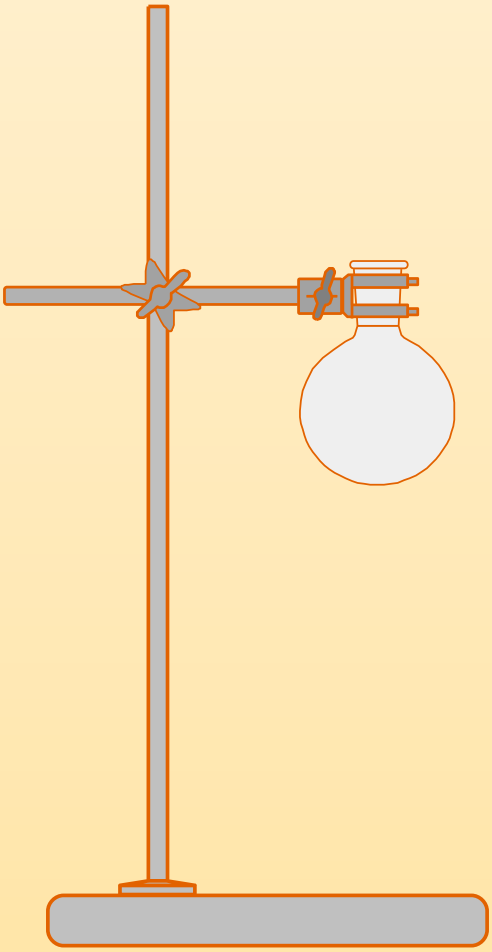

Chemical Calculations and Introduction to Laboratory Work in General and Inorganic Chemistry

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CHEMICAL CALCULATIONS

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IN

GENERAL AND INORGANIC CHEMISTRY

♦

Learning texts for foreign students

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CONTENT

PREFACE

This text is dedicated to the first-year students studying Pharmacy in the study programme in English language at the Faculty of Pharmacy, Comenius University Bratislava. Its contents involve topics presented in seminars of the main subject General and Inorganic Chemistry, including solved and unsolved problems and calculations, as well as instructions for laboratory experiments. Naturally, this text does not attempt to cover all aspects of the course and does not substitute a textbook of inorganic chemistry, nor the attendance at the seminars. We hope that the text will help the students to gain a better understanding of this challenging but rewarding subject.

We would like to thank all our colleagues who helped us with the development of the curriculum, both the seminar and the laboratory part, as well as with the preparation of the manuscript. We are particularly grateful to our long-time colleague and co-author doc. Mária Kohútová for her generous assistance, especially for sharing her profound knowledge and experience with the teaching of the subject Inorganic Chemistry and for providing the basis for this manuscript.

Authors

I SEMINAR PART

1 BASIC TERMS

Chemistry: The part of nature sciences studying reactvity, compositions, structure, ability to absorb or release energy in various forms and other chemical properties of compounds and materials.

Substance: A single, pure type of matter, either a compound or an element.

Element: A pure substance consisting of atoms with the same atomic number, and which cannot be broken down into simpler substances by ordinary chemical changes.

Atom: The smallest particle of an element that retains the chemical properties of the element. Atom consists of protons, neutrons and electrons. **Protons** (positively charged) and **neutrons** (without charge) placed in a core (nucleus) are responsible for mass of atoms, **electrons** (negatively charged) arranged around the nucleus determine the chemical behaviour and chemical properties of the corresponding element. Atoms are characterized using the terms *atomic* and mass *number*.

Atomic number represents the number of protons (in the neutral state also the number of electrons) written as a left side subscript ($_{8}O$, $_{16}S$, $_{29}Cu$).

Mass number represents the number of protons and neutrons written as a left side superscript (^{16}O, ^{32}S, ^{63}Cu).

Ion: A positively (cation) or negatively (anion) charged atom or group of bonded atoms.

Examples 1:
a) the atom of copper $^{63}_{29}Cu$ contains 29 protons, 29 electrons and 34 neutrons
the cation $^{63}_{29}Cu^{2+}$ contains 29 protons, 27 electrons and 34 neutrons,

b) the atom of sulfur $^{32}_{16}S$ contains 16 protons, 16 electrons and 16 neutrons
the anion $^{32}_{16}S^{2-}$ contains 16 protons, 18 electrons and 16 neutrons.

Nuclides: atoms of the same element with the same atomic and mass numbers.
Isotopes: atoms of the same element with the same atomic but different mass numbers ($^{16}_{8}O$, $^{17}_{8}O$, $^{18}_{8}O$).

Isobares: atoms of various elements, that means with different atomic number, but the same mass number ($^{12}_{5}B$, $^{12}_{6}C$, $^{12}_{7}N$).

Molecule: A definite and distinct, electrically neutral group of bonded atoms consisting of atoms with the same or different atomic and mass numbers; it is the smallest particle exhibiting the properties of a corresponding substance.

Compound: A pure substance which can be broken down into simpler substances (elements) using ordinary chemical changes. Compounds are composed of two or more elements combined in a fixed proportion.

Mixture: A combination of two or more pure substances in variable proportion, and without chemical bonds between them, which may be separated by a mere physical change.
Heterogeneous mixture (we can directly observe different components, e.g., mixture of sugar and sand).
Homogeneous mixture (we cannot make out individual components, e.g., sugar dissolved in water).

Chemical reaction: When a chemical change occurrs, the reacting substances (the reactants) disappear, and new substances, with entirely different properties, appear – the products. Because the elements are chemically combined to form a compound, a chemical change is necessary to separate them.

Atoms interact in two basic ways: one involves the sharing of electrons to produce **covalent bond**, the other involves the transfer of electrons to produce **ionic bond**.

1.1 RELATIVE ATOMIC AND MOLECULAR WEIGHTS

A single atom is too small to be weighed. So, as it was realized a long time ago, it is not necessary to weigh individual atoms. What we need to know are the masses of atoms in one element relative to atoms in other elements. The standard chosen for the atomic weight scale is the most abundant isotope of carbon, ${}^{12}_{6}C$.
In 1961, carbon-12 was assigned a mass of 12 atomic mass units (amu). Then the atomic masses of the other elements were determined by comparison to this unit.

$$1\ amu = \frac{1}{12} \times m({}^{12}_{6}C) = 1.66056 \times 10^{-27}\ kg = 1.66056 \times 10^{-24}\ g$$

The mass of the other elements (compounds) is determined relative to this value. It is known as the **relative atomic mass A_r** of an atom X and the **relative molecular mass M_r** of a molecule XY:

$$A_r(X) = \frac{m(X)}{1\ amu} \qquad M_r(X) = \frac{m(XY)}{1\ amu}$$

The values of relative atomic and molecular weights can be found in chemical data tables or in online sources.

The weight of a substance is directly proportional to its volume. The coefficient of proportionality is called **density** (and it is defined as the ratio of the weight *m*(A) of substance A and its volume *V*(A).

$$d(X) = \frac{m(X)}{V(X)}$$

The basic unit of density is *kilogram per cubic meter*, kg/m^3, but in laboratory practice the unit *gram per cubic centimeter*, g/cm^3 or g/mL is commonly used.

1.2 CHEMICAL AMOUNT

Chemical amount (the amount of substance) refers to the number of particles or elementary entities present in a sample. The unit 1 mol is used to express chemical amount.
The actual mass of a carbon-12 atom has been found to be 1.9926 × 10^{-23} grams. 12 grams of carbon-12 atoms represent 1 mole of carbon-12 atoms. Then, the number of atoms in 12 grams of carbon-12 is calculated as follows:

$$number\ of\ {}^{12}_{6}C\ atoms = \frac{12\ grams}{1{,}992\ \times\ 10^{-23} grams} = 6.022\ \times\ 10^{23} = 1\ mol$$

The number of objects (particles, atoms, molecules, ions) per mole which is equal to **6.022 × 10^{23} mol^{-1}** is called the **Avogadro constant** (number). It can be used to calculate the number of particles in a specific chemical amount. The following formulas apply:

$N(X) = n(X) \times N_A$ or $n(X) = \frac{N(X)}{N_A}$

where N_A is the Avogadro' constant, n(X) is the chemical amount of particle X and N(X) is the number of particles X in the sample.

The **average atomic weight** (found in chemical data tables) reflects the fact that elements are made up of atoms with different masses, i.e., isotopes.

1.3 MOLAR MASS

The *molar mass* of an element or a compound expresses the weight of 1 mole of this element or molecule. The unit used is grams per mole (g/mol). The formula for molar mass is:

$$M(X) = \frac{m(X)}{n(X)}$$

where M(X) is the molar mass of X in g/mol, m(X) is the mass of X, and n(X) is the chemical amount.

We can use this formula to calculate the chemical amount as:

$$\boldsymbol{n(X) = \frac{m(X)}{M(X)}}$$

Molar mass (M) is numerically equal to relative molecular mass (M_r) or relative atomic mass (Ar). The only difference is that molar mass has a unit (g/mol) while the relative mass does not have a unit.

Examples 2:

a) The mass of a fluorine atom is 3.155 × 10^{-23} g. We can calculate the molar mass of the fluorine atom because the value of molar mass is identical with the value of relative atom or molecule mass.

$$A_r(F) \approx M(F)$$

$$A_r(F) = \frac{m(F)}{1\ amu} = \frac{3.155\ \times\ 10^{-23}\ g}{1.66056 \times 10^{-24}\ g} = \ 19.00$$

where m(F) is the mass of the fluorine atom.

If relative atomic mass of fluorine atom $A_r(F)$ is 19.00, then the molar mass of fluorine atom M(F) is 19.00 g/mol.

b) The number of moles of F atoms in 22.5 g of fluorine can be calculated using the formula:

$$n(F) = \frac{m(F)}{M(F)} = \frac{22.5\ g}{19.00\ \frac{g}{mol}} = 1.18\ mol$$

c) The mass of CO_2 present in 3 moles of this compound, when molar mass of CO_2 is 44 grams/mol, can be calculated using the same formula:

$$M(CO_2) = \frac{m(CO_2)}{n(CO_2)}$$

but for mass calculation we need to use:

$$m(CO_2) = M(CO_2) \times\ n(CO_2) = \ 44.00\ \frac{g}{mol}\ \times 3\ mol = 132\ grams$$

d) We can calculate the molar mass of a CO_2 by summing the molar masses of the atoms the molecule is composed of. M(O) = 16 g/mol, M(C) = 12 g/mol

$$M(CO_2) = M(C) + 2\ \times M(O) = 12 + 2\ \times 16 = \ 44\frac{g}{mol}$$

1.4 MOLAR VOLUME

One mole of any gas occupies a fixed volume of **22.4 litres** at the standard temperature and pressure (1 atm ~ 101325 Pa, 0 °C). This value can be calculated using the ideal gas law.
We can use this value in the calculation of gas volumes:

$$V_M = \frac{V(gas)}{n(gas)} = 22.4\frac{L}{mol}$$

where V_M is the molar volume, V(gas) is the volume of the gas sample and n(gas) is the chemical amount of the gas.

Examples 3:

a) Calculate the volume occupied by 2.25 moles of chlorine at the standard conditions $V_M = \frac{V(gas)}{n(gas)}$ *can be transformed to:*

$$V(gas) = V_M \times n(gas) = 22.4\frac{L}{mol} \times 2.25\,mol = 50.4\,L$$

b) Calculate the number of moles and volume (at the standard conditions) occupied by 9.033×10^{23} particles of CO gas.

First, we use $n(X) = \frac{N(X)}{N_A}$ *to calculate the number of moles.*

$$n(CO) = \frac{N(CO)}{N_A} = \frac{9.033 \times 10^{23}}{6.022 \times 10^{23} mol^{-1}} = 1.5\,mol$$

Then we can use $V(gas) = V_M \times n(gas)$ *to calculate the volume of CO gas.*

$$V(CO) = V_M \times n(CO) = 22.4\,\frac{L}{mol} \times 1.5\,mol = 33.6\,L$$

1.5 PROBLEMS

1. Calculate the chemical amount in a) 0.5 g of hydrogen ($M_r(H_2)$= 2.016); b) 2.5 g of nitrogen dioxide ($M_r(NO_2)$ = 44.01).

2. Calculate the number of particles in a) 1.4 g of argon (A_r (Ar) = 39.95); b) 156 g of carbon monoxide (M_r (CO) = 28).

3. How many grams are contained in 1.45 moles of water (M_r = 18)?

4. What chemical amount corresponds to 50 g of H_2S? (M_r = 34)

5. How many molecules of NH_3 are there in 7.2 mol of NH_3?

6. Determine the chemical amount of Na_2SO_4 (M_r = 142.04) in 14.9 grams of this salt.

7. How many P atoms (A_r = 30.97) weigh 15.91 grams?

8. Calculate the number of atoms found in 1.00 g of pure iron (A_r = 55.85).

9. What is the chemical amount which corresponds to 75.8 g of Li_2S salt? $M_r(Li_2S)$ = 45.

10. Calculate the molar mass of silver nitrate $AgNO_3$ when 500 g of this compound represent 2.94 mol.

11. Calculate the volume occupied by 2.25 mol of chlorine gas (Cl_2).

12. Calculate the chemical amount and volume occupied by 9.033×10^{23} particles of CO gas.

13. State the chemical amount and volume (at standard conditions) of 18.066×10^{24} particles of SO_2 gas.

14. How many molecules of oxygen at normal conditions are in the volume of 10 litres?

15. Calculate the volume of 4 mol of mercury ($A_r = 200.6$) at 20 ºC. The density value for mercury at this temperature is equal to 13.55 g/mL.

16. How many molecules of water are there in 6 grams of H_2O? ($M_r = 18$)

17. Calculate the chemical amount of CN^- ($M_r = 26$) in 1.00 g of KCN ($M_r = 65.12$).

18. Calculate the chemical amount of water ($M_r = 18$) in 500 g of $CuSO_4 . 5H_2O$ ($M_r = 249.68$).

19. What mass of zinc ($A_r = 65.37$) is needed to obtain 2 mol of $ZnCl_2$ ($M_r = 36.28$)?

20. State the numbers of Cu and Cl atoms in 2 mol of $CuCl_2$.

Answers: *1*) a) 0.25 mol, b) 0.057 mol *2*) a) 2.11×10^{22}, b) 3.36×10^{24} *3*) 26.1 g *4*) 1.47 mol *5*) 4.34×10^{24} *6*) 0.105 mol *7*) 3.09×10^{23} *8*) 1.08×10^{22} *9*) 1.68 mol *10*) 170.07 g/mol *11*) 50.4 litres *12*) 1.5 mol, 33.6 L *13*) 30 mol, 672 litres *14*) 2.69×10^{23} *15*) 59.2 mL *16*) 2.0×10^{23} *17*) 0.015 mol *18*) 10 mol *19*) 130.74 g *20*) 1.2×10^{24} Cu, 2.408×10^{24} Cl

2 CHEMICAL FORMULAS

Chemical formulas are used to describe the composition of compounds. It is a simple way how to express the composition of a compound by using symbols of elements and the ratio of the elements in the compound using the number of atoms of the respective element indicated as a subscript.
A compound A_xB_y is made of elements A and B at the ratio x : y. For example, Al_2O_3 is made of Al and O and the ratio of Al : O = 2 : 3.

Empirical formulas were the first type of formulas used for compounds. They are the simplest chemical formulas that show the relative numbers of atoms of each element in a compound.
E.g.: HO (hydrogen peroxide), CH (benzene), NaCl, P_2O_5.
They show only the ratio, not the real number of atoms in a molecule.

Molecular formulas represent the actual number of atoms of elements (this fact must be experimentally proven). A combination of chemical symbols and subscripts shows the actual number of atoms of each element present in a molecule.
E.g.: C_6H_6 (benzene) instead of CH; P_4O_{10} instead of P_2O_5

Functional formulas are modified molecular formulas where some elements are presented in groups common for various compounds.
E.g.: $Ba(OH)_2$, NH_4NO_3, $CO(NH_2)_2$

Lewis formulas consist of element symbols and their valence electrons (more in the chapter *Lewis structure formulas*).

2.1 DETERMINATION OF EMPIRICAL FORMULAS

Empirical formulas can be determined using the percentage composition of the compounds. Overall, for a compound $A_xB_yC_z$ that contains some percentage of A (%A), B (%B) and C (%C), we can calculate the indexes expressing the ratio of these elements (x, y, z) using the formula:

$$x : y : z = \frac{\%A}{A_r(A)} : \frac{\%B}{A_r(B)} : \frac{\%C}{A_r(C)}$$

where $A_r(A)$, $A_r(B)$ and $A_r(C)$ are the relative atomic masses of elements A, B and C.

***Example 1**: Calculate the empirical formula for a compound containing 50.1% S (A_r = 32.1) and 49.9% O (A_r = 16.0).*

In this compound there are only two elements, so we use a shorter version of the formula:

$$x : y = \frac{\%S}{A_r(S)} : \frac{\%O}{A_r(O)}$$

and we replace A for S and B for O. We use it to calculate the composition of S_xO_y. After filling the percentages and the relative atomic masses of the atoms into the formula, we get:

$$x : y = \frac{50.1}{32.1} : \frac{49.9}{16}$$

The two fractions on the right side of the equation will give us the ratio values:

$$x : y = 1.56 : 3.12$$

Afterwards, the two numbers will be divided by the smaller one, in our case 1.56, and we get a new ratio, preferably with whole numbers (integers):

$$x : y = 1 : 2$$

As a result, the empirical formula of this compound is ***SO_2***.

2.2 PERCENTAGE COMPOSITION

According to the law of constant composition, a pure substance has a fixed and definite composition. It means that in each studied compound the proportion by weight of the element present is always the same,
e.g.: water is always 11.2% hydrogen and 88.8% oxygen, pure calcium carbonate (limestone) 40% calcium, 12% carbon, and 48% oxygen.

We can calculate the percentage of an element A in the compound A_xB_y using the weight percent formula:

$$\%A = \frac{x \times A_r(A)}{M_r(A_xB_y)} \times 100$$

where x is the coefficient of atom A, $A_r(A)$ is the relative atomic mass of atom A and $M_r(A_xB_y)$ is the relative molecular mass of the whole compound.

Example 2: Calculate the weight percentage of each element in calcium chloride, $CaCl_2$.
$A_r(Ca) = 40$; $A_r(Cl) = 35.5$; $M_r(CaCl_2) = 111$

$$\%Ca = \frac{1 \times 40}{111} \times 100 = \frac{40}{111} \times 100 = 0.36 \times 100 = 36\%$$

$$\%Cl = \frac{2 \times 35.5}{111} \times 100 = \frac{71}{111} \times 100 = 0.64 \times 100 = 64\%$$

2.3 PROBLEMS

Find the empirical formula for each of the following substances:

a) K (A_r = 39.10) 52.4%; Cl (A_r = 35.45) 47.6%
b) Na (A_r = 23) 16.2%; Mn (A_r = 55) 38.6%; O (A_r = 16) 45.2%
c) H (A_r = 1.01) 3.1%; P (A_r = 31) 31.5%; O (A_r = 16) 65.4%
d) K (A_r = 39) 56.6%; C (A_r = 12) 8.7%; O (A_r = 16) 34.7%
e) C (A_r = 12) 10.06%; H (A_r = 1.01) 0.84%; Cl (A_r = 35.45) 89.09%
f) Fe (A_r = 56) 69.94%; O (A_r = 16) 30.06%

g) Na (A_r = 23) 32.37%; S (A_r = 32) 22.57%; O (A_r = 16) 45.06%
h) K (A_r = 39.10) 31.90%, Cl (A_r= 35.45) 28.93%, O (A_r) = 16.00) 39.17%

Answers: *a*) KCl *b*) $NaMnO_4$ *c*) H_3PO_4 *d*) K_2CO_3 *e*) $CHCl_3$ *f*) Fe_2O_3 *g*) Na_2SO_4 *h*) $KClO_3$

Calculate the percentage by weight for each element in the following compounds:

a) H_2SO_4; M_r (H_2SO_4) = 98.08, A_r(H) = 1.01, A_r (S) = 32.06, A_r(O) = 16.00
b) CO; M_r (CO) = 28.01, A_r(C) = 12.01, A_r(O) = 16.00
c) CO_2; M_r (CO_2) = 44.01, A_r(C) = 12.01, A_r(O) = 16.00
d) $Al(OH)_3$; M_r ($Al(OH)_3$ = 78.00, A_r (Al) = 26.98, A_r(H) = 1.01 A_r(O) = 16.00
e) NaOH; M_r (NaOH) = 40.00, A_r (Na) = 22.99, A_r(O) = 16.00, A_r(H) = 1.01
f) Li_3PO_4; M_r (Li_3PO_4) = 115.47, A_r(Li) = 6.94, A_r (P) = 30.97, A_r(O) = 16.00
g) $ZnSO_4$; M_r ($ZnSO_4$) = 161.44, A_r(Zn) = 65.37, A_r (S) = 32.06, A_r(O) = 16.00
h) $HClO_4$; M_r ($HClO_4$) = 100.46, A_r(H) = 1.01, A_r (Cl) = 35.45, A_r(O) = 16.00

Answers: *a*) 2.06% H, 32.69% S, 65.25% O *b*) 42.88% C, 57.14% O *c*) 27.29% C, 72.71% O *d*) 34.59% Al, 61.53% O, 3.88% H *e*) 57.47% Na, 40.00%, O, 2.52% H, *f*) 17.98% Li, 26.75% P, 55.27% O *g*) 40.50% Zn, 19.86% S, 39.64% O *h*) 1.00% H, 35.29% Cl, 63.71% O

3 OXIDATION STATES OF ELEMENTS

When atoms bind with ionic or covalent bonds to form compounds, electrons are exchanged between them. The **more electronegative atom** takes electrons from the less electronegative atom completely to form an ionic bond or pulls the electrons closer to make a polar covalent bond.
This electron reposition is the reason why oxidation states (or oxidation numbers) are used in chemistry. They express how much more or less electrons the atoms have in compounds compared to the same atoms in elemental form. If an atom has more electrons, the oxidation state is negative, and vice versa. Oxidation states are usually written with Roman numerals (+II, -IV, +VII etc.)
The sum of all oxidative states must match the overall charge of the compound or ion. Consequently, for neutral compounds with charge 0, the sum of all oxidative states must be also 0.

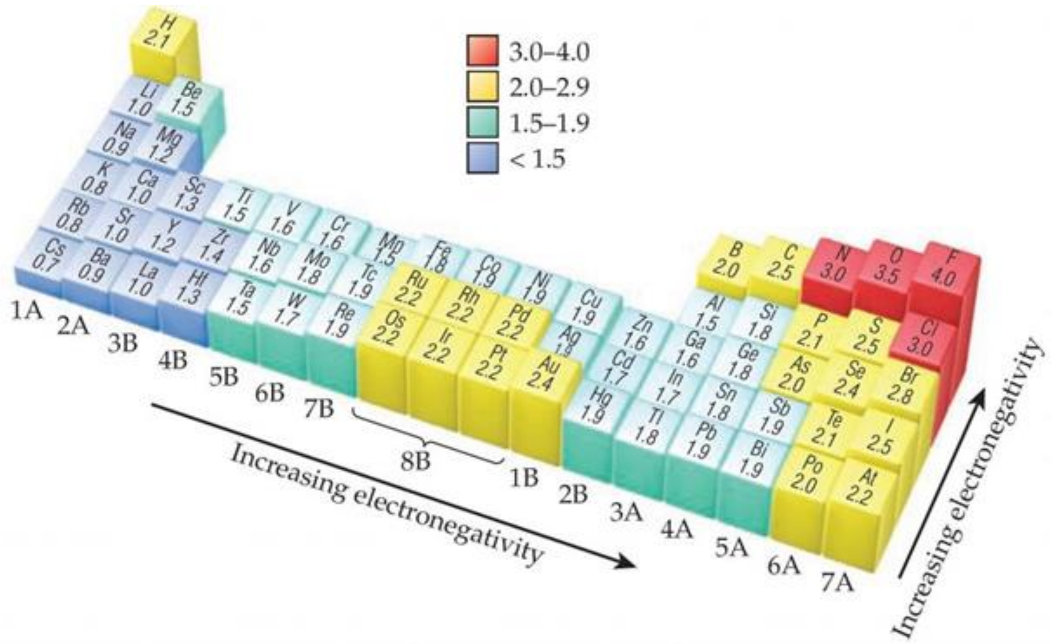
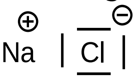


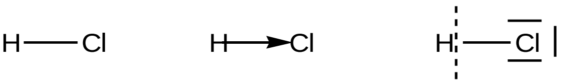
Figure 1 The distribution of electronegativities across the periodic table
Source: https://www.tollebild.com/bilden/electron-negativity-chart-1b.html

Example 1: *Na and Cl form the compound NaCl, which has one* ***ionic bond****. Na has the electronegativity EN = 1.0 and Cl EN = 2.8. So, Na will give its only valence electron to Cl and a cation Na^{+1} and an anion Cl^{-1} will form. In ionic compounds with simple ions the charge equals the oxidation state.*



Na: +I Cl: -I

Example 2: *H and Cl form the compound HCl, which has one* ***polar single covalent bond****. But Cl has the EN = 2.8 and H has EN = 2.1. As a result, Cl pulls the bonding pair towards it and Cl will have 1 electron more than in elemental form. So, its oxidation state will be -I and H will be at state +I.*



H: +I Cl: -I

If atoms of the same electronegativity form a covalent bond, there is no electron reposition present. Such bond is **nonpolar**, and the two electrons are split evenly between the two atoms. So, each atom retains one electron participating in the bond.

Example 3: *Hydrogen in elemental form creates H_2, which contains one* ***nonpolar single covalent bond****. Since the two H atoms have same electronegativity, the electrons are split equally. In this way, none of the two H atoms gain or lose electrons and the oxidation state of both is 0.*

H: 0

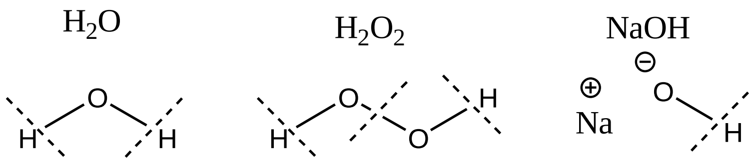
All atoms in elemental form have the oxidation state zero (0).

Example 4: *In* ***molecules made of more atoms****, each bond must be evaluated as ionic or polar covalent (between atoms of different electronegativity) or nonpolar covalent (atoms of the same electronegativity, or atoms of the same element). In molecules such as H_2O, H_2O_2, and NaOH, oxidation states can be determined by specifying atoms that take or lose the bonding electrons based on their electronegativity.*
EN(O) = 3.5, EN(H) = 2.1, EN(Na) = 1.0 *O > H > Na*

a) *In water (H_2O), O is the more electronegative element (EN = 3.5), so it pulls bonding electrons towards it and away from both H atoms. It gains 2 electrons so its oxidation state will be -II. Both hydrogens lose 1 electron, so they will have oxidation state +I.*

b) *In hydrogen peroxide (H_2O_2), there are 3 covalent bonds. Two of them are polar (between O and H), which is identical with the water structure. These two bonds cause that each hydrogen virtually loses one electron and their oxidation states are +I and oxygens gain one electron. The third bond is nonpolar (between 2 identical atoms), there is no shift of electrons. This means the oxygens have the oxidation state -I.*

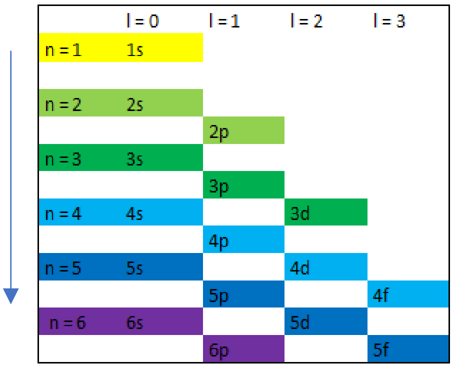
c) *In sodium hydroxide (NaOH) there are two bonds, one is ionic (between Na and O) and one is polar covalent (between O and H). In both cases O is the more electronegative atom. It takes one electron from Na and pulls the bonding pair away from H making it virtually lose one electron. These repositions give O the oxidation state -II, Na +I and H +I.*



This could be done also with **more complex compounds**, but it would make the process of the oxidation state determination very slow. Instead, an alternative method is used based on the number of electrons in atomic valence layer and the maximum number of electrons that an atom can gain or lose.

3.1 ELECTRON CONFIGURATIONS

Each element has some typical oxidation states**.** These states can be determined based on their **electron configuration.** The electron configuration describes how electrons occupy atomic orbitals (s, p, d, and f) from orbitals of low energy up to the orbitals with the highest energy:



The arrangement of atomic orbitals from the lowest to the highest energy is as follows: 1s < 2s < 2p < 3s < 3p < 4s ≈ 3d < 4p < 5s ≈ 4d …

The atomic orbitals with the same principal quantum number (n) belong to the same energy layer. The highest energy layer with occupied atomic orbitals is called **valence layer** (valence shell).

In most chemical applications, only electrons in valence layer can be taken to form positive oxidation states. If there is space for more electrons in the valence layer (the maximum electron number is not reached), electrons can be accepted, and negative oxidation states are formed.

Each atomic orbital type has a different maximum number of electrons occupying that orbital:
s 2 electrons, p 6 electrons, d 10 electrons, f 14 electrons

Example 5: *Carbon has the atomic number 6, which means it has 6 protons but also 6 electrons.*
Electron configuration is $C: 1s^2\ 2s^2\ 2p^2$
The electrons in layer 2 ($2s^2\ 2p^2$) belong to the valence layer. There are 4 electrons that can participate in bonding. This is the maximum number of electrons; therefore, the highest oxidation state of C is +IV. On the other hand, the 2p orbital has a maximum number of 6 electrons, so 4 electrons could be accepted by C and the lowest oxidation state for C could be -IV.
${}_6C(+IV): 1s^2\ 2s^0\ 2p^0$
${}_6C(+II): 1s^2\ 2s^2\ 2p^0$
${}_6C(-IV): 1s^2\ 2s^2\ 2p^6$
The typical oxidation states of C in inorganic compounds are +IV, -IV and also +II.

Example 6*: Magnesium has atomic number 12, so 12 electrons must be placed into atomic orbitals.*
Electron configuration is $Mg: 1s^2\ 2s^2\ 2p^6\ 3s^2$
The layer 3 ($3s^2$) is the valence layer. There are 2 electrons participating in bonds to other atoms. This is the maximum number of electrons available for bonding, therefore the highest oxidation state of Mg is +II.
$Mg(+II): 1s^2\ 2s^2\ 2p^6\ 3s^0$

3.2 NOBLE GAS CONFIGURATION

Atoms take or give electrons into their atomic orbitals in order to to reach the most stable configuration. For s- and p-elements (groups 1A-8A in periodic table) it is the configuration of noble gases (8A group). Noble gases have **completely filled valence layer** with electrons and are stable to the extent that they don't react with other elements to form compounds. This is the reason why only very few compounds composed of these elements exist.

The electron configurations of the elements of the 8A group are:
$_{2}$He: $\underline{1s^2}$
$_{10}$Ne: $1s^2$ $\underline{2s^2\ 2p^6}$ or $_{10}$Ne: [He] $\underline{2s^2\ 2p^6}$
$_{18}$Ar: $1s^2\ 2s^2\ 2p^6$ $\underline{3s^2\ 3p^6}$ or $_{18}$Ar: [Ne] $\underline{3s^2\ 3p^6}$
$_{36}$Kr: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$ $\underline{4s^2}$ $3d^{10}$ $\underline{4p^6}$ or $_{36}$Kr: [Ar] $\underline{4s^2}$ $3d^{10}$ $\underline{4p^6}$
$_{54}$Xe: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6$ $\underline{5s^2}$ $4d^{10}$ $\underline{5p^6}$ or $_{54}$Xe: [Kr] $\underline{5s^2}$ $4d^{10}\ 4f^{14}$ $\underline{5p^6}$
$_{86}$Rn: [Xe] $\underline{6s^2}$ $5d^{10}\ 5f^{14}$ $\underline{6p^6}$

The underlined parts belong to the valence layer. All 8A elements except for He have the configuration $\mathbf{ns^2\ np^6}$ of the valence layer.

The short version of electron configuration on the right side uses the electron configuration of the noble gas from the previous period (the row in periodic table) and adds the rest of the electrons in the energetically higher atomic orbitals. This can be used also for other elements:

$_{11}$Na: $1s^2\ 2s^2\ 2p^6$ $\underline{3s^1}$ or $_{11}$Na: [Ne] $\underline{3s^1}$
$_{17}$Cl: $1s^2\ 2s^2\ 2p^6$ $\underline{3s^2\ 3p^5}$ or $_{17}$Cl: [Ne] $\underline{3s^2\ 3p^5}$

Example 7: *Na and Cl can reach the stable noble gas configuration by accepting or giving an electron. Na has 1 electron in the 3s orbital; if this electron is removed and a cation Na^{+1} is formed, Na would acquire the electron configuration of Ne.*
$_{11}$Na(+I): $1s^2\ 2s^2\ 2p^6$ $\underline{3s^0}$ or $_{11}$Na(+I): [Ne]
Cl, on the other hand, can acquire the noble gas configuration most easily by accepting an electron and filling its valence layer completely. This would allow Cl to gain the electron configuration of Ar.
$_{17}$Cl(-I): $1s^2\ 2s^2\ 2p^6$ $\underline{3s^2\ 3p^6}$ or $_{17}$Cl(-I): [Ar]

3.3 TYPICAL OXIDATION STATES FOR S-ELEMENTS

The s-elements are elements of the 1A and 2A groups, which have the highest energy electrons placed in s atomic orbitals in the valence layer. Most of these elements are metals and have low electronegativity (alkali metals - 1A: Li, K, Na, Rb, Cs, Fr, alkaline earth metals - 2A: Be, Mg, Ca, Sr, Ba, Ra). The only exception is hydrogen which is also a gas.

