2S, HCN (in aqueous solutions)

anion: -ide

- monoprotic / diprotic acids

Acids (= oxoacids) cation: H^+ (pH < 7)

- the highest oxidative state per-..... -ic acid
- higher (or **only**) oxidative state **-ic acid**
- lower oxidative state -ous acid
- the lowest oxidative state hypo-... -ous acid

anion:

-ic acid → -ate
-ous acid → -ite

example:

HClO	hypochlorous acid	→	hypochlorite
$HClO_2$	chlorous acid	→	chlorite
$HClO_3$	chloric acid	→	chlorate
$HClO_4$	perchloric acid	→	perchlorate

The most important oxoacids:

H_2CO_3	carbon**ic** acid	→ carbon**ate**
H_2SiO_3	silic**ic** acid	→ silic**ate**
H_2CrO_4	chrom**ic** acid	→ chrom**ate**
H_3BO_3	bor**ic** acid	→ bor**ate**
H_3PO_4	phosphor**ic** acid	→ phosph**ate**
H_2SO_3	sulfurous acid	→ sulfite
H_2SO_4	sulfur**ic** acid	→ sulf**ate**
HNO_2	nitrous acid	→ nitrite
HNO_3	nitr**ic** acid	→ nitr**ate**
$HMnO_4$	permanganic acid	→ permanganate

Salts
are formed by neutralization:
acid + hydroxide → salt + water

cation: metal or NH_4^+
it is *derived from the hydroxide*
(= cation of the hydroxide)

anion: oxygen-free or polyatomic anion
it is *derived from the acid (= anion of the acid)*

acidic salts of ACIDS
- **„cation hydrogen anion“**

KH_2PO_4	potassium dihydrogen phosphate
K_2HPO_4	(di)potassium hydrogen phosphate
NH_4HCO_3	ammonium hydrogen carbonate
$Ca(HS)_2$	calcium hydrogen sulfide
K_3PO_4	*(tri)potassium phosphate (is not acidic)*

basic salts of ACIDS
- **„cation hydroxy anion“**

Mg(OH)Cl	magnesium hydroxychloride
$Sb(OH)_2(NO_3)$	antimony(III) dihydroxynitrate

Total charge of molecule is ZERO

double salts of ACIDS
a) „cation1 cation2 anion“

$KMgF_3$	potassium magnesium fluoride
$KLiSO_4$	potassium lithium sulfate

double salts of ACIDS
b) „cation anion1 anion2“

CaCl(ClO)	calcium chloride hypochlorite
$Cu_3(CO_3)_2F_2$	copper(II) carbonate fluoride

Total charge of molecule is ZERO

HYDRATES OF SALTS

- **„cation anion *multiple prefix* hydrate“**

$MgCl_2 . 6H_2O$ magnesium chloride hexahydrate

$CaHPO_4 . 2H_2O$
calcium hydrogen phosphate dihydrate

THIOACIDS AND THIOSALTS

- **„thio.... acid“ /„cation thio....anion“**

$H_2S_2O_3$ thiosulfuric acid (H_2SO_4 = sulfuric acid)
HSCN thiocyanic acid (HOCN = cyanic acid)

$K_2S_2O_3$ potassium thiosulfate
KSCN potassium thiocyanate

POLYACIDS AND SALTS

- **„*multiple prefix*.... acid“**

$H_2B_4O_7$	tetraboric acid
$H_2Cr_2O_7$	dichromic acid

- **„cation *multiple prefix*....anion“**

$Na_2B_4O_7$	sodium tetraborate
$K_2Cr_2O_7$	potassium dichromate

Symbols of elements

- symbols are derived from Latin names of elements

H = Hydrogenium = hydrogen
Na = Natrium = sodium
Ag = Argentum = silver

(Ar = Argon)

Important suffixes

ACIDS	acid name	salt suffixed by
oxygen-free	hydro-.....-ic acid	-ide
oxo-acid *lower ox.state*	-ous acid	-ite
oxo-acid *higher ox.state*	-ic acid	-ate
Binary compounds	**CATION**	**ANION** *-ide*
oxides	metal or nonmetal	O^{-II}
peroxides	H^{+I} or s^1 or s^2 metal	O_2^{-I}
oxygen-free acids / salts	H^{+I} / metal	S^{-II} $F^{-I}, Cl^{-I}, Br^{-I}, I^{-I}$
Ternary compounds	**CATION**	**ANION**
hydroxides	metal or NH_4^+	$(OH)^{-1}$ -ide
acids	H^{+I}	XO_n (X = central atom)
salts	metal (or NH_4^+)	XO_n (X = central atom)

Important prefixes

1	2	3	4	5	6	7	8	9	10	11	12
mono	di	tri	tetra	penta	hexa	hepta	octa	nona	deca	undeca	dodeca

Exercises

1) Make groups of compounds: oxides / hydroxides / peroxides / acids / salts

Na_2O, HCl, CO_2, Na_2O_2, $Ca(OH)_2$, KClO, HCN, HNO_2,

H_2S, H_2O_2, BaO_2, PbO_2, H_2SO_3, KOH, $MgSO_4$, NaF, NH_4HCO_3, HI,

$Al(OH)_3$, HIO_4, CdS, MgO_2, NaH_2PO_4

Solution:
Na_2O / sodium oxide, HCl / hydrochloric acid or hydrogen chloride, CO_2 / carbon dioxide, Na_2O_2 / sodium peroxide, $Ca(OH)_2$ / calcium hydroxide, KClO / potassium hypochlorite, HCN / hydrocyanic acid or hydrogen cyanide, HNO_2 / nitrous acid, H_2S / hydrosulfuric acid or hydrogen sulfide, H_2O_2 / hydrogen peroxide, BaO_2 / barium peroxide, PbO_2 / lead(IV) oxide or plumbic oxide, H_2SO_3 / sulfurous acid, KOH / potassium hydroxide, $MgSO_4$ / magnesium sulfate, NaF / sodium fluoride, NH_4HCO_3 / ammonium hydrogen carbonate, HI / hydroiodic acid or hydrogen iodide, $Al(OH)_3$ / aluminium hydroxide, HIO_4 / periodic acid or hyperiodic acid, CdS / cadmium sulfide, MgO_2 / magnesium peroxide, NaH_2PO_4 / sodium dihydrogen phosphate

2) Name the compounds:

a) CaO

b) Al_2O_3

c) Cu_2O

d) PbO_2

e) Na_2O_2

f) H_2O_2

g) BaO_2

h) $Al(OH)_3$

i) $Fe(OH)_2$

j) KOH

k) HCl (g)

l) HF (aq)

m) HCN (aq)

n) NH_4Cl

o) ZnS

p) H_2SO_3

q) $HClO_2$

r) H_2CO_3

s) HIO_4

t) $MgSO_4$

Solution:
a) calcium oxide, b) dialuminium trioxide, c) copper(I) oxide, d) lead(IV) oxide, e) sodium peroxide, f) hydrogen peroxide, g) barium peroxide, h) aluminium hydroxide, i) iron(II) hydroxide, j) potassium hydroxide, k) hydrogen chloride, l) hydrofluoric acid, m) hydrocyanic acid, n) ammonium chloride, o) zinc sulfide, p) sulfurous acid, q) chlorous acid, r) carbonic acid, s) periodic acid, t) magnesium sulfate

