APPENDIX B: EXERCISES

Molecular mass, the mole, and mass percent

Relative atomic and molecular mass

Relative atomic mass (A_r) is a constant that expresses the ratio of an exact atomic mass to the unified atomic mass unit (*amu*). It is unique for each element, and you can find it in the periodic table of the elements. Relative molecular mass (M_r) has similar meaning to A_r but for molecules. It is calculated as a sum of A_r of all atoms forming a molecule.

$$M_r\,(X_aY_b) = a\,A_r(X) + b\,A_r(Y)$$

The mole   n   [mol]

A single atom is so small that in order for any sample of matter to be large enough to be seen and manipulated it must consist of a huge number of atoms. Because of this, it is convenient to be able to specify the total number of atoms in a sample, not as individual atoms but rather in terms of "packages" consisting of a certain number of atoms. One mole is defined as the number equal to the number of carbon atoms in exactly 12 grams of pure ${}^{12}_{6}C$. This number is called Avogadro's number and it is equal to $6.023\cdot10^{23}$ particles. The mole expresses how many times the number of particles is greater than Avogadro's number.

Avogadro's number $N_A = 6.023\cdot10^{23}\ \text{mol}^{-1}$

$$n = \frac{N}{N_A}$$

N ········ number of particles

Molecular weight   M   [g/mol]

Molecular weight is the mass of 1 mole of any substance and is numerically equal to M_r.

$$M = \frac{m}{n}$$

m ·········· mass [g]

Example 1: How many moles are there in 200 grams of boron oxide?

$$M\,(B_2O_3) = 2\times10.8 + 3\times16 = 69.6\ \text{g}\cdot\text{mol}^{-1}$$

$$n = \frac{m}{M} = \frac{200\ \text{g}}{69.6\ \text{g mol}^{-1}} = 2.87\ \text{mol}$$

Mass percent

Mass percent expresses the fraction of atoms or a group of atoms in the mass of the whole molecule.

$$w(A) = \frac{m(A)}{m(A_xB)}\cdot 100\ \% = \frac{x\,M\,(A)}{M\,(A_xB)}\cdot 100\ \%$$

Example 2: What is the mass percent of elements in boron oxide?

$$w(B) = \frac{2\,M(B)}{M(B_2O_3)} = \frac{2\times 10.8}{69.6}\cdot 100\ \% = 31.03\ \%$$

$$w(O) = \frac{3\,M(O)}{M(B_2O_3)} = \frac{3\times 16}{69.6}\cdot 100\ \% = 68.97\ \%$$

Example 3: How many grams of boron are there in 200 grams of boron oxide?

a) To solve this problem we can use the result from the previous example.

$$m(B) = w(B)\ m(B_2O_3) = 0.3103 \times 200\ \text{g} = 62.06\ \text{g}$$

b) Another way is to apply direct proportion where the ratio of real masses is equal to the ratio of molecular weights and stoichiometric coefficients

$$B_2O_3 \longrightarrow 2\ B$$

1 mol ·········· 69.6 g ···················· 2×10.8 g
200 g ···················· x g

$$x = \frac{2\times 10.8}{69.6}\times 200 = 62.06\ \text{g}$$

Example 4: A rock contains 45 % of magnetite (Fe_3O_4). How many kg of iron can be obtained from 2 t of the rock? M(Fe) = 55.8 g/mol; M(Fe_3O_4) = 231.4 g/mol

Pure Fe_3O_4 is 0.45·2000 = 900 kg

$$Fe_3O_4 \longrightarrow 3\ Fe$$

1 mol ······ 231.4 g Fe_3O_4 ··········· 3×55.8 g Fe
900 kg Fe_3O_4 ············ x kg Fe

$$x = \frac{3\times 55.8}{231.4}\times 900 = 651.1\ \text{kg}$$

Problems to solve:

1. How many kg of pyrite (FeS_2) containing 5 % impurities are to be processed in order to obtain 442 kg of pure iron? [**999.42 kg**]
2. Calculate the mass percent of all elements in dolomite $CaCO_3{\cdot}MgCO_3$. [**21.8 % Ca, 13.2 % Mg, 13 % C, 52 % O**]
3. How many moles of water are present in 15 g of $FeSO_4{\cdot}7H_2O$? [**0.378 mol**]
4. Calculate the content of Zn in 324 g of white vitriol ($ZnSO_4{\cdot}7H_2O$). [**73.7 g**]
5. Calculate the percentage composition of the mineral merwinite ($3CaO{\cdot}MgO{\cdot}2SiO_2$). [**51.1 %CaO, 12.3 %MgO, 36.6 % SiO_2**]