<u>Hydrogen</u> has an electronegativity of 2.1 which allows it to take on electrons to form negative oxidation states with elements of low electronegativity. It is also able to give off its electron in the presence of more electronegative atoms.
<u>The other s-elements</u> have low electronegativity as well. They form +I or +II oxidation states according to their group number or the number of electrons in their s valence atomic orbital.

Example 8: *The electron configuration of hydrogen is* $_1H: 1s^1$.
In compounds with alkali metals, such as KH (potassium hydride), H is the more electronegative atom and has a negative oxidation state. It can accept only 1 electron to fill its valence layer. Therefore, the oxidation state can be -I only: $_1H(-I): 1s^2$.
Potassium in KH, on the other hand, loses one electron and gains the configuration: $_{19}K(+I): [Ar]\ 4s^0$
In compounds with more electronegative elements such as O, N, F, Cl etc., H will have a positive oxidation state. Since it has only one electron, it gains the oxidation state +I: $_1H(+I): 1s^0$.

3.4 TYPICAL OXIDATION STATES OF P-ELEMENTS

There are 6 groups within the p-elements (3A-8A) with 3 to 8 valence electrons. Their electronegativity ranges from 1.8 to 4.0. This is a very large range and makes the elements behave in very different ways.

The p-elements with the highest electronegativity belong to the upper sections of 5A – 7A groups (N, O, F, Cl) and they usually carry negative oxidation states (-I to -III). F is the element with the highest electronegativity, and it can only have the -I oxidation state. Oxygen usually acquires the -II oxidation state, except for peroxy-compounds such as H_2O_2 (see example 4) where the oxidation state is -I. Nitrogen atom can have the oxidation state -III. In compounds where bonds between N and O are present, it can also acquire positive oxidation states such as +V or +III. Oxidation state of Cl is similar to that of F which is -I. When bonded to oxygen, it can acquire also positive oxidation states such as +VII, +V, +III or +I.

The p-elements with average values of the electronegativity (EN = 2.0 – 3.0) can acquire both positive and negative oxidation states, depending on their bonding partners.

The p-elements with the lowest electronegativity belong to the 3A-5A groups in the lower periods. They have bonding properties similar to metallic s-elements, such as Al, Ga, In, Tl, Sn, Pb, Sb and Bi. These elements form compounds with positive oxidation states (+III, +IV, +V). Some of them have oxidation states smaller by 2 than their maximum oxidation number, e.g., Tl (+I), Sn and Pb (+II) or Sb and Bi (+III).

Group*	Valence electrons	Valence electron configuration	Typical oxidation states
1 A	1	$n\ s^1$	H **(+I or –I)** Li, Na, K, Rb, Cs, Fr **(+I)**
2 A	2	$n\ s^2$	All 2A elements **(+II)**
3 A	3	$n\ s^2\ n\ p^1$	All 3A elements **(+III)** Tl **(+I)**
4 A	4	$n\ s^2\ n\ p^2$	C **(-IV, - I, + II, +IV)** Si, Ge **(+IV)** Pb, Sn **(+II, +IV)**
5 A	5	$n\ s^2\ n\ p^3$	N, P **(-III, +I, +III, +V)** As **(-III, +III, +V)** Sb, Bi **(+III, +V)**

6 A	6	n s^2 n p^4	O **(-II, -I)** S **(-II, -I, +IV, +VI)** Se, Te (-II, +IV, +VI) Po (+IV, +VI)
7 A	7	n s^2 n p^5	F **(-I)** Cl, Br, I **(-I, +I, +III, +V, +VII)**
8 A	8	n s^2 n p^6	All 8A elements **(0),** rarely **+II**, **+IV**, **+ VI**, **+VIII**

* We use here the traditional numbering of the groups in the periodic table of elements; according to the new numbering scheme the groups are numbered 1-18.

Example 9: *The oxidation states of atoms in binary compounds of s- and p-elements can be most easily defined by knowing the typical oxidation states of at least some elements, while keeping the ratio of the atoms in the compound in mind. The sum of the oxidation states multiplied by the number of atoms in the compound must be 0, if the compound doesn't have a charge.*

$$CaCl_2 \qquad \overset{+II}{Ca}\ \overset{-I}{Cl_2} \qquad 1:2 \qquad \left.\begin{array}{l} Ca: 1 \text{ x } +II = 2 \\ O: 2x\ -I = -2 \end{array}\right\} 2-2 = 0$$

$$Al_2O_3 \qquad \overset{+III}{Al_2}\ \overset{-II}{O_3} \qquad 2:3 \qquad \left.\begin{array}{l} Al: 2 \text{ x } +III = 6 \\ O: 3x\ -II = -6 \end{array}\right\} 6-6 = 0$$

$$SO_3 \qquad S \quad \overset{-II}{O_3} \qquad \begin{array}{c} 1:3 \\ 2:? \end{array} \qquad \left.\begin{array}{l} O: 3x\ -II = -6 \\ S: 1x\ +IV = 6 \end{array}\right\} 6-6 = 0$$

$$!!! \quad NH_3 \qquad \overset{+I}{H_3} \quad N \qquad 1:3 \qquad \left.\begin{array}{l} H: 3 \text{ x } +I = 3 \\ O: 1x\ -III = -3 \end{array}\right\} 3-3 = 0$$

In $CaCl_2$ and Al_2O_3, there should not be any issues when determining the oxidation states. Ca and Al both have a positive oxidation number, which is the same as their group number. Also, Cl and O have their most typical oxidation numbers.
In SO_3, S can have multiple oxidation states (-II, -I, +IV, +VI). It will be the positive part since it has lower electronegativity than oxygen. Oxygen can be -II or -I. -I is related to peroxides$(O_2)_n$. If O is -II then S should be +VI to make up for the three oxygen atoms.
In ammonia (!!!), there is a confusing notation of writing the formula as NH_3 even though H is the positive part. H can only be +I here so N would be -III to compensate for the three H atoms.

3.5 OXIDATION STATES IN OXO-ACIDS AND THEIR SALTS

Oxo-acids are compounds consisting of:

a) several hydrogen atoms acquiring the oxidation state +I
b) one or more central atoms that are usually nonmetallic p-elements and have a positive oxidation number (I – VII)
c) multiple oxygen atoms with the oxidation number -II

The overall formula is: $H_nE_mO_p$ E can be: B, C, Si, N, P, As, S, Se, Cl, Br, I

Example 10: *To determine the central atom's oxidation number, a difference between the sum of the negative oxidation number on O atoms and the sum of positive oxidation* *numbers on H must be determined. If there is more than one central atom, the difference must be divided by the number of central atoms.*

H_2CO_3	*carbonic acid*	*2x H means there are 2x +I = +2* *3x O means there are 3x -II = -6* *6 – 2 = 4* *Oxidation number on C is +IV*
H_2SO_4	*sulfuric acid*	*2x H, so 2x +I = +2* *4x O, so 4x -II = -8* *8 – 2 = 6* *Oxidation number on S is +VI*
HNO_3	*nitric acid*	*1xH, so 1x +I = +1* *3x O, so 3x -II = -6* *6 – 1 = 5* *Oxidation number on N is +V*
$HClO_4$	*perchloric acid*	*1xH, so 1x +I = +1* *4x O, so 4x -II = -8* *8 – 1 = 7* *Oxidation number on Cl is +VII*
$H_2S_2O_7$	*disulfuric acid*	*2xH, so 2x +I = +2* *7xO, so 7x – II = -14* *14-2 = 12* *12 / 2xS = 6* *Oxidation number on both S is +VI*

Example 11: *In salts of oxo-acids, one or more hydrogen atoms are replaced by cations such as* Na^{+1} *or* Ca^{+2}*, but it can also be d-element cations or* NH_4^{+1} *cations. The number of hydrogens replaced equals the oxidation number of the cation atoms.*

$CaCO_3$	*calcium carbonate*	*1x Ca, so +2* *3x O means there are 3x -II = -6* *6 – 2 = 4* *Oxidation number on C is +IV*
$NaHCO_3$	*sodium hydrogencarbonate*	*1x H, so +1* *1x Na, so +1* *3x O means there are 3x -II = -6* *6 – (1+1) = 4* *Oxidation number on C is +IV*

Notice that the oxidation numbers of C in carbonic acids and salts derived from this acid (carbonates and hydrogencarbonates) are the same. This is true for all salts.
The salts of oxo-acids can be split in a cation and an anion. The cation in $CaCO_3$ is Ca^{2+} and the anion is $(CO_3)^{2-}$. This can also be used in determination of oxidation numbers.

K_2SO_4	*potassium sulfate*	*2x K, so 2x +I = +2* *4x O, so 4x -II = -8*

$8 – 2 = 6$
Oxidation number on S is +VI

NH_4NO_3	*ammonium nitrate*	*NH_4 must have the same charge as 1xH, so 1x +I = +1*
		3x O, so 3x -II = -6 *6 – 1 = 5* *Oxidation state on N in nitrate is +V*

NH_4^+ consists of 1x N and 4x H, where H has the lower electronegativity and will have the oxidation number +I. Since the sum of the oxidation numbers must be +1 to equal the charge, the oxidation number on the N can be calculated from the equation: $x + 4 = 1$, where x is the oxidation number of N. $-3 + 4 = 1$, so $x = -3$ and the oxidation number of N in NH_4^+ is -III.

$Mg(ClO_4)_2$	*magnesium perchlorate*	*1xMg, so +2* *8x O, so 8x -II = -16* *16 – 2 = 14* *14 / 2 = 7* *Oxidation number on Cl is +VII*
$Al(BrO_3)_3$	*aluminium bromate*	*1x Al, so +3* *9x O, so 9x -II = -18* *18 – 3 = 15* *15 / 3 = 5* *Oxidation number on Br is +V*

3.6 DETERMINATION OF OXIDATION STATES OF D-ELEMENTS

Most of the d-elements or transition elements can have more than one oxidation number. Since there is no simple key or rule what oxidation states these elements can acquire, learning and memorizing some of them is a good way to quickly determine the compound’s name. However, the oxidation number can be calculated if the oxidation numbers of the s- and p-elements are known.
d-Elements can be present in compounds usually as the cationic part, instead of Na, Ca, K or H. Only a few d-elements can have the role of central atoms in oxo-acid-like compounds. d-Elements never have negative oxidation numbers.

Example 12: *To determine the oxidation number of d-elements in binary compounds, the oxidation numbers or charges of the anionic part must be known.*

$FeCl_2$	*this is a chloride, where Cl has oxidation number -I* *2x – I = -2 so Fe must be +2 to compensate* *Fe has oxidation state +II*
Ni_2O_3	*this is an oxide, where O has oxidation number -II* *3x -II = -6, so 2x Ni must have +6, so 1x Ni has +3* *Ni has oxidation state +III*
$Cu(OH)_2$	*this is a hydroxide, where OH is an anion with the charge -1 (+I on H and -II on O)*

2x -1 = -2, so Cu must be +2
Cu has oxidation number +II

Ag_2S — *this is a sulfide, where S has oxidation number -II*
1x -II = -2, so 2x Ag must have +2, so 1x Ag has +1
Ag has oxidation number +I

$Zn(CN)_2$ — *this is a cyanide, where the anion CN^- has the charge -1 (+II on C and -III on N)*
2x -1 = -2, so Zn must be +2
Zn has oxidation number +II

***Example 13**: To determine the oxidation number of d-elements in oxo-acids, the oxidation numbers or charges of the anionic part must be known. The best way to tell the charge of the anion is to know how many H atoms have been replaced.*

$CuSO_4$ — *is a salt of H_2SO_4, so 2x H have been replaced, this means that the sulfate anion has the charge of -2: SO_4^{-2}*
To compensate for the negative charge, Cu must be +2
Cu has the oxidation number +II

$CoCO_3$ — *is a salt of H_2CO_3, so 2x H have been replaced, this means that the carbonate anion has the charge -2: CO_3^{-2}*
To compensate for the negative charge, Co must be +2
Co has the oxidation number +II

$Fe(NO_3)_3$ — *is a salt of HNO_3, so the nitrate anion can lose 1x H, this means that the nitrate anion has the charge -1: NO_3^{-1}*
but since there are 3x nitrate anions, the total negative charge is -3
To compensate for the negative charge, Fe must be +3
Fe has the oxidation number +III

$Ti(ClO_4)_4$ — *is the salt of $HClO_4$, so the perchlorate anion can lose 1x H, this means the perchlorate has the charge -1: ClO_4^{-1}*
But since there are 4x perchlorate anions, the total negative charge is -4
To compensate for the negative charge, Ti must be +4
Ti has the oxidation number +IV

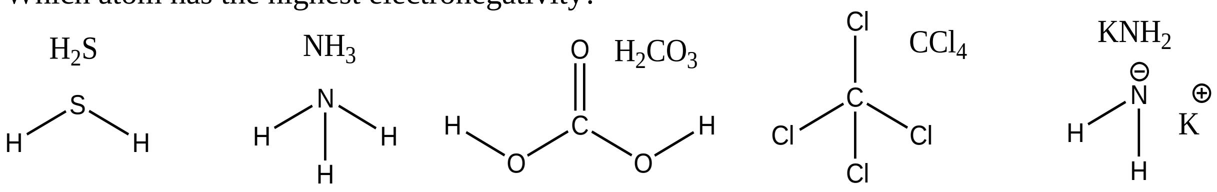
***Example 15:** Some d-elements can be in compounds in the role of central atoms of oxo-acid salts, such as chromate, permanganate, or vanadate. To calculate the oxidation number of the central atom in these compounds, the system identical to that applied to salts of p-element oxo-acids is used.*

K_2CrO_4	*potassium chromate*	*2x K, so +2* *4x O, so 4x -II = -8* *8 – 2 = 6* *Oxidation number of Cr is +VI*
$NaMnO_4$	*sodium permanganate*	*1x Na, so +1* *4x O, so 4x -II = -8* *8 – 1 = 7* *Oxidation number of Mn is +VII*

NH_4VO_3	*ammonium vanadate*	*1x $(NH_4)^{+1}$, so +1* *3x O, so 3x -II = -6* *6 – 1 = 5* *Oxidation number of V is +V*

3.7 Problems

1. For the following compounds, decide how their bonding electrons will be distributed. Which atom has the highest electronegativity?



2. Write the electron configuration (in full and short version) of the following atoms and ions:
a) $_{20}Ca$, $_{14}Si$, $_{9}F$, $_{33}As$, $_{16}S$, $_{37}Rb$, $_{15}P$, $_{13}Al$, $_{8}O$, $_{11}Na$
b) $_{20}Ca(+2)$, $_{14}Si(+4)$, $_{9}F(-1)$, $_{33}As(+3)$, $_{16}S(-2)$, $_{16}S(+6)$, $_{37}Rb(+1)$, $_{15}P(+5)$, $_{15}P(-3)$, $_{13}Al(+3)$, $_{8}O(-2)$, $_{11}Na(+1)$

3. Determine the oxidation states in the following binary compounds of s- and p-elements: NaCl, MgF_2, CaO, $Ca(O_2)$, H_2S, PH_3, KOH, $AlBr_3$, CsH, NO_2, NO, N_2O_5, BI_3, P_2S_5, SO_2, CO, CO_2, Ca_2C, $NaNH_2$, MgS, SiH_4, BH_3, PCl_3, TlCl, SbO_2, KCN, HCN, NH_4Cl

4. Determine the oxidation states of the central atoms in the following oxo-acids and their salts:
a) H_2CO_3, HNO_3, HNO_2, H_3PO_4, H_3PO_3, H_2SO_4, H_2SO_3, HIO_4, $HClO_4$, $HBrO_3$, $HClO_3$, $HClO_2$, HIO, $H_2S_2O_7$
b) $CaCO_3$, $NaHCO_3$, $Al(NO_3)_3$, KH_2PO_4, Na_2SO_4, Li_2SO_3, $Mg(ClO_3)_2$, $LiIO_2$, $Ca(ClO)_2$

5. Determine the oxidation states of the d-elements in the following compounds:
a) $CuCl_2$, $FeBr_2$, MnO_2, ZnO, NiS, $Co(OH)_2$, AgCN, $TiCl_4$, Fe_2O_3, $PdCl_2$, CuI
b) $Ni(NO_3)_2$, $CuSO_4$, $HgCO_3$, $Au(ClO_4)_3$, $Cd(BrO_3)_2$, $ZnSO_3$, $KMnO_4$, Na_2CrO_4

4 Chemical nomenclature

The universally understandable naming of chemical compounds is a key tool for communication in the chemical and pharmaceutical sciences, as well as for computer-based searching in scientific databases. Generally, there are two types of names: *systematic* names and *common* names. Common (or trivial) names often date back to the beginnings of chemistry as a science and are given to some common and wide-spread chemicals. They are traditional names based on historical discovery, properties, or chemical behaviour. They have little connection to the structure of the compounds but are simple and easy to remember. Systematic names, on the other hand, can be derived directly from the structure of the compound applying a set of rules. The large number of existing chemicals (currently millions) makes it impractical to assign a common name to every substance, hence the knowledge of systematic nomenclature is inevitable.

Today's naming system is based on the recommendations of the International Union of Pure and Applied Chemistry (IUPAC), an international organization dedicated in particular to the development of chemical nomenclature and terminology. IUPAC publishes regularly updated sets of rules, allowing to derive the chemical name of any compound from its structural formula, and *vice versa*, to construct a formula from the chemical name of a compound. These rules are referred to as the IUPAC nomenclature.

To correctly name an inorganic compound, the knowledge of the names and symbols of all chemical *elements* is a necessary requirement. The symbols of the elements consist of one or two letters (either one capital letter or one capital letter followed by a lower-case letter). For example, calcium is always Ca, never CA, ca, or cA. The symbols are not always derived from the English names of the elements but are sometimes of different origin (mainly from their Latin names). For example, the element potassium is denoted as K, from the Latin name of the element, *kalium*. Similarly, the element antimony has the symbol Sb (again, from the Latin name *stibium*). Thus, it is necessary to memorize them. The symbols of the elements are listed in Table 1 in the Appendix at the end of this booklet, together with their English, Latin, and Slovak names.

Two or several elements combine with each other to form *compounds*. Compounds are represented by formulas. The symbols of the combined elements are written without any space between them in a chemical formula. The formula provides the information not only on the elements that have been chemically combined to form the compound but also on the fixed proportion in which the chemical combination occurs (the *stoichiometry*). For example, in the molecule of ammonia (NH_3) the elements nitrogen and hydrogen combine at the ratio 1:3.

To write a proper formula for a compound, or to form a chemical name from a formula, it is very important to assign the correct *oxidation number* to each atom in the molecule, as described in detail in the previous chapter. To do this, the knowledge of the most common oxidation numbers for certain groups of elements is useful. Elements with high electronegativity tend to acquire additional electrons and form *anions* (or appear in negative oxidation numbers). For example, halogens often form negatively charged ions (F^-, Cl^-, Br^-, I^-). Elements with low electronegativity (i.e., electropositive elements) tend to lose electrons and provide positively charged *cations*. These are especially the elements of the IA and IIA groups. It is also good to remember that the maximum possible oxidation number of an element equals the number of the group in the periodic table. Therefore, the oxidation number of sodium or potassium (both Group IA) is +I (+1) while the oxidation number of calcium (Group IIA) is +II (+2). The highest oxidation number of carbon is thus +IV (+4). Some elements, especially from the d-block of the periodic table (transition metals), appear in several stable oxidation states.

Examples of typical oxidation numbers for some common chemical elements are given below.

Element	Typical oxidation number	Remark
Li, Na, K	+I	Forms only cations Li^+, Na^+, K^+
Mg, Ca, Ba	+II	Forms only cations Mg^{2+}, Ca^{2+}, Ba^{2+}
B, Al	+III	
C, Si	+IV	
F, Cl, Br, I	-I	Typically form anions F^-, Cl^-, Br^-, I^-
O	-II	
S	-II, +IV, +VI	
N, P	-III, +III, +V	
Cu, Hg	+II, +I	
Zn	+II	
Ag	+I	
Fe	+II, +III	

To write a formula or chemical name of a substance, it is necessary to distinguish between ionic and covalent (molecular) compounds. Although there is no sharp dividing line between ionic and molecular bonds and thus between ionic and molecular compounds, for purposes of nomenclature we use the simple generalization that metal and nonmetal combinations are ionic, and combinations of nonmetals are molecular. Especially compounds containing electropositive metals (like Na, K, Mg, Ca) are usually ionic. Sometimes, a molecule contains both ionic and covalent bonds. An example is $CaSO_4$, having an ionic bond between the cation (Ca^{2+}) and anion (SO_4^{2-}), but also covalent bonds (S-O bonds within the anion SO_4^{2-}). Even cations can be sometimes composed of several atoms, like in NH_4^+.

Cations are named exactly the same way as the metals from which they are derived, for instance:

hydrogen	H^+	magnesium	Mg^{2+}
potassium	K^+	calcium	Ca^{2+}
lithium	Li^+	barium	Ba^{2+}
sodium	Na^+	aluminium	Al^{3+}

Simple monoatomic anions are named by using the root name of the chemical element and adding to the root the suffix *-ide*, as shown below.

Element	Anion	Anion name
Fluorine	F^-	fluor*ide*
Chlorine	Cl^-	chlor*ide*
Bromine	Br^-	brom*ide*
Iodine	I^-	iod*ide*

Oxygen	O^{2-}	ox*ide*
	$(O_2)^{2-}$	perox*ide*
	$(O_2)^{-}$	hyperoxide (superoxide
Nitrogen	N^{3-}	nitr*ide*
	N_3^{-}	azide
Sulfur	S^{2-}	sulf*ide*
phosphorus	P^{3-}	phosph*ide*
Carbon	C^{4-}	carb*ide*
hydrogen	H^{-}	hydr*ide*

Compounds containing S can be written in two ways: either as sul*ph*ur, sul*ph*uric, sul*ph*ide etc., or as sul*f*ur, sul*f*uric, sul*f*ide, etc. The use of the latter form (with *f*) is recommended.

If the metal can occur in several stable oxidation states, its charge or oxidation number must be indicated in parentheses following the name of the element. The oxidation number is often given instead of the charge of an ion. This is because ions with high charges (higher than 2+ or 3+) are generally unstable and the bonds are in fact covalent, not ionic. For example, the compound CrO_3 is not ionic and does not contain any Cr^{6+} cations. Instead, it is a covalent compound containing chromium with the oxidation number +VI (denoted as Cr^{+VI}).

Fe^{2+}	iron(II)	Cu^{+}	copper(I)
Fe^{3+}	iron (III)	Cu^{2+}	copper(II)
Mn^{+VII}	manganese(VII)	Cr^{+VI}	chromium(VI)

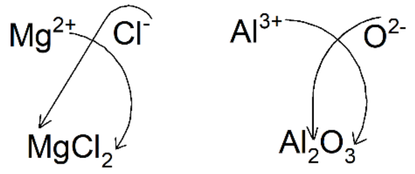
The simplest molecules are formed by only a single element. In this case, the chemical name is formed by combining the element's name with the appropriate multiplicative prefix indicating how many atoms of the same element are present. The examples are O_2 (dioxygen), N_2 (dinitrogen), S_8 (octasulfur), or P_4 (tetraphosphorus). It is necessary to learn at least the most common prefixes since they are used throughout the whole chemical nomenclature. The prefix mono- is generally omitted unless it is unavoidable.

1	(mono)	6	hexa
2	di	7	hepta
3	tri	8	octa
4	tetra	9	nona
5	penta	10	deka

4.1 BINARY COMPOUNDS

The simplest compounds are binary compounds, consisting of only two elements. We distinguish two main categories of binary compounds: binary compounds composed of a metal and a non–metal (e.g., NaCl, Mg_3P_2, Al_2O_3), and binary compounds consisting of two non-metals (e.g., CO_2, CCl_4, NH_3). The naming systems for each category are slightly different.

To write a formula of a chemical compound, the sum of the charges (oxidation numbers) of all participating atoms must equal to 0 (if it is an electroneutral molecule), or to the overall (net) charge in the case of a composite ion. The number of cations and anions in a compound can be established by a simple *crisscross method*. In this method, the numerical value of each of the ion charges is crossed over to become the subscript of the other ion, as shown below. Signs of the charges are dropped.



When a binary compound consists of a **metal** and a **non–metal**, the metal is always the less electronegative of the two elements. The name of the metal (cation) comes first, followed by the name of the non-metal (anion), like in *sodium chloride*. The name of the cation is the same as the name of the element, the name of the nonmetal anion is obtained by taking the root of the name and adding an *-ide* ending.

We can subdivide binary compounds into those having a metal with one possible oxidation state (NaCl), and those whose metallic element may exhibit varying oxidation states, such as iron or copper. If there is only one possible oxidation state for the metal, the name of the cation is simply the name of the element, for example:

Compound	Name	Cation	Anion
NaCl	sodium chloride	Na^+	Cl^-
LiH	lithium hydride	Li^+	H^-
Mg_3N_2	magnesium nitride	Mg^{2+}	N^{3-}
Ag_2O	silver oxide	Ag^+	O^{2-}

Some metals, especially the transition metals, may exhibit varying oxidation states. When the metallic element in question can exhibit more than one oxidation state, the name must specify the oxidation state. The naming is the same, the only difference is that here we include Roman numerals (in brackets) to indicate the oxidation state of the metal cation, e.g.:

CuBr	copper(I) bromide	HgO	mercury(II) oxide
FeS	iron(II) sulfide	Cu_2O	copper(I) oxide
CuO	copper(II) oxide	Co_3P_2	cobalt(II) phosphide
FeP	iron(III) phosphide	$SnCl_4$	tin(IV) chloride

According to an older naming convention that can still be found in the literature, metals with variable oxidation numbers are distinguished by assigning endings *-ic* or *-ous* to the Latin root of the metal name. When only two common oxidation numbers are possible, the lower oxidation number is indicated by the *-ous* suffix, the higher oxidation number by the *–ic* suffix, as shown below.

Metal	Name	Example	Name of the compound
iron(II)	ferrous	$FeBr_2$	ferrous bromide
iron(III)	ferric	$FeCl_3$	ferric chloride
copper(I)	cuprous	CuI	cuprous iodide
copper(II)	cupric	$CuCl_2$	cupric chloride
mercury(I)	mercurous	Hg_2O	mercurous oxide
mercury(II)	mercuric	HgO	mercuric oxide

Example 1: *Determine the chemical name for* ***K_2S****.*

The compound is a binary ionic compound, containing an element with high electronegativity (sulfur) and an electropositive metal (potassium). The cation is K^+ (potassium is in the group IA of the periodic table and has only one oxidation state, +I). Hence, we do not need to indicate the oxidation number (charge) of the cation. To compensate for the two K^+ cations, the sulfur carries the charge 2- (the anion is S^{2-}). We put first the name of the cation (the same as the name of the element, potassium), followed by the name of the anion (sulfide): ***potassium sulfide****.*

Example 2: *Determine the chemical name for* ***MnF_2****.*

The compound is a binary compound, composed of a highly electronegative element (fluorine) and a transition metal (manganese). The only oxidation state of fluorine in its compounds is -I, thus the anion is F^-. For the compound to be electrically neutral, the manganese cation must have the charge 2+. Since manganese as a transition metal can appear in several common oxidation states, its oxidation number must be indicated in its name. Thus, the name of the compound is ***manganese(II) fluoride****.*

Example 3: *Determine the formula for the compound named* ***iron(III) oxide****.*

Write the symbol and charge of the cation (metal) first and the anion (nonmetal) second, i.e., $Fe^{3+}O^{2-}$. The charges on the cation and on the anion differ, hence we need to adjust the number of the cations and the anions for the compound to be electroneutral (to have no net electric charge). We can do this using the simple crisscross method, obtaining the final formula ***Fe_2O_3****. Here the overall (net) charge of the cations ($Fe^{3+}{}_2$) is +6 while the net charge of the anions ($O^{2-}{}_3$) is -6, yielding an electrically neutral compound.*

Ionic compounds exist which contain several different cations or anions. They are named simply by putting the names of the ions in alphabetical order, as in the following examples:

$KAl(SO_4)_2$	aluminium potassium sulfate
NH_4MgCl_3	ammonium magnesium trichloride
$KMgCl(SO_4)$	magnesium potassium chloride sulfate
$Na_6ClF(SO_4)_2$	hexasodium chloride fluoride bis(sulfate)

Different type of nomenclature is used in the case of binary compounds consisting of **two non-metals**, where one non-metal is the more electropositive part (positive oxidation number) and the other one the more electronegative (negative oxidation number), like in HCl or CO_2. These are generally non-ionic, containing only covalent bonds. When naming these compounds, we indicate the number of the more electronegative elements by number prefixes (mono-, di-, tri-, tetra-, etc.). The name of the electropositive part is given in the same way as previously described (the name of the element). If there are several electropositive atoms, their number must be indicated as well. Unlike with metal-containing binary compounds, we do not put the oxidation number in the brackets. Examples include:

CO	carbon *mono*xide	PCl_3	phosphorus *tri*chloride
CO_2	carbon *di*oxide	PCl_5	phosphorus *penta*chloride
SO_2	sulfur *di*oxide	CS_2	carbon *di*sulfide
SO_3	sulfur *tri*oxide	SF_6	sulfur *hexa*fluoride
N_2O_5	*di*nitrogen *pent*oxide	As_2O_3	*di*arsenic *tri*oxide

Example 4: *Write the chemical name of* $\boldsymbol{B_2O_3}$.

The compound is an oxide of boron, containing oxide anions (O^{2-}). There are two boron atoms and three oxygen atoms. We use the numerical prefixes to indicate their number: ***diboron trioxide****.*

4.2 Binary compounds containing hydrogen

Specific type of binary compounds are the compounds of hydrogen with other elements, generally called **hydrides**. From the point of view of chemical nomenclature, they can be divided into three groups.

- Compounds containing hydrogen and an electropositive metal (metallic hydrides, mainly with groups IA and IIA of the periodic table). These contain hydrogen as an anion, (H^-). They are given names like common ionic binary compounds, adding the name *hydride* to the name of the metal cation, for instance:

NaH	sodium hydride
CaH_2	calcium hydride
LiH	lithium hydride

- Compounds containing hydrogen and a non-metal. These compounds are non-ionic, containing covalent bonds to hydrogen. They are named by appending the ending -*ane* to the root of the element's name.

H_2S	sulf*ane*
SiH_4	sil*ane*
PH_3	phosph*ane*

Some of these compounds have common names: H_2O (water), NH_3 (ammonia), CH_4 (methane), HN_3 (hydrogen azide or azoimide), N_2H_4 (hydrazine).

- Hydrides of halogens and some other elements are named in a different way. First comes the word *hydrogen* followed by the name of the more electronegative part.

HCl	hydrogen chloride	HI	hydrogen iodide

HF	hydrogen fluoride	H_2S	hydrogen sulfide

These substances are all gases. When dissolved in water, each of these substances forms an acidic solution.

HF	hydrofluoric acid	HBr	hydrobromic acid
HCl	hydrochloric acid	H_2S	hydrosulfuric acid

Hydrides of electronegative elements (e.g., HCl, H_2S) have acidic properties and dissociate into H^+ and the anion. The anions have the standard ending *-ide*. If more than one hydrogen is present (polyprotic acids), it is possible to remove only part of them, like in HS^- (hydrogensulfide). Some anions derived from these hydrides have common names:

hydride	anion	name
H_2O	OH^-	hydroxide
NH_3	NH_2^-	amide
	NH^{2-}	imide
HCN	CN^-	cyanide

Addition of H^+ to some covalent hydrides leads to cations: NH_4^+ (ammonium cation), H_3O^+(oxonium/hydronium), H_3S^+ (sulfonium), PH_4^+ (phosphonium).

Example 5: *Name the compounds a)* ***MgH_2****, b)* ***AsH_3****.*

a) *MgH_2 contains magnesium, a highly electropositive (low electronegativity) element from the group IIA (2), forming only Mg^{2+} cations. Thus, the hydride is of the ionic type and is named using the name of the cation (the same as the name of the element), followed by the name of the anion (hydride):* **magnesium hydride**.
b) *This hydride contains an element from the group VA (15); hence it is not ionic. It is named combining the root of the (Latin) name of the element (***ars***enic) with the ending -ane:* ***arsane****.*

4.3 NOMENCLATURE OF ACIDS AND BASES

An important category of compounds are the **hydroxides**, containing the OH^- ion. These compounds are bases, especially hydroxides of the groups IA and IIA of the periodic table.

NaOH	sodium hydroxide	$Ca(OH)_2$	calcium hydroxide
KOH	potassium hydroxide	$Ba(OH)_2$	barium hydroxide
$Al(OH)_3$	aluminium hydroxide	$Zn(OH)_2$	zinc hydroxide

Oxoacids (oxygen-containing acids) consist of three elements: hydrogen, a non-metal, and oxygen. They dissociate in water solution to form H^+ and an anion of the oxoacid. They are named using the stem name of the non-metal element and the appropriate ending. If there are only two common forms of the acid, suffixes *-ous* and *-ic* are used to denote different oxidation numbers of the non-metal. The *-ous* ending is used if the element is in its lower oxidation state, the *-ic* ending if the element is in its higher oxidation state.

HNO_3	nitr*ic* acid	H_2SO_4	sulfur*ic* acid
HNO_2	nitr*ous* acid	H_2SO_3	sulfur*ous* acid
H_3PO_4	phosphor*ic* acid	H_3PO_3	phosphor*ous* acid

The anions derived from oxoacids (the *oxoanions*) have the ending *-ate* or *-ite* attached to the stem of the acid's name. Some elements form several oxoanions that differ in the number of oxygen atoms. The name of the anion with more oxygen atoms ends in *-ate*, and the anion with fewer oxygen atoms ends in -ite. It is advisable to learn the names of common oxoanions by heart.

NO_3^-	nitrate	PO_4^{3-}	phosphate
NO_2^-	nitrite	CO_3^{2-}	carbonate
SO_4^{2-}	sulfate	SiO_3^{2-}	silicate
SO_3^{2-}	sulfite	BO_3^{3-}	borate

If more than two common oxidation states of the element exist, the anion with the greatest number of oxygen atoms (with the central atom in its highest oxidation state) is given the prefix *per*- and the suffix *-ate*, the anion with the least number of oxygens (lowest oxidation number of the central atom) is given the prefix *-hypo* and the suffix *-ite*, e.g., ClO_4^- (perchlorate) and ClO^- (hypochlorite). Another example is the permanganate anion MnO_4^-, e.g., in potassium permanganate $KMnO_4$. Here the central atom of manganese attains its highest possible oxidation number VII (+7).

