Stoichiometry and related calculations

Basic constants

Avogadro's Number $N_A = 6.022\,14 \times 10^{23}$ represents the number of atoms, molecules, or ions in one mole.

Atomic Mass Constant $1\ \text{amu} = \frac{m(^{12}\text{C})}{12} = 1.660\,538 \times 10^{-27}$ kg

Relative Atomic Mass the unified atomic mass unit or dalton (symbol: Da) is the standard unit that is used for indicating mass on an atomic or molecular scale (atomic mass). One unified atomic mass unit is approximately the mass of one nucleon (either a single proton or neutron) and is numerically equivalent to 1 g/mol.
It is defined by the means of Atomic Mass Constant – $A_r(\text{Li}) = \frac{m(\text{Li})}{\text{amu}}$

Molar volume $V_m = 22.413\,83\ \text{dm}^3 \cdot \text{mol}^{-1}$ – the volume, occupied by a 1 mol of any gas at the Standard Temperature and Pressure (273.15 K and 101.325 kPa)

Basic formulas

$$m = n \cdot M_r \quad n = \frac{m}{M_r} \quad m = \rho \cdot V \quad V = \frac{m}{\rho} \quad V_{gas} = n \cdot V_m \quad n = \frac{V_{gas}}{V_m}$$

where: m is mass; M_r is relative molecular weight; n is the mass of the substance (mol); V is the volume of a liquid; ρ is relative density (usually in $\text{g} \cdot \text{cm}^{-3}$); V_{gas} is volume of a gas; V_m is molar volume ($\text{dm}^3 \cdot \text{mol}^{-1}$)

Elemental analysis

Example 1. Calculate molar and mass ratio of elements in ammonia

Ammonia – NH_3 – Molar ratio of nitrogen and hydrogen in the molecule is 1 : 3. Based on this and the relative atomic masses we can calculate the mass ratio of particular elements. ($A_r(\text{N}) = 14.0067$; $A_r(\text{H}) = 1.008$)

The mass ratio can be calculated as $A_r(\text{N}) : 3 \times A_r(\text{H}) = 14.01 : 3.0237$. We usually calculate mass composition of a compound in mass percents.

$$w\%(element) = \frac{A_r(element) \times n}{M_r(compound)} \times 100 \qquad \text{where } n \text{ is a molar coefficient}$$

In case of the ammonia it is:

$$w\%\text{N} = \frac{14.01}{17.04} \times 100 = 82.25\ \% \quad w\%\text{H} = \frac{1.0079 \times 3}{17.04} \times 100 = 17.75\ \%$$

Ammonia contains 82.25 % of nitrogen and 17.75 % of hydrogen.

Example 2. We have a compound, which contains potassium, aluminium, sulfur, oxygen and hydrogen. The composition of the compound is showed below.

K	8.2418 %
Al	5.6877 %
S	13.5190 %
O	67.4530 %
H	5.0993 %

$A_r(\mathrm{K}) = 39.10$; $A_r(\mathrm{Al}) = 26.98$; $A_r(\mathrm{S}) = 32.065$; $A_r(\mathrm{O}) = 16.00$; $A_r(\mathrm{H}) = 1.008$

Calculate its stoichiometric formula.

We need calculate molar ratio of particular elements For this purpose, we can assume, that we have 100 g of a compound.

$$n = \frac{m}{A_r} \qquad n(\mathrm{K}) = \frac{8.2418}{39.098} = 0.2107985 \text{ mol}$$

$$n(\mathrm{Al}) = \frac{5.6877}{26.982} = 0.210796 \text{ mol} \quad n(\mathrm{S}) = \frac{13.519}{32.065} = 0.421612 \text{ mol}$$

$$n(\mathrm{O}) = \frac{67.453}{15.9994} = 4.21597 \text{ mol} \quad n(\mathrm{H}) = \frac{5.0993}{1.0079} = 5.05933 \text{ mol}$$

As the next step divide all obtained amounts of substances by the lowest number. We obtain:

K	1.0
Al	1.0
S	2.0
O	20.0
H	24.0

The stoichiometric formula of the compound is $KAlS_2O_{20}H_{24}$

Example 3. We have a compound, which contains carbon, hydrogen and bromine. The composition of the compound is showed below.