6. How many kg of sulphur are there in 10 kg of 38 % sulphuric acid? [**1.24 kg**]
7. How many moles make up 6.01 kg of SiO_2? [**100 mol**]
8. How many g and mol of aluminum are there in 30 g of Al_2O_3? [**15.88 g, 0.59 mol**]

Preparation of mixes and solutions and the calculation of concentration

General formula for mixing liquid and solid materials

The general formula for mixing liquid and solid materials is used for the calculation of concentration in percent or for the preparation of solutions or solid mixtures with a fixed percent of concentration. It is a mass balance, hence it is only allowed to take into account the relation between mass and mass percent.

$$m_1 w_1 + m_2 w_2 + \cdots + m_x w_x = (m_1 + m_2 + \cdots + m_x)\, w$$

m ········ mass (g, kg, t) w ·········· mass % or mass fraction

The left side of the equation represents components of the mixture and the right side represents the resulting mixture. The mass percent always refers to only one chemical substance in the mixture irrespective of the mixture component. If one of the components is a pure chemical, its concentration is 100 %.

Caution! If you mix two different liquids, the volume of the resulting mixture is not equal to the sum of the volumes of its components (different densities).

$$m_1 + m_2 = m \quad \text{but} \quad V_1 + V_2 \neq V$$

Example 1: What is the final mass concentration of a mixture prepared from 1t of material with 92% SiO_2 and 2 t of material with 9% SiO_2?

$$m_1 w_1 + m_2 w_2 = (m_1 + m_2)\, w$$
$$1\times92 + 2\times9 = (1 + 2)\, w$$
$$110 = 3\, w$$
$$w = 36.7\%$$

Example 2: How many grams of NaOH (1) it is necessary to dissolve in water (2), in order to obtain 920 mL of 10% NaOH? (ρ = 1.087 g/cm3)

$$m_1 w_1 + m_2 w_2 = m\, w$$
$$m_1\times100 + m_2\times0 = m\times10 \qquad m = V\rho$$
$$m_1\times100 + m_2\times0 = 920\times1.087\times10$$
$$m_1 = 100 \text{ g}$$

Example 3: How many g of $Na_2CO_3\cdot10H_2O$ (**1**) have to be added to 800 g of 15% Na_2CO_3 (**2**), in order to obtain a 20% solution?
$M(Na_2CO_3) = 106$ g/mol; $M(Na_2CO_3\cdot10H_2O) = 286$ g/mol

If $Na_2CO_3 \cdot 10H_2O$ is dissolved in water the hydrate decomposes and the crystalline water becomes part of the solvent. Therefore, the mass percent only refers to an Na_2CO_3 solution.

$$w_1 = \frac{M(Na_2CO_3)}{M(Na_2CO_3 \cdot 10H_2O)} = \frac{106}{286} \cdot 100\ \% = 37.1\ \%$$

$$m_1 w_1 + m_2 w_2 = (m_1 + m_2)\, w$$
$$m_1 \times 37.1 + 800 \times 15 = (m_1 + 800) \times 20$$
$$17.1 \times m_1 = 4000$$
$$m_1 = 233.9\ \text{g}$$

Problems to solve:

1. How many grams of $Al_2(SO_4)_3 \cdot 12H_2O$ and water have to be mixed in order to prepare 1 L of 1% solution? ($\rho = 1.008$ g/cm^3) M(Al) = 27 g/mol; M(S) = 32.1 g/mol; M(O) = 16 g/mol; M(H) = 1 g/mol [**16.44 g; 991.56 g**]
2. A mixture was prepared from the following raw materials: 6 t of 15.6% $CaCO_3$, 2.4 t of 32% $CaCO_3$, and 8.6 t of 25% $CaCO_3$. How many % of $CaCO_3$ does the final mixture contain? [**22.67%**]
3. How many g of $AgNO_3$ with 9% content of insoluble impurities are needed for the preparation of 5 kg of 10% solution of $AgNO_3$? [**549.5 g**]
4. How many mL of 65% HNO_3 ($\rho = 1.39$ g/cm^3) are necessary for the preparation of 500 mL of 30% HNO_3 ($\rho = 1.18$ g/cm^3)? [**196 mL**]
5. How many g of KI are needed for the preparation of 45 g of 5% solution?[**2.25 g**]
6. How many mL of 80% H_3PO_4 ($\rho = 1.633$ g/cm^3) are necessary for the preparation of 500 mL of 4% H_3PO_4 ($\rho = 1.020$ g/cm^3)? [**15.61 mL**]
7. How many g of KOH have to be added to 28 mL of 0.12% KOH in order to obtain a 0.39% solution? [**0.0756 g**]
8. How many mL of 98% H_2SO_4 ($\rho = 1.84$ g/cm^3) and water have to be mixed for the preparation of 2 L of 10% H_2SO_4 ($\rho = 1.20$ g/cm^3)? [**133.1 mL 98% H_2SO_4; 2155.1 mL H_2O**]