The names of ionic compounds (salts) containing oxo anions consist of the cation followed by the anion.

$CaCO_3$	calcium carbonate	$Al_2(SO_4)_3$	aluminium sulfate
K_3PO_4	potassium phosphate	$Fe(NO_3)_3$	iron(III) nitrate
Na_3BO_3	sodium borate		

Example 6: *Write the chemical name of the compound* ***K_3PO_4****.*

The compound is an ionic salt containing three cations K^+ and the anion of an oxoacid (phosphoric acid, H_3PO_4). To name the compound, we put the name of the cation (potassium) first, followed by the name of the anion (phosphate): ***potassium phosphate****.*

Example 7: *Determine the formula for* **aluminium nitrate***.*

The compound is an ionic salt with aluminium cation and the anion of an oxoacid of nitrogen (nitric acid, HNO_3). Nitrate ion has a single negative charge; the only common oxidation number of aluminium in its compounds is +III. Hence, we need three nitrate anions NO_3^- to compensate for the positive charge of the aluminium cation Al^{3+}, and the resulting formula is ***$Al(NO_3)_3$****.*

In the case of polyprotic oxoacids (several dissociable hydrogen atoms) we can have *acidic salts*, such as:

$NaHSO_4$	sodium hydrogensulfate
KH_2PO_4	potassium dihydrogenphosphate

The oxygen atoms (as =O or -OH groups) in the oxoacids can be replaced by other atoms. If this is the case, the substitution is indicated by prefixes before the name of the original acid:

- *Peroxoacids* – a hydroxy group is replaced by the *peroxo* group – O – O –
  H_2SO_4 sulfuric acid → H_2SO_5 *peroxo*sulfuric acid
  HNO_3 nitric acid → HNO_4 *peroxo*nitric acid

- *Thioacids* – the oxygen atom is replaced by a sulfur atom, and we use the prefix *thio*–
  H_2SO_4 sulfuric acid → $H_2S_2O_3$ *thio*sulfuric acid
  H_2CO_3 carbonic acid → H_2CS_3 *trithio*carbonic acid

- *Halogenoacids* – replacement of an oxygen by a halogen atom
  H_2SO_4 sulfuric acid → HSO_3Cl chlorosulfuric acid
  In some cases, they can also be named in a different way:
  $COCl_2$ carbonyl dichloride (common name *phosgene*)
  SO_2Cl_2 sulfuryl dichloride (dichlorosulfuric acid)

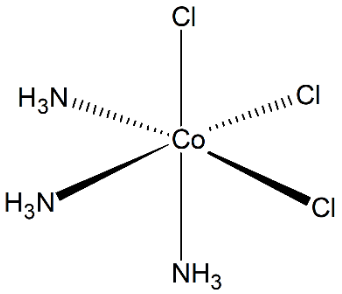
- Derivatives can be formed by the replacement of oxygen by a nitrogen-containing group, such as:
  $–NH_2$ amido group
  $=NH$ imido group
  $=N–$ nitrido group
  e.g.: HSO_3NH_2 amidosulfuric acid

Special type of compounds are the *hydrates*. They are solid substances with a number of bound water molecules at a specific ratio. The bound water molecules are called *water of hydration* or *water of crystallization*. To name these compounds, we use first the name of the salt, followed by the word hydrate. We must also indicate the number of water molecules present, e.g.:

Salt (anhydrous)	Number of H_2O	Formula hydrate	Name
$CuSO_4$	5	$CuSO_4 \cdot 5H_2O$	copper(II) sulfate *penta*hydrate
$NiSO_4$	6	$NiSO_4 \cdot 6H_2O$	nickel(II) sulfate *hexa*hydrate
$MnCl_2$	4	$MnCl_2 \cdot 4H_2O$	manganese(II) chloride *tetra*hydrate

4.4 Coordination compounds

Coordination compounds or metal complexes might be defined as compounds in which the so-called *central atom* or ion is attached to a group of ions or molecules (*ligands*) via donor–acceptor bonds, as shown in the following figure. The depicted complex contains a central metal ion of cobalt (Co^{3+}) and two types of ligands: the anionic ligand Cl^- and the neutral ammonia. The charges of the central atoms and ligands are normally not shown in the formulas of metal complexes.



This type of compounds is characterized by coordination number (total number of bonds formed between the central atom and the ligands) and coordination geometry (stereochemical arrangement of ligands). The above complex has the coordination number of the central cobalt atom 6, the coordination geometry of the complex is octahedral. A true coordination compound must have its coordination number higher than the oxidation number of the central atom.

The formulas of coordination compounds are often written in abbreviated form. The formula for the complex unit is by convention enclosed in square brackets, like in the above complex: $[CoCl_3(NH_3)_3]$. We distinguish between complex cation, complex anion, and neutral complex unit.

If the coordination unit is positively charged (complex cation), the whole complex must contain also negatively charged ions, so-called counterions, which are not connected directly to the central atom and whose function is only to compensate for the charge of the coordination unit, e.g., $[Cu(NH_3)_4]Cl_2$. In this complex, the coordination unit is endowed with twofold positive charge: $[Cu(NH_3)_4]^{2+}$. The electroneutrality is attained by two negatively charged counterions Cl^-.

The charge of negatively charged coordination units (complex anions) is neutralized by positively charged counterions, like in $K[HgI_3]$. Here, the negative charge of $[HgI_3]^-$ is counter-balanced by a K^+ cation.

In a neutral complex unit, the positive charge of the central metal atom (cation) is exactly counter-balanced by the negative charges of the ligands, as in the complex $[PtCl_2(NH_3)_2]$, with the central platinum(II) cation (Pt^{2+}), two Cl^- anionic ligands, and two neutral NH_3 ligands. In this case, there are no counterions.

The names of the ligands in coordination chemistry often differ from their normal chemical names as separate compounds. Negatively charged ligands generally have the ending *-o*, whereas neutral ligands have various other endings. Some examples of common ligands are given below.

Ionic ligands		Neutral ligands	
Cl^-	*chlorido*	NH_3	*ammine*
I^-	*iodido*	H_2O	*aqua*
F^-	*fluorido*	NO	*nitrosyl*
OH^-	*hydroxido*	CO	*carbonyl*
N_3^-	*azido*	C_5H_5N	*pyridine*
NO_3^-	*nitrato*	PH_3	*phosphine*
SCN^-	*thiocyanato*	PPh_3	*triphenylphosphine*
$(COO)_2^{2-}$	*oxalato*	2,2’-bipyridine	*2,2’-bipyridine*
CH_3COO^-	*acetato*	ethane-1,2-diamine	*ethylenediamine*
CN^-	*cyanido*	1,10-phenanthroline	*1,10-phenanthroline*

When naming a complex, whether it is cationic, anionic, or neutral, first the ligands are listed in alphabetical order, regardless of charge, then the central metal is mentioned followed by a Roman numeral in parentheses giving its oxidation state. The number of the ligands of the same type must be indicated. If the complex is an anion, the suffix –ate is attached to the (Latin) name of central atom.

Negatively charged metal	Name of the complex anion
cobalt	cobaltate
aluminium	aluminate
copper	cuprate
iron	ferrate
chromium	chromate

If several oxidation states of the central metal atom are possible, this suffix can be followed by the oxidation number (in parentheses) for better understanding.

The following are some examples of naming the metal complexes:

$[Cu(H_2O)_4]NO_3$	tetraaquacopper(II) nitrate	
$[Cu(NH_3)_4]SO_4 \cdot H_2O$	tetraamminecopper(II) sulfate monohydrate	
$[Pt(NH_3)_6]Cl_4$	hexaammineplatinum(IV) chloride	
$[Co(NH_3)_6]^{3+}$	hexaammine cobalt(III) cation	
$[Cr(NH_3)_2(H_2O)_2Cl_2]Cl$	diamminediaquadichloridochromium(III) chloride	
$[PtCl_6]^{2-}$	hexachloridoplatinate(IV) anion	
$Fe(CN)_6]^{4-}$	hexacyanidoferrate(II) anion	
$K_3[Fe(CN)_6]$	potassium hexacyanidoferrate(III)	
$K_2[Cr(NH_3)(CN)_5]$	potassium pentacyanidoamminechromate(III)	
$K_2[PtCl_6]$	potassium hexachloridoplatinate(II)	
$[Co(NH_3)_3Cl_3]$	triamminetrichloridocobalt(III)	
$[Ir(NH_3)_3(NO_2)_3]$	triamminetrinitritoiridium(III)	
$[B(NH_3)F_3]$	amminetrifluoroboron(III)	
$[Ni(CO)_4]$	tetracarbonylnickel	*oxid. Number Ni(0)*
$[Co_2(CO)_8]$	octacarbonyldicobalt	*oxid. Number Co(0)*

Example 8: *Write the chemical name of* ***[Co(H₂O)(NH₃)₅]Cl₂****.*

This is a metal complex with a cationic coordination unit, $[Co(H_2O)(NH_3)_5]^{2+}$. It contains six ligands: five molecules of ammonia (named ***ammine****) and a molecule of water (named* ***aqua****). First, we name the ligands in alphabetical order (without spaces), followed by the name of the central metal atom (****cobalt****). We indicate the oxidation number of the central atom in brackets. Since both ligands are electroneutral, and we have two counterions (Cl^-), the oxidation number of cobalt must be* ***II****. Finally, we add the name of the simple anion (the counterion),* ***chloride****. The complete name is* ***pentaammineaquacobalt (II) chloride****.*

Example 9: *Write the chemical name of* ***$[PtCl_2(NH_3)_2]$****.*

The coordination compound is electroneutral, with the charge of the ligands fully compensating for the charge of the central atom, so there are no counterions. We name the ligands in alphabetical order, along with their number. Finally, we specify the name of the metal atom and its oxidation number: ***diamminedichloridoplatinum(II)****.*

Example 10: *Determine the formula of* ***pentaammineiodidocobalt (III) sulfate****.*

The compound consists of a positively charged coordination unit and negatively charged sulfate counterions. We put the coordination unit first, followed by the sulfate anions. There are two types of ligands within the coordination unit: five molecules of ammonia (the ammine ligands) and one iodide anion (the iodido ligand). Inside the square brackets, we write first the symbol of the central atom and then the formulas of the ligands in alphabetical order: ***$[Co(NH_3)_5I]SO_4$****.*

4.5 Problems

Give the names for the following elements:
H, O, N, S, Si, Se, B, Be, Br, Po, P, F, Ac, Ar, As, Sb, Sr, He, Ne, Ni, Ag, Au, C, Cu, Zr, Zn, Sn,Tl, Pb, Bi, Rn, Ra, Rb, Mn, Mo, Mg, Ce, Cs, Co, Cr, La, Li, Xe, Kr, Fr, Os, I.

Give the names for the following compounds:
K_2O, H_2O_2, BaO, $Ba(OH)_2$, CaO, $CaCl_2$, FeS_2, CuCl, $CuCl_2$, MnO, MnO_2, Al_2O_3, BeO, B_2O_3, CrO_3, H_2SeO_4, $NaHCO_3$, $NaNO_3$, $KMnO_4$, K_2MnO_4, $PtCl_4$, $ZnSO_3$, H_3PO_4, H_2S_2, H_2SO_5, $BaCS_3$, $HgCl_2$, Cu_2O, CuO, $KHSO_4$, Li_3PO_4, $PbCrO_4$, H_4SiO_4, $LiNO_2$, $K_2Cr_2O_7$.

Give the symbols for the following elements:
Magnesium, manganese, gold, iodine, indium, iridium, iron, chromium, calcium, boron, neon, fluorine, palladium, silicium, silver, gold, antimony, sodium, scandium, polonium, potassium, copper, cadmium, lanthanum, arsenium, titanium, mercury, lead, aluminium.

Give the formula for the following compounds:
boric acid, trihydrogen boric acid, sulfuric acid, nitric acid, nitrous acid, sodium hydroxide, hydrogen peroxide, peroxosulfuric acid, trithiocarbonic acid, sodium peroxide, calcium carbonate, iron(II) disulfide, potassium iodide, barium nitrate, strontium nitrite, beryllium chloride, lithium hydrogen carbonate, lead(II) tetrasulfide.

State the name, coordination number and oxidation state of the central atom in the following coordination compounds:
$[Cu(H_2O)_4]SO_4 \cdot H_2O$, $[Co(NH_3)_6]Cl_3$, $K_2[PtCl_6]$, $K_4[Fe(CN)_6]$, $[Cd(CN)]^+$, $[Cd(CN)_3]^-$, $[Fe(CO)_5]$, $[PtCl_4]^{2-}$, $[AlF_6]^{3-}$, $[Co(H_2O)_3(NH_3)_3]Cl_3$, $[Cu(NH_3)_4]^{2+}$, $[Cr(H_2O)_6]Cl_3$,

$Na_2[Sn(OH)_4]$, $K_2[OsCl_5N]$, $[Ag(H_2O)_2]^+$, $[Cu(CN)_4]^{3-}$, $[Pt(NH_3)_4][PtCl_4]$, $[Fe(CN)_6]^{3-}$, $[Pt(NH_3)_4Cl_2]Br_2$, $[Co(NH_3)_4Cl_2]NO_2$, $[Co(NH_3)_4Cl(NO_2)]Cl$, $[Co(NH_3)_6][Cr(CN)_6]$.

Write the chemical formula for the following metal complexes:
Tetraamminepalladium(II) chloride
Tetraamminediaquacopper(II) sulfate
Hexaaquacopper(II) cation
Potassium diaquatetrahydroxidoaluminate

5 SOLUTIONS

Solutions are homogeneous mixtures of two or more substances. In order for the mixture to be truly homogeneous, the particles of the intermixed substances must be ionic or molecular in size.
The substance dissolved is called the *solute*. The substance doing the dissolving is the *solvent*. In general, the solute is the component that is present in lesser amount in solution. So, in a NaCl solution in water, NaCl is the solute and water is the solvent.
solute + solvent = solution

The most common solutions are those in which the solvent, or dissolving medium, is a liquid. Solutes, which are the substances dissolved, may be either gases, liquids, or solids. In all homogeneous mixtures

a) the composition of solution is variable;
b) the solute and the solvent may be separated by physical means without any chemical change;
c) the solute particles must be uniformly distributed among the solvent particles;
d) the solute particles will not settle down;
e) the solution has the same chemical and physical properties in its entire volume.

Miscible liquids dissolve in each other in all proportions.
Immiscible liquids are completely insoluble in one another regardless of the proportions involved.

The maximum amount of solute which can be dissolved in some given amount of solvent at a given temperature is called **solubility.**
(The experimentally found values at various temperatures are gathered in chemical data table books or on-line.)

A solution in which no more solute can dissolve at a given temperature is called **saturated solution.**

Solubility <u>depends on temperature.</u> It is defined as the amount of solute dissolved in a specific amount of solvent at a specific temperature. For most compounds, the solubility rises with increased temperature. This means more solute can be dissolved at an elevated temperature.
e.g. 34.2 grams of KCl in 100 grams of water at 20°C
56.3 grams of KCl in 100 grams of water at 100°C

The solution process in general involves an intermingling of solute and solvent particles and hence, solubility depends greatly on the similarity of the intermolecular forces of the components in the solution. Polarity of the compound, pressure, particle size and stirring affect the solution process as well.
Ionic compounds dissolve in water through the action of water molecules surrounding cations and anions in the hydration process. Solutions that contain ions conduct electricity and are known as **electrolytes**. Solutions are classified as strong electrolytes, weak electrolytes, or non-electrolytes, depending on the concentration of ions.
Soluble ionic compounds form strong electrolyte solutions because they completely dissociate in water. Most molecular compounds are non–electrolytes but they may form strong or weak electrolyte solutions through ionization reactions.

5.1 COMPOSITION OF SOLUTIONS

The composition of a solution can vary, depending on the chemical amount of the dissolved compound in the specified amount of solvent. There are two main ways to express the composition:

a) by percentage (fraction)
b) by molar concentration (molarity).

To calculate the percentage, the ratio of the amount of solute and of the whole solution is determined. Depending on whether mass units or volume units are used, we can use:

a) *weight/weight %,. or fraction*
b) *volume/volume %, or fraction*
c) *weight/volume %, or fraction*

The most used and most precise physical quantity is the *weight/weight* % w(%), or fraction w with the following formulas:

$$\boldsymbol{w}(\%) = \frac{\boldsymbol{mass\ of\ solute}}{\boldsymbol{mass\ of\ solution}} \times \mathbf{100}$$

$$\boldsymbol{w}(\boldsymbol{X}) = \frac{\boldsymbol{mass\ of\ solute}}{\boldsymbol{mass\ of\ solution}} = \frac{\boldsymbol{m}(\boldsymbol{X})}{\boldsymbol{m}(\boldsymbol{sol.})}$$

$$w(\%) = w(X) \times 100$$

The mass of the solution is the sum of all parts the solution is made of:

$$mass\ of\ solution = mass\ of\ solute + mass\ of\ solvent$$
$$m(sol.) = m(X) + m(water)$$

Example 1: *Calculate the weight/weight % w(%) and fraction w of a solution made from 12 grams of NaCl and 100 grams of water.*

The mass of the whole solution must be calculated:

$$m(sol.) = m(NaCl) + m(water) = 12 + 100 = 112\ g$$

$$w = \frac{mass\ of\ solute}{mass\ of\ solution} = \frac{12}{112} = 0.107$$

$$w(\%) = 0.107 \times 100 = 10.7\%$$

Alternatively, the V/V % and w/V % are calculated in a similar way, only volumes are used instead of masses:

$$\frac{\boldsymbol{V}}{\boldsymbol{V}(\%)} = \frac{\boldsymbol{volume\ of\ solute}}{\boldsymbol{volume\ of\ solution}} \times \mathbf{100} \qquad \frac{\boldsymbol{w}}{\boldsymbol{V}(\%)} = \frac{\boldsymbol{mass\ of\ solute}}{\boldsymbol{volume\ of\ solution}} \times \mathbf{100}$$

The V/V % is used only for solutions which are mixtures of liquids. For example, a water solution of alcohol might be labeled 45 V/V%. This indicates 45 mL of alcohol per 100 mL of solution.

Molar concentration or **molarity** is defined as a specific chemical amount of solute dissolved in a specific volume of solution, e.g., 1 mol of HCl in 1 liter of solution. The unit of molar concentration is mol/L or mol/dm^3, often abbreviated as M.
The respective formula is as follows:

$$molar\ concentration = \frac{moles\ of\ solute}{volume\ of\ solution}$$

In the abbreviated form:

$$\boldsymbol{c(X)} = \frac{\boldsymbol{n(X)}}{\boldsymbol{V(sol.)}}$$

Example 2: *Calculate the chemical amount of KCl dissolved in 250 mL (equals 0.25 litres) of the solution with the concentration of 1.5 mol/L.*

$$c(KCl) = \frac{n(KCl)}{V(sol.)} \Rightarrow 1.5\frac{mol}{L} = \frac{n(KCl)}{0.25\ L} \Rightarrow n(KCl) = 1.5\frac{mol}{L} \times 0.25\ L = 0.375\ mol$$

5.1.1 Transformation between weight fraction and molar concentration

In some calculations, it is necessary to change weight fractions w to the concentration c or *vice versa*. It can be done by combining multiple formulas:

a) $c(X) = \frac{n(X)}{V(sol.)}$ will be combined with the formula for chemical amount $n(X) = \frac{m(X)}{M(X)}$ to receive: $c(X) = \frac{m(X)}{M(X) \times V(sol.)}$

b) Then, the formula for weight fraction $w = \frac{m(X)}{m(sol.)}$ is used in the form: so $m(X) = w(X) \times m(sol.)$ to obtain: $c(X) = \frac{w(X) \times m(sol.)}{M(X) \times V(sol.)}$

c) Finally, the formula for density $d(sol.) = \frac{m(sol.)}{V(sol.)}$ is used to replace this division and we receive the formula:

$$\boldsymbol{c(X)} = \frac{\boldsymbol{w(X)} \times \boldsymbol{d(sol.)}}{\boldsymbol{M(X)}}$$

This formula uses the molar concentration in mol/L or mol/dm^3 units. The density is usually given in g/mL or g/cm^3, so the units must be changed to be the same. The easiest way how to unify different units is to convert the density into g/L. This is done by multiplying the value by 1000:
1 g/mL = 1000 g/L

Examle 3: *State the concentration (mol/L) of a 20% solution of HNO_3 (M_r = 63.02, d = 1.115 g/cm^3).*
1.115 g/mL = 1115 g/L; w = 0.2 (or 20/100)

$$c(HNO_3) = \frac{w(HNO_3)\ \times\ d(sol.)}{M(HNO_3)} = \frac{0.2\ \times 1115\frac{g}{L}}{63.02\frac{g}{mol}} = 3.54\frac{mol}{L}$$

Example 4: *State the weight percentage of a 4.55 M solution of HNO_3 (M_r = 63.02, d = 1.147 g/mL).*
1.147 g/mL = 1147 g/L

Here we calculate w. Therefore, we need to separate it in the formula above:

$$w(HNO_3) = \frac{c(HNO_3)\ \times\ M(HNO_3)}{d(sol)} = \frac{4.55\frac{mol}{L} \times 63.02\frac{g}{mol}}{1147\frac{g}{L}} = 0.25$$

$$w(\%) = 0.25\ \times 100 = 25\%$$

5.2 Change of solution composition – Balancing equations

Another method for preparing solutions of a desired molarity is through the process of:

a) addition of solute
b) mixing two different solutions
c) addition of solvent (dilution)

To calculate the final concentration, the mass balancing is used. When mixing a solution containing 10 grams of a solute and adding extra 10 grams of the same solute, we get the sum of the two masses. The same situation happens when mixing two different solutions with each containing some mass of the solute. The final solution will contain the sum of the original masses from the two initial mixtures. We can write the mass balance equation:

$$m_1(X) +\ m_2(X) =\ m_3(X)$$

where $m_1(X)$ and $m_2(X)$ is the mass of the solute in the two initial systems and $m_3(X)$ is the mass of the solute in the final mixture.
For each of the $m_{1\text{-}3}(X)$ we can write the formula for the weight fraction:

$$w_1 = \frac{m_1(X)}{m_1(sol.)} \qquad \text{Or} \qquad m_1(X) = w_1 \times\ m_1(sol.)$$

Upon inserting these multiplications into the mass balance equation, a new formula is obtained:

$$m_1(sol.) \times w_1 +\ m_2(sol.) \times w_2 =\ m_3(sol.) \times w_3$$

which can be rewritten as:

$$\boldsymbol{m_1 w_1 +\ m_2 w_2 =\ m_3 w_3}$$

where $m_{1\text{-}3}$ are the masses of the mixtures and $w_{1\text{-}3}$ are the weight fractions of the mixtures.

Similarly, we can write the molar balance equation using chemical amounts:

$n_1(X) + n_2(X) = n_3(X)$

where $n_1(X)$ and $n_2(X)$ is the number of moles of the solute in the two initial systems and $n_3(X)$ is the chemical amount of the solute in the final mixture.
For each of the $n_{1\text{-}3}(X)$ we can write the formula for molar concentration:

$c_1(X) = \frac{n_1(X)}{V_1(sol.)}$ or $n_1(X) = c_1(X) \times V_1(sol.)$

After the substitution of the multiplications into the mass balance equation, a new formula is obtained:

$$c_1(X) \times V_1(sol) + c_2(X) \times V_2(sol) = c_3(X) \times V_3(sol)$$

The abbreviated form is as follows:
$\boldsymbol{c_1V_1 + c_2V_2 = c_3V_3}$

where $c_{1\text{-}3}$ are the molar concentrations of the mixtures and $V_{1\text{-}3}$ are the volumes of the mixtures.

Example 5: *State the weight percentage obtained after mixing two solutions:*
(I) 50 grams solution with weight percentage 10%
(II) 20 grams of solution with weight percentage 25%

$m_1 = 50\ g$, $w_1 = 0.1$, $m_2 = 20\ g$, $w_2 = 0.25$

Not only can the masses of solute be summed but also the masses of whole solutions. By doing this, we can get the mass of the final solution: $m_3 = m_1 + m_2 = 50 + 20 = 70\ g$

Now we can use the mass balance equation for weight fractions:
$m_1w_1 + m_2w_2 = m_3w_3$

$$50 \times 0.1 + 20 \times 0.25 = 70 \times w_3$$

$$w_3 = \frac{50 \times 0.1 + 20 \times 0.25}{70} = \frac{10}{70} = 0.143$$

The percentage is $0.143 \times 100 = 14.3\%$

Example 6: *State the concentration obtained after mixing two solutions:*
(I) 5 litres solution with concentration 0.5 mol/L
(II) 3 litres solution with concentration 0.2 mol/L

$V_1 = 5\ L$, $c_1 = 0.5M$, $V_2 = 3\ L$, $c_2 = 0.2M$

Not only can the masses be summed but also the volumes of solutions. By doing this, we get the volume of the final solution: $V_3 = V_1 + V_2 = 5 + 3 = 8\ g$

Now we can use the balance equation for concentrations:
$c_1V_1 + c_2V_2 = c_3V_3$

$0.5 \times 5 + 0.2 \times 3 = c_3 \times 8$

$$c_3 = \frac{0.5 \times 5 + 0.2 \times 3}{8} = \frac{3.1}{8} = 0.388M$$

Example 7: *State how many grams of solute were added to 100 grams of solution with weight percentage 10% to get a 25% solution?*

In this case, pure solute (100%) was added to the first solution. If a pure solute is used, we can use $w_2 = 1$*. We know only the % of all 3 systems (initial solution, added solute and final solution) and the mass of the initial solution.*

$m_1 = 100$ *g*, $w_1 = 0.1$, $w_2 = 1$, $w_3 = 0.25$

$m_1 w_1 + m_2 w_2 = m_3 w_3$

In this equation there are now two unknown quantities – m_2 *and* m_3*. To get rid of one of them (*m_3*), we can use the substitution* $m_3 = m_1 + m_2$*. Then, we get:*

$m_1 w_1 + m_2 w_2 = (m_1 + m_2) w_3$

$100 \times 0.1 + m_2 \times 1 = (100 + m_2) \times 0.25$

$100 \times 0.1 + m_2 = 100 \times 0.25 + m_2 \times 0.25$

$10 + m_2 = 25 + m_2 \times 0.25$

$(1 - 0.25) m_2 = 15$

$$m_2 = \frac{15}{0.75} = 20\ g$$

20 grams of solute must be added to the 10% solution to obtain 25% solution.

Example 8: *State how many grams of water must be added to 167 grams of solution with the weight percentage 15% to get a 5% solution.*

In this case, pure water that doesn't contain any solute (0%) was added to the first solution. If pure water is used, then $w_2 = 0$*. We know only the % of all 3 systems (initial solution, added water and final solution) and the mass of the initial solution.*

$m_1 = 167$ *g*, $w_1 = 0.15$, $w_2 = 0$, $w_3 = 0.05$

$m_1 w_1 + m_2 w_2 = m_3 w_3$

When we replace the quantities with known values, we get:

$167 \times 0.15 + m_2 \times 0 = m_3 \times 0.05$

$167 \times 0.15 + 0 = m_3 \times 0.05$

$$25 = m_3 \times 0.05$$

$$m_3 = \frac{25}{0.05} = 500\ g$$

The final solution must have the mass of 500 grams to be 5%. To calculate the mass of water added to the initial solution – m2, we need to make the difference:
$m_2 = m_3 - m_1 = 500 - 167 = 333\ grams$

Thus, 333 grams of water were added to the initial solution to dilute it from 15% to 5%.

5.3 PROBLEMS

1. In a laboratory, 12.0 grams of $AgNO_3$ are dissolved in 26.0 g of H_2O. What is the percentage by weight of $AgNO_3$ in the solution?

2. How would you prepare 50 grams of a 32% solution of KBr in water?

3. How many grams of NaOH are contained in 0.5 L of its 10% solution (d = 1.115 g/mL)?

4. State the volume of a 10% H_2SO_4 solution containing 18.5 grams of pure H_2SO_4 (solution density d = 1.070 g/mL).

5. How many grams of H_3PO_4 (M_r = 98.02) do we need to prepare 500 mL of its solution with the concentration 0.2 mol/L?

6. State the chemical amount of KBr which is dissolved in 35.8 mL of a 0.172 M solution.

7. How many grams of NaOH (M_r = 40) are dissolved in 250 mL of a 0.343 M solution?

8. How many mL of 60% H_2SO_4 (M_r = 98.08) do we need to prepare 1 liter of its 1 molar solution (60% solution density d = 1.4983 g cm^{-3})?

9. How many litres of a 0.643 M solution contain 114 grams of NaF (M_r = 42)?

10. State the concentration (mol dm^{-3}) of a solution containing 71 g of Na_2SO_4 (M_r = 142) in 10 litres of solution.

11. State the concentration (mol dm^{-3}) of the solution containing 28 g of KOH (M_r = 56) in 500 mL.

12. State the concentration (mol dm^{-3}) of a 10% solution of HNO_3 (M_r = 63, d = 1.050 g/mL).

13. A 500 mL solution of $Ba(NO_3)_2$ (M_r = 261.34) was prepared by dissolving 20 grams of the substance in water. Determine the molar concentration.

14. Determine the molarity of the following solutions: a) 4 moles of NaCl are dissolved in a sufficient amount of water to make 2 L of solution, b) 58.8 g of KOH (M_r = 56) are dissolved in enough water to make 700 mL of solution.

15. What is the molarity of the solution prepared by adding 2 litres of water to 2 litres of a 0.5 M KOH solution?

16. What volume of a 0.34 M $MgCl_2$ solution is required to make 450 mL of a 0.10 M solution by dilution?

17. In a laboratory, 500 mL of water is added to 250 mL of a 0.75 M NaOH solution. Determine the molarity of the resulting solution.

18. A solution was prepared by dissolving 18.3 grams of KNO_3 in 75.0 grams of water at 20 °C. What is the percentage weight/weight of this solution?

19. State the weight fraction of 1.4 molar solution of $AgNO_3$ (M_r = 169.8, d = 1.180 g/mL).

20. How many grams of KNO_3 do we need to prepare 3 litres of its 5% solution (d = 1.080 g/mL)?

21. What is the weight percentage of the solution formed by adding of 20 g of 62% solution of HNO_3 to 30 g of water?

22. How many mL of 10% H_2SO_4 solution (d = 1.065 g cm^{-3}) do we need to prepare its 25% solution from 300 grams of 50% H_2SO_4?

23. We want to prepare 1.5 dm^3 of a 5% hydrochloric acid solution (d = 1.023 g/mL). Calculate the volume of 30% HCl (d = 1.149 g/mL) and the volume of water which must be added.

24. How many grams of pure KOH must be added to 200 grams of its 10% solution to obtain a 25% solution?

25. Calculate the final concentration after mixing 250 mL solution with the concentration 2 M and a 0.5 M solution? The total volume after mixing is 7.5 litres.

26. State the weight fraction of the solution prepared by adding 25 g of NaOH to 450 g of a 3% solution.

27. Determine the molar concentration of the solution which was added to 2 litres of 0.5 molar solution to obtain 10 litres of a 1.5 molar solution.

28. 10 mL of 12 molar HCl was diluted to 250 mL. State the concentration of the final solution.

29. Calculate the weight percentage of a 2.0 molar solution of NaOH (M_r = 40, d = 1.080 g/mL).

30. 44.8 g of KOH (M_r = 56) was dissolved in a sufficient amount of water to make 1.2 litres of solution. State the molar concentration.

Answers: *1*) 31.58% *2*) 16 g of KBr and 34 g of H_2O *3*) 55.75 g *4*) 172.9 mL *5*) 9.80 g *6*) 0.0062 moles *7*) 3.43 g *8*) 109 mL *9*) 4.24 litres *10*) 0.05 mol dm^{-3} *11*) 1 M *12*) 1.66 M *13*) 0.153 M *14*) 2 M (a), 1.5 M (b) *15*) 0.25 M *16*) 0.132 L *17*) 0.25 M *18*) 19.6% *19*) 0.2 *20*) 162 g *21*) 24.8% *22*) 469.48 mL *23*) 255.7 g (222.54 mL) of 30% HCl, 1278.75 g of water *24*) 40 g *25*) 0.55 M *26*) 0.10 *27*) 1.75 M 28) 0.48 M 29) 7.4% *30*) 1.5 M

6 STOICHIOMETRIC CALCULATIONS

The main goal of chemistry is the study of chemical reactions defined as the combination of the elements and their compounds to give new compounds.

a A + b B ⟵⟶ c C + d D

where
A, B: reactants, C, D: products
a, *b*: stoichiometric coefficients defining the molar ratio of reacting particles
c, *d*: stoichiometric coefficients defining the molar ratio of particles formed

The written representation of a chemical reaction is the chemical equation showing the reactants (A, B) and the products (C, D), as well as the direction (⟵⟶) in which the reaction proceeds. In other words, reactants mean the material put into the reaction, products are the material obtained.
The relationship between chemical amounts of chemical reactants and products is called stoichiometry and the multiplying numbers (*a*, *b*, *c*, *d*) in a balanced equation are the stoichiometric coefficients. **Stoichiometric coefficients represent the molar ratio of the given substances**.
In chemical reactions, mass is always conserved. Balancing an equation ensures that the same number of atoms of each element appear on both sides.

How to approach the calculations:

1. Determine the chemical amount of one of the products or reactants from given mass, solution data or gas volumes.
2. Using the stoichiometric coefficients, calculate the chemical amount of the other compounds in the chemical reaction.
3. Calculate the required data and yields.