2) Write formulas of the compounds:

a) sodium carbonate

b) calcium sulfite

c) potassium hypochlorite

d) silver chlorate

e) iron(III) sulfate

f) potassium dihydrogen phosphate

g) lithium ammonium sulfate

h) magnesium chloride hexahydrate

i) calcium hydrogen phosphate dihydrate

j) cupric oxide

k) ferrous hydroxide

l) hydrosulfuric acid

m) sulfuric acid

n) nitrous acid

o) mercury(II) chloride

p) sodium sulfite

q) potassium permanganate

r) ammonium hydrogen carbonate

s) iron(II) sulfate heptahydrate

Solution:
(a) Na_2CO_3 (b) $CaSO_3$ (c) $KClO$ (d) $AgClO_3$ (e) $Fe_2(SO_4)_3$ (f) KH_2PO_4 (g) $Li(NH_4)SO_4$ (h) $MgCl_2 . 6 H_2O$ (i) $CaHPO_4 . 2 H_2O$
(j) CuO (k) $Fe(OH)_2$ (l) H_2S (m) H_2SO_4 (n) HNO_2 (o) $HgCl_2$ (p) Na_2SO_3 (q) $KMnO_4$ (r) NH_4HCO_3 (s) $FeSO_4 . 7 H_2O$

Appendix 3

Organic compounds

<u>Important terms</u>:

- **constitution** = the type and the arrangement of both atoms and bonds in a molecule; it doesn´t describe spatial arrangement
- **conformation** = any of the large number of possible shapes of a molecule resulting from rotation of one part of the molecule around a single bond
- **configuration** = the spatial arrangement of atoms or groups in a molecule
- **saturated hydrocarbon** = hydrocarbon in which there are no carbon-carbon double or triple bonds (all carbon atoms are bound to the maximum number of hydrogen atoms)
- **alkyl** = hydrocarbon rest = a group formed by removing a hydrogen from an alkane, e.g. methyl group CH_3–, derived from methane CH_4; ending -yl
- **aryl** = a group formed by removing a hydrogen from an aromatic compound, e.g. phenyl group C_6H_5–, derived from benzene C_6H_6
- **acyl** = rest of a carboxylic acid = a group **R-CO**– formed by removing OH from R-COOH
- **isomers** = compounds that have the same molecular formula but differ in physical properties, because their different structures

<u>example</u>:	a) ethanol (= alcohol)	or	b) dimethyl ether (= ether)
C_2H_6O can be	$CH_3 — CH_2 — OH$		$CH_3 — O — CH_3$

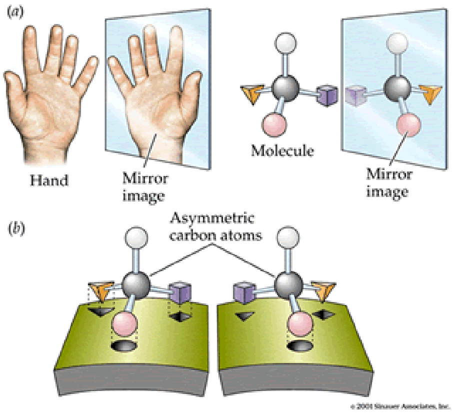
- **stereoisomers** (different configuration of molecules)

1. **<u>cis-trans isomers</u>** (geometrical isomers)

   cis-but-2-ene / *trans*-but-2-ene

2. **<u>enantiomers</u>** (optical isomers = mirror images)

   L-amino acid / D-amino acid



<u>Important prefixes</u>:

	1	2	3	4	5	6	7	8	9	10
number of C	meth-	eth-	prop-	but-	pent-	hex-	hept-	oct-	non-	dec-
number of substituents	mono	di	tri	tetra	penta	hexa	hepta	octa	nona	deca

	11	12	13	20
number of C	undec-	dodec-	tridec-	eicosa-

cyclo- = ring in a structure

Naming organic compounds

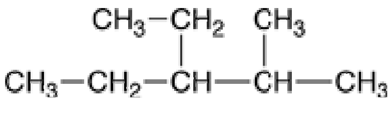
1) **common names** = trivial names - mostly no rules, originally assigned to compounds on the basis of their origin or properties; the structure of the compound cannot be derived from the trivial name
   example: CH_3CHO acetaldehyde, CH_3COCH_3 acetone, CHCH acetylene
2) **systematic names** = IUPAC names - based on exact rules of naming (locants, prefixes, suffixes), describes the structure of the compound
   a) *substitutional principle* - the name of the compound is derived from the name of the basic unbranched hydrocarbon - MOST SUITABLE
   b) *radical-functional principle* - the structure is characterized by a single typical group of atoms (functional group), to which the rest of the molecule (hydrocarbon rest) is attached

   example: a) ethanol
   b) ethyl alcohol

Numbering the hydrocarbon chain

1) find the longest unbranched chain containing the most principal functional goups that can be indicated by specific suffix
2) or find the longest unbranched chain containing the most double bonds (double bonds take precedence over triple bonds)
3) or find the longest unbranched chain (= parent chain)
4) the principal functional groups, multiple bonds and the other substituents must obtain the lowest-number locants as possible
5) the root of the name of the compound is that of the hydrocarbon with the suffix giving the degree of unsaturation
6) the suffix expressing the presence of the principal functional group is the last part of the compound name (the presence of additional functional groups is expressed by the prefixes)
7) the root is preceded by prefixes indicating the presence of other hydrocarbon rests or non-hydrocarbon components in the molecule: these prefixes are listed alphabetically
8) the presence of several identical components is indicated by the multiple prefixes: bi-, tri-, tetra, etc., for simple substituents, and bis-, tris-, tetrakis-, etc., for complex substituents
9) each prefix and suffix is preceded by the locant giving the position on the parent hydrocarbon; the numbers are separated from the rest of the word by a hyphen
10) the spatial arrangement is given by special affix placed prior to the whole name of the compound

examples:



$CH_3-CH_2-CH(CH_2CH_3)-CH(CH_3)-CH_3$

3-**ethyl**-2-**methyl**pentane
(pent = C5 in the parent chain, -ane = saturated)

$\mathbf{CH_3\text{-}CH_2\text{-}}CH(CH_2CH_2CH_3)\text{-}CH{=}CH\text{-}C(\mathbf{CH_3})_2\text{-}CH_3$

5-**ethyl**-2,2-di**methyl**oct-3-ene
(oct = C8 in the parent chain, -ene = unsaturated)