Calculation of pH

Water is the most common amphoteric substance. It undergoes partial autoionisation, which involves the transfer of a proton from one water molecule to another to produce a hydroxide anion and a hydronium ion.

$$2\ H_2O \rightleftharpoons H_3O^+ + OH^-$$

This reaction leads to the equilibrium expression

$$K_w = c(H_3O^+)\, c(OH^-) = c(H^+)\, c(OH^-) = 10^{-14}\ \text{mol}^2\ \text{L}^{-2}$$

Since the concentration of hydrogen ions in an aqueous solution is quite small, the pH scale provides a convenient way to represent solution acidity. The pH is a base 10 logarithmic scale. The pOH that represents solution basicity is expressed in a similar way. To calculate the pH of strong acids and bases we can just use the three following equations:

$$pH = -\log c(H^+)$$
$$pOH = -\log c(OH^-)$$
$$pH + pOH = 14$$

Example 1: Calculate the pH value of an HCl solution when c(HCl) = 0.01 mol/L!

HCl – strong acid, completely dissociates => $HCl \longrightarrow H^+ + Cl^-$

$c(H^+) = c(HCl)$
$pH = -\log c(H^+) = -\log c(HCl) = -\log 0.01 = 2$

Example 2: Calculate the pH value of a $Ca(OH)_2$ solution when $c(Ca(OH)_2) = 0.005$ mol/L!

$Ca(OH)_2$ – completely dissociates => $Ca(OH)_2 \longrightarrow Ca^{2+} + 2\,OH^-$

$c(OH^-) = 2\,c(Ca(OH)_2)$
$pOH = -\log c(OH^-) = -\log 2\,c(Ca(OH)_2) = -\log 2\times0.005 = 2$
$pH = 14 - pOH = 14 - 2 = 12$

Example 3: Calculate the concentration of an HCl solution when pH = 4!

HCl – strong acid, completely dissociates => $c(H^+) = c(HCl)$

$4 = -\log c(HCl)$ => $c(HCl) = 10^{-4} = 0.0001$ mol/L

Problems to solve:

1. Calculate the pH values of HNO_3 solution of the following concentrations:
   a) $3.5\cdot10^{-5}$
   b) $2\cdot10^{-4}$
   c) $7.8\cdot10^{-10}$ [**4.46; 3.7; 9.11**]
2. Calculate concentrations of H^+ and OH^- ions, if the pH value equals:
   a) 9.55 [$\mathbf{2.82\cdot10^{-10}; 3.55\cdot10^{-5}}$]
   b) 6.20 [$\mathbf{6.31\cdot10^{-7}; 1.58\cdot10^{-6}}$]
   c) 4.3 [$\mathbf{5.01\cdot10^{-5}; 1.99\cdot10^{-10}}$]
3. What is the pOH value of an HCl solution when $c(HCl) = 1.94\cdot10^{-5}$ mol/L?**[9.29]**
4. Calculate the pH values of an NaOH solution when c(NaOH) = 0.2068 mol/L! [**13.32**]
5. Calculate the pH of a sulphuric acid solution with a concentration of 0.02 mol/L? [**1.4**]
6. What is the concentration of an HCl solution when the pOH is 12,2? [$\mathbf{1.58\cdot10^{-2}}$ **mol/L**]
7. Calculate the pH values of an NaOH solution when c(NaOH) = 0.6 mol/L![**12.8**]

Calculations from chemical equations

The first thing that we must do in calculations involving chemical reactions is to write the balanced chemical equation. The ratio of the moles of any two compounds from an equation is equal to the ratio of the corresponding stoichiometric coefficients.

$$\boldsymbol{a}\,\mathbf{A} + \boldsymbol{b}\,\mathbf{B} \longrightarrow \boldsymbol{c}\,\mathbf{C} + \boldsymbol{d}\,\mathbf{D}$$

a, b, c, d ······· stoichiometric coefficients

$$\frac{n(C)}{n(A)} = \frac{c}{a}$$

→ this expression can also be transformed into the rule of proportion

$a\ M(\mathrm{A})$ ·························· $c\ M(\mathrm{C})$

$m(\mathrm{A})$ ·························· $m\,(\mathrm{C})$

$$\frac{m(A)}{a\,M(A)} = \frac{m(C)}{c\,M(C)}$$

$$m(C) = \frac{c\,M(C)}{a\,M(A)}\,m(A)$$

Example 1: How many tons of burnt lime can be obtained from 16 t of pure limestone?