For the calculations under part 1, we need to use the basic relationships to calculate chemical amount:
$n(X) = \frac{m(X)}{M(X)}$ (when mass of a compound is known)
$c(X) = \frac{\boldsymbol{n(X)}}{V(sol.)}$ (when concentration and volume of a solution is known)
$n(X) = \frac{V(X)}{V_M}$ (when volume of a gas is known)
$n(X) = \frac{N(X)}{N_A}$ (when number of particles is known)

For the calculations under part 2, we can use the ratio:

$$\boldsymbol{\frac{a}{b} = \frac{n(A)}{n(B)}}$$

If we know the chemical amount of B, we can use this relationship to calculate the chemical amount of A, using:

$$\boldsymbol{n(A) = \frac{a}{b} \times n(B)}$$

Example 1: *Calculate how many grams of zinc and sulfuric acid are needed for the preparation of 1 mol of $ZnSO_4$. How many litres of hydrogen gas can be prepared? M(Zn) = 65.38 g/mol, M(H_2SO_4) = 98.08 g/mol*

$Zn + H_2SO_4 \rightarrow ZnSO_4 + H_2$

All these compounds are at the ratio 1 : 1 with $ZnSO_4$. That means they will have same chemical amount, because:

$$\frac{n(A)}{n(ZnSO_4)} = \frac{1}{1}$$

$$m(Zn) = n(Zn) \times M(Zn) = \ 1\,mol\ \times 65.38\frac{g}{mol} = 65.38\ g$$

$$m(H_2SO_4) = n(H_2SO_4) \times M(H_2SO_4) = \ 1\,mol\ \times 98.08\frac{g}{mol} = 98.08\ g$$

H_2 is a gas, therefore the molar volume can be used to calculate the volume of the gas produced:

$$V(H_2) = n(H_2) \times V_M = 1\,mol\ \times 22.4\frac{L}{mol} = 22.4\ L$$

Example 2: *State the volume of a 25% sulfuric acid needed to prepare 1 gram of $ZnSO_4$. M($ZnSO_4$) = 161.45 g/mol, M(H_2SO_4) = 98.08 g/mol, density of 25% H_2SO_4 is 1.1783 g/mL*

$Zn + H_2SO_4 \rightarrow ZnSO_4 + H_2$

We can calculate the chemical amount of $ZnSO_4$ from its mass - 1 gram.

$$n(ZnSO_4) = \frac{m(ZnSO_4)}{M(ZnSO_4)} = \frac{1}{161.45} = 0.0062\,mol$$

Again, the chemical amount of H_2SO_4 is the same as that of $ZnSO_4$ because their ratio is 1 : 1. The mass of pure H_2SO_4 can be calculated as follows:

$$m(H_2SO_4) = n(H_2SO_4) \times M(H_2SO_4) = \ 0.0062\,mol\ \times 98.08\frac{g}{mol} = 0.608\ g$$

Now the mass of the 25% solution (w = 0.25) of sulfuric acid can be calculated:

$$w(25\%\ H_2SO_4) = \frac{m(H_2SO_4)}{m(25\%\ H_2SO_4)}$$

$$0.25 = \frac{0.608}{m(25\%\ H_2SO_4)}\ \ so\ m(25\%\ H_2SO_4) = \frac{0.608}{0.25} = 2.432\ g$$

The volume of this solution can be calculated using the density:

$$d(25\%\ H_2SO_4) = \frac{m(25\%\ H_2SO_4)}{V(25\%\ H_2SO_4)}$$

$$1.1783\frac{g}{mL} = \frac{2.432\ g}{V(25\%\ H_2SO_4)} \quad so\ V(25\%\ H_2SO_4) = \frac{2.432\ g}{1.1783\frac{g}{mL}} = 2.04\ mL$$

Example 3: *Calculate the mass of phosphoric acid, calcium hydroxide and water needed to prepare 5 grams of calcium phosphate. M(H_3PO_4) = 98.00 g/mol, M($Ca(OH)_2$) = 74.09 g/mol, M($Ca_3(PO_4)_2$) = 310.18 g/mol, M(H_2O) = 18.02 g/mol*

2 H_3PO_4 + 3 $Ca(OH)_2$ → $Ca_3(PO_4)_2$ + 6 H_2O

First, we calculate the chemical amount of calcium phosphate from the mass:

$$n(Ca_3(PO_4)_2) = \frac{m(Ca_3(PO_4)_2)}{M(Ca_3(PO_4)_2)} = \frac{5}{310.18} = 0.0161\ mol$$

Second, we need to calculate the chemical amounts of the other compounds using the stoichiometric coefficients:

$$\frac{2}{1} = \frac{n(H_3PO_4)}{n(Ca_3(PO_4)_2)}$$

$$n(H_3PO_4) = \frac{2}{1} \times n(Ca_3(PO_4)_2) = \frac{2}{1} \times 0.0161 = 0.0322\ mol$$

$$m(H_3PO_4) = n(H_3PO_4) \times M(H_3PO_4) = 0.0322 \times 98.00 = 3.16\ g$$

$$\frac{3}{1} = \frac{n(Ca(OH)_2)}{n(Ca_3(PO_4)_2)} \quad so \quad n(Ca(OH)_2) = \frac{3}{1} \times 0.0161 = 0.0483\ mol$$

$$m(Ca(OH)_2) = n(Ca(OH)_2) \times M(Ca(OH)_2) = 0.0483 \times 74.09 = 3.57\ g$$

$$\frac{6}{1} = \frac{n(H_2O)}{n(Ca_3(PO_4)_2)} \quad so \quad n(H_2O) = \frac{6}{1} \times 0.0161 = 0.0966\ mol$$

$$m(H_2O) = n(H_2O) \times M(H_2O) = 0.0966 \times 18.02 = 1.74\ g$$

6.1 Calculation of reaction yields

Theoretical yield is the maximum number of grams of product that can be obtained based on the balanced chemical reaction.
Practical yield represents the actual amount of product collected in a laboratorory preparation. It is always smaller than the theoretical yield.
Percentage yield is expressing the practical yield at the ratio to the theoretical yield:

$$\boldsymbol{percentage\ yield = \frac{practical\ yield}{theoretical\ yield} \times 100}$$

or

$$\boldsymbol{\gamma}(\%) = \frac{\boldsymbol{m_P}}{\boldsymbol{m_T}} \times \mathbf{100}$$

Example 3: *Calculate the percentage yield of a reaction for the preparation of 15 grams of $CaCO_3$, when only 10.5 grams were actually prepared.*
m_P = 10.5 g, m_T = 15 g

$$\gamma(\%) = \frac{m_P}{m_T} \times 100 = \frac{10.5}{15} \times 100 = 70\%$$

Example 4: Calculate the theoretical and percentage yield of the preparation of potassium sulfate from potassium hydroxide and sulfuric acid, if 5.6 grams of potassium hydroxide are used. The practical yield of the reaction was 5.23 grams. M(KOH) = 56.11 g/mol, M(K_2SO_4) = 174.26 g/mol

$2\ KOH + H_2SO_4 \rightarrow K_2SO_4 + 2\ H_2O$

The chemical amount of KOH can be calculated from its mass.

$$n(KOH) = \frac{m(KOH)}{M(KOH)} = \frac{5.6}{56.11} = 0.10\, mol$$

The chemical amount of K_2SO_4 can be calculated from the stoichiometric ratio:

$$\frac{1}{2} = \frac{n(K_2SO_4)}{n(KOH)} \quad so \quad n(K_2SO_4) = \frac{1}{2} \times n(KOH) = \frac{1}{2} \times 0.10 = 0.05\, mol$$

The mass of K_2SO_4 can be calculated from the chemical amount. The mass will be also the theoretical yield of the reaction.

$$m(K_2SO_4) = n(K_2SO_4) \times M(K_2SO_4) = 0.05 \times 174.26 = 8.71\ g = m_T$$

Now the percentage yield can be calculated, when m_P = 5.23 g:

$$\gamma(\%) = \frac{m_P}{m_T} \times 100 = \frac{5.23}{8.71} \times 100 = 60\%$$

6.2 Problems

1. How many moles and how many litres of hydrogen are formed in the reaction of 50 grams of zinc (A_r = 65.39) with sulfuric acid (M_r = 98.08)?

2. How many grams of zinc (A_r = 65.39) and how many grams of 20% sulfuric acid (M_r = 98.08) solution do we need for the preparation of 56 litres of hydrogen?

3. H_2SO_4 (M_r = 98.08) reacted with impure zinc (A_r = 65.39) and produced 224 mL of hydrogen gas. The impure zinc mixture weighed 0.8 grams. What was the mass fraction of pure zinc in the impure mixture?

4. To a solution containing 0.2 mol of $FeCl_3$ 0.24 mol of NaOH were added. Calculate the chemical amount of $Fe(OH)_3$ formed. Which reactant was in excess and was left partially unreacted? Calculate the chemical amount of the unreacted reactant.

5. Calculate the chemical amount of products formed by thermal decomposition of 20 grams of $CaCO_3$ (M_r = 100). ($CaCO_3 \rightarrow CaO + CO_2$)

6. Zinc reacts with HCl to form $ZnCl_2$ and H_2. How many grams of zinc (A_r = 65.39) and how many mL of 20% HCl (M_r = 36.46, d = 1.098 g cm^{-3}) do we need to prepare 112 L of hydrogen?

7. How many litres of hydrochloric acid (c = 0.5 mol dm^{-3}) are needed for the neutralization reaction of 250 grams of 25% KOH (M_r = 56.11) and how many grams of KCl (M_r = 74.55) are formed?

8. We want to prepare 25 grams of K_2SO_4 (M_r = 174.26) by the reaction of KOH (M_r = 56.11) with 96% H_2SO_4 (M_r = 98.08). State the volumes of 96% sulfuric acid (d = 1.8355 g/mL) and 20% KOH solutions (d = 1.1818 g cm^{-3}) which must be used in this reaction.

9. State the chemical amount of water formed after the reduction of 200.0 g of copper(II) oxide (M_r = 79.54) to metallic copper. ($CuO + H_2 \rightarrow Cu + H_2O$)

10. State the volumes (mL) of 36% solution of HCl (M_r = 36.46, d =1.1790 g/mL) and 25% solution of NH_3 (M_r = 17, d = 0.9070 g/mL) required for the preparation of one gram of NH_4Cl (M_r = 53.46). ($HCl + NH_3 \rightarrow NH_4Cl$)

11. How many litres of 15% KOH (M_r = 56.11, d = 1.137 g/mL) solution are equal to 2 litres of 20% solution of H_2SO_4 (M_r = 98.08, d = 1.139 g/mL), (neutralization reaction). How many grams of K_2SO_4 (M_r = 174.26) are formed?

12. A mixture of 30.0 g of Al (A_r = 27) and 80 g of Fe_2O_3 (M_r = 160) is prepared. The mixture is heated and a vigorous single replacement reaction occurs according to the following equation: $Fe_2O_3 + 2\ Al \rightarrow Al_2O_3 + 2\ Fe$
What is the mass of iron (A_r(Fe) = 55.9) produced?

13. How many grams of magnesium nitride Mg_3N_2 (M_r = 100.9) are produced when 63 grams of Mg (A_r = 24.3) and 41 grams of N_2 (A_r = 14) react with each other?
($3\ Mg + N_2 \rightarrow Mg_3N_2$)

14. What is the mass of SO_3 (M_r = 80.06) produced when 3.60 g of SO_2 (M_r = 64.06) are combined with 2.40 g of O_2 (A_r = 16)?

15. How many mL of a 50% NaOH (M_r = 40, d = 1.5253 g/mL) solution do we need for the neutralization of 1 litre of a 20 % H_2SO_4 solution (M_r = 98.08, d = 1.3980 g/mL)?

16. Metallic magnesium reacts with hydrochloric acid to form magnesium chloride and hydrogen. State the number of millilitres of 3.0 molar HCl needed for the preparation of 136.6 mL of hydrogen gas. ($Mg + 2\ HCl \rightarrow MgCl_2 + H_2$)

17. Into the solution containing 27 grams $CuCl_2$ (M_r = 134.44), 12 grams of iron powder (A_r = 55.83) were added. How many grams of copper (A_r = 63.54) were formed? ($CuCl_2 + Fe \rightarrow Cu + FeCl_2$)

18. How many grams of lithium (A_r = 6.94) are required to react completely with 161 grams of sulfur (A_r = 32), assuming Li_2S is produced?

19. Sodium iodide (M_r = 148.89) can be prepared in the laboratory by combining metallic sodium (A_r = 22.99) and iodine (A_r = 125.9). How many grams of I_2 are required to obtain 225 grams of NaI? ($2\ Na + I_2 \rightarrow 2\ NaI$)

20. Ammonia can be prepared by direct reaction of nitrogen and hydrogen according to the equation $N_2 + 3\ H_2 \rightarrow 2\ NH_3$. How many moles of ammonia are formed from 12 moles of hydrogen?

21. State the weight fraction of $Ca(OH)_2$ (M_r = 74.09) in 50.0 grams of lime water, if 1.50 grams of $CaCO_3$ (M_r = 100) were obtained after the reaction of this solution with CO_2. ($Ca(OH)_2 + CO_2 \rightarrow CaCO_3 + H_2O$)

22. In preparation of HCl, 10 dm^3 of chlorine gas react with 0.80 g of hydrogen (M_r = 2.016). State the chemical amount of both and determine which of the reactants is in excess.

23. How many kilograms of iron (A_r = 55.85) and sulfur (A_r = 32.06) do we need to prepare 1 000 kilograms of FeS (M_r = 87.91)?

24. After burning 60 grams of carbon in the air, 220 grams of carbon dioxide were formed. Calculate the mass of CO_2 created after burning 90 g of carbon.

25. Calculate the volume of a 20% solution of NaOH (M_r = 40, d = 1.2191 g/mL) and volume of CO_2 necessary for the preparation of 100 grams of Na_2CO_3 (M_r = 106). ($2\ NaOH + CO_2 \rightarrow Na_2CO_3$)

26. A neutralization reaction between $Mg(OH)_2$ (M_r = 58.3) and H_3PO_4 (M_r = 98.0) represents the equation $3\ Mg(OH)_2 + 2\ H_3PO_4 \rightarrow Mg_3(PO_4)_2 + 6\ H_2O$. How many grams of $Mg_3(PO_4)_2$ (M_r = 262.9) are produced after the reaction of 50 grams of $Mg(OH)_2$ and 70 grams of H_3PO_4?

27. How many grams of NaOH (M_r = 40) do we need for the neutralization of a solution containing 0.2 moles of sulfuric acid (M_r = 98.08) and how many grams of Na_2SO_4 (M_r = 142.02) can be prepared?
$H_2SO_4 + 2\ NaOH \rightarrow Na_2SO_4 + 2\ H_2O$

28. State the volume of 0.75 M solution of HCl (M_r = 36.46) equal to 250 grams of 25% solution of KOH (M_r = 56.1).

29. How many grams of iron (M_r = 55.85) "dissolve" in 700 mL of 32% H_2SO_4 (M_r = 98.08, d = 1.1353 g/mL) and how many litres of hydrogen evolve during the reaction $Fe + H_2SO_4 \rightarrow FeSO_4 + H_2$?

30. How many grams of CaO (M_r = 56.08) react with 275 mL of 0.523 M solution of HCl (M_r = 36.46)? ($CaO + 2\ HCl \rightarrow CaCl_2 + H_2O$)

Answers:
1) 0.765 mol, 17.13 L *2*) 163 g of Zn, 1226 g of 20% H_2SO_4 *3*) 0.813, 81.3% *4*) 0.08 mol $Fe(OH)_3$, 0.12 mol of $FeCl_3$ stay unreacted *5*) 0.2 mol of both *6*) 326.8 g Zn, 1660.3 mL of 20% HCl *7*) 2.23 litres of HCl solution, 83.0 g of KCl *8*) 68.11 mL of 20% KOH, 7.99 mL of 96% H_2SO_4 *9*) 2.51 mol *10*) 1.4 mL of 25% NH_3, 1.6 mL of 36% HCl *11*) 3.056 litres, 809 g of K_2SO_4 *12*) 55.9 g *13*) 87 g *14*) 4.49 g of SO_3 *15*) 299 mL *16*) 3.7 mL *17*) 12.71 g Cu *18*) 69.83 g of Li *19*) 95.13 g of I_2 *20*) 8 mol *21*) 0.022 *22*) 0.446 mol of Cl_2 and 0.397 mol of H_2, so Cl_2 is in excess *23*) 635.3 kg of Fe, 364.7 kg of S *24*) 330 g *25*) 21.1 litres of CO_2, 309.5 mL of 20% NaOH *26*) 75.15 g of $Mg_3(PO_4)_2$ *27*) 16 g of NaOH, 28.4 g of Na_2SO_4 *28*) 1.485 L *29*) 144.65 g of Fe, 58.08 L of H_2 *30*) 4.033 g

7 HYDROGEN EXPONENT

The concept of hydrogen exponent is based on the so–called **autoionization of water**, that means on **autoprotolytic** reaction between two water molecules. In this reaction the proton is being transferred from one water molecule to another and hydronium (H_3O^+) and hydroxide ($OH^–$) ions are produced.

$H_2O + H_2O \leftrightarrow H_3O^+ + OH^–$

The equilibrium constant expression for this reaction is as follows

$$K = \frac{c(H_3O^+) \times c(OH^-)}{c(H_2O)^2}$$

The concentration of undissociated water molecules is high and can be considered to be constant, so it can be simplified to:

$$K_w = c(H_3O^+) \times c(OH^-) = 1 \times 10^{-14}$$

Ionisation constant of water: $K_w = 10^{-14}$ (experimentally determined)

In pure water or in a solution with pH = 7 the concentrations of H_3O^+ and OH^- are equal: $c(H_3O^+) = c(OH^–) = 10^{-7}$ M

As the concentrations of $c(H_3O^+)$ and $c(OH^–)$ are practically very low, the concept of so-called hydrogen exponent (pH) was proposed and developed.

Thus, we define the pH of a solution as:

$$\boldsymbol{pH = -log\ c(H_3O^+)}$$

For example, if the concentration of H_3O^+ is 10^{-3} mol/L, then pH = 3.

For the concentration of OH^-, the pOH is used:

$$\boldsymbol{pOH = -log\ c(OH^-)}$$

There is a relationship between pH and pOH based on the K_w constant:

$$K_w = c(H_3O^+) \times c(OH^-) = 1 \times 10^{-14}$$

$$-logK_w = -log\ c(H_3O^+) - -log\ c(OH^-) = 14$$

So, the relationship of pH and pOH is:

$$\boldsymbol{pK_w = pH + pOH = 14}$$

where: $pK_w = -\log K_w = 14$

It can be concluded that in an aqueous solution of any solute at 25 °C the sum of pH and pOH is always 14.

Solutions of acids and bases have pH higher or lower than 7. This happens because acids can produce more H_3O^+ in solutions and bases form OH^-. These reactions are called protolytic (proton, H^+ is being moved between compounds).

$HCl + H_2O \rightarrow H_3O^+ + Cl^-$ pH < 7, pOH > 7 acidic solution
(concentration of H_3O^+ above 10^{-7} mol dm^{-3})

$NaOH \rightarrow Na^+ + OH^-$ pH > 7, pOH < 7 basic solution
(concentration of OH^- above 10^{-7} mol dm^{-3})

If the solution contains solutes that don't undergo protolytic reactions or contain no solute, the solution is neutral and pH = pOH = 7.

However, the product of concentration of H_3O^+ and OH^- ions in water must remain constant and is equal to $K_w = 10^{-14}$.

The relations between molar concentration of $c(H_3O^+)$ and $c(OH^-)$ ions and original molar concentration of corrresponing undisociated acids or bases (c) are as follows:

$HCl + H_2O \rightarrow H_3O^+ + Cl^-$ $c(H_3O^+) = c(HCl)$

$NaOH \rightarrow Na^+ + OH^-$ $c(OH^-) = c(NaOH)$

$H_2SO_4 + 2\,H_2O \rightarrow 2\,H_3O^+ + SO_4^{2-}$ $c(H_3O^+) = 2 \times c(H_2SO_4)$

$Ba(OH)_2 \rightarrow Ba^{2+} + 2\,OH^-$ $c(OH^-) = 2 \times c(Ba(OH)_2)$

Thus, the stoichiometry reflects the overall concentration of H_3O^+ in acidic solutions and OH^- in basic solutions.

Examples 1*: State the pH value of the following solutions:*
a) H_2SO_4 with concentration 10^{-4} mol/L

This is an acid, so we can calculate pH directly from the concentration of the acid. The stoichiometry must be considered:
$H_2SO_4 + 2\,H_2O \rightarrow 2\,H_3O^+ + SO_4^{2-}$ $c(H_3O^+) = 2 \times c(H_2SO_4)$

$C(H_3O^+) = 2 \times c(H_2SO_4) = 2 \times 10^{-4}$ *mol/L*

$pH = -\log(2 \times 10^{-4}) = 3.7$

b) KOH with concentration 0.003 mol/L

This is a base. Therefore, pOH can be calculated from the concentration of KOH. After that, pH can be calculated from K_w.

$KOH \rightarrow K^+ + OH^-$ $c(OH^-) = c(KOH)$

$pOH = -\log(3 \times 10^{-3}) = 2.5$
$pH + pOH = 14 \Rightarrow pH = 14 - pOH = 14 - 2.5 = 11.5$

pH can be used in the calculations of solutions and in the determination of properties of acidic and basic solutions. E.g., how much acid or base is needed to obtain a solution of a specific pH or how much solution of an acid is needed to neutralize a basic solution with the known concentration values or pH.

In these calculations, it is often necessary to calculate the concentration of H_3O^+ from pH or OH ions from pOH. The following formulas can be used:

$$\boldsymbol{c(H_3O^+) = 10^{-pH}}$$

$$\boldsymbol{c(OH^-) = 10^{-pOH}}$$

Example 2: *Calculate the mass of $Ca(OH)_2$ which is needed to obtain 0.5 liter solution with pH = 11.4. $M(Ca(OH)_2)$ = 74.09 g/mol*

$Ca(OH)_2 \rightarrow Ca^{2+} + 2\ OH^-$ *$c(OH^-) = 2 \times c(Ca(OH)_2)$*

First, the concentration of OH- can be calculated from pOH.

pOH = 14 – pH = 2.6

$$c(OH^-) = 10^{-pOH} = 10^{-2.6} = 0.0025 \frac{mol}{L}$$

$$c(Ca(OH)_2) = \frac{c(OH^-)}{2} = \frac{0.0025}{2} = 0.00125 \frac{mol}{L}$$

$$n(Ca(OH)_2) = c(Ca(OH)_2) \times V(sol.) = 0.00125 \frac{mol}{L} \times 0.5\ L = 6.25 \times 10^{-4}\ mol$$

$$m(Ca(OH)_2) = n(Ca(OH)_2) \times M(Ca(OH)_2) = 6.25 \times 10^{-4}\ mol \times 74.09 \frac{g}{mol}$$

$$\boldsymbol{m(Ca(OH)_2) = 0.046\ g = 46\ mg}$$

Example 3: *Calculate the pH value of the solution of perchloric acid with the weight fraction w = 0,01. $M(HClO_4)$ = 100,458, d (1%) = 1,005 g/mL = 1005 g/L*

$HClO_4 + H_2O \rightarrow H_3O^+ + ClO_4^-$ *$c(H_3O^+) = c(HClO_4)$*

This is a calculation where w is transformed into c and then, pH is calculated.

$$c = \frac{n}{V\odot} = \frac{m}{M \times V\odot} = \frac{w \times m\odot}{M \times V\odot} = \frac{wd\odot}{M} = \frac{0.01 \times 1005}{100.458} = 0.1\ M$$

$$pH = -\log 0.1 = \mathbf{1}$$

Example 4: *For the neutralization of 200 mL of NaOH solution a HCl solution of 100 mL and pH = 1 was used. Calculate the pH of the NaOH solution!*

NaOH + HCl → NaCl + H₂O
c(OH⁻) = c(NaOH)

*This is the case of neutralization, where an acidic and a basic solution are mixed together to obtain a neutral solution. For this type of calculation, the condition of **equivalent chemical amounts of H_3O^+ and OH^-** must be used:*

$$\boldsymbol{n(H_3O) = n(OH)}$$

HCl solution: pH = 1, $[\boldsymbol{H_3O^+}] = \boldsymbol{10^{-pH}} = \boldsymbol{10^{-1}} = \boldsymbol{0.1\,\frac{mol}{L}}$

$$n(H_3O^+) = [H_3O^+] \times V(HCl\,sol.) = 0.1 \times 0.1 = 0.01\,mol$$
$$n(H_3O^+) = n(OH^-) = 0.01\,mol$$

$$[OH-] = \frac{n(OH^-)}{V(NaOH\ sol)} = \frac{0.01}{0.2} = 0.05\ \frac{mol}{L}$$

$$pOH = -\log 0.05 = 1.3$$

$$pH = 14 - pOH = 14 - 1.3 = 12.7$$

7.1 PROBLEMS

1. Determine the pH value of the following solutions:
   a) $c(H_3O^+) = 10^{-2}$ M
   b) $c(OH^-) = 10^{-2}$ M
   c) $c(H_3O^+) = 3.3 \times 10^{-8}$ M
   d) $c(OH^-) = 5.7 \times 10^{-3}$ M

2. Determine the concentration (M) of H_3O^+ ions from pH or OH^- ions from pOH in solutions with:
   a) pH = 2
   b) pH = 4.6
   c) pH = 11.3
   d) pOH = 6.5
   e) pOH = 12.3

3. Calculate the pH of a solution with H_3O^+ concentration 0.004 mol/L.

4. State the pH value of fully dissociated 0.001 molar hydrochloric acid.

5. State the pH value of a solution with OH^- concentration 2.5×10^{-2} mol/L.

6. State the pH value of H_2SO_4 with the concentration 4×10^{-4} mol/L.

7. Calculate the pH value of a 0.025 M solution of NaOH.

8. Calculate the pH value of the NaOH ($M_r = 40$) solution containing 1 gram of NaOH in 200 mL of solution.

9. Calculate the pH value of the 1% solution of NaOH ($M_r = 40$, $d = 1.0095$ g/mL).

10. State the pH value of a solution containing 0.2 g $Ba(OH)_2$ (M_r = 171.35) in one liter of solution.

11. Calculate the pH value of a 2% HCl (M_r = 36.46) solution (d = 1.008 g/mL).

12. State the pH value of the solution prepared by dilution of 100 mL of 0.1 M $Ba(OH)_2$ to 500 mL final volume.

13. Calculate the pH value of a 0.61% solution of NaOH (M_r = 40, d = 1.007 g/mL).

14. A solution was prepared by dissolving 25.0 grams of NaOH (M_r = 40) in 1 liter of water. State the pH value.

15. State the pH value of a solution with OH^- concentration 3×10^{-2} mol/mL.

16. Determine the concentration of the H_2SO_4 solution with pH = 2.42.

17. State the pH value of a KOH (M_r = 56.11) solution containing 6 g of this substance in 3 L of solution.

18. State the pH value of a solution containing 0.1 g of $Ba(OH)_2$ (M_r = 171.35) in 100 mL of solution.

19. By mistake, two solutions of two different acids were mixed together. The first solution contained HCl at the 0.05 M concentration and had a volume of 0.5 L. The second one contained H_2SO_4 at the 0.02 M concentration. After mixing, the mixture had 750 mL volume. Calculate the pH of the final solution.

20. To a solution with pH = 3.5 and the volume of 2 litres a 0.2 M solution of HCl with the volume of 100 mL was added. What pH was obtained after mixing them together?

21. To a solution of $Ca(OH)_2$ with the concentration 0.0025 M and the volume 500 mL a solution with pH = 12.3 was added. The total volume after the addition was 600 mL. Determine the pH of the final basic solution.

22. 500 mL of 0.1 M solution of $Ba(OH)_2$ were diluted with distilled water to the volume of 800 mL. State the pH value of the resulting solution.

23. Calculate the pH value of a solution prepared by adding 3 L of water to 2 L of a solution with a pH = 2.25.

24. A solution was prepared by diluting 10.0 mL of a 6.00 M HCl to the final volume 0.5 L. State the pH value.

25. To one litre of sulfuric acid with the concentration of 0.1 M one litre of water was added. State the pH value of the solution formed.

26. Calculate the pH value of the solution prepared by dilution of 100 mL of 0.1 molar H_2SO_4 to 250 mL final volume.

27. State the pH value of the solution prepared by the dilution of 5 mL of 35% HCl (M_r = 36.46, d = 1.1740 g/mL) with distilled water to 1 litre final volume.

28. Two litres of a solution with pH = 2.25 were neutralized with a basic solution of three litres volume. Calculate the pH and the concentration of OH^- ions of the basic solution.

29. For the neutralization of 100 mL of an H_2SO_4 solution with pH = 2 we need 200 mL of KOH solution. State the pH value of the KOH solution.

30. State the pH value of hydrochloric acid when it is known that 100 mL of this solution are equal to 200 mL of a KOH solution with the pH value of 9.

Answers:
1) a) 2, b) 12, c) 7.48, d) 11.76 *2*) a) 10^{-2}, b) 2.5×10^{-5}, c) 5×10^{-12}, d) 3.16×10^{-7}, e) 5×10^{-13} *3*) 2.4 *4*) 3 *5*) 12.4 *6*) 3.1 *7*) 12.4 *8*) 13.1 *9*) 13.4 *10*) 11.37 *11*) 0.26 *12*) 12.6 *13*) 13.19 *14*) 13.8 *15*) 12.5 *16*) 1.9×10^{-3} *17*) 12.56 *18*) 12.07 *19*) 1.33 *20*) 2 *21*) 11.88 *22*) 13.1 *23*) 2.65 *24*) 0.92 *25*) 1 *26*) 1.1 *27*) 1.25 *28*) pH = 11.57, c(OH^-) = 3.7×10^{-3} M *29*) 11.7 30) 4.7

8 THEORY OF ACIDS AND BASES

In simplest terms, acids and bases are categories of substances which cause acidic or basic reaction of their aqueous solutions. The property of *acidity* of a solution is related to the presence of H_3O^+ cations (called *hydronium* ions, or sometimes also oxonium or hydroxonium ions) in these solutions, as described in the previous chapter. They were originally named after their sharp, sour taste. The basicity of a solution, on the other hand, is associated with the presence of OH^- anions.

8.1 ARRHENIUS THEORY

Multiple theories exist which describe these compounds and their behaviour in solution. The oldest, and simplest theory describing these substances, is the *Arrhenius theory*. According to this theory, acids are compounds that produce hydrogen cations in solution, whereas bases are compounds containing OH^- ions which they dissociate into upon dissolution. A typical Arrhenius acid is hydrochloric acid:

$$HCl \rightarrow H^+ + Cl^-$$

Acids can be divided into *monoprotic* acids which generate only one H^+ per one molecule of acid (e.g., HCl, HNO_3), and *polyprotic* acids, generating several H^+ ions (e.g., H_2SO_4, H_3PO_4).

A single hydrogen cation (H^+) is in fact only the tiny nucleus of the hydrogen atom, consisting of a proton. Hence, the H^+ ion is sometimes called simply *proton* and its transfer reactions *protolysis*. The charge of this ion is concentrated in a very small volume, leading to high charge density. Thus, the particle is highly reactive and is attracted to any molecule with an excess of negative charge. In an aqueous solution, this molecule is water, and the product is *hydronium cation*. There is a donor-acceptor bond between the cation and the lone electron pair on oxygen (the non-bonding electron orbital).

$$H^+ + H_2O \rightarrow H_3O^+$$

Although a bare hydrogen cation is not stable in solution, it is often used in chemical equations for the sake of simplicity.

Typical Arrhenius bases are the hydroxides of the groups IA and IIA, dissociating into metal cations and hydroxide anions:

$$NaOH \rightarrow Na^+ + OH^-$$

When both the acid and the base are present in the solution, **neutralisation** reaction occurs. Ionic salts and neutral molecules of water are formed, e.g.:

$$NaOH + HCl \rightarrow NaCl + H_2O$$

The underlying neutralisation reaction is the recombination of hydroxide and hydronium ions:

$$H_3O^+ + OH^- \rightarrow H_2O$$

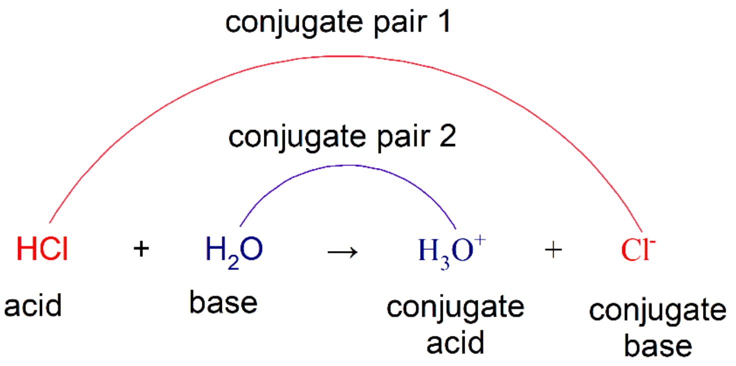
The simple Arrhenius theory does not explain why some substances that do not contain any hydroxide ions in their molecules still generate basic (alkaline) solutions in water. The typical example of such compounds is ammonia (NH_3).

8.2 Brønsted-Lowry theory

To provide explanations for this and similar disagreements, a more advanced theory is needed. The *Brønsted-Lowry theory* expands the Arrhenius theory to cover also acids and bases which do not contain hydrogen or hydroxide ions. This theory states:

- An acid is a *donor* of hydrogen cation (proton, H^+).
- A base is an *acceptor* of hydrogen cation (proton, H^+).

According to Brønsted-Lowry theory, a compound manifests itself as an acid only in a reaction with a base, e.g.:



Here HCl acts as a Brønsted-Lowry acid; it splits off H^+ and gives it to a water molecule, leaving behind a Cl^- anion. This anion is then called *conjugate base* (of HCl). The water molecule, on the other hand, accepts (binds) the hydrogen cation and turns itself into H_3O^+. Thus, the water molecule acts as a Brønsted-Lowry base and hydronium as a *conjugate acid* of this base.