Derivatives of hydrocarbons – overview

derivative	formula	prefix	suffix
carboxylic acid	**- COOH**	**carboxy-**	**-oic acid**
sulfonic acid	**- SO_3H**	**sulfo-**	**-sulfonic acid**
aldehyde	**- CHO**	**formyl-**	**-al**
ketone	**>C=O**	**oxo-**	**-one**
alcohol	**- OH**	**hydroxy-**	**-ol**
thiol	**- SH**	**sulfanyl-**	**-thiol**
amine	**- NH_2**	**amino-**	**-amine**
ether	**- O -**	**R-oxy-**	**ether**
sulfide	**- S -**	**R-thio-**	**sulfide**
halogen derivative	**- F, -Cl, -Br, -I**	***halogeno-***	**-**
nitro derivative	**- NO_2**	***nitro-***	**-**

The name of a hydrocarbon derivative is derived from the name of the basic unbranched hydrocarbon + locants, prefixes and suffixes:

- principal functional group (the one found in the highest possition in the table above)
  ⇒ type of the derivative ≈ suffix
- other functional groups
  ⇒ expressed by special prefixes + locants

example:	CH_3-CO-CH_3	propan**one**	(**ketone**)
	CH_3-CO-COOH	2-**oxo**propanoic acid	(**oxo** carboxylic **acid**)

Chemical formulas of organic compounds:

a) **molecular formula** - very brief one, it gives information about the number of different atoms present in the molecule, but no information about the structure; it is used to calculate molar mass or to detect isomers (their molecular formulas are identical)

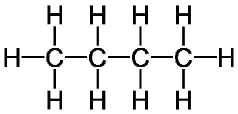
b) **full structural formula** - all bonds are described

c) **rational structural formula** = condensed structural formula, very useful, the best one for understanding medical chemistry !

d) **scientific depiction** - real shape of the carbon skeleton

examples:

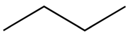
a) C_4H_{10}

b) 

$$\begin{array}{ccccccccccc} & & H & & H & & H & & H & & \\ & & | & & | & & | & & | & & \\ H & - & C & - & C & - & C & - & C & - & H \\ & & | & & | & & | & & | & & \\ & & H & & H & & H & & H & & \end{array}$$

c) CH_3-CH_2-CH_2-CH_3

or $CH_3CH_2CH_2CH_3$ or $CH_3(CH_2)_2CH_3$

d) 

Acids and bases in organic chemistry

- **acids** *(H^+ bound to oxygen can dissociate)*
  - it occurs in alcohols (-OH), carboxylic acids (-COOH) and sulfonic acids ($-SO_3H$)
  - alcohols do not dissociate in aqueous solutions, but can react with hydroxides (phenols are more acidic than alcohols, hence phenol former name „carbolic acid")
  - carboxylic acids and their substitutional derivatives are week acids, they are partially dissociated in aqueous solutions (α-hydroxy-acids and α-oxo-acids are stronger than carboxylic acids; amino acids have at least two ionisable functional groups: -COOH and $-NH_2$, hence they act also as bases)
  - sulfonic acids are stronger than carboxylic acids (their functional group is derived from sulfuric acid, H_2SO_4)
- **bases** *(Lewis bases = they contain free electron pair on nitrogen that can accept H^+)*
  - amines ($-NH_2$, -NH-, -N-) and amino acids ($-NH_2$)
  - N-containing heterocyclic compounds (only if the free electron pair of nitrogen is not involved in the aromatic character of their molecule as „delocalized electrons")
  - **organic compounds containing hydroxyl group** (-OH) **are NOT basic** – this group does not dissociate as hydroxide group (OH^{-1}) of inorganic hydroxides

- **dissociation of carboxylic acids:** $-COOH \leftrightarrow -COO^- + H^+$

  carboxylic acid → carboxylate + H^+ *(= simplification)*

  carboxylic acid + H_2O → carboxylate + H_3O^+

- **neutralization of carboxylic acids** converts acid to its salt (e.g. -COONa)

  carboxylic acid + NaOH → sodium carboxylate + H_2O

- **protonation of nitrogen** (in amines and some heterocyclic compounds)

  amine + H^+ ↔ ammonium cation of a hydrocarbon or amino acid

  $-NH_2 + H^+ \leftrightarrow -NH_3^+$

  $-NH- + H^+ \leftrightarrow -NH_2^+-$

Important chemical reactions of organic compounds:

1. **substitution** *(= replacement)*
   $CH_4 + Cl_2 \rightarrow CH_3Cl + HCl$

2. **addition** *(multiplicity of chemical bond is lowered)*
   $CH_2{=}CH_2 + H_2O \rightarrow CH_3\text{-}CH_2\text{-}OH$ addition of water = **hydration**
   $CH_3\text{-}CO\text{-}COOH + 2\,H \rightarrow CH_3\text{-}CH(OH)\text{-}COOH$ addition of hydrogen = **hydrogenation**

3. **elimination** *(new multiple bond is often formed, small molecule is released)*
   $CH_3\text{-}CH_2\text{-}OH \rightarrow CH_2{=}CH_2 + H_2O$ elimination of water = **dehydration**
   $CH_3\text{-}CH(OH)\text{-}COOH \rightarrow CH_3\text{-}CO\text{-}COOH + 2\,H$ elimination of hydrogen = **dehydrogenation**

4. **rearrangement** *(= formation of an isomer, isomerization)*
   $CH_2{=}C(OH)\text{-}COOH \rightarrow CH_3\text{-}CO\text{-}COOH$

oxidation: **dehydrogenation (- 2 H), hydration (+ H_2O)**
complete oxidation (= burning) of a hydrocarbon skeleton → **CO_2 + H_2O**

reduction: **hydrogenation (+ 2 H), dehydration (- H_2O)**

EXERCISES

1) Add structural formulas and choose water soluble compounds

a) butane

b) methanol

c) isoprene

d) octanol

e) benzene

f) glycerol

g) ethyl propyl ether

h) benzene-1,2-diol

i) cyclohexane

j) dimethyl ether

2) Name or draw the following constitution isomers:

a)	CH_3-CH=CH-CH_3	CH_3-CH_2-CH=CH_2
b)	CH_3-CH_2-CH_2-Cl	CH_3-CHCl-CH_3
c)	1,2-dimethylbenzene (= o-xylene)	1,3-dimethylbenzene (m-xylene)
d)	2,2-dimethylbutane	2,3-dimethylbutane
e)	propanal	propanone
f)	2-oxopropanoic acid	2-hydroxyprop-2-enoic acid

3) Draw the following configuration isomers (stereoisomers):

a) *cis* but-2-ene   *trans* but-2-ene

b) 2-aminopropanoic acid (two possible spatial structures)

4) Draw structural formulas of the molecules and explain their differences:

a) cyclohexane   b) cyclohexene   c) benzene

5) Finish the following chemical reactions („addition reactions“):