$$CaCO_3 \longrightarrow CaO + CO_2$$

1×100.1 g/mol $CaCO_3$ ················ **1**×56.1 g/mol CaO

16 t $CaCO_3$ ··························· *x* t CaO

$$x = \frac{1\times 56.1}{1\times 100.1}\times 16 = 8.97\ \mathrm{t}$$

Problems to solve:

1. How many kg of CaO can be obtained by burning of 730 kg of limestone containing 5% impurities? [**388.6 kg**]
2. How many g of SO_2 will be formed by burning 12 g of sulphur? [**24 g**]
3. How many g of quick-setting plaster can be obtained by heating 7.5 kg of gypsum with a 2.5% content of impurities? [**6.16 kg**]
4. How many tons of slaked lime are formed by slaking 6.5 t of burnt lime containing 2.5% impurities? [**8.28 t**]
5. How many tons of burnt lime can be obtained from 20 t of 90% $CaCO_3$? [**10.09 t**]
6. How many g of aluminum hydroxide are formed by precipitating 18 g of aluminum sulphate with sodium hydroxide? [**8.21 g**]
7. How many tons of MgO can be obtained from 250 tons of magnesite containing 85% $MgCO_3$? [**104 t**]
8. How many tons of lime hydrate are formed by slaking 100 tons of air lime that contains 13% impurities? [**114.9 t**]

Volume of dilute solutions

Many reactions occur in the liquid phase as water solutions (neutralisation, hydrolysis). However, it is always necessary to consider only pure chemicals for calculations from chemical equations.

Example 2: How many grams of NaOH are necessary for the neutralisation of 50 mL of 21% H_2SO_4 ($\rho = 1.47$ g/cm^3)?

$$m(H_2SO_4) = V\rho\, w = \underbrace{50 \times 1.47}_{m(21\%\ H_2SO_4)} \times 0.21 = 15.435 \text{ g} \rightarrow \text{mass of pure } H_2SO_4$$

m(21% H_2SO_4) → mass of the solution

$$2\ NaOH + H_2SO_4 \longrightarrow Na_2SO_4 + 2\ H_2O$$

1 × 98 g/mol H_2SO_4 .... **2** × 40 g/mol NaOH

15.435 g H_2SO_4 .... x g NaOH

$$x = \frac{2 \times 40}{1 \times 98.1} \times 15.435 = 12.6 \text{ g}$$

Problems to solve:

1. How many mL of 21% HCl ($\rho = 1.008$ g/cm^3) are necessary for the neutralisation of 15 g of solid NaOH? [**64.7 mL**]
2. How many kg of NaOH are necessary for the neutralisation of 550 L of 70% H_2SO_4 ($\rho = 1.61$ g/cm^3)? [**505.5 kg**]
3. How many mL of 5% HNO_3 ($\rho = 1.03$ g/cm^3) are necessary for the neutralisation of 5 g of solid NaOH? [**152.9 mL**]
4. How many g of NaOH are necessary for the neutralisation of 100 mL of 36% HCl ($\rho = 1.1789$ g/cm^3)? [**46.51 g**]
5. How many litres of 20% HCl ($\rho = 1.1$ g/cm^3) are necessary for the neutralisation of 8.4 L of 10% NaOH ($\rho = 1.109$ g/cm^3)? [**3.86 L**]
6. How many litres of 25% KOH ($\rho = 1.29$ g/cm^3) are necessary for neutralisation of 8 L 14% HCl ($\rho = 1.07$ g/cm^3)? [**5.71 L**]
7. How many litres of 30% NaOH ($\rho = 1.328$ g/cm^3) are necessary for the neutralisation of 82 L of 62% H_2SO_4 ($\rho = 1.520$ g/cm^3)? [**158.2 L**]
8. How many g of KOH are necessary for the neutralisation of 50 mL of 24% H_2SO_4 ($\rho = 1.173$ g/cm^3)? [**16.12 g**]
9. How many mL of 5% HNO_3 ($\rho = 1{,}0256$ g cm^{-3}) are needed for the neutralisation of 9 g of NaOH ? [**276.4 mL**]
10. How many L of 12% KOH ($\rho = 1{,}13$ g·cm^{-3}) are necessary for the neutralisation of 2.5 litres of 10% H_2SO_4 ($\rho = 1{,}095$ g·cm^{-3})? [**2,31 l**]

Volume of gases

Some components in chemical reactions are gaseous. It is more convenient and customary to calculate their volumes. The volume of gases depends only on temperature and pressure conditions and is directly proportional to the number of moles of gas. The volume of 1 mole of gas is called the **molar volume**. Its value for normal temperature and pressure is given by the ideal gas law.