An acid and its conjugate base, as well as a base and its conjugate acid, form a *conjugate pair*. Both species within this conjugate acid-base pair differ only in one hydrogen.

This theory also explains why there are hydroxide ions in the aqueous solution of ammonia:

$$NH_3 + H_2O \rightarrow NH_4^+ + OH^-$$

Ions of weak acids and bases can also undergo protolytic reactions. Ions of polyprotic acids like carbonic or phosphoric acid can act as both acids and bases, they are *amphoteric*.

$HCO_3^- + H_2O \rightarrow CO_3^{2-} + H_3O^+$ (HCO_3^- acts as an acid)

$HCO_3^- + H_3O^+ \rightarrow H_2CO_3 + H_2O$ (HCO_3^- acts as a base)

$H_2PO_4^- + H_2O \rightarrow HPO_4^{2-} + H_3O^+$ ($H_2PO_4^-$ acts as an acid)

$H_2PO_4^- + H_3O^+ \rightarrow H_3PO_4 + H_2O$ ($H_2PO_4^-$ acts as a base)

Even water can act as an amphoteric compound, as it is evident from its self-ionisation equation. Here one molecule of water acts as a base while the second one acts as an acid.

$$H_2O + H_2O \rightarrow H_3O^+ + OH^-$$

Example 1: *In the following reaction, decide which compound is an acid and which is a base. Also, identify their conjugate acid and conjugate base.*

$$HClO \ + \ H_2O \ \rightarrow \ ClO^- \ + \ H_3O^+$$

HClO loses a hydrogen ion, so it is an acid. What remains of this acid after the elimination of H^+, is the hypochlorite anion (ClO^-), which is the conjugate base of HClO. H_2O receives the H^+ ion, hence it is a base. The product of the addition of H^+ to water is the hydronium cation, which is the conjugate acid of H_2O.

8.2.1 Strength of acids and bases

An important property of acids and bases is their *strength*. It refers to the degree of ionization which the acid or base undergoes. They are strong if they are ionized completely in solution, e.g., a strong acid like $HClO_4$ exists in an aqueous solution only as ions. There are no non-ionized molecules of $HClO_4$ present in the solution, only perchlorate anions and hydronium cations.

$$HClO_4 \ + \ H_2O \ \rightarrow \ ClO_4^{--} \ + \ H_3O^+$$

Typical strong acids are H_2SO_4 (sulfuric acid), HCl (hydrochloric acid), HBr (hydrobromic acid), $HClO_4$ (perchloric acid), and HNO_3 (nitric acid). Strong bases include NaOH (sodium hydroxide), KOH (potassium hydroxide), and $Ca(OH)_2$ (calcium hydroxide).

A weak acid or base is ionized only partially. In an aqueous solution, an equilibrium is created between the ionized and non-ionized (neutral) forms, as indicated by the double arrow, e.g.:

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

Thus, the water solution of acetic acid contains a mixture of hydronium cations, acetate anions (CH_3COO^-), and non-ionized molecules of acetic acid (CH_3COOH). The amount of hydronium ions that you get in solutions of this acid is much less than it is with a strong acid. In a one molar aqueous solution of acetic acid, only about 0.4% of the acid dissociates into ions, that is, most of the acetic acid remains in the combined (neutral) form CH_3COOH. Other examples of weak acids are boric acid (H_3BO_3), carbonic acid (H_2CO_3), and hydrosulfuric acid (H_2S). A typical weak base is ammonia (NH_3).

The equilibrium between the ionized and non-ionized form in a solution of a weak acid (base) can be described by the *dissociation fraction α*.

$$\alpha = \frac{c_i}{c'}$$

In this equation, c_i is the concentration of the ionized form of the acid while c‘ is the overall concentration of the weak acid (the so-called *formal concentration*). In the case of acetic acid, concentration of the ionized form $c_i = c(CH_3COO^-) = c(H_3O^+)$. The formal concentration is the sum of concentrations of all forms of acetic acid, i.e., ionized (CH_3COO^-/ H_3O^+) and non-ionized (CH_3COOH) forms.

Example 2: *Calculate the concentration of hydronium ions in a 1 molar solution of acetic acid. The dissociation fraction of acetic acid at this concentration is 0.004, that is, 0.4% of the acid is dissociated into ions.*

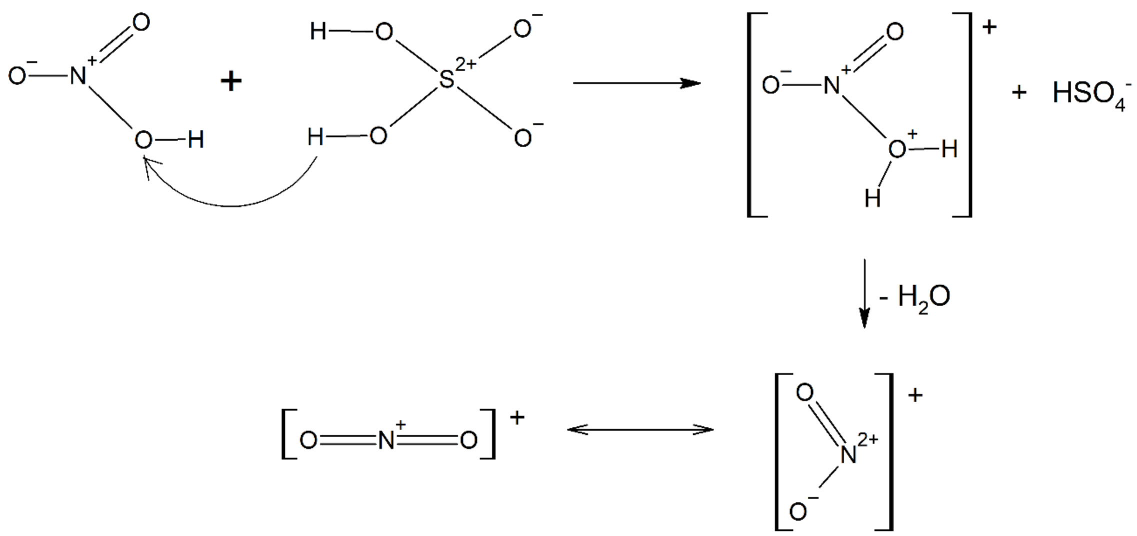
According to the ionization reaction of acetic acid, the concentration of the ionized form $c_i = c(CH_3COO^-) = c(H_3O^+)$. The formal concentration of acetic acid (regardless of its form) is 1M. Hence, the concentration of hydronium ions is given as

$c_i = c(H_3O^+) = \alpha \times c' = 0.004 \times 1 = 0.004M$

The strength of acids and bases according to the Brønsted-Lowry theory is always *relative*, always depending on the environment, i.e., on the second partner in the reaction. E.g., in the following reaction HNO_3 acts as an acid towards the base H_2O. The reason for this is that H_2O, although amphoteric, is a much weaker acid than HNO_3. Thus, it acts as a base within this conjugated pair.

$$HNO_3 + H_2O \rightarrow NO_3^- + H_3O^+$$

On the other hand, if we combine HNO_3 and H_2SO_4, the latter acid is stronger than HNO_3. Hence, sulfuric acid is ionized preferentially, splits off H^+ and thus acts as an acid. Meanwhile, nitric acid is the acceptor of H^+, acting as a base. The protonation of HNO_3 leads to *nitronium ion* NO_2^+, which is an important active agent in organic chemistry (aromatic nitration). The following mechanism describes the formation of nitronium ions:



A quantitative measure of the degree of dissociation of an acid or a base is given by its equilibrium constant. The higher the equilibrium constant, the greater the degree of dissociation of the acid or base. Therefore, a higher equilibrium constant means a stronger acid or base. For the general ionization reaction of an acid with water

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

the equilibrium constant is given as

$$K = \frac{c(H_3O^+) \times c(A^-)}{c(HA) \times c(H_2O)}$$

Since the concentration of H_2O (the solvent) is much higher than the concentrations of the ions, it can be considered constant and incorporated into the value of K. In this way, we obtain a new constant called the **acid dissociation constant** (K_a):

$$K_a = \frac{c(H_3O^+) \times c(A^-)}{c(HA)}$$

Similarly, the dissociation of a base B is described by the equation:

$$B + H_2O \rightleftharpoons HB^+ + OH^-$$

The **base dissociation constant** is then given as

$$K_b = \frac{c(HB^+) \times c(OH^-)}{c(B)}$$

The ionization of polyprotic acids like H_3PO_4 occurs in several steps:

$$H_3PO_4 \rightarrow H_3O^+ + H_2PO_4^-$$

$$H_2PO_4^- \rightarrow H_3O^+ + HPO_4^{2-}$$

$$HPO_4^{2-} \rightarrow H_3O^+ + PO_4^{3-}$$

For each step we can write its own acid dissociation constant (*stepwise constant*). Generally, the first step of this and similar reactions has the highest dissociation constant, that is, the strongest acid is in this case H_3PO_4. Consequently, the weakest acidity exhibits HPO_4^{2-}.

As the values of acid dissociation constants are rather small and difficult to deal with, we often use pK_a (pK_b) values instead:

$$pK_a = - \log(K_a)$$

For instance, the K_a value for acetic acid is 1.8×10^{-5}, so its pK_a value is 4.74.

8.2.2 Hydrolysis of salts

Neutralisation reactions between acids and bases provide ionic salts. If both the acid and the base are strong, the resulting solution is neutral. For example, sodium chloride (NaCl) is the product of a reaction between a strong acid (HCl) and a strong base (NaOH). Hence, the solution of sodium chloride in water is neutral. On the other hand, when one or both of the reacting partners are weak, the resulting salt solution has the pH value different from 7. E.g., the solution of sodium acetate is basic, and the solution of ammonium chloride is acidic. The reason for this is the *hydrolysis* (reaction with water) of the corresponding ions. Thus, ions derived from weak acids hydrolyse, producing hydroxide anions which cause the basic reaction of the solution. An example is the CN^- (cyanide) ion, derived from the weak acid HCN.

$$CN^- + H_2O \rightarrow HCN + OH^-$$

Cations derived from weak bases react with water producing hydronium ionswhich cause the solution to become acidic:

$$NH_4^+ + H_2O \rightarrow NH_3 + H_3O^+$$

If one of the ions in the salt is derived from a strong acid or base and the other from a weak one, the pH of the resulting salt solution is determined by the stronger acid or base. For instance, sodium carbonate Na_2CO_3 is the salt of the weak carbonic acid (H_2CO_3) and the strong base NaOH, the stronger partner (sodium hydroxide) prevails and the solution is basic. This is caused by the hydrolysis of the anion (the cation Na^+ does not hydrolyse):

$$CO_3^{2-} + H_2O \rightarrow HCO_3^- + OH^-$$

In the case both the acid and the base are weak, the resulting pH is determined by the stronger of them, although this is not so obvious as in the previous case and the table values of pK_a/pK_b need to be consulted.

Example 3: *Decide whether the aqueous solution of potassium sulfide is acidic or basic, and state the reason.*

Potassium sufide (K_2S) is the salt of the strong base potassium hydroxide (KOH) and the weak acid hydrogen sulfide (H_2S). Hence, the resulting solution of the salt is basic. The reason for this is the hydrolysis of the sulfide anion (the potassium cation does not hydrolyse).

$$S^{2-} + H_2O \rightarrow HS^- + OH^-$$

Salts containing ions of weak acids and bases are also part of **buffer solutions**. A buffer is a solution which can withstand pH change upon the addition of an acid or a base. It consists of a mixture of a *weak acid* and its *conjugate base*, or a mixture of a *weak base* and its *conjugate acid*. Buffers are able to neutralize small amounts of added acids or bases, keeping the pH value of the solution nearly constant. Consider the ionization of a generalized weak acid in solution:

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

This is an equilibrium reaction, the solution consists of all three components (HA, H^+, and A^-). Upon addition of a strong acid to the buffer, the excess of H^+ reacts with the anion A^-, and the reaction equilibrium is shifted to the left. On the other hand, when adding a strong base, the released OH^- anions neutralize the weak acid HA. An example is the buffer containing acetic acid and sodium acetate. The active principles of this buffer system are acetic acid CH_3COOH and its conjugate base, CH_3COO^-. The reactions following the addition of an acid or a base, respectively, are as follows:

Addition of an acid: $CH_3COO^- + H^+ \rightarrow CH_3COOH$

Addition of a base: $CH_3COOH + OH^- \rightarrow CH_3COO^- + H_2O$

Buffers are important in biochemical reactions as well as in various technological applications where there is a need to maintain constant pH. They are characterized by their *capacity*, that is, by the maximum amount of an acid or a base which can be added to the buffer solution without a radical change of the pH value. They also have a typical working pH range which is maintained upon the addition of small amounts af acid or base.

Example 4: *Write the reactions in the ammonia / ammonium chloride buffer after the addition of hydronium cations and hydroxide anions, respectively.*

This buffer contains a weak base (NH_3) and its salt with a strong acid (NH_4Cl). After the addition of an acid, ammonia reacts with the added H_3O^+ ions:

$$NH_3 + H_3O^+ \rightarrow NH_4^+ + H_2O$$

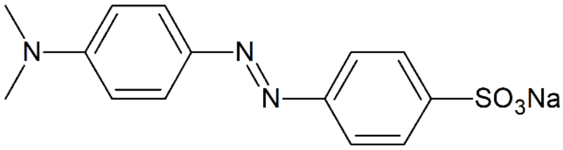
So the excess of the acid is neutralized and the pH of the solution does not change. If a base is added to the solution, it produces OH^- ions upon dissociation. These ions react with the ammonium ions. Again, a neutral molecule of water is produced and the pH does not change significantly.

$$NH_4^{+,} + OH^- \rightarrow NH_3 + H_2O$$

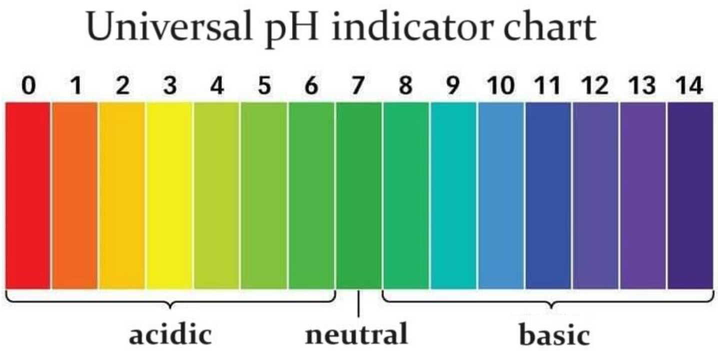
8.2.3 Measuring the pH

Today, the acidity and basicity of a solution (its pH value) is most often measured instrumentally, with the help of precise pH-meters. However, chemical methods for quick assesssment of pH are stillwidely used. A simple method employs substances which change their colour according to the pH of the solution, the **pH indicators**. These can be added in small amounts to the solution, or they can be used as dye-infused paper strips which can be dipped into the solution. The pH is then determined visually observing the colour of the solution or of the paper strip, and comparing it with a colour/pH key.

The indicators are either weak acids or bases. Their chemical structures usually involve alternating (conjugated) carbon-carbon double bonds. An example is the indicator *methyl orange*, changing its colour with increasing pH from red to orange to yellow. That is, in an acidic medium, methyl orange is red, and in a basic medium, it is yellow.



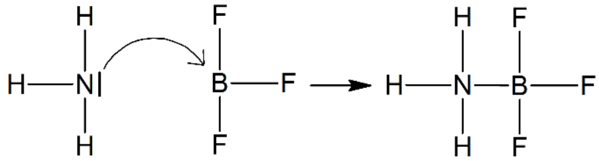
Common pH indicator is the *universal indicator*, used mainly on paper strips. It contains a mixture of several compounds that exhibit various smooth colour changes over a wide range of pH. The pH/colour code for this indicator is given below:



8.3 LEWIS THEORY

A completely different approach to acidity/basicity than the previous two theories provides the *Lewis theory*. According to this theory, *Lewis acid* is a compound that accepts a pair of electrons to form a covalent bond. *Lewis base*, on the other hand, is a compound that donates a pair of electrons to form a covalent (donor-acceptor) bond. Thus, a Lewis acid-base reaction means a transfer of a pair of electrons (a lone pair) from a base to an acid (unlike the reactions of Arrhenius and Brønsted-Lowry acids/bases, which are based on the transfer of H^+).

Lewis bases are molecules or ions containing a lone pair of electrons, e.g., NH_3, H_2O, Cl^- and OH^-. Typical Lewis acids are molecules with a lack of electrons (electron-deficient). They have an empty orbital which is capable of accepting an electron pair from a Lewis base to form a *Lewis adduct*. Examples include electron-deficient molecules like $AlCl_3$ or BF_3. The reaction between NH_3 as a Lewis base and boron trifluoride (BF_3) as a Lewis acid is shown below.



A large number of Lewis acids are cations, e.g., H^+, Fe^{3+}, or Al^{3+}. These are of special importance in coordination chemistry, as the formation of a metal complex is basically an interaction between a Lewis acid (the central metal atom) and a Lewis base (the donor atom of a ligand).

Example 5: *Explain the reaction between aluminium hydroxide and the OH^- ion.*

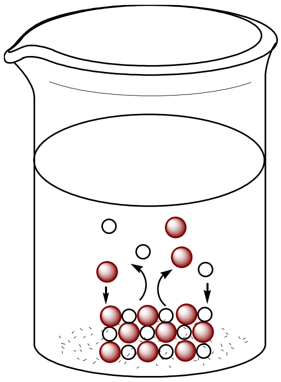
Aluminium hydroxide contains aluminium(III) atom which is a strong Lewis acid, acting as an electron pair acceptor. Hydroxide ion contains a lone electron pair, which can be used to form a donor-acceptor bond, i.e., it is a Lewis base. The product of their reaction is the tetrahydroxidoaluminate(1-).

$Al(OH)_3 \quad + \quad OH^- \quad \rightarrow \quad [Al(OH)_4]^-$

8.4 PROBLEMS

1. Find the correct conjugated acid or base for the following compounds acting as Brønsted-Lowry acids (A) or bases (B):
   HSO_4^- (B): .... (conj. A)
   NH_3 (A): .... (conj. B)
   H_2O (A): .... (conj. B)
   ClO_4^- (B) .... (conj. A)
2. Write both dissociation steps for sulfurous acid (H_2SO_3), together with their stepwise dissociation constants.
3. The value of the dissociation fraction α for a given weak acid is 0.11. How much of the acid in solution (in %) remains undissociated?
4. Which ion in the salt NaOCl (sodium hypochlorite) does undergo hydrolysis? Write the hydrolysis of this ion (its reaction with water).
5. Classify the two species, Br^- and $AlBr_3$, as either a Lewis base or a Lewis acid. Write their mutual reaction according to the Lewis acid-base theory.
6. Explain the reaction between $Zn(OH)_2$ and the OH^- ion

9 HETEROGENOUS EQUILIBRIUM – SOLUBILITY PRODUCT



In saturated solutions, a dynamic equilibrium exists where ions are constantly released from the solid to dissolve in the solvent and dissolved ions are returning to the solid at the same rate.

$A_xB_y(s) \leftrightarrow x\ A^+(aq) + y\ B^-(aq)$

The equilibrium constant for this heterogeneous equilibrium is called the **solubility product** (K_{sp})

$$\boldsymbol{K_{sp} = c_A^x \times c_B^y}$$

where c_A and c_B are the equilibrium concentrations of the cation A^+ and the anion B^-, powered by their stoichiometric coefficients x and y from the equilibrium chemical equation above.

Solubility product constant (K_{sp}) is an equilibrium constant that is equal to the mathematical product of the molar concentrations (activities) of the solvated ions powered to its stoichiometric coefficient and tells us the maximum concentration (in mol dm^{-3}) of ions that can coexist in saturated solution.
*K_{sp} value remains always **constant**, and it is used for poorly **soluble salts**.*

Example 1: *Write the K_{sp} formulas for the following compounds: AgI, $CaCO_3$, $Zn(OH)_2$, Li_3PO_4, Sb_2S_3.*

$AgI \leftrightarrow Ag^+ + I^-$	$K_{sp} = c_{Ag}^1 \times c_I^1 = c_{Ag} \times c_I$
$CaCO_3 \leftrightarrow Ca^{+2} + CO_3^{-2}$	$K_{sp} = c_{Ca}^1 \times c_{CO3}^1 = c_{Ca} \times c_{CO3}$
$Zn(OH)_2 \leftrightarrow Zn^{+2} + 2\ OH^-$	$K_{sp} = c_{Zn}^1 \times c_{OH}^2 = c_{Zn} \times c_{OH}^2$
$Li_3PO_4 \leftrightarrow 3\ Li^+ + PO_4^{-3}$	$K_{sp} = c_{Li}^3 \times c_{PO4}^1 = c_{Li}^3 \times c_{PO4}$
$Sb_2S_3 \leftrightarrow 2\ Sb^{+3} + 3\ S^{-2}$	$K_{sp} = c_{Sb}^2 \times c_S^3$

It demonstrates whether the solution is unsaturated, saturated or contains too much of the solute depending on whether the mathematical product number is lower, equal, or higher than the value of K_{sp}.
For example, for $AgCl \leftrightarrow Ag^+ + Cl^-$

$c(Ag^+) \times c(Cl^-) < K_{sp}$	the solution is unsaturated, no precipitate is formed
$c(Ag^+) \times c(Cl^-) = K_{sp}$	the solution is saturated, the maximum amount of the substance is dissolved, and no precipitate is formed
$c(Ag^+) \times c(Cl^-) > K_{sp}$	the amount of solute is higher than the amount in saturated solution, solid AgCl is formed

Example 2: *Calculate the concentrations of the salts and their ions from K_{sp}.*

a) ***AgCl, K_{sp}*** = $\mathbf{1 \times 10^{-10}}$

$AgCl \leftrightarrow Ag^{+} + Cl^{-}$ $\qquad\qquad$ $K_{sp} = c_{Ag} \times c_{Cl}$

The stoichiometric ratio of AgCl, Ag^{+} and Cl^{-} is 1 : 1 : 1, which means the chemical amount of these 3 particles dissolved will be the same.
Since the solution doesn't undergo any changes, such as the change of overall volume or concentration, we can also conclude that the concentrations of these 3 particles will be the same too:
$c_{Ag} = c_{Cl} = c_{AgCl} = c$ $\qquad$ *so we can replace them:* $\qquad$ $K_{sp} = c_{Ag} \times c_{Cl} = c^2$

Since K_{sp} is a known value, we can calculate the concentrations as:

$$c = \sqrt{K_{sp}} = \sqrt{1 \times 10^{-10}} = \mathbf{1 \times 10^{-5}}\ \boldsymbol{M} = c_{Ag} = c_{Cl} = c_{AgCl}$$

b) ***PbF_2, K_{sp}*** = $\mathbf{3.2 \times 10^{-8}}$

$PbF_2 \leftrightarrow Pb^{+2} + 2\,F^{-}$ $\qquad\qquad$ $K_{sp} = c_{Pb} \times c_F^2$

The stoichiometry of PbF_2 and Pb^{+2} is 1 : 1, so we can write: $c_{Pb} = c_{PbF2} = c$
The stoichiometry of PbF_2 and F^{-} is 1 : 2, so we can write: $c_F = 2 \times c_{PbF2} = 2c$

So when we replace them, we get:
$K_{sp} = c_{Pb} \times c_F^2 = c \times (2c)^2 = 4c^3$

To calculate the concentration c, we use the 3rd root:

$$c = \sqrt[3]{K_{sp}/4} = \sqrt[3]{(3.2 \times 10^{-8})/4} = \sqrt[3]{8 \times 10^{-9}} = 0.002\ M$$

$c_{Pb} = c_{PbF_2} = \mathbf{0.002}\ \boldsymbol{M}$ $\qquad$ $c_F = 2c = \mathbf{0.004}\ \boldsymbol{M}$

c) ***Li_3PO_4, K_{sp}*** = $\mathbf{3.36 \times 10^{-9}}$

$Li_3PO_4 \leftrightarrow 3\,Li^{+} + PO_4^{-3}$ $\qquad\qquad$ $K_{sp} = c_{Li}^3 \times c_{PO_4}$

The stoichiometry of Li_3PO_4 and Li^{+} is 1 : 3, so we can write: $c_{Li} = 3 \times c_{Li_3PO_4} = 3c$
The stoichiometry of Li_3PO_4 and PO_4^{-3} is 1 : 3, so we can write: $c_{PO_4} = c_{Li_3PO_4} = c$

Upon the substitution, we get:
$K_{sp} = c_{Li}^3 \times c_{PO_4} = c \times (3c)^3 = 27c^4$

To calculate the concentration c, we use the 4th root:

$$c = \sqrt[4]{K_{sp}/27} = \sqrt[4]{(3.36 \times 10^{-9})/27} = \sqrt[4]{8 \times 10^{-9}} = 3.34 \times 10^{-3}\ M$$

$c_{PO_4} = c_{Li_3PO_4} = \mathbf{3.34 \times 10^{-3}\ M}$ $c_{Li} = 3c = \mathbf{0.01\ M}$

K_{sp} can be calculated if the concentrations are known. The calculations using the K_{sp} values can be used to calculate the properties of the solutions, such as the mass of dissolved solute or the volume needed to dissolve the poorly soluble solute and other quantities.

Example 3: The solubility product of AgBr (M_r = 187.77) is 3.6 × 10^{-13}. State:
a) the concentration of this salt (mol dm^{-3}),
b) the mass of AgBr in 100 litres of solution,
c) the number of Ag^+ particles in 100 litres of solution,
d) the weight fraction and percentage of AgBr in its saturated solution (*d* = 1.00 g/mL = 1.00 kg/L).

a) $AgBr \leftrightarrow Ag^+ + Br^-$ $\qquad K_{sp} = c_{Ag} \times c_{Br}$

$c_{Ag} = c_{Br} = c$ $\qquad K_{sp} = c_{Ag} \times c_{Br} = c^2$

$c = \sqrt{K_{sp}} = \sqrt{3.6 \times 10^{-13}} = \mathbf{6 \times 10^{-7}\ M}$

b) $n = c \times V(sol.) = 6 \times 10^{-7} \times 100 = 6 \times 10^{-5}\ mol$

$m_{AgBr} = n \times M_r = 6 \times 10^{-5} \times 187.77 = 0.0112\ g = \mathbf{11.2\ mg}$

c) $n_{Ag} = n_{Br} = n$
$N = n \times N_A = 6 \times 10^{-5} \times 6.022 \times 10^{23} = 3.613 \times 10^{19}$ Ag^+ particles

d) $m(sol.) = V(sol.) \times d(sol.) = 100\ L \times 1.00 \frac{kg}{L} = 100\ kg = 100\ 000\ g$

$w = \frac{m_{AgBr}}{m(sol.)} = \frac{0.0112}{100\ 000} = 1.12 \times 10^{-7}$ so $w(\%) = w \times 100 = 1.12 \times 10^{-5}\%$

Note: As the concentration of solutions in question is very low, the density (d) is considered to be 1 g/mL.

Since K_{sp} is always a constant, there is one interesting implication: If a well soluble salt of one ion (for example KCl) is added to a saturated solution of a badly soluble salt (for example AgCl), it causes AgCl to precipitate. This si caused by the fact that if the concentration of chloride anions is high, so the concentration of silver ions must decrease.

9.1 PROBLEMS

1. Write the dissociation reaction and expression of the solubility product for the following substances: $Bi(OH)_3$, $BaCO_3$, PbF_2, AgOH, Sb_2S_3, $PbCrO_4$, $CaSO_4$, HgS, CaF_2, $Mg(OH)_2$.

2. The solubility product of AgCl is 10^{-10}. State the concentration of this salt.

3. The solubility product of PbF_2 is 3.2×10^{-8}. State the concentration of both ions (Pb^{2+} and F^-) in its saturated solution.

4. Solubility of $Mg(OH)_2$ (M_r = 58.33) in water is 0.00912 g in 1 liter. State the solubility product.

5. The solubility product of AgOH is 1.5×10^{-8}. State the concentration of the hydroxide ion and the pH value in its saturated solution.

6. For dissolving of 1.0 gram of $PbCl_2$ (M_r = 278) we need 2.27 dm^3 of water. Determine the solubility product.

7. The concentration of Pb^{2+} cations in saturated solution of PbI_2 is 1.5×10^{-3} mol/L. State the solubility product.

8. The solubility product of AgBr (M_r = 187.8) is 5.04×10^{-3}. State the concentration of this salt. How many grams of this salt are in 200 mL of its solution?

9. The solubility product of Ag_2S is $K_{sp} = 5.7 \times 10^{-51}$. Determine the number of Ag^+ particles in 1 litre and 100 mL of its saturated solution.

10. The molar concentration of Li_3PO_4 is 3.34×10^{-3} mol/L. State the solubility product.

11. How many grams of ZnS (M_r = 97.4) are in 2 litres of its solution, when the solubility product is equal to 4.0×10^{-2}?

12. State the concentration of Ni^{2+} cations in a saturated solution of NiS with the solubility product $K_{sp} = 1.0 \times 10^{-24}$.

13. The solubility product of $CaCO_3$ (M_r = 100) at 25 ˚C is 8.70×10^{-9}. Calculate the number of grams of $CaCO_3$ in 100 mL of its saturated solution.

14. The solubility product of PbF_2 is 3.2×10^{-8}. State the number of Pb^{2+} cations in one litre of its saturated solution.

15. 100 mL of $PbCrO_4$ contain 1.11×10^{-5} grams of Pb^{2+} (A_r = 207.2) particles. State the solubility product of this salt.

16. The concentration of $SrSO_4$ in saturated solution at 18 °C is 1.67×10^{-4} mol/L. State the solubility product.

17. In 500 mL of a saturated solution of CaF_2 (M_r = 78.07) (at 25 °C), 11.71 miligrams of this salt are dissolved. State the solubility product.

18. Determine the solubility product of PbI_2 in its saturated solution at 18 °C in which concentration of I^- anions was found to be 3×10^{-3} mol dm^{-3}.

19. 100 mL of Li_3PO_4 (M_r = 115.79) solution contain 0.0387 g of this salt. State the solubility product.

20. 200 mL of a saturated solution of PbI_2 (M_r = 461.0) contain 0.14 g of this salt. State the solubility product.

21. The saturated solution of $Cd(OH)_2$ (M_r = 146.43, d = 1 g/mL) corresponds to 2.6×10^{-4}%. State the solubility product.

22. Solubility product of SrF_2 (M_r = 125.62) has the value $K_{sp} = 3 \times 10^{-9}$. Calculate the concentration of this salt, as well as the concentrations of Sr^{2+} and F^- ions in saturated solution.

23. State the volume of water required for dissolving of 1.0 gram of $BaCO_3$ (M_r = 197.34), when $K_{sp} = 1.9 \times 10^{-9}$.

24. Calculate the concentration of Ag^+ and CrO_4^{2-} ions in a saturated solution of Ag_2CrO_4 at 20 °C, when the value of $K_{sp} = 1.1 \times 10^{-12}$.

25. The concentration of F^- anions in a saturated solution of CaF_2 at 18 °C has the value 4×10^{-4} mol/L. Determine the concentration of Ca^{2+} cations and the value of solubility product.

26. To dissolve 1g of $PbCrO_4$ (M_r = 323.2), 500 litres of solvent are necessary. State the solubility product.

27. State the number of mg of silver (A_r = 107.87) in 20 L of saturated aqueous solution of AgBr (M_r = 187.77) at 25 °C, when solubility product is equal to 3.6×10^{-13}.

28. Concentration of Cu_2S (M_r = 159.15) in its saturated solution at 25 °C is 5×10^{-8} mol/L. State the concentrations of the individual ions.

29. Solubility product of $CaSO_4$ is equal to 2.0×10^{-4}. Determine whether after mixing of equivalent volumes of solutions of $CaCl_2$ and Na_2SO_4 (concentration in both is 1×10^{-2} mol/L) the solid $CaSO_4$ will be formed.

30. Solubility product of Ag_2SO_4 is equal to 7.0×10^{-5}. Decide whether after addition of 0.01 M solution of H_2SO_4 to the same volume of 0.1 M solution of $AgNO_3$ the precipitation of Ag_2SO_4 will take place.

Answers:
2) 10^{-5} M *3*) 2×10^{-3} M, 4×10^{-3} M *4*) 1.53×10^{-11} *5*) 1.22×10^{-4} M, pH = 10.08 *6*) 1.59×10^{-8} *7*) 1.35×10^{-8} *8*) 0,071 M, 2.67 g *9*) 1.36×10^{7}, 1.36×10^{6} *10*) 3.4×10^{-9} *11*) 38.96 g *12*) 10^{-12} M *13*) 9.35×10^{-4} g *14*) 1.2×10^{21} *15*) 2.87×10^{-13} *16*) 2.79×10^{-8} *17*) 1.08×10^{-10} *18*) 1.35×10^{-8} *19*) 3.36×10^{-9} *20*) 1.4×10^{-8} *21*) 2.2×10^{-14} *22*) 9.08×10^{-4}, 1.816×10^{-3} *23*) 116 litres *24*) c(Ag^+) = 1.3×10^{-4} M, c(CrO_4^{-2}) = 6.5×10^{-5} M *25*) c(Ca^{2+}) = 2×10^{-4} M, 3.2×10^{-11} *26*) 3.83×10^{-11} *27*) 1.29 mg *28*) c(Cu^+) = 10^{-7} M, c(S^{2-}) = 5×10^{-8} M *29*) no *30*) no

10 OXIDATION–REDUCTION REACTIONS

Oxidation–reduction (redox) reactions involve the transfer of one or more electrons from one species to another. If one substance is oxidized, another one must be reduced.

Oxidation is a chemical change in which an atom, ion, or molecule **loses** electrons. Giving electrons away also results in a shift of oxidation state to higher values – ***oxidation state on at least one atom is increased***.

Reduction is a chemical change in which an atom, ion, or molecule **gains** electrons. Accepting electrons also results in a shift of oxidation state to lower values – ***oxidation number on at least one atom is decreased***.