C	29.9509 %
H	3.6306 %
Br	66.4185 %

$A_r(\mathrm{C}) = 12.01$; $A_r(\mathrm{H}) = 1.008$; $A_r(\mathrm{Br}) = 79.904$

Calculate its stoichiometric formula.

According the procedure, described previously we obtain the molar ratios of the particular elements

C	3.000
H	4.333
Br	1.000

In this case we have to multiply the coefficients by three to obtain the whole numbers. The stoichiometric formula of the compound is $C_9H_{13}Br_3$

Chemical equation based calculations

There is chemical reaction of compounds A and B, compounds C and D arise
$\mathrm{a\,A + b\,B \longrightarrow c\,C + d\,D}$,
the letters a, b, c, and d represents molar coefficients of particular compounds in the chemical equation. Based on the equation is possible to calculate masses of all particular compounds in the reaction using general formulas

$$m(\mathrm{A}) = a \cdot n \cdot M_r(\mathrm{A}), \quad m(\mathrm{B}) = b \cdot n \cdot M_r(\mathrm{B}), \quad m(\mathrm{C}) = c \cdot n \cdot M_r(\mathrm{C}), \quad m(\mathrm{D}) = d \cdot n \cdot M_r(\mathrm{D})$$

where n is amount of substance of one equivalent in the particular preparation. To be able to calculate the masses is necessary to know mass of at least one compound.

Exercises

1. Calculate number of atoms, which contains 1 mg of pure silver.
   $A_r(\mathrm{Ag}) = 107.87$

2. The atom of an element has mass of 3.2395×10^{-25} kg. Calculate its relative atomic mass A_r. What is the name of the element?

3. Calculate relative atomic mass of a gas, if 25 litres of the gas weights 31.258 g at standard conditions.

4. Calculate content of vanadium and oxygen (in mass %) in the vanadium(V) oxide.
   $A_r(\mathrm{V}) = 50.94$; $A_r(\mathrm{O}) = 15.9994$

5. Calculate content of all particular elements as mass percents in the compound, which molecular formula is $C_{23}H_{29}N_3O_4$. For the result use four decimal places.
   $A_r(\mathrm{C}) = 12.01$; $A_r(\mathrm{H}) = 1.008$; $A_r(\mathrm{N}) = 14.0067$; $A_r(\mathrm{O}) = 15.9994$

6. Determine stoichiometric formula of an oxide, which contains 72.3591 % of iron and 27.6409 % of oxygen.
   $A_r(\mathrm{Fe}) = 55.845$; $A_r(\mathrm{O}) = 15.9994$

7. Determine stoichiometric formula of a compound, which contains 11.9847 % of aluminium, 2.6866 % of hydrogen, 63.9635 % of oxygen and 21.3653 % of sulphur.
   $A_r(\mathrm{Al}) = 26.98$; $A_r(\mathrm{H}) = 1.008$; $A_r(\mathrm{O}) = 15.9994$, $A_r(\mathrm{S}) = 32.065$

8. In an analysator, 21 mg of an organic compound was burned and 30.75 mg of CO_2 and 12.60 mg of H_2O arise. Determine stoichiometric and summary formula of the compound of $M_r = 60$.
   $A_r(\mathrm{H}) = 1.008$; $A_r(\mathrm{C}) = 12.01$; $A_r(\mathrm{O}) = 15.9994$

9. Calculate content of the iron (in mass %) in $FeCO_3$. Calculate mass of iron, which can be obtained from 1000 kg of the compound with 10 % of impurities.
   $A_r(\mathrm{Fe}) = 55.845$; $M_r(\mathrm{FeCO_3}) = 115.86$

10. Calculate amount of water, which can be evaporated from 250 g of sodium carbonate decahydrate.
$M_r(Na_2CO_3 \cdot 10\,H_2O) = 286.141$; $M_r(Na_2CO_3) = 105.99$

11. A hydrate of iron(II) chloride was dried to constant mass. The starting mass of the hydrate was 25 g, the final mass was 15.9385 g. Determine composition of this hydrate.
$M_r(FeCl_2) = 126.751$; $M_r(H_2O) = 18.016$