1 mol ······· *M = m/n* [g/mol] ··········· V_m = *V/n* [dm^3/mol]
molecular weight *molar volume*

$$V_m = \frac{RT}{p} = \frac{8.314\, J\, mol^{-1}\, K^{-1} \times 273.15\, K}{101325\, Pa} = 0.02241\, m^3\, mol^{-1}$$

> In equations:
>
> 1 g/mol ≅ 1 L/mol, dm^3/mol
> 1 kg/mol ≅ 1 m^3/mol
>
> **Remember**
> **V_m = 22.4 L·mol^{-1} !!!**

Example 3: How many litres of hydrogen are formed by the reaction of 20 g of zinc with hydrochloric acid?

$$Zn + 2\,HCl \longrightarrow ZnCl_2 + H_2$$

1 × 65.4 g/mol Zn ················ **1** × 22.4 L/mol H_2

20 g Zn ··························· x L H_2

$$x = \frac{1 \times 22.41\ \mathrm{L\,mol^{-1}}}{1 \times 65.4\ \mathrm{g\,mol^{-1}}} \times 20\ \mathrm{g} = 6.85\ \mathrm{L}$$

Problems to solve:

1. How many m^3 of CO_2 are formed by the decomposition of 12 t of $MgCO_3$ containing 15% of impurities? [**2711 m^3**]
2. How many litres of CO_2 can be formed by the decomposition of 500 g of limestone containing 3% of impurities? [**108.68 L**]
3. How many litres of hydrogen are formed by the reaction of 30 g of zinc with hydrochloric acid? [**10.28 L**]
4. How many litres of SO_2 are formed by the combustion of 8.7 kg of coal, which contains 2.8% of sulphur? [**170 L**]
5. How many m^3 of oxygen are needed for the combustion of 2 m^3 of methane (CH_4)? [**4 m^3**]
6. How many m^3 of CO_2 are formed by the combustion of 2.3 t of coal, which contains 8% of impurities? [**3950 m^3**]
7. How many m^3 of HF are formed by the reaction of 1 t of fluorite containing 85% CaF_2 with sulphuric acid? [**488 m^3**]

APPENDIX C: TABLE OF THE ELEMENTS

Name	Symbol	Atomic number	M [g·mol^{-1}]	Electronegativity
Aluminum	Al	13	26.98	1.5
Antimony	Sb	51	121.75	1.9
Arsenic	As	33	74.92	2.0
Barium	Ba	56	137.33	0.9
Bismuth	Bi	83	208.98	1.9
Boron	B	5	10.81	2.0
Bromine	Br	35	79.90	2.8
Cadmium	Cd	48	112.41	1.7
Calcium	Ca	20	40.08	1.0
Carbon	C	6	12.01	2.5
Cesium	Cs	55	132.91	0.7
Chlorine	Cl	17	35.45	3.0
Chromium	Cr	24	52.00	1.6
Cobalt	Co	27	58.93	1.9
Copper	Cu	29	63.55	1.9
Fluorine	F	9	19.00	4.0
Gold	Au	79	196.97	2.4
Hydrogen	H	1	1.01	2.1
Iodine	I	53	126.90	2.5
Iron	Fe	26	55.85	1.8
Lead	Pb	82	207.2	1.8
Magnesium	Mg	12	24.31	1.2
Manganese	Mn	25	54.94	1.5
Mercury	Hg	80	200.59	1.9
Nickel	Ni	28	58.69	1.8
Nitrogen	N	7	14.01	3.0
Oxygen	O	8	16.00	3.5
Phosphorus	P	15	30.97	2.1
Potassium	K	19	39.10	0.8
Selenium	Se	34	78.96	2.4
Silicon	Si	14	28.09	1.8
Silver	Ag	47	107.87	1.9
Sodium	Na	11	23.00	0.9
Strontium	Sr	38	87.62	1.0
Sulphur	S	21	32.07	2.5
Tin	Sn	50	118.71	1.8
Titanium	Ti	22	47.88	1.5
Zinc	Zn	30	65.39	1.6