For example, in the reaction of metallic sodium with chlorine gas, sodium is oxidized (change of oxidation state from 0 to +I) and chlorine is reduced (change of oxidation state from 0 to -I).

$$2\ Na + Cl_2 \rightarrow 2\ Na^+ + 2\ Cl^-$$

An electron is transferred from the sodium atom to the chlorine atom. ***Oxidation and reduction processes always occur simultaneously.***

Oxidation agent is a compound able to accept electrons from another compound. By accepting electrons, the oxidation agent is reduced, and the other compound is oxidized. **Reduction agent** does the opposite – it gives electrons to another compound, so reduction agent is oxidized while the other compound is reduced.
In other words, oxidation agent reacts with a reduction agent.

In the sodium–chlorine reaction, sodium is the reducing agent and chlorine is the oxidizing agent.

While studying the redox reactions, we can split each reaction into two **half reactions** – one for oxidation and one for reduction.

For the sodium–chlorine reaction, they are:
oxidation $2\ Na - 2\ e^- \rightarrow 2\ Na^+$
reduction $2\ Cl + 2\ e^- \rightarrow 2\ Cl^-$

Oxidation process must be always accompanied by a reduction process, it means the overall ***number of electrons released must be equal to the number of electrons received***.

Example 1: *Determine how many electrons are transferred in the following reaction:*
$CuSO_4 + Zn \rightarrow ZnSO_4 + Cu$

First, we need to figure out the oxidation states (see the chapter Oxidation States of Elements) and where the change of oxidation state is present. In this reaction, there is a change on Cu and Zn:
$Cu^{II} + Zn^0 \rightarrow Cu^0(s) + Zn^{II}$

Zn^0 *loses electrons (is oxidized) and is a reducing agent:*
$Zn^0 - 2\ e^- \rightarrow Zn^{2+}$

Cu^{2+} accepts electrons (is reduced) and is an oxidizing agent
$Cu^{2+} + 2\,e^{-} \rightarrow Cu^{0}$

In this reaction, 2 electrons ate transferred from Zn to Cu.

***Example 2:** Determine how many electrons are transferred in the following reaction:*
$Fe + Cl_2 \rightarrow FeCl_3$

The changes of oxidation states are:
$Fe^{0} + Cl_2^{0} \rightarrow Fe^{+III} + Cl_3^{-I}$

Oxidation is present on Fe and since there is one Fe atom on each side, we can write the half reaction directly:

$Fe^{0} - 3\,e^{-} \rightarrow Fe^{III}$

Reduction occurs on Cl, but there are not equal number of atoms in the reaction. Therefore, we must multiply the number of Cl atoms to have same number – 6 atoms:

$3\,Cl_2^{0} + 6\,e^{-} \rightarrow 2\,Cl_3^{-I}$

But in the oxidation half reaction, there are 3 electrons, and in the reduction 6 electrons. We must balance these numbers so that there is the same number of given and accepted electrons. If the oxidation reaction is multiplied by 2, we get 6 given electrons which would match 6 accepted electrons:

$Fe^{0} - 3\,e^{-} \rightarrow Fe^{III} \qquad \times 2$
$3\,Cl_2^{0} + 6\,e^{-} \rightarrow 2\,Cl_3^{-I}$

In this way we get:
$2\,Fe^{0} - 6\,e^{-} \rightarrow 2\,Fe^{III}$
$6\,Cl^{0} + 6\,e^{-} \rightarrow 6\,Cl^{-I}$

In this reaction, 6 electrons are transferred from 2 iron atoms to 6 chlorine atoms.

To successfully balance the redox reaction problems, the following steps are recommended:

1. Find the proper **oxidation numbers of elements** in question.

2. Write the **half reactions** with the exchange of electrons. Keep in mind that there must be the same number of atoms of reactants and products in the half reactions.

2. **Balance the number of gained and lost electrons** in half reactions by multiplying the half reactions.

3. If reaction contains compounds where no changes of oxidation numbers occurred, they must be balanced too by using stoichiometric coefficients.

4. **Water** can be an additional reactant or product not mentioned in the original reaction assignment. Balance the number of oxygen and hydrogen atoms by adding of H_2O, if needed.

5. **Check the number of all atoms** on both sides of equation. Usually, this can be done by summing the number of O atoms on each side of the reaction.

Example 3: *Balance the following redox reaction:* $Cu + HNO_3 \rightarrow Cu(NO_3)_2 + NO$

Oxidation state changes: Cu is oxidized, N is reduced.

$Cu^{0} + HN^{+V}O_3 \rightarrow Cu^{+II}(N^{+V}O_3)_2 + N^{+II}O$

Half reactions:

Ox: $Cu^{+0} - 2\,e^{-} \rightarrow Cu^{+II}$ / × 3

Red: $N^{+V} + 3\,e^{-} \rightarrow N^{+II}$ / × 2

Ox: $3\,Cu^{+0} - 6\,e^{-} \rightarrow 3\,Cu^{+II}$

Red: $2\,N^{+V} + 6\,e^{-} \rightarrow 2\,N^{+II}$

Sum: $3\,Cu^{+0} + 2\,N^{+V} \rightarrow 3\,Cu^{+II} + 2\,N^{+II}$

The numbers of atoms in the sum reaction above give the stoichiometric coefficients for the compounds of the reduced and oxidized atoms:

$3\,Cu + 2\,HNO_3 \rightarrow 3\,Cu(NO_3)_2 + 2\,NO$

In the new reaction, the numbers of N atoms don't match. The left side contains 2 N atoms, the right side 8 N atoms. No extra N-containing compound is added to the left side of the equation. On the right side of the equation, there are 6 atoms of N that do not change their oxidation number. The only molecule with N on the left side is HNO_3*. Therefore, we must add 6 molecules of* HNO_3 *to the left side of the equation:*

$3\,Cu + 8\,HNO_3 \rightarrow 3\,Cu(NO_3)_2 + 2\,NO$

Now, there are matching numbers of Cu (3x) and N (8x) on both sides of the reaction. But the numbers of H and O don't match: H – 8 on left side, 0 on right side, O – 24 on left side, 20 on right side.
This means that 4 water molecules must be added to the right side:

$3\,Cu + 8\,HNO_3 \rightarrow 3\,Cu(NO_3)_2 + 2\,NO + 4\,H_2O$

Now there are 8x H and 24x O on each side.

In some reactions, atoms of ***two different elements can be oxidized simultaneously within a single molecule***. Therefore, both atoms are reducing agents. or the whole compound is a reducing agent. If this is the case, it is crucial for solving the redox reaction to ***keep the ratio of the two elements in the compound constant in the calculations***.

Example 2: *Balance the following redox reaction:* $FeS_2 + O_2 \rightarrow Fe_2O_3 + SO_2$

Redox changes:

$Fe^{+II}S_2^{-I} + O_2^{0} \rightarrow Fe_2^{+III}O_3^{-II} + S^{+IV}O_2^{-II}$

In FeS_2*, both Fe and S are oxidized. The two elements are in the* ***ratio 1 : 2****, so this ratio must be kept also in the half reactions. The half reactions must be multiplied by the same number, not separately!*

Half reactions:

Ox1:	$2\ Fe^{+II} - 2e^{-} \rightarrow Fe_2^{+III}$	$\times\ 2$
Ox2:	$4\ S^{-I} - 20e^{-} \rightarrow 4\ S^{+IV}$	$\times\ 2$
		must be 4x S, if Fe is 2x to keep ratio
Red:	$O_2^{0} + 4e^{-} \rightarrow 2\ O^{-II}$	$\times\ 11$

Ox1: $4\ Fe^{+II} - 4e^{-} \rightarrow 2\ Fe_2^{+III}$
Ox2: $8\ S^{-I} - 40e^{-} \rightarrow 8\ S^{+IV}$

Red: $11\ O_2^{0} + 44e^{-} \rightarrow 22\ O^{-II}$

Sum: $4\ Fe^{+II} + 8\ S^{-I} + 11\ O_2^{0} \rightarrow 2\ Fe_2^{+III} + 8\ S^{+IV} + 22\ O^{-II}$

$4\ FeS_2 + 11\ O_2 \rightarrow 2\ Fe_2O_3 + 8\ SO_2$

On each side there are 4x Fe, 8x S, 22x O.

10.1 Problems

Balance the following reactions using the oxidation number method.

1. $Pb + O_2 \rightarrow PbO$
2. $HNO_3 + HI \rightarrow NO + I_2 + H_2O$
3. $Cr_2O_3 + KNO_3 + KOH \rightarrow K_2CrO_4 + KNO_2 + H_2O$
4. $As_2O_3 + Zn + H_2SO_4 \rightarrow AsH_3 + ZnSO_4 + H_2O$
5. $Br_2 + KOH \rightarrow KBr + KBrO_3 + H_2O$
6. $Ti + HNO_3 + HCl \rightarrow TiCl_4 + NO + H_2O$
7. $NH_3 + Br_2 \rightarrow NH_4Br + N_2$

8. Fe_2O_3 + C → FeO + CO_2

9. Bi_2O_3 + C → Bi + CO

10. HF + Si → SiF_4 + H_2

11. SnO_2 + C → Sn + CO

12. Mg + CO_2 → MgO + C

13. PbS + H_2O_2 → $PbSO_4$ + H_2O

14. Ag_2O + H_2 → Ag + H_2O

15. NO + O_2 → N_2O_5

16. $Mn(NO_3)_2$ + PbO_2 + HNO_3 → $Pb(NO_3)_2$ + $HMnO_4$ + H_2O

17. Cu + H_2SO_4 → $CuSO_4$ + SO_2 + H_2O

18. Zn + H_2O + NaOH → $Na_2[Zn(OH)_4]$ + H_2

19. Na_2O_2 + Na → Na_2O

20. CuS + HNO_3 → $Cu(NO_3)_2$ + NO_2 + H_2SO_4 + H_2O

21. $K_2Cr_2O_7$ + HCl → KCl + $CrCl_3$ + Cl_2 + H_2O

22. $KMnO_4$ + NH_3 → KNO_3 + MnO_2 + KOH + H_2O

23. Cu_2S + HNO_3 → $CuSO_4$ + $Cu(NO_3)_2$ + NO_2 + H_2O

24. KNO_3 + S + C → K_2S + N_2 + CO_2

25. AsI_3 + H_2O_2 → H_3AsO_4 + I_2 + H_2O

26. As_2S_3 + HNO_3 → H_3AsO_4 + S + NO_2 + H_2O

27. Write a balanced equation for the reaction of potassium permanganate with hydrogen peroxide in the medium of sulfuric acid. Oxygen, potassium sulfate, manganese(II) sulfate and water are formed as products.

28. The industrial production of nitrogen monoxide is based on catalytic reaction of ammonia with atmospheric oxygen. Water is produced as a secondary product. Write a balanced chemical reaction.

29. Oxidation of sulfur with diluted nitric acid is followed by formation of sulfur dioxide, nitrogen monoxide, and water. Write a balanced chemical equation.

30. In the reduction process of calcium sulfate with carbon, calcium sulfide and carbon monoxide were found to be formed. Write a balanced chemical equation.

31. The oxidation–reduction process between phosphorus and nitric acid in water results in the formation of trihydrogen phosphoric acid and nitrogen monoxide. Write a balanced equation.

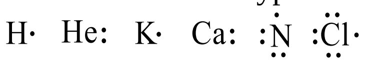
Answers:

1. $2 + 1 \rightarrow 2$
2. $2 + 6 \rightarrow 2 + 3 + 4$
3. $1 + 3 + 4 \rightarrow 2 + 3 + 2$
4. $1 + 6 + 6 \rightarrow 2 + 6 + 3$
5. $3 + 6 \rightarrow 5 + 1 + 3$
6. $3 + 4 + 12 \rightarrow 3 + 4 + 8$
7. $8 + 3 \rightarrow 6 + 1$
8. $2 + 1 \rightarrow 4 + 1$
9. $1 + 3 \rightarrow 2 + 3$
10. $4 + 1 \rightarrow 1 + 2$
11. $1 + 2 \rightarrow 1 + 2$
12. $2 + 1 \rightarrow 2 + 1$
13. $1 + 4 \rightarrow 1 + 4$
14. $1 + 1 \rightarrow 2 + 1$
15. $4 + 3 \rightarrow 2$
16. $2 + 5 + 6 \rightarrow 5 + 2 + 2$
17. $1 + 2 \rightarrow 1 + 1 + 2$
18. $1 + 2 + 2 \rightarrow 1 + 1$
19. $1 + 2 \rightarrow 2$
20. $1 + 10 \rightarrow 1 + 8 + 1 + 4$
21. $1 + 14 \rightarrow 2 + 2 + 3 + 7$
22. $8 + 3 \rightarrow 3 + 8 + 5 + 2$
23. $1 + 12 \rightarrow 1 + 1 + 10 + 6$
24. $2 + 1 + 3 \rightarrow 1 + 1 + 3$
25. $2 + 5 \rightarrow 2 + 3 + 2$
26. $1 + 10 \rightarrow 2 + 3 + 10 + 2$
27. $5\ H_2O_2 + 2\ KMnO_4 + 3\ H_2SO_4 \rightarrow 5\ O_2 + 2\ MnSO_4 + K_2SO_4 + 8H_2O$
28. $4\ NH_3 + 5\ O_2 \rightarrow 4\ NO + 6\ H_2O$
29. $3\ S + 4\ HNO_3 \rightarrow 3\ SO_2 + 4\ NO + 2\ H_2O$
30. $CaSO_4 + 4\ C \rightarrow CaS + 4\ CO$
31. $3\ P + 5\ HNO_3 + 2\ H_2O \rightarrow 3\ H_3PO_4 + 5\ NO$

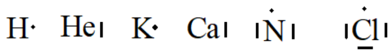
11 LEWIS STRUCTURE FORMULAS

Structure formulas show every atom separated and bound to other atoms by covalent or ionic bonds.
In **Lewis structure formulas,** each atom must have specified the <u>number of valence electrons</u> surrounding it – either in bond pairs or lone electron pairs localized on the atom.

A **Lewis symbol** consists of the chemical symbol of an element and a dot for each of its valence electrons. Typical examples are:



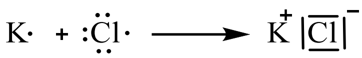
A pair of dots represents an electron pair called lone electron pair (LEP). It is usually written as a line:



11.1 IONIC COMPOUNDS

Ionic bonds are formed between one metal and one non-metal element with large difference in electronegativity.
To work out the formula of an ionic compound, we first have to decide which is the less electronegative atom. This atom will give one or more electrons, depending on the oxidation state, to the more electronegative.

In KCl for example, K is the less electronegative and it is in group 1A of the periodic table. Therefore, the oxidation state can only be +I and potassium is able to give its only valence electron to Cl. In this way, K has 0 valence electronsand the cation K^{+1} is formed. Cl has 8 electrons and the anion Cl^{-1} is formed.



In calcium chloride, Ca is a low electronegativity metal from 2A group, it has 2 valence electrons and can give them away to more electronegative atoms, such as Cl. Since Cl has only one “empty slot“ for an electron (Cl: [Ne] $3s^2$ $3p^5$) to become Cl^{-1} (Cl^{-1}: [Ne] $3s^2$ $3p^6$), there must be two Cl atoms to accommodate the two electrons supplied by one Ca atom:

In each case, the transfer of electrons results in the formation of an **octet of electrons** (an ns^2 np^6 electron configuration) on each of the atoms. Hydrogen, lithium and beryllium are exceptions to this rule, because the n = 1 shell is complete with only two electrons.

When s–block metal atom forms a cation, it loses all its valence electrons and is left with only its core. That core has the octet configuration of the preceeding noble gas element. For anions, the $(n\text{-}1)s^2$ $(n\text{-}1)p^6$ configuration applies. Hydrogen is the only s-element that can also take an electron to form a negatively charged hydride (**doublet** $1s^2$, which is the electron configuration of the noble gas helium).

Cations of s-elements and anions of p-elements usually acquire electron configurations of noble gases. For example, oxygen anion in ionic oxides O^{-2} has the same electron configuration as Ne noble gas.

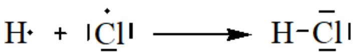
11.2 COVALENT COMPOUNDS

Lewis's octet rule: In covalent bonds, atoms share electrons to reach noble gas configuration – ns^2 np^6 (or $1s^2$ for H).

Consider molecular hydrogen H_2. Each atom completes its helium-like doublet by sharing its electron with the other:

$$H\cdot + \cdot H \longrightarrow H{-}H$$

In the HCl molecule, there is one single covalent bond made of two electrons. These two electrons are shared by both atoms:



In this way, H has 2 electrons and forms a doublet and Cl has 8 electrons (2 from bond pair, 6 from lone electron pairs) and forms an octet.

A single shared pair of electrons is called a **single** bond. However, atoms can share two or three electron pairs. A **double** bond, e.g. O = O contains 4 electrons and a **triple** bond, e.g., N ≡ N contains 6 electrons. Collectively, double and triple bonds are called **multiple** bonds.
Covalent bonds are formed between atoms of relatively similar values of electronegativity. Generally, these atoms belong to nonmetal elements.

11.3 DRAWING OF LEWIS STRUCTURE FORMULAS

To draw Lewis structure formula follow these recommendation:
1. Central atom: As a rule, the central atom is the p-element atom with the lowest electronegativity.

For covalent compounds containing only two elements, the central atom is the one that appears only once in the formula (H is never a central atom).
For covalent compounds containing H, O and a third element, the central atom is the third element. For example in H_2CO_3, it is C.

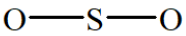
For example, in SO_2 it is sulfur. Arrange the other atoms symmetrically around the central atom: O S O

2. Total number of valence electrons: Count the total number of valence electrons on each atom and determine the number of electron pairs in the molecule.

In SO_2: S belongs to 6A group, it has 6 electrons
2x O belonging to 6A group, it has 6 x 2 = 12 electrons
In total: 18 electrons or 9 electron pairs

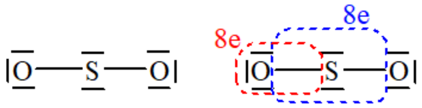
If a molecule is not electroneutral, i.e., it is a cation, it has less electrons. A cation with the charge +2 would have 2 electrons less. If a molecule is an anion, it has more electrons.

3. **Connect atoms with single bonds:** put bond pairs between the atoms.



4. **Complete the octet** (or doublet in the case of H): Put the remaining electrons around the atoms to fullfill the octet rule.

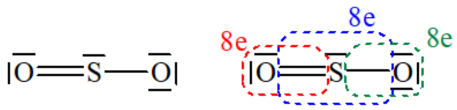
Option 1:



10 electron pairs, 20 electrons

5. **Check the number of electrons:** Count how many electrons are present in the molecule. If the number is too high, it means there will be some double or triple bonds.

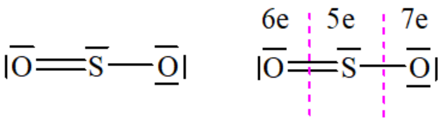
Option 2:



9 electron pairs, 18 electrons

According to the experimental findings both bond distances are the same, so the real structure is proposed to exist somewhere between these two. This type of structure is called **resonance structure**.

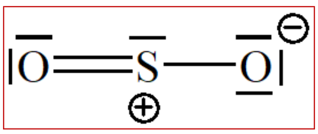
6. **Formal charges:** Formal charges represent the difference between the number of valence electrons of the element and the number of electrons in the close vicinity of the atom. To do this, the bonds are split in half and the number of electrons is counted:



S should have 6 electrons but has 5 in the formula. Therefore, it has 1 electron less and its formal charge will be +1.

O should have 6 electrons, but the oxygen bound via a single bond has 7 electrons in the formula. As a result, it has 1 electron more and its fomal charge will be -1.

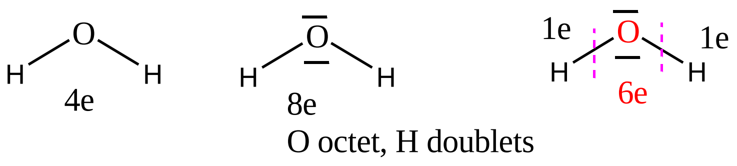
The final formula will be:



11.3.1 Simple covalent compounds

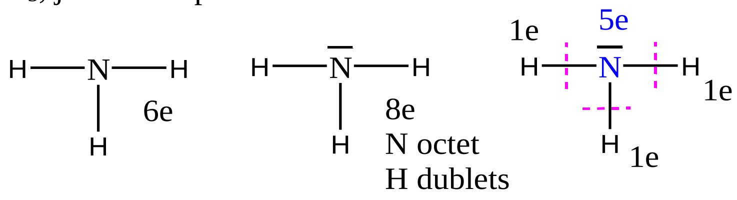
H_2O and **H_2S** have similar formulas, just S takes the place of O, since both S and O belong to the same group – 6A and they have similar electronegativities. 8 electrons are placed in 4 electron pairs, 2 in bonding pairs and 2 as lone electron pairs on oxygen to fill the octet. When bonds are split, each atom has the same number of electrons as in its elemental form, so there are no formal charges.

H_2O
O 6A 6e
H 1A 1e x2
together 8e



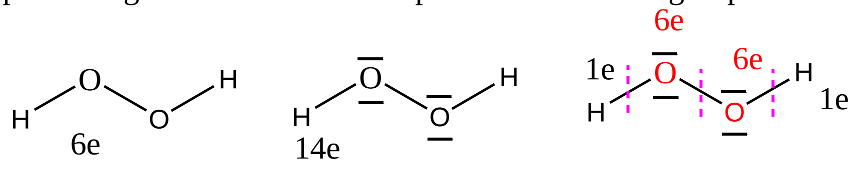
NH_3 has N as the only p-element, so it will be located in the center, surrounded by three H atoms. 6 electrons are used in 3 bonding pairs and the last two as LEP on N to fullfill the octet. Again, there are no formal charges in this molecule. The molecule **PH_3** has the same formula as NH_3, just N is replaced with the P atom.

NH_3
N VA 5e
H IA 1e x 3
together 8e

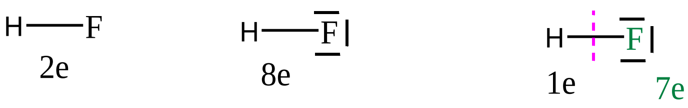


H_2O_2 and **H_2S_2**: These two compounds contain a bond between two equal p-elements O-O or S-S. These types of fragments are also called peroxo or disulfido groups.

H_2O_2
O VIA 6e x2
H IA 1e x2
together 14e

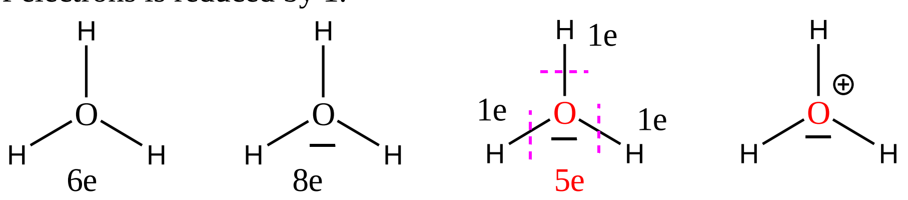


HF, **HCl**, **HBr** and **HI** have all a similar formula, just the halogen (7A group element) is changed.
HF
F 7A 7e
H 1A 1e
together 8e



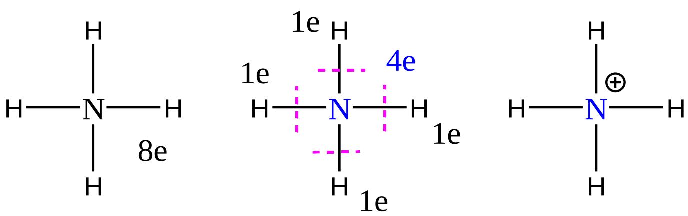
The **oxonium cation H_3O^+** is formed when a proton (H+) makes a new bond with water using one of the lone electron pairs on oxygen. Since it is a cation with charge +1, the overall number of electrons is reduced by 1.

H_3O^+
O VIA 6e
H IA 1e x3
cation -1e
together 8e



The **ammonium cation NH_4^+** is formed when ammonia makes a 4th N-H bond with H^+(similar as in H_3O^+ cation). The lone electron pair on nitrogen is used to form this bond. Again, the number of electrons in this molecule is not 9 but 8, because it is a cation with charge +1. Ammonium cation forms stable salts with many anions, such as halogenides of oxo-acid anions.

NH_4^+
N VA 5e
H IA 1e x 4
cation -1e
together 8e



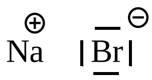
11.3.2 Simple ionic compounds

Most ionic compounds are obtained by a chemical reaction of an acid with a base, in a reaction called neutralization, e.g., $HCl + NaOH \rightarrow NaCl + H_2O$.
In this reaction, an H atom covalently bound to a p-element is removed as H^+ cation, so the p-element keeps the electron from H (s^1) and it is replaced by a cation, e.g., $H\text{-}Cl + Na^+ \rightarrow Na^+Cl^- + H^+$.

Ionic **fluorides**, **chlorides**, **bromides,** and **iodides** contain anions with 8 electrons. They have 1 more electron than in their elemental form., Therefore, they carry the formal charge -1. If the cation has also the charge +1 like in Na, K, NH_4, Li etc., then such salt has the ratio 1:1. If the cation has higher charge, then the number of halogen anions must be multiplied ($CaCl_2$, $MgBr_2$ etc.)

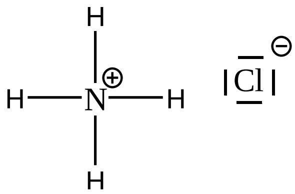
NaBr
Na 1A 1e
Br 7A 7e
together 8e

salt of HBr - ionic



NH_4Cl
N 5A 5e
H 1A 1e x4
Cl 7A 7e
together 16e

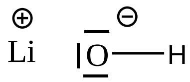
salt of HCl - ionic



The water molecule H_2O can form an anion losing one or both H^+ ions. If one is lost, the **hydroxide anion OH^{-1}** is produced, if both, the **oxide anion O^{-2}** is formed.

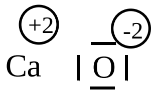
LiOH
Li 1A 1e
O 6A 6e
H 1A 1e
together 8e

salt of H_2O - ionic



CaO
Ca 2A 2e
O 6A 6e
together 8e

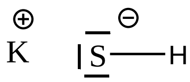
salt of H_2O - ionic



Similarly, H_2S can also lose one or both H^+ cations and hydrogensulfide SH^{-1} or sulfide S^{-2} is produced.

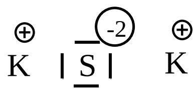
KSH
K 1A 1e
S 6A 6e
H 1A 1e
together 8e

salt of H_2S - ionic



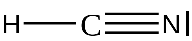
K_2S
K 1A 1e x2
S 6A 6e
together 8e

salt of H_2S - ionic



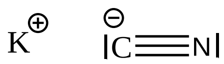
Cyanides (CN^{-1}) are stable salts formed from cyanic acid, **HCN**:

HCN
C IVA 4e
N VA 5e
H IA 1e
together 10e



KCN
C IVA 4e
N VA 5e
K IA 1e
together 10e

salt of HCN - ionic

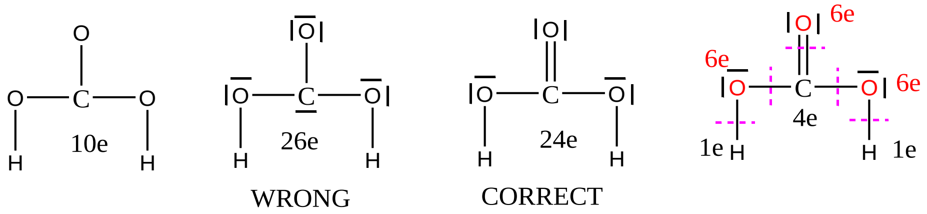


11.3.3 Oxo-acids

In oxo-acids, the central atom (CA) is surrounded by O atoms, the H atoms are bonded with only few exceptions to the O atoms: O – CA – O – H

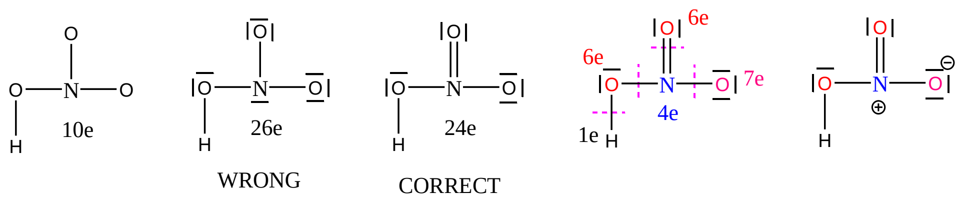
Carbonic acid, **H_2CO_3**, has C as the central atom (4A element). This molecule has 5 covalent bonds. If LEP are placed around every atom to observe the octet rule, a molecule with 26 electrons is obtained. To reduce the number of electrons, a double bond is placed between C and the only oxygen that doesn't bind to an H atom. Two LEP mut be removed from the formula. In this way, we get the correct formula.

H_2CO_3
C 4A 4e
O 6A 6e x3
H 1A 1e x2
together 24e



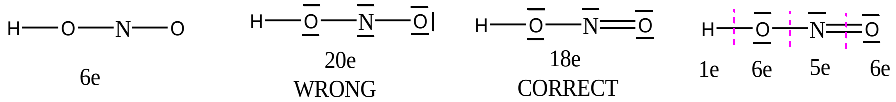
Nitric acid, **HNO_3**, has N as the central atom (5A element). Again, if LEP are placed on every p-element to have 8 electrons, a molecule with 2 extra electrons is formed. By using two LEP to make a double bond between N and O, we receive the right formula.
A **double bond** can be placed only between the central atom and an *oxygen without a bonded H*.

HNO_3
N 5A 5e
O 6A 6e x3
H IA 1e
together 24e



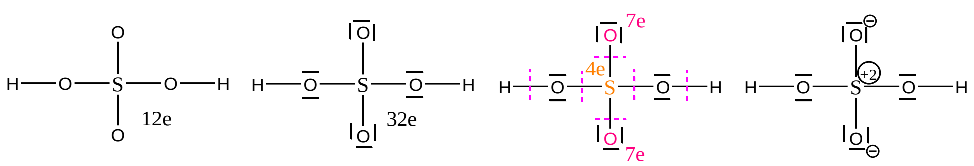
Nitrous acid, **HNO_2**, has one oxygen less:

HNO_2
N 5A 5e
O 6A 6e x2
H 1A 1e
together 18e



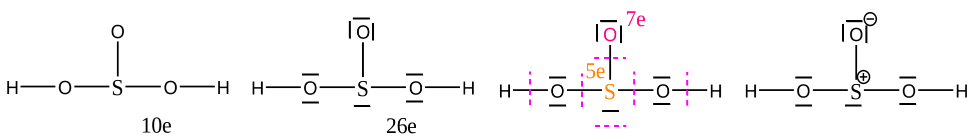
Sulfuric acid, **H_2SO_4**, has S as a central atom (6A element). In this molecule, no LEP need to be removed. There are no double bonds here:

H_2SO_4
S 6A 6e
O 6A 6e x4
H 1A 1e x2
together 32e



Sulfurous acid, **H_2SO_3**, has one oxygen less:

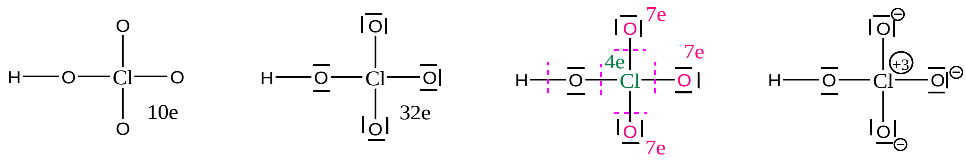
H_2SO_3
S 6A 6e
O 6A 6e x3
H 1A 1e x2
together 26e



Oxo-acids of halogens (7A group elements) are known for Cl, Br and I and include acids such as:

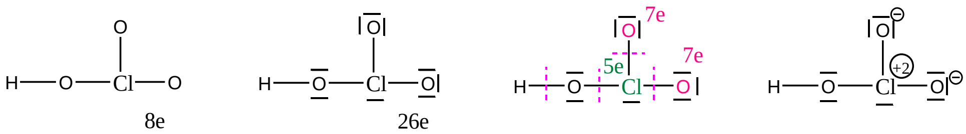
Perchloric acid, **$HClO_4$**, perbromic acid, **$HBrO_4$**, and periodic acid **HIO_4**

$HClO_4$
Cl 7A 7e
O 6A 6e x4
H 1A 1e
together 32e



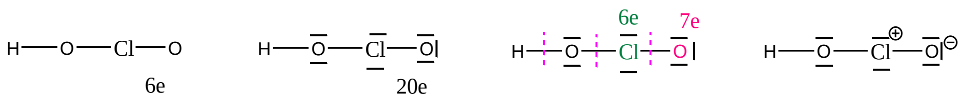
Chloric acid, **$HClO_3$**, bromic acid, **$HBrO_3$**, and iodic acid, **HIO_3**

$HClO_3$
Cl 7A 7e
O 6A 6e x3
H 1A 1e
together 26e



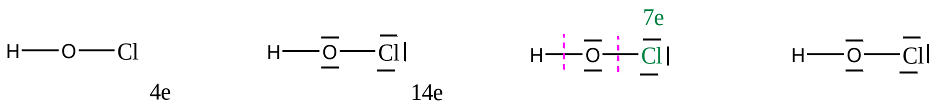
Chlorous acid, **$HClO_2$**, bromous acid, **$HBrO_2$**, and iodous acid, **HIO_2**

$HClO_2$
Cl 7A 7e
O 6A 6e x2
H 1A 1e
together 20e



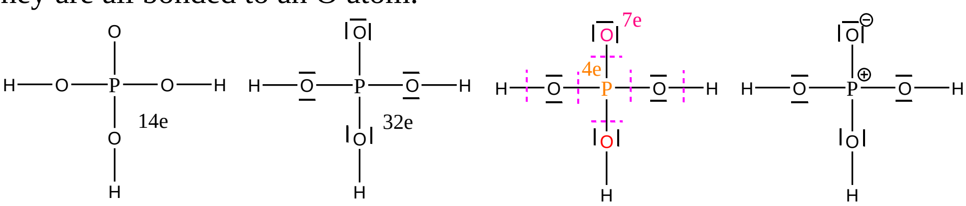
Hypochlorous acid, **HClO**, hypobromous acid, **HBrO**, and hypoiodous acid, **HIO**

HClO
Cl 7A 7e
O 6A 6e
H 1A 1e
together 14e



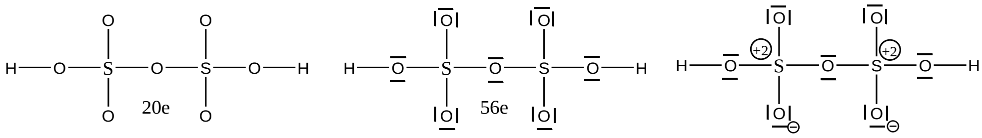
Phosphoric acid, **H_3PO_4**, has P as central atom. This acid is unusual because it has 3 hydrogens. They are all bonded to an O atom.