$CH_3\text{-}CH_2\text{-}CH{=}CH_2 + H_2 \rightarrow$

$CH_3\text{-}CH_2\text{-}CH{=}CH_2 + H_2O \rightarrow$

6) Add structural formulas to the following <u>important common names</u>:

acetylene (= ethyne)   **chloroform** (= trichloromethane)   **vinyl chloride**

isoprene   **toluene** (= methylbenzene)   **styrene**

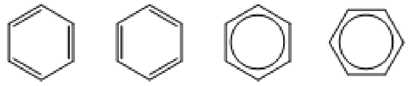
all isomers of xylene
(o-xylene, m-xylene, p-xylene)

all isomers of benzenediol
(pyrocatechol, resorcinol, hydroquinone)

Solution:

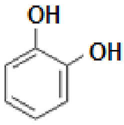
1) water soluble = (S): a) $CH_3-CH_2-CH_2-CH_3$, b) CH_3-OH (S), c) $CH_2=C(CH_3)-CH=CH_2$, d) $CH_3-(CH_2)_6-CH_2-OH$,

e) benzene (all forms):

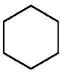


f) $HO-CH_2-CH(OH)-CH_2-OH$ (S), g) $CH_3-CH_2-O-CH_2-CH_2-CH_3$

h) benzene-1,2-diol (S)



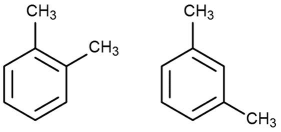
i) cyclohexane



j) CH_3-O-CH_3

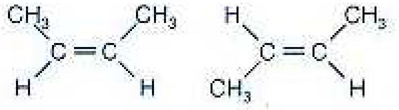
2) a) but-2-ene / but-1-ene, b) 1-chloropropane / 2-chloropropane,

c) o-xylene, m-xylene

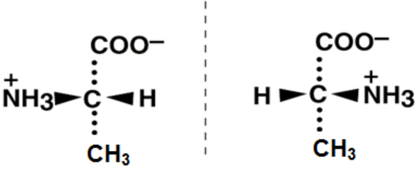


d) $CH_3-C(CH_3)_2-CH_2-CH_3$ / $CH_3-CH(CH_3)-CH(CH_3)-CH_3$, e) CH_3-CH_2-CHO / $CH_3-CO-CH_3$,
f) $CH_3-CO-COOH$ / $CH_2=C(OH)-COOH$

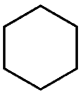
3) a) *cis* but-2-ene, *trans* but-2-ene

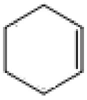


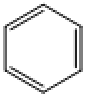
b) L-2-aminopropanoic acid D-2-aminopropanoic acid



4) a) cyclohexane cyclohexene benzene (the only aromatic)



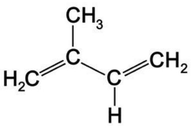




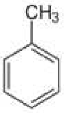
5) $CH_3-CH_2-CH_2-CH_3$, $CH_3-CH_2-CH(OH)-CH_3$ or $CH_3-CH_2-CH_2-CH_2-OH$

6) $H-C\equiv C-H$, $CHCl_3$, $CH_2=CH-Cl$,

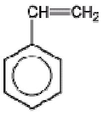
isoprene



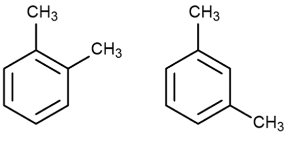
toluene



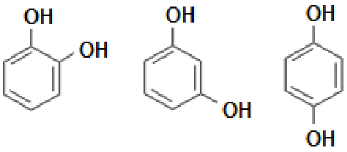
styrene



o-xylene, m-xylene, p-xylene



pyrocatechol, resorcinol, hydroquinone



Results of Tasks 1.1 – 1.23

1.1 a) 60 kg, b) 36 kg	**1.13** 1 000 / 10^3 mmol 1 000 000 / 10^6 µmol 1 000 000 000 / 10^9 nmol 1 000 000 000 000 / 10^{12} pmol 0.001 / 10^{-3} mol 0.000 001 / 10^{-6} mol
1.2 10, 1, 0.1, 0.01, 0.001 mol / 10, 1, 0.1, 0.01, 0.001 g	**1.14** O_2: 21 000 Pa, CO_2: 40 Pa
1.3 a) 5%, b) 0.5%, c) 5%, d) 0.5%	**1.15** 5.2 mmol/l
1.4 a) 1 mol/l, b) 2 mol/l, c) 0.5 mol/l, d) 1 mol/l	**1.16** 1.69×10^{22}
1.5 a) 4 g, b) 11.7 g, c) 1 g, d) 2 g	**1.17** 11.3 g
1.6 1, 2, 3, 4, 5, 6, 7	**1.18** 6.1 mmol/l, 133 µmol/l, 5.0 mmol/l
1.7 a) 10^{-11}/base, b) 10^{-7}/water, c) 10^{-5}/acid, d) 10^{-12}/base a) $[OH^-] = 10^{-3}$ / pH=11, b) $[OH^-] = 10^{-7}$ / pH=7, c) $[OH^-] = 10^{-9}$ / pH=5, d) $[OH^-] = 10^{-2}$ / pH=12	**1.19** 0.6 mmol/l
1.8 a) pH = 1, b) 0.0005 M, c) pH = 12, d) 0.005 M	**1.20** 2.8 mmol/l
1.9 **$[OH^-]$** 10^{-13}, 10^{-11}, 10^{-9}, 10^{-7}, 10^{-5}, 10^{-3}, 10^{-1} **$[H^+]$** 10^{-1}, 10^{-3}, 10^{-5}, 10^{-7}, 10^{-9}, 10^{-11}, 10^{-13} **K** 10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}, 10^{-10}, 10^{-12}, 10^{-14}	**1.21** a) 0.35%, 2%, 0.25%, 0.15% b) in mmol/l: 59.8, 111.1, 29.8, 20.1 c) in mmol/l: Na^+ = *89.6*, Cl^- = *79.9,* HCO_3^- = *29.8*, K^+ = *20.1*
1.10 a) pH = 1, b) pH = 3 / 100x diluted c) pH = 13, d) pH = 11 / 100x diluted	**1.22** *0.3%, 0.4%, 0.02%, 0.1%, 0.1%*
1.11 a) 4x, b) 2 l	MW(g/mol): *NaCl = 58.5, glc = 180* $NaHCO_3$ = *84* (HCO_3^- = *61), KCl = 74.5*
1.12 450 mmol/l	**1.23** glucose > iron > testosterone > estradiol

Answers to tasks 2.1 - 2.25

2.1 Inorganic compounds contain any element of the periodic table, in organic compounds C, H, O, N are the most common elements.

2.2 One-carbon containing inorganic compounds: CO, CO_2, HCN, HOCN, H_2CO_3, HCO_3^-

2.3 a) The molecule (C) consists of 6 carbons, b) its molecular formula is $C_6H_{13}NO_2$, c) x

d) The number of valence electrons involved in individual bonds is 4 for carbon, 1 for hydrogen, 2 for oxygen and 3 for nitrogen atom; oxygen has two more pairs of electrons and nitrogen has one more electron pair not involved in a bond formation (= free unbonded electrons).

e) Electronegativity differences are 0.0 for C-C and 0.3 for C-H bond (these bonds are nonpolar covalent bonds) whereas the differences are 0.6 for C-N, 0.9 for N-H, 1.0 for C-O and 1.3 for O-H bond (these bonds are polar covalent bonds, shared electrons occur closer to the more electronegative element resulting in partial charges on these atoms).

