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 of a substance.

Atomic Mass Constant 1 amu = $1.660\,538 \times 10^{-27}$ kg – 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.

Molar volume $V_m = 22.413\,83\ \mathrm{dm^3 \cdot mol^{-1}}$ – 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 $\mathrm{g \cdot cm^{-3}}$); V_{gas} is volume of a gas; V_m is molar volume ($\mathrm{dm^3 \cdot mol^{-1}}$)

Avogadro's Number

1. 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?

2. Calculate relative atomic mass of nitrogen, if 25 litres of nitrogen weights 31.258 g at standard conditions

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(N) = 14.01; A_r(H) = 1.0079)

The mass ratio can be calculated as $A_r(\mathrm{N}) : 3 \times A_r(\mathrm{H}) = 14.01 : 3.0237$. 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:

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

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 %

$A_r(\mathrm{K}) = 39.10$; $A_r(\mathrm{Al}) = 26.98$; $A_r(\mathrm{S}) = 32.07$; $A_r(\mathrm{O}) = 15.9994$; $A_r(\mathrm{H}) = 1.0079$
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 %

$A_r(\mathrm{C}) = 12.01$; $A_r(\mathrm{H}) = 1.0079$; $A_r(\mathrm{Br}) = 79.904$
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 thic case we have to multiply the coeficients to obtain the whole numbers. The stoichiometric formula of the compound is $C_9H_{13}Br_3$

Tasks

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

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

3. Determine stoichiometric formula of a compound, which contains 25 % of hydrogen and 75 % of carbon.
   $A_r(\mathrm{H}) = 1.0079$; $A_r(\mathrm{C}) = 12.01$

4. 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 stochimetric and summary formula of the compound of $M_r = 60$.
   $A_r(\mathrm{H}) = 1.0079$; $A_r(\mathrm{C}) = 12.01$; $A_r(\mathrm{O}) = 15.9994$

5. 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.
   $A_r(\mathrm{Fe}) = 55.845$; $M_r(\mathrm{FeCO_3}) = 115.86$

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

7. 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.
   $M_r(\mathrm{FeCl_2}) = 126.751$; $M_r(\mathrm{H_2O}) = 18.016$

8. 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.
   $A_r(\mathrm{N}) = 14.01$; $A_r(\mathrm{O}) = 15.9994$

Calculation based on chemical equations

1. 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.
   $M_r(\mathrm{CaCO_3}) = 100.09$; $M_r(\mathrm{CaO}) = 56.08$; $M_r(\mathrm{CO_2}) = 44.01$
   $\mathrm{CaCO_3 \longrightarrow CaO + CO_2}$

2. Zinc reacts with a diluted sulfuric acid and gives zinc(II) sulfate and hydrogen.
   $\mathrm{Zn + H_2SO_4 \longrightarrow ZnSO_4 + H_2}$
   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.
   $A_r(\mathrm{Zn}) = 65.39$; $M_r(\mathrm{H_2SO_4}) = 98.08$; $M_r(\mathrm{ZnSO_4 \cdot 7\,H_2O}) = 287.55$

3. 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 $\rho = 1.066\ \mathrm{g \cdot cm^{-3}}$

4. The gaseous ammonia reacts with 500 g of 15% solution of sulfuric acid and ammonium sulfate was obtained. Calculate volume (at the standard conditions) of gaseous ammonia, needed for this reaction.
   $\mathrm{2\,NH_3 + H_2SO_4 \longrightarrow (NH_4)_2SO_4}$

Calculate volumes of ammonia (at the standard conditions) and the sulfuric acid solution
($\rho = 1.11\ \text{g} \cdot \text{cm}^{-3}$), needed for preparation of 60 g of the ammonium sulfate.
$M_r(H_2SO_4) = 98.08$; $M_r(NH_3) = 17.03$; $M_r((NH_4)_2SO_4) = 132.14$

5. 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.
$3\,Cl_2 + 6\,KOH \longrightarrow 5\,KCl + KClO_3 + 3\,H_2O$
$M_r(Cl_2) = 70.90$; $M_r(KOH) = 56.11$; $M_r(KCl) = 74.55$; $M_r(KClO_3) = 122.55$

6. Based on the previous reaction calculate volume of chlorine (at the standard conditions), which can react with 500 g of 15% solution of KOH.
$M_r(H_2SO_4) = 98.08$