Calculations involving concentrations, stoichiometry

MUDr. Jan Pláteník, Ph.D.

Metric System Units

- Meter (m), gram (g), liter (l), second (s)
- Prefixes:

mega-	M	1,000,000 (10^6)
kilo-	k	1000 (10^3)
deci-	d	0.1 (10^{-1})
centi-	c	0.01 (10^{-2})
milli-	m	0.001 (10^{-3})
micro-	µ	0.000001 (10^{-6})
nano-	n	0.000000001 (10^{-9})
pico-	p	0.000000000001 (10^{-12})

Significant figures in calculations:

- **Multiplication or division:**

Keep smallest number of significant figures in answer

- **Addition or subtraction**:

Keep smallest number of decimal places in answer

Mole

- Unit of amount of substance
- **The amount of substance containing as many particles (atoms, ions, molecules, etc.) as present in 12 g of the carbon isotope ^{12}C**
- This amount equals 6.02×10^{23} particles (**Avogadro's Number**)

(Relative) Atomic Mass

- Atomic mass unit (u): 1/12 of the mass of one atom of the carbon isotope ^{12}C

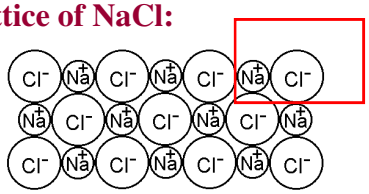
  $1\ u = 1.66057 \times 10^{-27}\ kg$

- Relative atomic mass (atomic weight, AW): mass of an atom expressed in u
- Molecules: (relative) molecular mass (molecular weight, MW)
- Substances that do not form true molecules (ionic salts etc.):

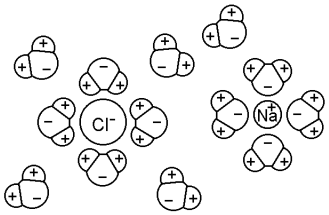
  (relative) formula weight (FW)

Ionic salts: no true molecule

- **Crystal lattice of NaCl:**



- **Dissolution of NaCl in water: electrolytic dissociation producing hydrated independent ions Na^+, Cl^-**



Molar Mass

- Mass of one mole of given substance
- Expressed in g/mol
- **The molar mass of a substance in grams has the same numerical value as its relative atomic (molecular) mass**

Solution

- Homogeneous dispersion system of two or more chemical entities whose relative amounts can be varied within certain limits
- Solvent + solute(s)
- Gaseous (e.g. air)
- Liquid (e.g. saline, NaCl dissolved in water)
- Solid (e.g. metal alloy)

Concentration of a solution

- Mass concentration: grams of dissolved substance per liter of solution (g/l)
- Molar concentration: moles of dissolved substance per liter of solution (mol/l or M)

Conversion from mass to molar

Task: Calculate molar concentration of $(NH_4)_2SO_4$ solution c = 33 g/l.
(AW of N: 14, S: 32, O: 16, H: 1)

Conversion from molar to mass

Task: Calculate how many g of $K_2HPO_4 . 3H_2O$ is needed for preparation of 250 ml of 0.1 M solution. (AW of K: 39, P: 31, O: 16, H: 1)

Concentration of a solution in %

% weight per weight (w/w): grams of substance in 100 g of mixture

= (mass of solute/mass of solution) × 100

% weight per volume (w/v): grams of substance in 100 ml of solution

= (mass of solute in g/volume of sol. in ml) × 100

% volume per volume (v/v): ml of substance in 100 ml of solution

= (volume of solute/volume of solution) × 100

Conversion from % to molarity

Task: The physiological saline is NaCl 0.9 % (w/v)
What is molar concentration of NaCl in this solution?
(AW of Na: 23, Cl: 35.5)

Diluting solutions

Task: How many ml of stock solution of NaCl 0.5 mol/l will be needed in order to get two liters of physiological saline (0.15 mol/l) by dilution ?

Diluting solutions

Example II: How many ml of water need to be added to 10 ml of concentrated HCl (12 M) in order to get 0.1 M HCl ?

Molar Volume

One mole of any gaseous substance occupies the same volume at the same temperature and pressure

..22.414 litres at 101.325 kPa, 0 °C (273.15 K)

(Avogadro's Law)

$P \times V = n \times R \times T$

P: pressure in kPa

V: volume in dm^3 (l)

n: number of moles

R: universal gas constant (8.31441 $N.m.mol^{-1}.K^{-1}$)

T: temperature in K

Task: What is volume of one mole of gas at 101.325 kPa and 25 °C ?

$$P \times V = n \times R \times T$$

$$V = \frac{n \times R \times T}{P} = \frac{1 \times 8.31441 \times (273.15+25)}{101.325} =$$

$$= 24.465\ dm^3$$

Calculations with molar volume

Task: What volume (in liters) would by occupied by 1 kg of gaseous oxygen at atmospheric pressure and ambient temperature ?