*The structure (A) describes the molecule of **but**ane; (B) can be called „isobutane“ (= an isomer of butane), but names of isomers do not often start by the prefix iso-, the recommended name of (B) is 2-**meth**yl**prop**ane because the branch (called methyl-) is attached to the second carbon of the linear chain containing three carbons; the hydrocarbon derivative (C) is mostly called by its common name: **leucine**; (D) is cyclo**prop**ane*

2.4
C_6H_{14} / 5 isomers of hexane: n-hexane (linear), isohexane = 2-methylpentane, 3-methylpentane, 2,3-dimethylbutane, 2,2-dimethylbutane, respectively:
$CH_3-CH_2-CH_2-CH_2-CH_2-CH_3$, $CH_3-CH(CH_3)-CH_2-CH_2-CH_3$, $CH_3-CH_2-CH(CH_3)-CH_2-CH_3$, $CH_3-CH(CH_3)-CH(CH_3)-CH_3$, $CH_3-CH_2-CH(CH_3)_2-CH_3$

C_6H_{12} / 8 cyclic isomers: cyclohexane, methylcyclopentane, 1,2-dimethylcyclobutane, 1,3-dimethylcyclobutane, ethylcyclobutane, 1,2,3-trimethylcyclopropane, 1-ethyl-2-methylcyclopropane, propylcyclopropane

2.5 1) C=C found in caffeine, but-2-ene-1-thiol, vitaminA
2) caffeine contains a heterocycle (with 4 nitrogens), vitamin A has cyclohexene ring in its structure
3) methyl branches occur in caffeine and vitamin A
4) fructose: –OH groups 5x and =O group 1x; acetic acid: –COOH group 1x; glutamic acid: –COOH group 2x; caffeine: =O group 2x; vitamin A: -OH group 1x
5) glutamic acid: $-NH_2$ group 1x; caffeine: 4 heterocyclic nitrogens
6) but-2-ene-1-thiol contains –SH group

2.6 a) alcohol (hydroxyl) –OH functional group, b) two cyclohexane rings and one cyclopentane ring, c) one cyclohexene ring, d) two methyl groups attached to the rings, one to the hydrocarbon chain (up on the rihgt) e) 8 carbons containing branched hydrocarbon attached on the top of the structure: $-CH(CH_3)-CH_2-CH_2-CH_2-CH(CH_3)_2$, f) $C_{27}H_{46}O$

2.7 **eth**anoic acid, **prop**yl amine, cyclo**hex**ane, **meth**yl **eth**anoate, potassium **but**anoate, sodium **eth**anoate, **meth**ane, **eth**yne, **hex**anol, **oct**adecanoic acid, (the prefix expressing the number of carbons is **bold-written**, specific suffix related to the type of the hydrocarbon or its derivative is underlined)

2.8 propane, C_3H_8, exists only as a linear structure ($CH_3-CH_2-CH_3$), no branching is possible, because single bonds are freely rotating – but in the space it is not a stright line (see later);
pentane, C_5H_{12}, forms one linear and two branched structures called: 2-**meth**yl**but**ane (=isopentane) or 2,2-di**meth**yl**prop**ane, the position of a branch always gets the lowest locant as possible (3-methylbutane is a wrong name - its chain must be numbered from the other end); $CH_3-CH_2-CH_2-CH_2-CH_3$, $CH_3-CH(CH_3)-CH_2-CH_3$, $CH_3-CH(CH_3)_2-CH_3$

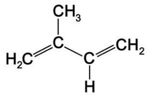
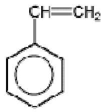
2.9 a) C_2H_6O and c) C_3H_6O

2.10 by hand it is better to draw the structures without parentheses: -C(=O)-O-H, $-S(=O)(O-H)_2$, -C(=O)-H, >C=O, -O-H, -S-H, -N(H)-H, a) oxygen, b) $O^{(-)} \cdots\cdots {}^{(+)}H-O^{(-)}-H^{(+)}$, c) -NH2 → $-NH_3^+$

2.11 3) propane, 4) butyne, 5) pentanol, 6) hexene, 7) cycloheptane, 8) octane, 9) nonyne, 10) decanol, 12) dodecene, 14) tetradecane

2.12 a) propane-1,2,3-triol, b) cyclohexanol, c) cyclohexene

2.13 CH_3CH_3 / CH_3CH_2-, $CH_3CH_2CH_3$ / propyl, butyl / $CH_3CH_2CH_2CH_2$-, $CH_3CH_2CH_2CH_2CH_3$ / pentyl / $CH_3CH_2CH_2CH_2CH_2$-, $CH_3CH_2CH_2CH_2CH_2CH_3$ / hexyl / $CH_3CH_2CH_2CH_2CH_2CH_2$-, $CH_3CH_2CH_2CH_2CH_2CH_2CH_3$ / $CH_3CH_2CH_2CH_2CH_2CH_2CH_2$-, $CH_3(CH_2)_6CH_3$ / octyl, $CH_3(CH_2)_7CH_3$ / nonyl, $CH_3(CH_2)_7CH_2$-, decyl / $CH_3(CH_2)_8CH_2$-

2.14 a)  b) 

2.15 c) estradiol, f) serotonin, g) phenylalanine, h) tryptophan, j) histidine (its free electron pair on the lower nitrogen is involved in the aromatic character – delocalized electrons), k) adrenaline

2.16 CH_3-COOH, methanesulfonic acid, CH_3-CH_2-CH_2-CHO, butanone or ethyl methyl ketone, CH_3-OH, methanol or methyl alcohol, pentane-1-thiol, CH_3-CH_2-CH_2-CH_2-CH_2-CH_2-NH_2, hexan-1-amine or hexyl amine, diethyl ether, CH_3-S-CH_3, 2-chlorobutane, CH_3-$CH(NO_2)$-CH_3

2.17 CH_3-CHCl-CH_2-CH_3, its 2nd carbon binds four different substituents, hence it is chiral

2.18 $HCl < Cl_2 < HClO < HClO_2 < HClO_3 < HClO_4$ (oxidation states of chlorine: -I, 0, +I, +III, +V, +VII)

2.19 A) is oxidation, B) is reduction; they are reverse processes
A) a) dehydrogenation, b) hydration, c) dehydrogenation, d) hydration + dehydrogenation;
B) a) hydrogenation + dehydration, b) hydrogenation, c) dehydration, d) hydrogenation

2.20 A) ethane → ethene → ethanol → ethanal → ethanoic acid
B) ethanoic acid → ethanal → ethanol → ethene → ethane

2.21 oxidation (dehydrogenation): number of hydrogens in reactants lowers;
methanethiol + methanethiol → dimethyl disulfide + hydrogen molecule

2.22 reduction: number of oxygen atoms lowers and number of hydrogen atoms increases hydrogenation = b) d) e), dehydration = c)