H_3PO_4
P 5A 5e
O 6A 6e x4
H 1A 1e x3
together 32e



Disulfuric acid, **$H_2S_2O_7$**, has two central atoms. It can be obtained by partial dehydratation of two sulfuric acid molecules ($2\ H_2SO_4 - H_2O \rightarrow H_2S_2O_7$).

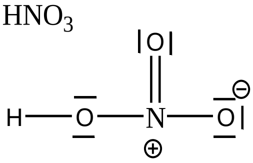
$H_2S_2O_7$
S 6A 6e x2
O 6A 6e x7
H 1A 1e x2
together 56e



11.3.4 Salts of oxo-acids

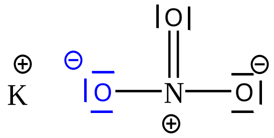
Similarly, as in salts of simple compounds, salts of oxo-acids are formed by replacing the H atom bonded to O with a cation:
$K^+ + H\text{-}O\text{-}CA \rightarrow K^+O^-\text{-}CA + H^+$

HNO_3

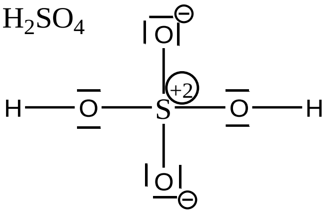


KNO_3

K 1A 1e
N 5A 5e
O 6A 6e x3
together 24e

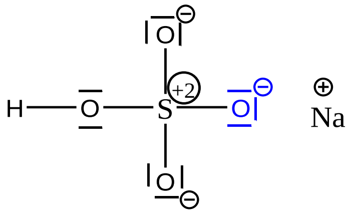


H_2SO_4



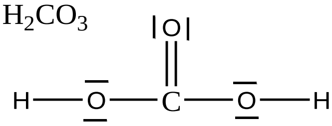
$NaHSO_4$

Na 1A 1e
H 1A 1e
S 6A 6e
O 6A 6e x4
together 32e



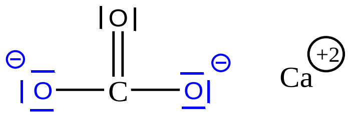
If an acid has several O-H groups, more of the H^+ can be replaced:

H_2CO_3

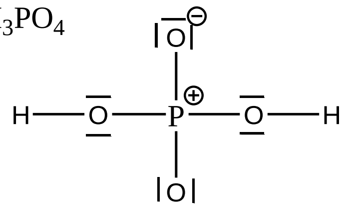


$CaCO_3$

Ca 2A 2e
C 4A 4e
O 4A 6e x3
together 24e

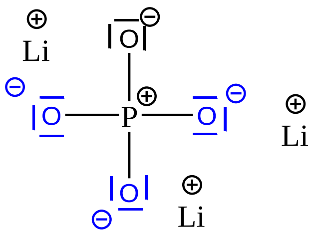


H_3PO_4



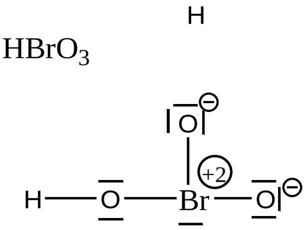
Li_3PO_4

Li 1A 1e x3
P 5A 5e
O 6A 6e x4
together 32e



Also, NH_4^+ can be used as a cation:

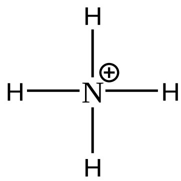
$HBrO_3$

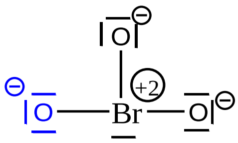


NH_4BrO_3

H 1A 1e x4
N 5A 5e

Br 7A 7e
O 6A 6e x3
together 34e





11.3.5 Derivatives of oxo-acids and their salts

Derivatives of oxo-acids include:

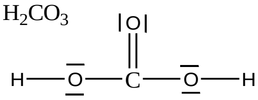
a) ***thio***- and ***peroxo***-derivatives
b) ***halogeno***- (***fluoro***-, ***chloro***-, ***bromo***-) and ***amido***-derivatives

Thioderivatives are obtained by replacing an *O atom with an S atom*.

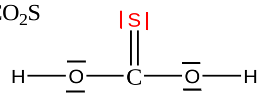
Peroxoderivaties are obtained by replacing an *O atom with the O-O group* (peroxo group).

Carbonic acid / Thiocarbonic acid / Peroxocarbonic acid

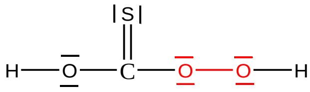
H_2CO_3



H_2CO_2S

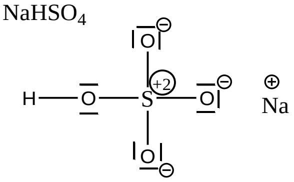


H_2CO_4

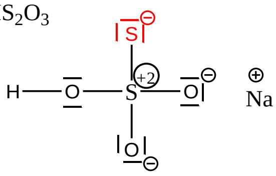


Sodium hydrogensulfate / Sodium hydrogenthiosulfate / Sodium hydrogenperoxosulfate

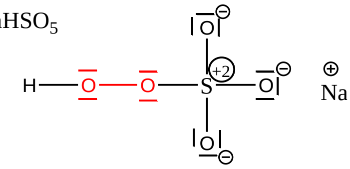
$NaHSO_4$



$NaHS_2O_3$



$NaHSO_5$

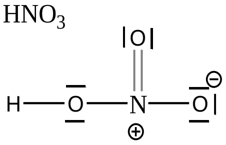


*Halogeno*derivatives are obtained by replacing *O-H group with a halogen* (F, Cl or Br).

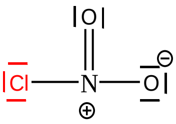
*Amido*derivaties are obtained by replacing *O-H group with NH_2 group* (amido group).

Nitric acid / Nitryl chloride / Nitryl amide

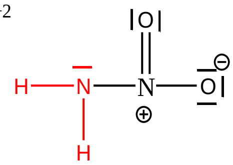
HNO_3



NO_2Cl

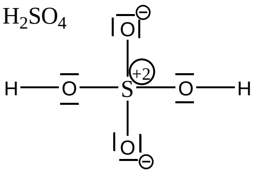


NO_2NH_2

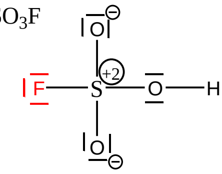


Sulfuric acid / Fluorosufuric acid / Amidosulfuric acid / Sulfuryl diamide

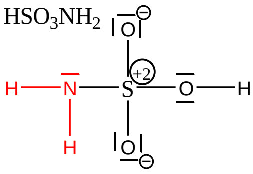
H_2SO_4



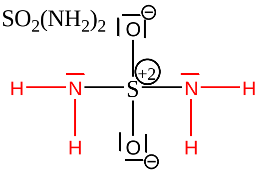
HSO_3F



HSO_3NH_2



$SO_2(NH_2)_2$



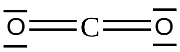
11.3.6 Covalent oxides

Covalent oxides are oxides of p-elements such as C, N, S, P, and others. Their structure is variable and not easy to learn.

Oxides of carbon:

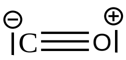
CO_2

C 4A 4e
O 6A 6e x2
together 16e



CO

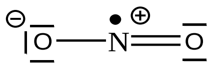
C 4A 4e
O 6A 6e
together 10e



Oxides of nitrogen – *radicals*:

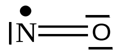
NO_2

N 5A 5e
O 6A 6e x2
together 17e - 1 unpaired e!



NO

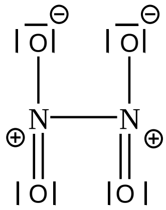
N 5A 5e
O 6A 6e
together 11e - 1 unpaired e!



Oxides with two nitrogens:

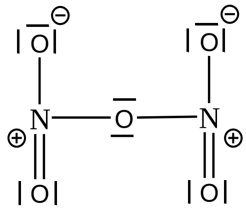
N_2O_4

N 5A 5e x2
O 6A 6e x4
together 34e



N_2O_5

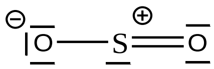
N 5A 5e x2
O 6A 6e x5
together 40e



Oxides of sulfur:

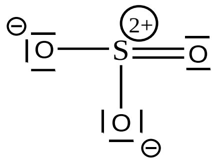
SO_2

S 6A 6e
O 6A 6e x2
together 18e



SO_3

S 6A 6e
O 6A 6e x3
together 24e



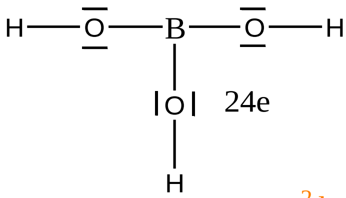
11.3.7 Exceptions to the octet rule

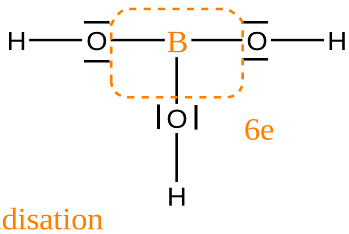
There are a few compounds of p-elements where the octet rule cannot be applied.

One of the p-elements forming such compounds is *boron*. Boron is in the 3A group and has only 3 electrons which it can use for bonds, so there are compounds where boron forms 3 bonds and doesn't have any other electrons around it. This means, it shares only 6 electrons.

Boric acid, **H_3BO_3**

H_3BO_3
H 1A 1e x3
B 3A 3e
O 6A 6e x3
together 24e

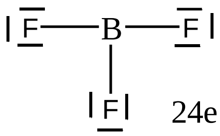


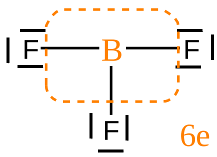


sp^2 hybridisation

Boron trifluoride, **BF_3**

BF_3
B 3A 3e
F 7A 7e x3
together 24e

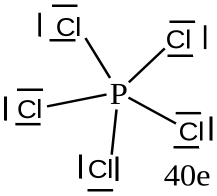




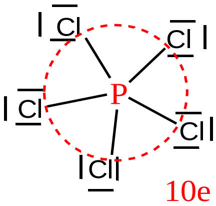
Some elements of the 3rd period of periodic table, such as S or P, can form more than 4 bonds and also combine the d-atomic orbitals to make additional bonds. More bonds mean more than 8 electrons.

Phosphorus pentachloride, **PCl_5**

PCl_5
P 5A 5e
Cl 7A 7e x5
together 40e



40e

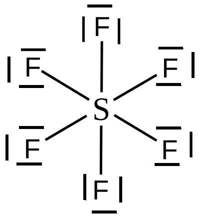


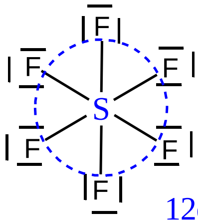
10e

sp^{3}d hybridisation

Sulfur hexafluoride, **SF_6**

SF_6
S 6A 6e
F 7A 7e x6
together 48e





12e

sp^{3}d^2 hybridisation

11.4 Problems

Draw the Lewis structure formula for

a) O_2, Br_2, N_2, HF, NaI, LiO_2, Cl_2O, H_2S, Na_2S, $Ca(OH)_2$, CCl_4, PH_3, NH_4OH, KHS, HCN, NaCN

b) H_2SO_3, HNO_2, H_3PO_4, KH_2PO_4, $KBrO_4$, K_2SO_4, $Ca(NO_3)_2$, $NaIO_2$, NH_4NO_3, $NaHSO_4$, HBrO, $KBrO_3$, $K_2S_2O_7$, $NaHCO_3$

c) H_2SO_5, H_2CS_3, KNO_4, HCO_2F, $COCl_2$, NO_2NH_2, $NaSO_3Cl$

d) CO, NO, NO_2, SO_3, CO_2, N_2O_4

II EXPERIMENTAL PART

1 SAFETY AND GENERAL PRECAUTIONS IN THE CHEMISTRY LABORATORY

Chemistry laboratories are the places where chemical experiments are conducted, and students can practically observe how different chemicals interact with each other. Although there is an interesting interactive activity performed in the laboratory, students should not forget that a couple of safety precautions must be respected to evade the hazardous character of some experiments. Discipline is mandatory in a chemistry laboratory to avoid injury to yourself or your coworkers. As a first step in the chemistry laboratory, you might remember that for this place, the <u>rules are set NOT to be broken</u>!
During a chemistry laboratory class, students may handle chemicals that can be flammable, poisonous, carcinogenic, and skin-harmful. Some materials and equipment used in the laboratory may also cause severe burns, cuts, or bruises if handled improperly or carelessly. Usually, the accidents that occur in the chemistry laboratory, result from negligence, impatience, or improper usage of materials and equipment. To minimize the chances of an accident during the experiments in the chemistry laboratory, certain rules and regulations must be obeyed.

1. Appropriate clothing must be worn at all times while working in the chemistry laboratory. The wearing of a full-length protective laboratory coat, sparing shoes, and other protective clothing is strictly required. To minimize the risk of exposure to chemicals and prevent yourself from any accident, eye protection (eye safety glasses) or a face shield must be worn. Some of the chemicals are absorbed through the skin, therefore wearing rubber gloves is expected as well as heat-resistant gloves to protect your hands from hot glassware or other devices used in experiments.
2. Unconditionally it is necessary to know the location and proper use of fire extinguishers, fire blankets, safety showers, and first aid kits.
3. The safest approach is to regard all chemicals other than water as toxic and to treat them as such unless their safety is established. Chemicals are supplied in bottles (glass or plastic) and containers (powder bottle, wide neck bottle) labelled with the information on content, purity grade (*technical grade, pure, analytical grade chemically pure, substances with special applications*), and some necessary data concerning their physical and chemical properties. Chemicals should not be handled with bare fingers, for this purpose use a spoon or spatula. To state the weight of solid substances, the electric balance available in the laboratory is usually used. Never place chemicals directly on the balance pan, use a proper weighing container to weigh a chemical. To measure the volume of liquid substances, special calibrated bottles or graduated cylinders are used. Before removing a chemical from a bottle, read the label carefully to be sure that you have the correct substance and never return unused chemicals to their original bottle (unless directed to do so by a supervisor).

For safe experimental work, the following regulations must be obeyed:

- never taste the chemicals. If you are instructed to smell a chemical, gently fan the vapors toward your face. Eating and drinking are not allowed in a chemistry laboratory.
- never pour water into concentrated acid, always pour the acid slowly into the water while stirring constantly (very exothermic reaction).
- in the case of alkali solution, add water to basic substances or their concentrated solutions.

- when heating a substance in a test tube, never direct the open end of the test tube toward yourself or anyone else near you.
- all reactions involving dangerous or volatile materials either as reactants or products should be carried out in a fume hood, this recommendation concerns also heating with concentrated acid, evaporation to dryness, as well as works with corrosive and poisonous gases. The fume hoods must be always used when toxic or irritating vapors are involved.
- using laboratory glassware for personal purposes is forbidden.
- do not place anything that is not directly required for the experiment on laboratory desks. Personal belongings should be placed in the free cupboards as you enter the laboratory.
- when using pipettes, mouth suction is never used to fill a pipette.
- before leaving the chemistry laboratory, make sure your work area is clean and dry and all gas, water, and vacuum valves are completely turned off.
- do not initiate and perform unauthorized experiments in the chemistry laboratory alone.

In the case of any accident, report any injury, even a minor one, to your supervising teacher immediately and follow his/her instructions!
Your supervisors are available for any assistance you may need.

For treating burns caused by heat, use the running tap water first to cool the affected area and then, use an adequate vaseline or ointment. Large blisters or places with the destruction of tissue must be covered with sterile gauze. Ask for medical assistance immediately. Burns caused by chemicals must be cooled using running tap water. Then, acid burns should be treated with 1 – 2% sodium hydrogen carbonate solution, while alkali burns treating with a diluted solution of trihydrogen boric acid (or diluted solution of acetic acid).
Chemicals penetrated into the eyes must be washed up with distilled water using a special eye cup and then using trihydrogen boric acid solution for alkali damage and sodium hydrogen carbonate solution for acid damage.
Cuts should be disinfected with a 3% solution of hydrogen peroxide, ethanol, or iodine tincture.
Toxic fumes: the person must take a deep breath of fresh air.

For a successful and safe experimental work, always come to the laboratory thoroughly prepared for the day's experiment.

2 SEPARATION AND PURIFICATION METHODS IN CHEMISTRY

2.1 FILTRATION

Through this method, solid substances are separated from liquids. The liquid separated by filtration is called filtrate. Practically, we recognize two types of filtrations:

a) gravity filtration when the filtrate passes through the filter medium under the force of gravity. A funnel with a long stem and simple (smooth) or fluted filter paper are used (see **Figures 1** and **2**)

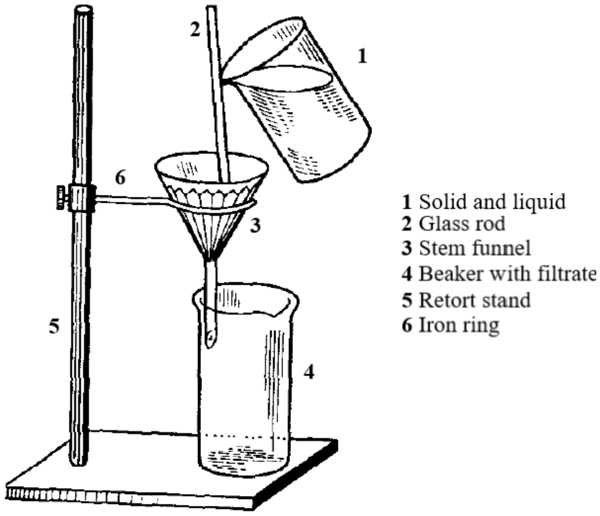


Figure 1 Gravity filtration
(Original picture belongs to MIR Publishers 1987, Practical Inorganic Chemistry, O.I. Vorobyova et al.)

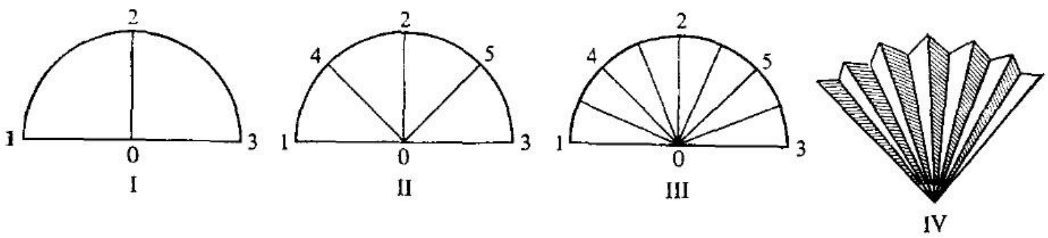


Figure 2 Folding a fluted filter paper
(Original picture belongs to MIR Publishers 1987, Practical Inorganic Chemistry, O.I. Vorobyova et al.)

b) vacuum filtration (suction filtration) when reduced pressure is maintained. In comparison with gravity filtration, the rate of vacuum filtration is higher. In this procedure, the Büchner funnel, suction flask (side-arm flask), and a laboratory water-jet pump apparatus providing the lower pressure are used (see **Figure 3**).

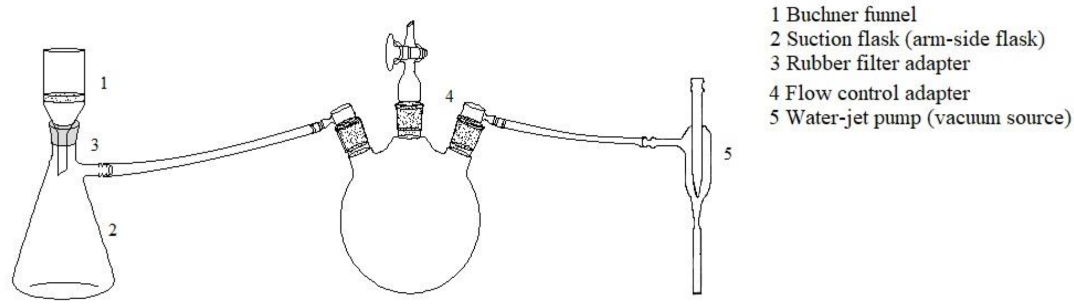


Figure 3 Vacuum filtration apparatus

2.2 WASHING AND DECANTATION

Washing and decantation are used to remove the excess liquid phase and soluble impurities present in the precipitate. The solvent used for washing is supposed to be miscible with the liquid phase and does not dissolve any appreciable amounts of precipitate. The procedure of washing usually follows the process of filtration. On the other hand, decantation can be applied in the case of "heavier" substances settled down at the bottom of the beaker. The procedure consists of mixing and rinsing the precipitate with a particular solvent in the original container followed by a careful pouring the used solvent out of the mixture. In both cases (washing and decantation), it is recommended to carry out several washings with a small volume of liquid because they are more effective than a single washing using a large volume of liquid.

2.3 CRYSTALLIZATION

Crystallization is a purification method for solid substances. It is a technique that separates a solid from its solution by increasing its concentration (evaporation of solute by heating). This process (a) is often used as a purification method based on different solubilities of substances in question. Another (b) way to achieve this effect is to employ temperature dependence of solubility.

a) The mixture of substances is stirred with a volume of the chosen solvent; the dissolved component (mostly impurities) is separated by filtration. After evaporation of the solvent, the pure substance is recovered.

b) Using the data available in published collections of chemical data, the prepared solutions at a higher temperature are firstly filtered and then cooled down to room temperature. While the solution is slowly cooling down, the pure component is crystallizing, and the recovered crystals can be separated by suction filtration.

For better separation of substances, it is recommended to repeat the dissolving and crystallization processes to eliminate all the impurities. This process is also called recrystallization.

Crystallization occurs when the solvent evaporates slowly. A rapid formation of finely divided powder (precipitate) in a chemical reaction is called precipitation.

The purification of a chemical compound can be performed either from water (**Figure 4a**) or from a particular organic solvent (**Figure 4b**). In each case, several steps in the crystallization process must be followed:

1. Choose an appropriate solvent.

2. Dissolve the solid compound in the solvent by increasing the temperature until the solid visually “disappears“.

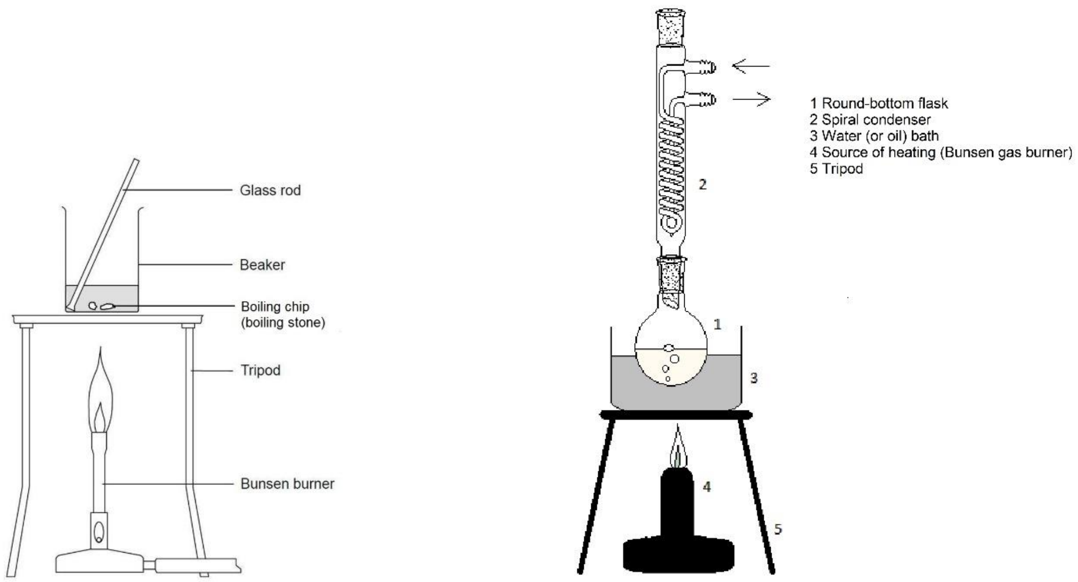
3. Add a small amount of activated carbon to the solution (activated carbon removes impurities and contaminants through the chemical process of adsorption)

4. Make a simple filtration using a long stem funnel and a fluted filter paper. Warning! The glassware used in the filtration (the beaker and the funnel) must be hot to avoid the crystallization of the pure product on the glassware

5. Cool the filtrate to crystallize the pure product

6. Make a vacuum filtration (by suction) to separate the crystals from the mother liquor.

7. Dry the crystals and weigh the product.



(a) (b)

Figure 4 Crystallization from water (**a**), and from a particular organic solvent (**b**)
(Source: Royal Society of Chemistry/www.rsc.org)

2.4 SUBLIMATION

Some of the inorganic or organic compounds can be purified also by sublimation. This method depends on the ability of solids to achieve a high vapor pressure at a temperature below their melting points, which means that the molecules of a solid can pass directly to a gaseous state. These solid–gas changes occur at the sublimation point. The procedure consists of heating the substance or the mixture followed by a subsequent cooling of the formed vapors (this process can be carried out at atmospheric or low pressure).

The best known examples are iodine (I_2), mercury(II) chloride ($HgCl_2$), carbon dioxide (CO_2) in solid state (dry ice), and some organic compounds like benzoic acid or naphthalene.

Within the Inorganic Chemistry Laboratory session, the sublimation of iodine is demonstrated by placing a mixture of iodine and sand (SiO_2) in a beaker covered with a round bottom flask filled with cold water or ice cubes (cooling system) (**Figure 5**). When the iodine pellets are heated up, a purple gas is evolved. In contact with the cooling system, these vapors start to crystallize. The newly formed crystals are the purified iodine.

Figure 5 Sublimation apparatus
(Source: Stanislav.nevyhosteny, CC BY-SA 4.0 <https://creativecommons.org/licenses/by-sa/4.0>, via Wikimedia Commons)

2.5 DISTILLATION

Distillation is a method of purification and separation of liquid substances. By this process, a liquid can be separated from a solid or another liquid. This method is very successful in the separation of liquids with different boiling points. The principle of the method consists of the vaporization of the liquid followed by condensation of the formed vapors. In other words, the liquid is transformed by heating to gaseous state and then cooled (condensed) using a condenser. In general, we recognize two types of distillation: at normal (atmospheric) pressure (**Figure 6**) and at diminished (lowered) pressure, or vacuum pressure (**Figure 7**).
The choice of a proper distillation type is based on the value of the boiling point and other properties of a relevant liquid. The boiling point is defined as the temperature at which the liquid vapor pressure achieves the pressure of the surrounding atmosphere. Therefore, the boiling points change proportionally with the changes in the surrounding atmosphere pressure. This premise is useful in cases when the value of the boiling point is too high, or the substance is very unstable and decomposes at a temperature below this point. In such cases, we use the distillation at a diminished pressure because the lowering of surrounding pressure results in a lowering of boiling temperature.
Both distillation methods, at normal pressure as well as at diminished pressure, follow the same principle, the vaporization-condensation cycle. The only difference appears in the apparatus used for distillation. In the case of vacuum distillation, a vacuum source (in the laboratory the water jet vacuum pump) and a manometer are mandatory.

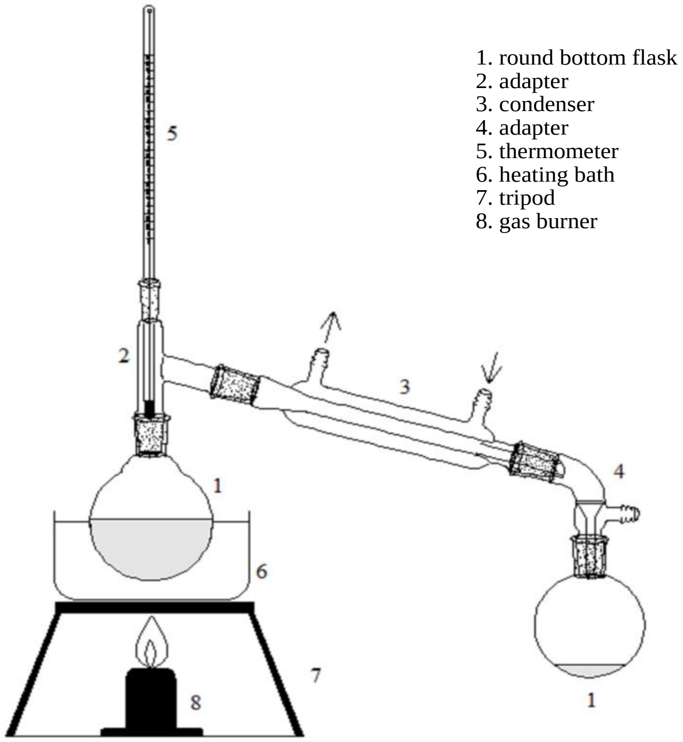


Figure 6 Simple distillation (at atmospheric pressure) apparatus

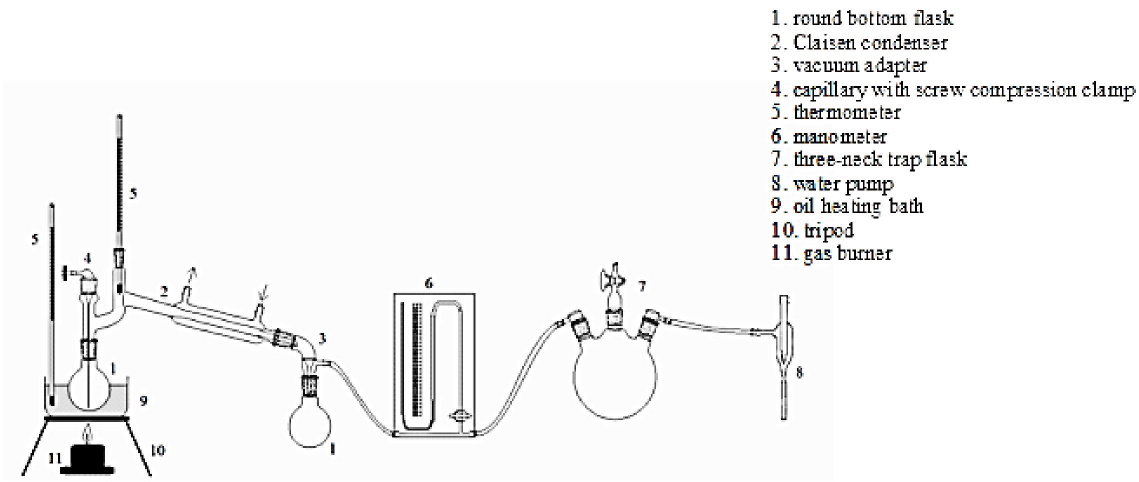


Figure 7 Vacuum distillation apparatus

For more details see the handbook for laboratory practice (reference 16).

3 LABORATORY REPORT

In the laboratory report required for all practical laboratory work, the following information should be included:

1. Name of the student, date, and title of the experiment
2. Purpose (principle and chemical equations of the experiment)
3. Procedure and methods applied
4. Equipment used (with simple hand-drawn schemes)
5. Necessary calculations
6. Results

4 SEPARATION AND PURIFICATION EXPERIMENTS

4.1 PURIFICATION OF SODIUM CHLORIDE

The purification process is based on good water solubility of sodium chloride followed by evaporation of water.

Chemicals needed: mixture of NaCl and active carbon.

Dissolve the whole mixture in enough amount of distilled water at room temperature, then use simple filtration to separate the active carbon from the colorless solution. Use a porcelain evaporating dish and a water bath to evaporate the water. The final product obtained after the evaporation of water is the pure white powder of NaCl, known as table salt.

4.2 SEPARATION OF A TERNARY HETEROGENEOUS MIXTURE

potassium chloride (KCl) – calcium carbonate ($CaCO_3$) – sand (SiO_2)

To separate a given mixture of more compounds into its components, their different physical and chemical properties might be utilized. First of all, the solubility in water. In this mixture, only KCl is water soluble, while the other two components are not. To separate calcium carbonate and silica sand, the chemical reaction with HCl might be applied. As it is known, only calcium carbonate will react with HCl.

$$CaCO_3 + 2\,HCl \rightarrow CaCl_2 + CO_2\uparrow + H_2O$$

Chemicals needed: mixture (KCl, $CaCO_3$, SiO_2), diluted HCl (1:1 by volume), distilled water.

Suppose that the whole mixture is only KCl. The found solubility of KCl is 34.2 g in 100 mL of water. Calculate the amount of water needed for dissolving KCl. Using simple filtration and folded filter paper, separate the solution of KCl in water from the rest of the solids ($CaCO_3$ and SiO_2). To obtain the solid KCl and remove the water, use the evaporating dish and the water bath. After the simple filtration of the KCl solution, make a hole at the bottom of the filter paper and rinse the solid with a minimum amount of distilled water. This operation helps to collect back into the initial beaker the traces of $CaCO_3$ and SiO_2 which remained on the filter paper during the filtration operation. Over the two solids remaining in the beaker add in small portions the diluted hydrochloric acid until it has reacted completely with $CaCO_3$. During this exothermic reaction, the liberation of gaseous CO_2 can be observed. At the end, at the bottom of the beaker remains only SiO_2 (sand). Wash with distilled water (3 times) and decantate it. Then, let it dry in a drying laboratory oven.