(Molar volume 24.465 l/mol, AW of O: 16)

Stoichiometric calculations

Calculations based on a chemical equation

E.g.: $A + B \rightarrow C + D$

Amount of A given, how much B reacts?
Amount of C desired, how much A needed?
Amount of A given, how much C is formed?
…

Titration

- Reaction: A + B → C
  - Acid-base reaction (neutralisation)
  - Precipitation reaction
  - Redox reaction
  - (...)
- **Substance A:** unknown concentration, amount (solution volume) known
- **Substance B:** known concentration, is used to determine concentration of A

Neutralisation (acid-base) titration

E.g. $HCl + NaOH \rightarrow NaCl + H_2O$

ionic: $H^+ + OH^- \rightarrow H_2O$

HCl: amount is known, but concentration unknown

NaOH: concentration known, added gradually until the reaction is just completed, and the used amount is recorded.

An **indicator,** e.g. phenolphthalein (in acid colorless, but violet in alkali) needed to show that the reaction has reached completion.

Titration calculations

Example: An unknown sample of sulfuric acid H_2SO_4 was titrated with the known KOH solution. It was found that 12 mL of the KOH c=0.1 mol/L was needed for just complete neutralisation of 10 mL H_2SO_4 unknown sample.

What is concentration of sulfuric acid in the sample?

Assumption of the Virgin by Titian
(Fig. from Wikipedia)

Cinnabar (Vermillion)

$Hg + S \rightarrow \mathbf{HgS}$

Mercury(II) sulfide

Stoichiometric calculations

Task: How many grams of solid mercury(II) sulfide can be prepared from 10 ml of liquid mercury with an excess of powdered elemental sulfur? Take into account that about 25% of the product will be lost. (AW of mercury: 200.6, sulfur: 32.1, density of mercury 13.534 g/cm^3)

equation: Hg + S → HgS

Mass of Hg: 10 ml × 13.534 g/ml = 135.34 g

Moles of Hg: 135.34/200.6 = 0.6747 mol

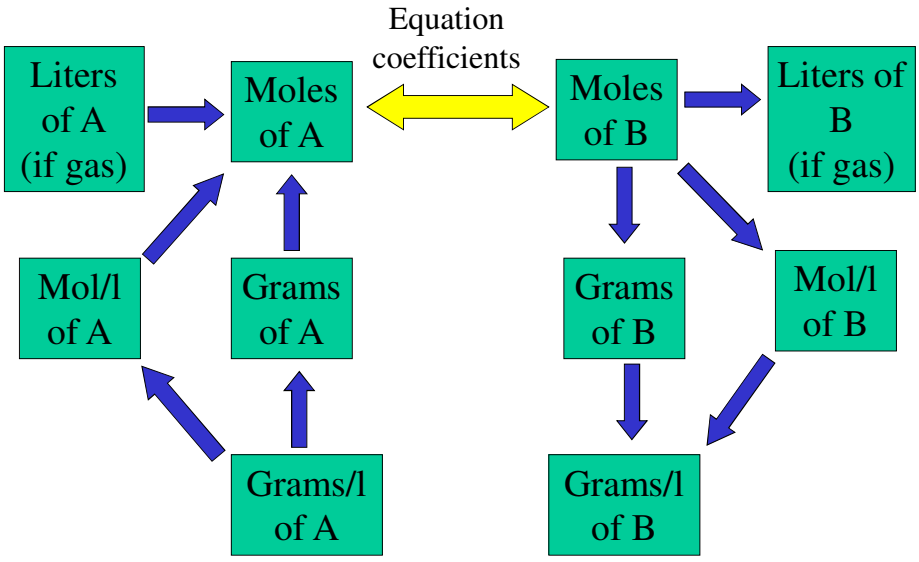
Moles of HgS: the same as moles of Hg …. 0.6747 mol

MW HgS: 200.6 + 32.1 = 232.7 g/mol

Mass of HgS: 0.6747 × 232.7 = 157.00 g

25% loss: (157/100) × 75 = **117.75 g**

Stoichiometric calculations



Stoichiometric calculations