2.23 more oxidized is in bold: A) **methanesulfonic**, methanethiol; B) methanol, **methanal,** C) **methanoic acid**, methanal; D) ethane, **ethene;** E) methyl amine, **nitromethan**

2.24 inorganic acids: a) c) e); strong acids: c) e); monoprotic: b) c) d); diprotic: a) e) f)

a) step-1: $H_2CO_3 + H_2O \rightarrow HCO_3^- + H_3O^+$ step-2: $HCO_3^- + H_2O \rightarrow CO_3^{-2} + H_3O^+$

b) step-1: $CH_3\text{-}COOH + H_2O \rightarrow CH_3\text{-}COO^- + H_3O^+$

c) step-1: $HCl + H_2O \rightarrow Cl^- + H_3O^+$

d) step-1: $CH_3\text{-}CH_2\text{-}CH_2\text{-}COOH + H_2O \rightarrow CH_3\text{-}CH_2\text{-}CH_2\text{-}COO^- + H_3O^+$

e) step-1: $H_2SO_4 + H_2O \rightarrow HSO_4^- + H_3O^+$ step-2: $HSO_4^- + H_2O \rightarrow SO_4^{-2} + H_3O^+$

f) step-1: $HOOC\text{-}CH_2\text{-}COOH + H_2O \rightarrow HOOC\text{-}CH_2\text{-}COO^- + H_3O^+$
step-2: $HOOC\text{-}CH_2\text{-}COO^- + H_2O \rightarrow {}^-OOC\text{-}CH_2\text{-}COO^- + H_3O^+$

2.25 similarity: in all reactions water is produced (and also one of reactants contains OH group and the other is an acid); a) c) organic acid, b) d) inorganic acid reaction

a) ethanoic acid + sodium hydroxide	→ sodium ethanoate (salt) + water	neutralization
b) nitric acid + sodium hydroxide	→ sodium nitrate (salt) + water	neutralization
c) ethanoic acid + methanol	→ methyl ethanoate (ester) + water	esterification
d) nitric acid + methanol	→ methyl nitrate (ester) + water	esterification

(ethanoic acid = acetic acid, sodium ethanoate = sodium acetate)

Answers to tasks 3.1 - 3.27

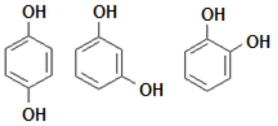
3.1 ethanol or ethyl alcohol, ethanal or acetaldehyde, ethanoic acid or acetic acid; butanal or butyraldehyde, butanoic acid or butyric acid

3.2 hexan-1-ol, octanal, decan-1-ol, tetradecanoic acid, tetradecan-1-ol, hexadecanoic acid, hexadecan-1-ol, octadecanoic acid, octadecan-1-ol, eicosanal, eicosan-1-ol, docosanal, docosan-1-ol

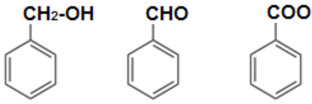
3.3 a) 2-aminoethanol, b) 2-hydroxyethanal, c) ethan-1,2-diol, d) ethanoic acid; alcohols: a) c)

3.4 a) $H^{(+)}\text{-}O^{(-)}\text{-}H^{(+)} \cdots\cdots O^{(-)}\text{-}(H^{(+)})_2$ b) $CH_3\text{-}CH_2\text{-}O^{(-)}\text{-}H^{(+)} \cdots\cdots O^{(-)}(\text{-}H^{(+)})\text{-}CH_2\text{-}CH_3$
c) $CH_3\text{-}CH_2\text{-}O^{(-)}\text{-}H^{(+)} \cdots\cdots O^{(-)}\text{-}(H^{(+)})_2$ d) $CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}O^{(-)}\text{-}H^{(+)} \cdots\cdots O^{(-)}\text{-}(H^{(+)})_2$

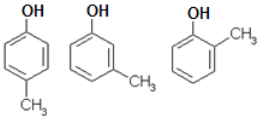
3.5 benzene-1,4-diol = hydroquinone
benzene-1,3-diol = resorcinol
benzene-1,2-diol = pyrocatechol
(or catechol)



3.6 benzyl alcohol → benzaldehyde → benzoic acid



3.7 4-methylphenol = p-cresol (p- = para-)
3-methylphenol = m-cresol (m- = meta-)
2-methylphenol = o-cresol (o- = ortho-)

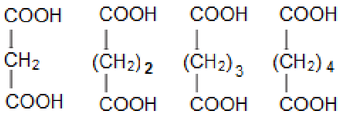


3.8 a) $HO\text{-}CH_2\text{-}CH(OH)\text{-}CH_2\text{-}OH$ → $HO\text{-}CH_2\text{-}CH(OH)\text{-}CHO$ → $HO\text{-}CH_2\text{-}CH(OH)\text{-}COOH$
propane-1,2,3-triol = glycerol
2,3-dihydroxypropanal = glyceraldehyde
2,3-dihydroxypropanoic acid = glyceric acid

b) $HO\text{-}CH_2\text{-}CH(OH)\text{-}CH_2\text{-}OH$ → $HO\text{-}CH_2\text{-}CO\text{-}CH_2\text{-}OH$
1,3 dihydroxypropanone = glycerone = dihydroxyacetone

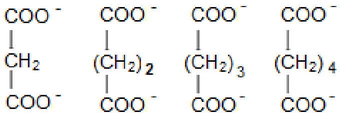
3.9 butyric acid (164 ℃), caproic acid (206 ℃), caprylic acid (240 ℃), capric acid (269℃), lauric acid (298 ℃), myristic acid (326 ℃), palmitic acid (351 ℃), stearic acid (361 ℃)

3.10 propanedioic acid, butanedioic acid, pentanedioic acid, hexanedioic acid



$$\begin{array}{c}COOH\\ |\\ CH_2\\ |\\ COOH\end{array}\quad\begin{array}{c}COOH\\ |\\ (CH_2)_2\\ |\\ COOH\end{array}\quad\begin{array}{c}COOH\\ |\\ (CH_2)_3\\ |\\ COOH\end{array}\quad\begin{array}{c}COOH\\ |\\ (CH_2)_4\\ |\\ COOH\end{array}$$

3.11

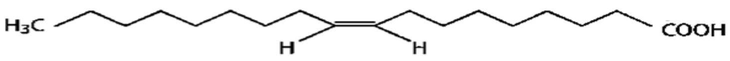


$$\begin{array}{c}COO^-\\ |\\ CH_2\\ |\\ COO^-\end{array}\quad\begin{array}{c}COO^-\\ |\\ (CH_2)_2\\ |\\ COO^-\end{array}\quad\begin{array}{c}COO^-\\ |\\ (CH_2)_3\\ |\\ COO^-\end{array}\quad\begin{array}{c}COO^-\\ |\\ (CH_2)_4\\ |\\ COO^-\end{array}$$