4.3 CRYSTALLIZATION FROM WATER (OF BORIC ACID)

Crystallization of H_3BO_3 as a purification method is based on a good temperature-dependent solubility of trihydrogen boric acid in water.

Solubility of H_3BO_3 (according to chemical table data)

20 °C . . . 5 g in 100 g of water
80 °C . . . 23.6 g in 100 g of water

In this experiment, we use the Erlenmayer flask to avoid the evaporation of heated water. Calculate the amount of water needed for the dissolving of H_3BO_3 at 80 °C. When H_3BO_3 is completely dissolved in water by heating, filtrate the solution using simple filtration and fluted filter paper and let the filtrate cool down to room temperature. By cooling down white crystals of pure H_3BO_3 are formed. Separate the crystals from the solution by vacuum filtration and dry the final product.

4.4 CRYSTALLIZATION FROM AN ORGANIC SOLVENT

Crystallization of an organic compound (benzoin or dibenzylideneacetone) follows the same steps as the crystallization from water. In the laboratory, we will use 2 grams of an organic compound (benzoin or dibenzylideneacetone) and 30-40 mL of ethanol (as the organic solvent used in crystallization).
The apparatus for crystallization from an organic solvent differs from that used in the crystallization from water (**Figure 4b** - Separation and purification methods in chemistry – Crystallization). The organic compound is dissolved in ethanol by heating it in a round bottom flask in a water bath. The use of a condenser is required to avoid the evolution of flammable ethanol vapors in the atmosphere. When the organic material is completely dissolved, remove the heating source, add a small amount of activated carbon, and then filter off the solution by using hot glassware (use a simple filtration). By cooling down the filtrate you will observe the formation of crystals of the purified organic product. Separate the crystals from the mother liquor by vacuum filtration and dry the product under low pressure on a Büchner funnel.

5 PREPARATIVE PART

5.1 PREPARATION OF COPPER

Metallic copper can be prepared by a substitution reaction of zinc with an acidic solution of copper(II) sulfate pentahydrate (cupric sulfate pentahydrate).

$Zn + CuSO_4 \rightarrow \mathbf{Cu} + ZnSO_4$

Chemicals needed: copper(II) sulfate pentahydrate, powdered zinc, concentrated sulfuric acid, distilled water.

From the calculated amount of $CuSO_4 \cdot 5\ H_2O$, prepare a 10% solution of copper(II) sulfate in distilled water. After filtration (using simple filtration), add a 3% solution of H_2SO_4 (5 mL for 20 grams of $CuSO_4 \cdot 5\ H_2O$ are recommended). After a gentle heating of the prepared solution, add the calculated amount of powdered zinc in small portions under continuous stirring. The powdered copper deposits at the bottom of the beaker as a result of the reaction.
Unreacted zinc powder (grey-colored) should be removed using decantation with a diluted solution of H_2SO_4 (3%) according to the following reaction

$Zn + H_2SO_4 \rightarrow ZnSO_4 + H_2\uparrow$

As the metallic copper prepared is very sensitive to moisture and oxygen, it must be stored under diluted sulfuric acid. Don't weigh the product!

Properties: Compact copper is a bright metal of pink to yellowish–red color. At the ambient (room) temperature and in a dry (moisture-free) atmosphere it is stable, otherwise it oxidizes to CuO. Copper belongs to noble metals, and it is insoluble in mineral acids.

5.2 TRIHYDROGEN BORIC ACID

The preparation of trihydrogen boric acid is based on a replacement reaction between its salt (borax) and a stronger mineral acid, e.g., hydrochloric acid (HCl).

$Na_2B_4O_7 \cdot 10\ H_2O + 2\ HCl \rightarrow 4\ H_3BO_3 + 2\ NaCl + 5\ H_2O$

Chemicals needed: borax, concentrated hydrochloric acid.

Firstly, the saturated solution of borax must be prepared by dissolving the calculated amount of this salt in hot distilled water (add it in small portions). After that, filter off and reheat the borax solution. Carefully add the calculated amount of 37% solution of HCl to the hot borax solution. Using universal indicator paper, check the pH value of the reaction mixture, which must have the value 0 – 1. In the case of a higher pH value, add some drops of HCl solution. After cooling the reaction mixture, trihydrogen boric acid crystallizes as fine white crystals. Separate the crystals using filtration at reduced pressure and allow the product to dry in the air.

Solubility of $Na_2B_4O_7 \cdot 10H_2O$ (at 60 ^{0}C) is 20 g in 100 mL of H_2O.

Properties: H_3BO_3 crystallizes in white shiny needles linked together by hydrogen bonds to form infinite layers of nearly hexagonal symmetry. It is used as a disinfection agent.

5.3 NICKEL(II) HYDROXIDE

$Ni(NO_3)_2 \cdot 7\ H_2O\ +\ 2\ KOH\ \rightarrow\ Ni(OH)_2\ +\ 2\ KNO_3\ +\ 7\ H_2O$
$Ni^{2+}\ +\ 2\ OH^{-}\ \rightarrow\ Ni(OH)_2$

Chemicals needed: nickel(II) nitrate heptahydrate, potassium (sodium) hydroxide, distilled water, ammonia solution

Add a 20% solution of KOH (in 20% stoichiometric excess) to a heated (at 30 – 40 °C) and filtered 25 % solution of $Ni(NO_3)_2 \cdot 7\ H_2O$. Wash the formed precipitate with warm water and decantate (3 times). To the last portion of washing water add some mL of 25% ammonia solution because the reaction medium must be basic. Use universal pH indicator paper to check it. After decantation, dry the product on a porcelain evaporating dish in a water bath.

Properties: $Ni(OH)_2$ represents stable microcrystalline light green powder, very poorly soluble in water.

5.4 POTASSIUM CHLORIDE

Potassium chloride can be prepared by the neutralization reaction of hydrochloric acid with potassium hydroxide in aqueous medium according to the reaction

$HCl + KOH\ \rightarrow\ KCl + H_2O$

Chemicals needed: concentrated HCl solution (37%), KOH.

In this synthesis, 20% solutions of both chemicals are used. KOH solution is poured in small portions into the HCl solution under stirring. The resulting reaction mixture must exhibit a pH of about 8 (weakly basic). Check the pH with universal indicator paper. After evaporation of water using an evaporating dish in a water bath, the product is obtained as a white powder.

Properties: KCl forms white crystals, which are water-soluble and stable in air.

5.5 AMMONIUM CHLORIDE

The preparation of the title compound is based on a neutralization reaction between concentrated solutions of hydrochloric acid (HCl) and ammonium hydroxide (NH_4OH). It is very important to achieve a neutral value of pH. Check the value of pH by using universal indicator paper.

$NH_3 + HCl\ \rightarrow\ NH_4Cl$

Chemicals needed: concentrated hydrochloric acid, ammonium hydroxide.

Add about one-half of the calculated amount of ammonium hydroxide solution to the calculated amount of concentrated hydrochloric acid. The rest of NH_4OH must be added in small portions until the reaction mixture exhibits a neutral pH value. The whole process should be carried out in a fume cupboard due to the toxicity and breathing danger. The resulting solution must be clear without any crystals. For isolation of the product use a water bath.

Properties: Ammonium chloride (NH_4Cl) crystallizes in colorless crystals with cubic symmetry. It is well soluble in water, and less soluble in alcohol.

5.6 CALCIUM(II) CARBONATE

Calcium carbonate is usually prepared by precipitation reaction of soluble calcium(II) salts with alkaline carbonates (Na_2CO_3, K_2CO_3) according to the following reaction

$$Ca^{2+} + CO_3^{2-} \rightarrow CaCO_3\downarrow$$

$$CaCl_2 + Na_2CO_3 \rightarrow CaCO_3\downarrow + 2\,NaCl$$

Chemicals needed: calcium chloride, sodium carbonate.

Prepare an 8% solution of $CaCl_2$ in waterat elevated temperature. After filtration (using folded filter paper) and heating, add the warm 10% water solution of Na_2CO_3 (in 30% excess). After cooling, wash out the precipitated $CaCO_3$ using decantation with distilled water (three times). Separate the white powder of $CaCO_3$ by suction filtration and dry it on an evaporating dish heated on a water bath.

Properties: Calcium carbonate precipitates as a white microcrystalline powder, practically insoluble in water and common organic solvents. It decomposes to CaO and CO_2 at temperatures over 800 ºC.

$$CaCO_3 \rightarrow CaO + CO_2$$

6 Preparation of coordination compounds

6.1 Diaqua-bis(salicylato)copper(II) monohydrate

$[Cu(H_2O)_2(C_6H_4OHCOO)_2]\cdot H_2O$

Synthesis of this complex is based on the reaction between the aqueous solutions of tetraaquacopper(II) sulfate monohydrate and sodium salicylate at ambient temperature. During the reaction, a substitution of two water molecules in the parent copper(II) complex takes place.

$$[Cu(H_2O)_4]SO_4\cdot H_2O + 2\ C_6H_4OHCOONa \rightarrow [Cu(H_2O)_2(C_6H_4OHCOO)_2]\cdot 2\ H_2O + Na_2SO_4 + H_2O$$

Chemicals needed: tetraaquacopper(II) sulfate monohydrate, sodium salicylate, distilled water.

Prepare a 7% solution of tetraaquacopper(II) sulfate monohydrate and a 9% solution of sodium salicylate in distilled water. Then, mix the solutions by pouring the solution of sodium salicylate into the solution of copper(II) sulfate. Let the reaction mixture settle at room temperature. The greenish-blue crystals appear within 1 hour. Separate them using the suction filtration and a Büchner funnel, wash them out with cold distilled water, and dry them in the air at laboratory temperature.

Properties: The formed complex diaqua-bis(salicylato)copper(II) dihydrate crystallizes in the form of turquoise-colored needles. It has good solubility in ethanol but it is less soluble in water. It is stable up to 60 ºC.

6.2 Tetraammincopper(II) sulfate monohydrate

$[Cu(NH_3)_4]SO_4\cdot H_2O$

The preparation is based on the substitution reaction of all four coordinated water molecules with ammonia.

$$[Cu(H_2O)_4]SO_4\cdot H_2O + 4\ NH_3 \rightarrow [Cu(NH_3)_4]SO_4\cdot H_2O + 4\ H_2O$$

Chemicals needed: copper(II) sulfate pentahydrate, ammonium, ethanol, distilled water.

Dissolve the powdered copper(II) sulfate in a concentrated solution of NH_3 used in 25% excess. The colour of the formed solution is changed to deep blue. Then, add distilled water (2/3 of ammonia volume used) and filtrate using gravity filtration and folded filter paper. To obtain crystals of the complex, the so-called *salting–out* process can be applied. It means to add ethanol to the NH_3 solution very slowly at the ratio of 1:2 (by volume). Ethanol is well miscible with water and accelerates the crystal deposition in this way. After about one hour, separate the precipitated crystals using suction filtration and the Büchner funnel. Wash out first with 50 mL of a mixture of ethanol and ammonium hydroxide (1:1 by volume). The second washing must be done with 25 mL of ethanol and the final product is afterwards dried in the air at laboratory temperature.

Properties: The product is a deep blue water-soluble crystal material. This reaction is used for the analytical determination of copper.

6.3 BIS(PYRIDINE)-BIS(SALICYLATO)COPPER(II) COMPLEX

$[Cu(C_5H_5N)_2(C_6H_4OHCOO)_2]$

The synthesis of the title compound is based on the substitution reaction in which two water molecules coordinated in the parent copper(II) complex are displaced by two molecules of pyridine according to the following reaction

$$[Cu(H_2O)_2(C_6H_4OHCOO)_2]\cdot 2\,H_2O\ +\ 2\,C_5H_5N\ \rightarrow\ [Cu(C_5H_5N)_2(C_6H_4OHCOO)_2]\ +\ 4\,H_2O$$

Chemicals needed: diaqua-bis(salicylato)copper(II) dihydrate, pyridine, salicylic acid, ethanol.

From the calculated amount of the parent copper(II) complex, prepare a 9% solution in ethanol (use Erlenmayer flask) and add an equimolar amount of salicylic acid. To form a deep blue solution, add a molar ratio of 1:1.5 pyridine mixed with ethanol 1:3 (by volume). After some minutes, the deposition of deep blue crystals of the prepared copper(II) complex is observed. Separate them using suction filtration and dry them in the air at ambient temperature.

Properties: The title Cu(II) complex crystallizes in deep blue plates and is well soluble in ethanol, but practically water-insoluble.

APPENDIX

Table 1 Elements of the Periodic Table

English	Latin	Slovak	Symbol	Atomic number	A_r
actinium	actinium	aktínium	Ac	89	227.03
aluminium	aluminium	hliník	Al	13	26.98
americium	americium	americícium	Am	95	(243)
antimony	stibium	antimón	Sb	51	121.75
argon	argon	argón	Ar	18	39.95
arsenic	arsenicum	arzén	As	33	74.92
astatine	astatium	astát	At	85	215.00
barium	barium	bárium	Ba	56	137.34
beryllium	beryllium	berýlium	Be	4	9.01
berkelium	berkelium	berkélium	Bk	97	(247)
bismuth	bismuthum	bizmut	Bi	83	208.98
boron	borum	bór	B	5	10.81
bromine	bromum	bróm	Br	35	79.90
cadmium	cadmium	kadmium	Cd	48	112.40
caesium	caesium	cézium	Cs	55	132.90
calcium	calcium	vápnik	Ca	20	40.08
californium	californium	kalifornium	Cf	98	(251)
carbon	carboneum	uhlík	C	6	12.011
cerium	cerium	cér	Ce	58	140.12
chlorine	chlorum	chlór	Cl	17	35.45
chromium	chromium	chróm	Cr	24	51.99
cobalt	cobaltum	kobalt	Co	27	58.93
copper	cuprum	meď	Cu	29	63.54
curium	curium	curium	Cm	96	(247)
dysprosium	dysprosium	dysprózium	Dy	66	162.5
einsteinium	einsteinium	einsteinium	Es	99	162.5
erbium	erbium	erbium	Er	68	167.26
europium	europium	európium	Eu	63	151.96
fermium	fermium	fermium	Fm	100	(257)
fluorine	florum	fluór	F	9	18.99
francium	francium	francium	Fr	87	223.02
gadolinium	gadolinium	gadolínium	Gd	64	157.25
gallium	gallium	gálium	Ga	31	69.72
germanium	germanium	germánium	Ge	32	72.59
gold	aurum	zlato	Au	79	196.97
hafnium	hafnium	hafnium	Hf	72	178.49
helium	helium	hélium	He	2	4.00
holmium	holmium	holmium	Ho	67	164.93
hydrogen	hydrogenium	vodík	H	1	1.008
indium	indium	indium	In	49	114.82
iodine	iodum	jód	I	53	126.90
iridium	iridium	irídium	Ir	77	192.22
iron	ferrum	železo	Fe	26	55.85
krypton	krypton	kryptón	Kr	36	83.80
kurchatovium	kurchatovium	kurčatovium	Ku	104	(264)

English	Latin	Slovak	Symbol	Atomic number	A_r
lanthanum	lanthanum	lantán	La	57	138.90
lawrentium	lawrentium	lawrencium	Lr	103	(256)
lead	plumbum	olovo	Pb	82	207.19
lithium	lithium	lítium	Li	3	6.94
lutetium	lutetium	lutécium	Lu	71	174.97
magnesium	magnesium	horčík	Mg	12	24.31
manganese	manganum	mangán	Mn	25	54.94
mendelevium	mendelevium	mendelevium	Md	101	(258)
mercury	hydrargyrum	ortuť	Mg	80	200.59
molybdenum	molybdenum	molybdén	Mo	42	95.94
neodymium	neodymium	neodým	Nd	60	144.24
neon	neon	neón	Ne	10	20.18
neptunium	neptunium	neptúnium	Np	93	237.05
nickel	niccolum	nikel	Ni	28	58.70
niobium	niobium	nióbium	Nb	41	92.91
nitrogen	nitrogenium	dusík	N	7	14.01
nobelium	nobelium	nobelium	No	102	(255)
osmium	osmium	osmium	Os	76	190.2
oxygen	oxygenium	kyslík	O	8	15.99
palladium	palladium	paládium	Pd	46	106.44
phosphorus	phosphorus	fosfor	P	15	30.97
platinum	platinum	platina	Pt	78	195.09
plutonium	plutonium	plutónium	Pu	94	(244)
polonium	polonium	polónium	Po	84	(210)
potassium	kalium	draslík	K	19	39.10
praseodymium	praseodymium	prazeodým	Pr	59	140.91
promethium	promethium	prométium	Pm	61	(145)
protactinium	protactinium	protaktínium	Pa	91	231.03
radium	radium	rádium	Ra	88	226.02
radon	radon	radón	Rn	86	(222)
rhenium	rhenium	rénium	Re	75	186.21
rhodium	rhodium	ródium	Rh	45	102.90
rubidium	rubidium	rubídium	Rb	37	85.47
ruthenium	ruthenium	ruténium	Ru	44	101.07
samarium	samarium	samárium	Sm	62	150.36
scandium	scandium	skandium	Sc	21	44.96
selenium	selenium	selén	Se	34	78.96
silicon	silicium	kremík	Si	14	28.08
silver	argentum	striebro	Ag	47	107.87
sodium	natrium	sodík	Na	11	22.99
strontium	strontium	stroncium	Sr	38	87.62
sulfur	sulphur	síra	S	16	32.06
tantalum	tantalum	tantal	Ta	73	180.95
technetium	technetium	technécium	Tc	43	98.91
tellurium	tellurium	telúr	Te	52	127.60
terbium	terbium	terbium	Tb	65	158.92

English	Latin	Slovak	Symbol	Atomic number	A_r
thallium	thallium	tálium	Tl	81	204.37
thorium	thorium	tórium	Th	90	232.04
thulium	thulium	túlium	Tm	69	168.93
tin	stannum	cín	Sn	50	118.69
titanium	titanium	titán	Ti	22	47.90
tungsten	wolframium	volfrám	W	74	183.85
uranium	uranium	urán	U	92	238.03
vanadium	vanadium	vanád	V	23	50.94
xenon	xenon	xenón	Xe	54	131.30
ytterbium	ytterbium	yterbium	Yb	70	173.04
yttrium	yttrium	ytrium	Y	39	88.91
zinc	zincum	zinok	Zn	30	65.37
zirconium	zirconium	zirkónium	Zr	40	91.22

Table 2 Densities of HCl solutions

w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]
1	1.0031	11	1.0526	22	1.1083
2	1.0081	12	1.0576	24	1.1185
3	1.0130	13	1.0626	26	1.1288
4	1.0179	14	1.0676	28	1.1391
5	1.0228	15	1.0726	30	1.1492
6	1.0278	16	1.0777	32	1.1594
7	1.0327	17	1.0828	34	1.1693
8	1.0377	18	1.0878	36	1.1791
9	1.0426	19	1.0929	38	1.1886
10	1.0476	20	1.0980	40	1.1977

Table 3 Densities of H_2SO_4 solutions

w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]
1	1.0049	22	1.1554	62	1.5200
2	1.0116	24	1.1714	64	1.5421
3	1.0183	26	1.1872	66	1.5646
4	1.0250	28	1.2031	68	1.5874
5	1.0318	30	1.2191	70	1.6105
6	1.0385	32	1.1353	72	1.6338
7	1.0453	34	1.2518	74	1.6574
8	1.0522	36	1.2685	76	1.6810
9	1.0591	38	1.2855	78	1.7043
10	1.0661	40	1.3028	80	1.7272
11	1.0731	42	1.3205	82	1.7491
12	1.0802	44	1.3386	84	1.7693
13	1.0874	46	1.3570	86	1.7872
14	1.0947	48	1.3759	88	1.8022
15	1.1020	50	1.3952	90	1.8144
16	1.1094	52	1.4149	92	1.8240
17	1.1169	54	1.4351	94	1.8312
18	1.1245	56	1.4558	96	1.8355
19	1.1321	58	1.4770	98	1.8361
20	1.1398	60	1.4987	100	1.8305

Table 4 Densities of HNO_3 solutions

w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]
1	1.0037	15	1.0840	40	1.2463
2	1.0091	16	1.0901	42	1.2591
3	1.0146	17	1.0963	44	1.2719
4	1.0202	18	1.1025	46	1.2847
5	1.0257	20	1.1150	48	1.2975
6	1.0314	22	1.1277	50	1.3100
7	1.0370	24	1.1406	52	1.3219
8	1.0427	26	1.1536	54	1.3336
9	1.0485	28	1.1668	56	1.3449
10	1.0543	30	1.1800	58	1.3560
11	1.0620	32	1.1934	60	1.3667
12	1.0660	34	1.2071	62	1.3769
13	1.0720	36	1.2205	64	1.3866
14	1.0780	38	1.2335	65	1.3913

Table 5 Densities of H_3PO_4 solutions

w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]
1	1.0038	11	1.0589	22	1.1263
2	1.0092	12	1.0647	24	1.1395
3	1.0146	13	1.0705	26	1.1528
4	1.0200	14	1.0765	28	1.1665
5	1.0254	15	1.0825	30	1.1804
6	1.0309	16	1.0885	32	1.1945
7	1.0363	17	1.0947	34	1.2089
8	1.0418	18	1.1009	36	1.2236
9	1.0474	19	1.1071	38	1.2385
10	1.0531	20	1.1135	40	1.2536

Table 6 Densities of NH_3 solutions

w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]
1	0.9938	11	0.9538	21	0.9196
2	0.9895	12	0.9502	22	0.9164
3	0.9853	13	0.9466	23	0.9132
4	0.9811	14	0.9431	24	0.9101
5	0.9770	15	0.9396	25	0.9070
6	0.9730	16	0.9361	26	0.9040
7	0.9690	17	0.9327	27	0.9010
8	0.9651	18	0.9294	28	0.8980
9	0.9613	19	0.9361	29	0.8950
10	0.9575	20	0.9228	30	0.8920

Table 7 Densities of NaOH solutions

w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]
1	1.0095	11	1.1199	22	1.2412
2	1.0207	12	1.1309	24	1.2631
3	1.0138	13	1.1419	26	1.2848
4	1.0428	14	1.1530	28	1.3064
5	1.0538	15	1.1640	30	1.3277
6	1.0648	16	1.1751	32	1.3488
7	1.0758	17	1.1861	34	1.3697
8	1.0869	18	1.1971	36	1.3901
9	1.0979	19	1.2082	38	1.4102
10	1.1089	20	1.2192	40	1.4299

Table 8 Densities of KOH solutions

w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]	w/w [%]	Density [g/mL]
1	1.0068	11	1.0966	22	1.2014
2	1.0155	12	1.1059	24	1.2210
3	1.0242	13	1.1153	26	1.2408
4	1.0330	14	1.1246	28	1.2609
5	1.0419	15	1.1341	30	1.2813
6	1.0509	16	1.1435	32	1.3020
7	1.0599	17	1.1531	34	1.3230
8	1.0690	18	1.1626	36	1.3444
9	1.0781	19	1.1722	38	1.3661
10	1.0873	20	1.1818	40	1.3881

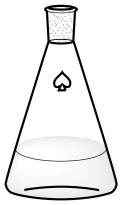
Table 9 Solubilities of some selected substances at various temperatures (g of substance for 100 g of water)

Compound	0 °C	20 °C	50 °C	80 °C	100 °C
$AgNO_3$	127	210	446 (60 °C)	585	719
$Al_2(SO_4)_3$	31	36	50	-	89
$Al_2(SO_4)_3 \cdot 18\ H_2O$	86	108	220	508	1 108
$BaCl_2$	31.6	35.7	40.7 (*40 °C*)	45.9	51.2
$BaCl_2 \cdot 2H_2O$	38.6	45	50	-	77
$Ba(NO_3)_2$	5.0	9.0	177.1	27.0	34.2
$CaCl_2 \cdot 2H_2O$	97.6	130.1	326 (*60 °C*)	373.6	437
$CaCl_2 \cdot 6H_2O$	283	564	-	-	-
$Ca(HCO_3)_2$	16.2	16.6	17.5 (*60 °C*)	17.9	18.4
$Ca(NO_3)_2 \cdot 4H_2O$	258	444	-	-	-
$Cu(NO_3)_2 \cdot 6H_2O$	248.5	785	-	-	-
$CuSO_4$	14.3	20.7	33.3	55	75.4
$CuSO_4 \cdot 5H_2O$	24	35.5	80		205
$FeCl_3$	74.4	91.8	315.1	528.8	554
$FeCl_3 \cdot 6H_2O$	245.9	395	-	-	-
$FeSO_4 \cdot 7H_2O$	33	61.5	180.5 (*56°C*)	-	-
H_3BO_3	2.7	5.0	11.5	23.6	37.6
$HgCl_2$	3.8	6.2	16	-	55.4
KBr	65.11	75.92	86.03	95.18	103.26
KCl	28.1	34.2	42.651.1	51.1	56.2
$KClO_4$	1.71	3.67	7.23	13.27	22.95
$KHCO_3$	22.9	33.2	60	-	-
KI	127.5	144	168	192	208
KNO_3	13.3	31.6	85.5	169	246
KOH	97	112	140	-	178
KSCN	223.29	286.38	373.01	497.07	686.12
K_2CO_3	105.5	110.5	121	-	156
K_2CrO_4	56	63.8	66.8	72.1	79.6
$K_2Cr_2O_7$	4.5	12.2	34.5	73	95.6
K_2SO_4	7.35	11.11	14.8 (*14 °C*)	-	-
$Na_2B_4O_7 \cdot 10H_2O$	1.3	2.7	20.3 (*60 °C*)	-	-
NaCl	35.6	35.9	37.0	38.4	39.2
$NaHCO_3$	6.9	9.6	14.45	-	23.8
$NaNO_3$	71	88	114	148	180
NaOH	42	109	145	-	347
Na_2CO_3	-	21.5	-	-	45.5
Na_2SO_4	-	-	46.53	43.31	42.21
$Na_2SO_4 \cdot 10H_2O$	5.0	19.4	-	-	-
NH_4Cl	29.4	37.2	50.4	65.6	77.3
$NiCl_2 \cdot 6H_2O$	174.50	239.75	-	-	-
$PbCl_2$	0.67	0.99	1.70	2.64	3.34
$Pb(NO_3)_2$	38.8	56.5	85	115	127
$ZnSO_4 \cdot 7H_2O$	-	165.6	-	-	390

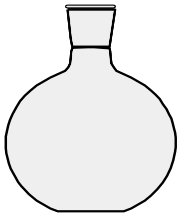
GLASSWARE (A) AND EQUIPMENT (B) COMMONLY USED IN CHEMICAL LABORATORY

A (glassware)

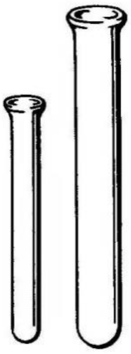
beaker



Erlenmayer flask



boiling flat-bottom flask

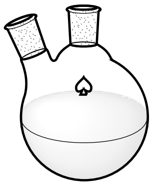


test tubes

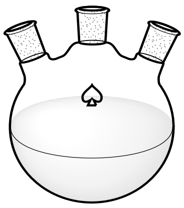
watch glass

evaporating dish (porcelain)

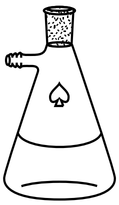
distillation round-bottom flask



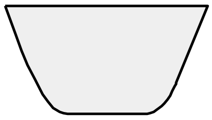
distillation two-necked flask



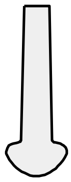
three-necked flask



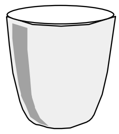
suction flask



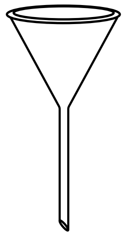
mortar



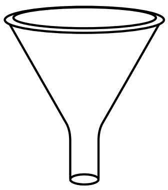
pestle



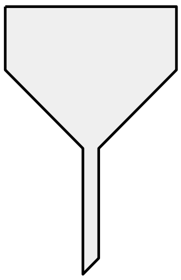
porcelain crucible



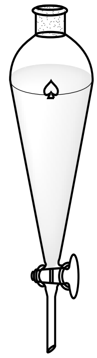
funnel with a long stem



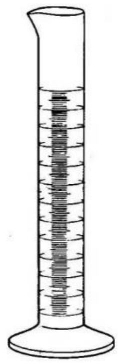
fluted funnel



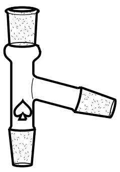
Büchner funnel



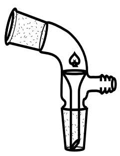
separatory funnel



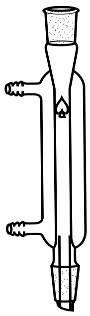
graduated cylinder



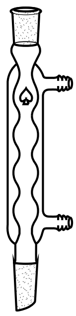
adapter



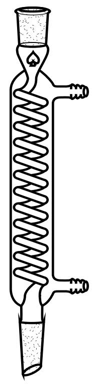
vacuum adapter



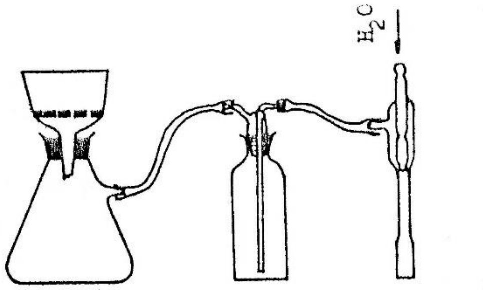
Liebig condenser



bulb condense



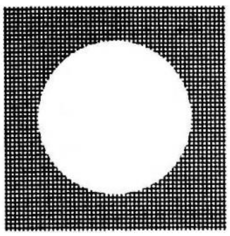
spiral condenser



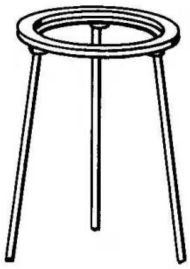
trap flask jet-water pump

Büchner funnel
suction flask

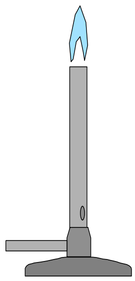
B (equipment)



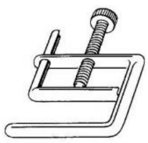
wire gauze with Teflon center



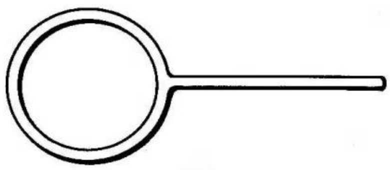
tripod



gas burner

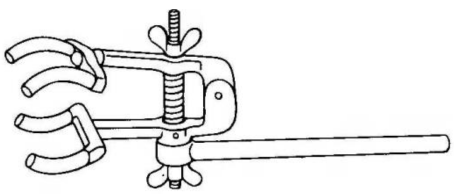


screw clamp

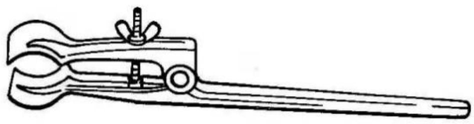


iron ring

iron ring with clamp



condenser holder



flask holder

ENGLISH-SLOVAK VOCABULARY

acid	kyselina
base	zásada
beaker	kadička
boil	vrieť
burner	kahan
flask	banka, nádoba
coat	plášť
chemical	chemikália, chemický
chemistry	chémia
clamp	svorka
composition	zloženie
compound	zlúčenina
condenser	chladič
cool	chladný, chladiť
crucible	téglik
cylinder (graduated)	valec (odmerný)
decomposition	rozklad
distillation	destilácia
dish	miska
dissolved	rozpustený
dry	suchý
element	prvok
equation	rovnica
evaporate	odparovať
filtration	filtrácia
flame	plameň
flask	nádoba, banka
formula	vzorec
fume cupboard	digestor
funnel	lievik
gas	plyn
glass	sklo
glasses	okuliare
gloves	rukavice
grade	stupeň
ground glass joint	zábrus
heat	teplo
holder	lapák
ice	ľad
lamp	lampa
liquid	kvapalina
matches	zápalky
melt (to)	tavenina, (taviť)
moist	vlhký
moisture	vlhkosť
oil	olej
oil bath	olejový kúpeľ
oven	pec, sušiareň
paper	papier

point	bod
powder	prášok
precipitate	zrazenina
precipitation	zrážanie
pressure	tlak
reaction	reakcia
ring	kruh
salt	soľ
sand	piesok
scissors	nožnice
solid	pevný, teleso
solubility	rozpustnosť
solution	roztok, riešenie
solute	rozpustená látka
solvent	rozpúšťadlo
spatula	lopatka (špachtľa)
spoon	lyžica
stand	stojan
state	stav, skupenstvo
substance	látka
temperature	teplota
test tube	skúmavka
tongs	kliešte
volatile	prchavý
warm	horúci
water	voda
water bath	vodný kúpeľ
water pump	vodná výveva
wire gauze	sieťka

condenser	chladič
Dimroth c.	
Liebig c.	
reflux c.	spätný
spiral c.	špirálový

filtration	filtrácia
at normal pressure	za normálneho tlaku
at diminished pressure	za zníženého tlaku
vacuum f.	vákuová

flask	banka
boiling f.	varná
distillation f.	destilačná
flat-bottom f.	s plochým dnom
round-bottom f.	s guľatým dnom
suction f.	odsávacia
trap f.	poistná

funnel	lievik
Büchner f.	Büchnerov
with long stem	s dlhou stopkou

glasses	okuliare
protecting g.	ochranné
gloves	rukavice
heat resistant g.	tepluvzdorné
protecting g.	ochranné
point	bod
boiling p.	varu
dew p.	rosný
melting p.	topenia
pressure	tlak
normal, atmospheric p.,	normálny
lowered, diminished p.	znížený
temperature	teplota
ambient (room) t.	laboratórna
lowered t.	znížená
elevated t.	zvýšená

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