12. In 15 g of an oxide of nitrogen was found 5.52811 g of nitrogen. Determine stoichiometric formula of the oxide and write the name of this compound.
$A_r(N) = 14.0067$; $A_r(O) = 15.9994$

13. Calculate mass of calcium oxide and volume of carbon dioxide (at the standard conditions), which can be obtained by thermal decomposition of 900 kg of pure calcium carbonate.
$M_r(CaCO_3) = 100.09$; $M_r(CaO) = 56.08$; $M_r(CO_2) = 44.01$
$CaCO_3 \longrightarrow CaO + CO_2$

14. Zinc reacts with a diluted sulfuric acid and gives zinc(II) sulfate and hydrogen.
$Zn + H_2SO_4 \longrightarrow ZnSO_4 + H_2$
Calculate mass of Zinc(II) sulfate heptahydrate, which arises from 20 g of the zinc. Calculate volume of hydrogen (at the standard conditions), arising by this reaction.
$A_r(Zn) = 65.38$; $M_r(H_2SO_4) = 98.08$; $M_r(ZnSO_4 \cdot 7\,H_2O) = 287.55$

15. Based on the previous reaction calculate volume of 10% sulfuric acid, needed for reaction with 130 g of the zinc.
Relative density of the 10% solution of H_2SO_4 $\rho = 1.066\ g \cdot cm^{-3}$

16. Iodine can be prepared by the reaction of potassium iodide with potassium chlorate and sulfuric acid. Calculate masses of potassium iodide, potassium chlorate and volume of 15% sulfuric acid solution ($\rho = 1.11\ g \cdot cm^{-3}$) needed for preparation of 25 g of iodine. **Assume 75% yield** of the process.
$6\,KI + KClO_3 + 3\,H_2SO_4 \longrightarrow KCl + 3\,I_2 + 3\,K_2SO_4 + 3\,H_2O$
$M_r(KI) = 166.00$; $M_r(KClO_3) = 122.55$; $M_r(H_2SO_4) = 98.08$; $A_r(I) = 126.904$

17. By reaction of gaseous chlorine with aqueous solution of potassium hydroxide arise potassium chloride and potassium chlorate. Calculate mass of the 10% solution of KOH, needed for reaction with 10 L of chlorine (at standard conditions). Calculate mass of both salts, arising by this reaction.
$3\,Cl_2 + 6\,KOH \longrightarrow 5\,KCl + KClO_3 + 3\,H_2O$
$M_r(Cl_2) = 70.90$; $M_r(KOH) = 56.11$; $M_r(KCl) = 74.55$; $M_r(KClO_3) = 122.55$

18. Based on the previous reaction calculate volume of chlorine (at the standard conditions), which can react with 500 g of 15% solution of KOH.
$M_r(KOH) = 56.11$

Results

1. 9.27×10^{-6} mol; 5.583×10^{18} atoms of Ag
2. A_r = 195.092; platinum
3. 28.02 is relative molecular mass (N_2) 14.0098, nitrogen
4. $M_r(V_2O_5)$ = 181.877; 56.01588 % of vanadium; 43.9841 % of oxygen
5. $M_r(C_{23}H_{29}N_3O_4)$ = 411.4797; 67.13089 % of carbon; 7.10412 % of hydrogen; 10.21195 % of nitrogen; 15.55304 % of oxygen
6. Fe_3O_4
7. $Al_2H_{12}O_{18}S_3$
8. $C_2H_4O_2$
9. 48.2004 % of iron; 433.804 kg of iron
10. 157.397 g of water
11. $FeCl_2 \cdot 4\,H_2O$
12. N_2O_3; dinitrogen trioxide
13. 504.27 kg of CaO; 201.51 m^3 of CO_2
14. 87.963 g of $ZnSO_4 \cdot 7\,H_2O$; 6.855 L of H_2
15. 1829.45 mL of 10% H_2SO_4
16. 43.603 g of KI; 5.365 g of $KClO_3$; 77.36 mL of 15% H_2SO_4
17. 500.76 g of 10% KOH; 55.44 g of KCl; 18.23 g of $KClO_3$
18. 14.98 L of Cl_2