3.12 C2 oxalate, C3 malonate, C4 succinate, C5 glutarate, C6 adipate

3.13 C2 ethanoic acid, acetate, acetyl; C3 propanoic acid, propionate, propionyl; C4 butanoic acid, butyrate, butyryl, C5 pentanoic acid, valerate, valeryl; C6 hexanoic acid, caproate, caproyl; C8 octanoic acid, caprylate, caprylyl; C10 decanoic acid, caprate, capryl; C12 dodecanoic acid, laurate, lauryl; tetradecanoic acid, myristate, myristyl; C16 hexadecanoic acid, palmitate, palmityl; C18 octadecanoic acid, stearate, stearyl;
dicarboxylic: C3 propandioic acid, malonate, malonyl; C4 butanedioic acid, succinate, succinyl; C5 pentanedioic acid, glutarate, glutaryl; C6 hexandioic acid, adipate, adipyl

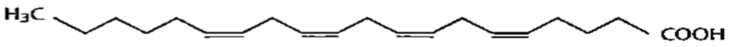
3.14 a)



b)

c)

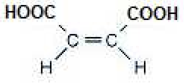
d)

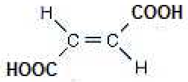


3.14 a) oleate, oleyl; b) linoleate, linoleyl; c) α-linolenate, α-linolenyl; d) arachidonate, arachidonyl

3.15 20:4; 5,8,11,14 eicosa-5,8,11,14-tetraenoic acid
20:5; 5,8,11,14,17 eicosa-5,8,11,14,17-pentaenoic acid
22:6; 4,7,10,13,16,19 docosa-4,7,10,13,16,19-hexaenoic acid

3.17 *cis* but-2-endioic acid, *trans* but-2-endioic acid; anions: maleate, fumarate; acyls: maleyl, fumaryl





3.18 a) CH_3-CH_2-CH_2-CO– b) HCO– c) CH_3-CO– d) HOOC-CH_2-CH_2-CO–
e) HOOC-CH_2-CO – f) CH_3-$(CH_2)_{16}$-CO– g) CH_3-CH_2-CO–
h) HOOC-CH_2-CH_2-CH_2-CO–

3.19 CH_3-OH → HCHO → HCOOH (methanal = formaldehyde, methanoic acid = formic acid)
CH_3-CO-CH_3 → CH_3-CH(OH)-CH_3 (propan-2-ol = isopropanol)
CH_3-CH_2-CH_2-CH_2-OH → CH_3-CH_2-CH=CH_2 (but-1-ene) + H_2O
CH_2=CH_2 + H_2O → CH_3-CH_2-OH (ethanol)
CH_3-COOH → CH_3-COO^- + H^+ (acetate, proton)

3.20 acetyl, acetate; formyl, formate; propionyl, propionate; stearoyl, stearate; succinyl, succinate; oxalyl, oxalate; palmityl, palmitate

3.21 a) methanoic acid = formic acid, b) ethanedioic acid = oxalic acid, c) butanoic = butyric acid

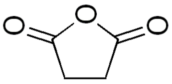
3.22 a) butyric acid + methyl alcohol = methanol; CH_3-CH_2-CH_2-COOH + CH_3-OH
b) butyric acid + pentyl alcohol = penthanol; CH_3-CH_2-CH_2-COOH + CH_3-CH_2-CH_2-CH_2-CH_2-OH
c) acetic acid + pentyl alcohol = penthanol; CH_3-COOH + CH_3-CH_2-CH_2-CH_2-CH_2-OH
d) butyric acid + ethyl alcohol = ethanol; CH_3-CH_2-CH_2-COOH + CH_3-CH_2-OH
e) formic acid + ethyl alcohol = ethanol; HCOOH + CH_3-CH_2-OH

3.23 palmitic acid, oleic acid, stearic acid

3.24 CH_3-CO-O-CH_2-CH_2-$^+N(CH_3)_3$
tetravalent nitrogen (forming four bonds) is charged because the forth bond has been made by its free electron pair, normally present unbounded; only 4 valence electrons of N → cation N^+

3.25 a) ester: methyl butyrate, b) ethyl methyl ether, c) palmitic acid, d) salt: sodium butyrate, e) salt: calcium (di)propionate, f) ester: ethyl formate

3.26 a) CH_3-**CO-O-OC**-CH_3 , b) H-**CO-O-OC**-H, c) CH_3-**CO-O-OC**-H,
d) CH_3-CH_2-**CO-O-PO**-$(OH)_2$, e) succinic anhydride is cyclic:



3.27 a) two anhydride bonds connecting two terminal phosphoric acids, which are released by the anhydride bonds cleavage
b) it connects the third phosphoric acid with the cyclic sugar molecule (ribose)
c) phosphoric acid and alcohol (hydroxyl) group of ribose
d) the nitrogen containing, it is called adenine (purine derivative)

Answers to tasks 4.1 - 4.26

4.1 a) 2-hydroxypropanoic acid → $\mathrm{CH_3{-}CO{-}COOH}$, 2-oxopropanoic acid
b) 3-hydroxybutanoic acid → $\mathrm{CH_3{-}CO{-}CH_2{-}COOH}$, 3-oxobutanoic acid
c) 2-hydoxybutanedioic acid → $\mathrm{HOOC{-}CH_2{-}CO{-}COOH}$, 2-oxobutanedioic acid
d) 2-hydroxypentanedioic acid → $\mathrm{HOOC{-}CH_2{-}CH_2{-}CO{-}COOH}$, 2-oxopentanedioic acid

4.2 a) 2-oxopropanoic acid → $\mathrm{CH_3{-}CH(OH){-}COOH}$, 2-hydroxypropanoic acid
b) 3-oxobutanoic acid → $\mathrm{CH_3{-}CH(OH){-}CH_2{-}COOH}$, 3-hydroxybutanoic acid
c) 2-oxobutanedioic acid → $\mathrm{HOOC{-}CH_2{-}CH(OH){-}COOH}$, 2-hydoxybutanedioic acid
d) 2-oxopentanedioic acid → $\mathrm{HOOC{-}CH_2{-}CH_2{-}CH(OH){-}COOH}$, 2-hydroxypentanedioic acid

4.3 a) $\mathrm{CH_3{-}CH(NH_2){-}COOH}$, 2-aminopropanoic acid
b) $\mathrm{HOOC{-}CH_2{-}CH(NH_2){-}COOH}$, 2-aminobutanedioic acid
c) $\mathrm{HOOC{-}CH_2{-}CH_2{-}CH(NH_2){-}COOH}$, 2-aminopentanedioic acid

4.4	a) $\mathrm{CH_3{-}CH(NH_3)^+{-}COO^-}$	monocarboxylic
4.5	b) $\mathrm{{}^-OOC{-}CH_2{-}CH(NH_3)^+{-}COO^-}$	dicarboxylic, negative charge predominates
	c) $\mathrm{{}^-OOC{-}CH_2{-}CH_2{-}CH(NH_3)^+{-}COO^-}$	dicarboxylic, negative charge predominates

4.6 C3 lactate, lactyl; C4 β-hydroxybutyrate, β-hydroxybutyryl; C4 malate, malyl; 6 citrate, citryl; C6 salicylate, salicylyl; C3 pyruvate, pyruvyl; C4 acetoacetate, acetoacetyl; C4 oxaloacetate, oxaloacetyl; C5 α-ketogultarate, α-ketoglutaryl; C2 glycyl; C3 alanyl; C3 β-alanyl; C9 phenylalanyl; C4 aspartate, aspartyl; C5 glutamate, gluatamyl

4.6	$\mathrm{CH_3{-}CH(OH){-}COOH}$	2-hydroxypropanoic acid = lactic acid	C3
	$\mathrm{CH_3{-}CO{-}COOH}$	2-oxopropanoic acid = pyruvic acid	C3
	$\mathrm{CH_3{-}CH(NH_2){-}COOH}$	2-aminopropanoic acid = alanine	C3

4.7	$\mathrm{HOOC{-}CH_2{-}CH_2{-}COOH}$	butanedioic acid = succinic acid	C4
	$\mathrm{HOOC{-}CH_2{-}CH(OH){-}COOH}$	2-hydroxybutanedioic acid = malic acid	C4
	$\mathrm{HOOC{-}CH_2{-}CO{-}COOH}$	2-oxobutanedioic acid = oxaloacetic acid	C4
	$\mathrm{HOOC{-}CH_2{-}CH(NH_2){-}COOH}$	2-aminobutanedioic acid = aspartic acid	C4

4.8	$\mathrm{HOOC{-}CH_2{-}CH_2{-}CH_2{-}COOH}$	pentanedioic acid = glutaric acid	C5
	$\mathrm{HOOC{-}CH_2{-}CH_2{-}CO{-}COOH}$	2-oxopentanedioic acid = α-ketoglutaric acid	C5
	$\mathrm{HOOC{-}CH_2{-}CH_2{-}CH(NH_2){-}COOH}$	2-aminopentanedioic acid = glutamic acid	C5

4.9	$\mathrm{{}^-OOC{-}CH_2{-}CH(NH_3)^+{-}COO^-}$	net charge -1 +1 -1 = -1 (negative)
	$\mathrm{{}^-OOC{-}CH_2{-}CH_2{-}CH(NH_3)^+{-}COO^-}$	net charge -1 +1 -1 = -1 (negative)

4.10 a) 4-aminobutanoic acid = γ-aminobutyric acid, b) 3-oxobutanoic acid = acetoacetic acid,
c) 4-hydroxybutanoic acid = β-hydroxybutyric acid, d) ethyl propanoate = ethyl propionate,
e) 2-oxopropanoic acid = pyruvic acid, f) diethyl ether, g) butanone = ethyl methyl ketone,
h) octadecanoic acid = stearic acid, i) potassium butanoate = potassium butyrate,
j) magnesium ethanoate = magnesium acetate, methyl methanoate = methyl formate

4.11 a) lactic acid → $\mathrm{CH_3{-}CO{-}COOH}$, pyruvic acid
b) formic acid + ethyl alcohol → $\mathrm{H{-}CO{-}O{-}CH_2{-}CH_3}$, ethyl formate
c) oxalic acid + calcium hydroxide → $\mathrm{(COO^-)_2Ca}$, calcium oxalate
d) but-2-enedioic acid + water → $\mathrm{HOOC{-}CH_2{-}CH(OH){-}COOH}$, malic acid

4.12 a) ammonia, b) amine, c) amino acid, d) amide, e) substituted amide

4.13 $\mathrm{NH_3 + H_2O \rightarrow NH_4^+OH^-}$ (ammonium hydroxide)

4.14 a) methyl amine, b) butyl propyl amine, c) ethyl methyl propyl amine, d) 1,4-butanediamine

4.15 a) 2 phenol groups, 1 alcohol (hydroxyl) group, 1 primary amino group
b) 2 phenol groups, 1 alcohol (hydroxyl) group, 1 secondary amino group
c) ester group, quarternary ammonium group

4.16 a) ethyl amine, b) isopropyl amine, c) ethyl methyl propyl amine, d) secondary butyl amine, e) 2-aminopropan-1-ol (not amine but alcohol), f) propylene diamin = 1,3-propanediamine, g) 2-aminobutanoic acid (not amine), h) dimethyl amine, i) ethyl methyl propyl amine
primary amines: a) b) d) f), secondary amine: h), teriary amine: c) = i)

4.17 a) H-CO-NH_2 formamide, b) $\text{CH}_3\text{-CO-NH}_2$ acetamide,
c) $\text{CH}_3\text{-CH}_2\text{-CO-NH}_2$ propionamide, d) $\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-CO-NH}_2$ butyramide,
e) $\mathbf{H_2N\text{-}CO}\text{-CH}_2\text{-CH}_2\text{-CH(NH}_2\text{)-COOH}$ glutamine

4.18 $\text{H}_2\text{N-CH(CH}_3\text{)}\mathbf{\text{-CO-NH}}\text{-CH}_2\text{-COOH}$

4.19 $\text{H}_2\text{N-CH}_2\mathbf{\text{-CO-NH}}\text{-CH(CH}_3\text{)}\mathbf{\text{-CO-NH}}\text{-CH}_2\text{-COOH}$ glycyl-alanyl-glycine

4.20 amide group / amino group / carboxylic acid group
amide group hydrolysis → NH_3 (ammonia) + $\text{HOOC-CH}_2\text{-CH}_2\text{-CH(NH}_2\text{)-COOH}$ (glutamic acid)

4.21 a) on the left, b) bottom, c) -CO-O- (on the right) d) -CO-NH- (in the middle)
hydrolysis → $\text{HOOC-CH}_2\text{-CH(NH}_2\text{)-COOH}$ (aspartic acid)
+ phenyl-$\text{CH}_2\text{-CH(NH}_2\text{)-COOH}$ (phenylalanine) + methyl alcohol (= methanol)

4.22 a) ammonia + water → ammonium hydroxide,
methyl amine + water → methyl ammonium hydroxide
b) ammonia + hydrochloric acid → ammonium chloride
methyl amine + hydrochloric acid → methyl ammonium chloride

4.23 -SH group
$\text{HOOC-CH(NH}_2\text{)-CH}_2\mathbf{\text{-S-S-}}\text{CH}_2\text{-CH(NH}_2\text{)-COOH}$ this disulfide is called **cystine**

4.24 1) pyrimidine, 2) purine, 3) pyridine, 4) indol, 5) imidazole, 6) pyrrole

4.25 fructose contains „furane“ ring, glucose contains „pyrane“ ring

4.26

- pyrrole in bilirubin; functional groups and substituents from the left: oxo, methyl, vinyl, methyl, propionate, propionate (carboxylic acid group), methyl, methyl, vinyl, oxo group
- imidazole in histidine; amino and carboxylic acid groups
- indol in tryptophan; amino and carboxylic acid groups
- pyridine in nicotinamide; amide group
- purine in adenine; amino group
- tetrahydrofuran in ribose; alcohol (hydroxyl) groups

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