Calculations involving concentrations, stoichiometry

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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 Weight

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

  1 u = 1.66057 x 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)

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) weight**

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)

$P \,.\, V = n \,.\, R \,.\, T$

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

Example: what is volume of one mole of gas at 101.325 kPa and 25 °C ?

$$P.V = n.R.T$$

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

= 24.465 dm^3

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 substance per litre of solution
- molar concentration: moles of substance per litre of solution
- in %:
  - **% (w/v):** weight per volume, grams of substance per 100 ml of solution
  - **% (v/v)** volume per volume, ml of substance per 100 ml of solution

Conversion from mass to molar

Example: Calculate molar concentration of Na_2HPO_4 solution c = 21 g /l.
(AW of Na: 23, P: 31, O: 16, H: 1)

FW of Na_2HPO_4 : 46+1+31+4x16 = 142

Molar concentration = Mass conc. (g/l) / FW

= 21 / 142 = 0.15 mol/l

Conversion from molar to mass

Example: Calculate how many g of $KClO_4$ is needed for preparation of 250 ml of 0.1 M solution.
(AW of K: 39, Cl: 35.4, O: 16)

FW of $KClO_4$: 39 + 35.4 + 4x16 = 138.4

Mass conc. = molar conc. x FW

we need 138.4 x 0.1 x 0.25 = 3.46 g $KClO_4$

Conversions between mass and molarity: Summary

- Always distinguish between amount of substance in moles (grams) and concentration of substance in mol/l (g/l)
- For conversion from mass to molarity divide the mass (g or g/l) with molar mass (relative AW/MW/FW)
- For conversion from molarity to mass multiply the molarity (mol or mol/l) with molar mass (relative AW/MW/FW)

Conversion from % to molarity

Example: 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)

FW of NaCl : 23+35.45 = 58.5

0.9 % (w/v) is 0.9 g/100 ml = Mass conc. 9 g/l

Molar concentration = Mass conc. (g/l) / FW

= 9/58.5 = 0.154 mol/l

Diluting solutions

Example: How many ml of water should be added to 100 ml of NaCl 1 mol/l, in order to get 0.15 mol/l ('physiological saline') ?

$$c_1 . v_1 = c_2 . v_2$$

$$1 \times 100 = 0.15 \times v_2$$

$$v_2 = 100/0.15 = 666.67 \text{ ml}$$

Volume that needs to be added:

666.67 ml - 100 ml = **566.67 ml**

Diluting solutions

Example II: You need to prepare 1 liter of 0.1 M HCl. How many ml of concentrated HCl (12 M) do you need to take ?

$c_1 \cdot v_1 = c_2 \cdot v_2$

$12 \times v_1 = 0.1 \times 1000$

$v_1 = 100/12 =$ **8.33 ml**

What is molarity of pure water?

Molar concentration: moles of substance per liter of solution

1 liter of water weighs 997 g at 25 °C

FW of H_2O: 2+16=18

997 g H_2O is 997/18 = 55.4 moles

Molarity of pure water is **55.4 mol/l**

Calculations with molar volume

Example: What is weight (in grams) of 1 liter of oxygen at atmospheric pressure and ambient temperature ?

(AW of O: 16)

Molar volume at 101.325 kPa and 25 °C: 24.5 l/mol

1 liter of oxygen is 1/24.5 = 0.040816 mol

Conversion to mass: 0.040816 x 32 = **1.306 g**

Stoichiometric calculations

Example: In the reaction between barium nitrate and sodium sulfate, how many grams of barium sulfate can be prepared from 10 ml of 10 % (w/v) barium nitrate? Take into account that about 5% of the product is lost.
(AW of barium: 137.3, sulfur: 32.1, nitrogen: 14.0, oxygen: 16.0)

equation: $Ba(NO_3)_2 + Na_2SO_4 \rightarrow BaSO_4 + 2NaNO_3$

FW $Ba(NO_3)_2$: 261.3 FW $BaSO_4$: 233.4

10 ml of 10% (w/v) $Ba(NO_3)_2$: 1 g ... 1/261.3 = 0.003827 moles

amount of $BaSO_4$ formed: 0.003827 moles ....

... 0.003827 x 233.4 = 0.8932 g (theoretical yield, 100%)

Actual yield: 0.8932 x 0.95 = **0.849 g**

Stoichiometric calculations

Example II: Reaction between hydrochloric acid and solid zinc can be used to prepare hydrogen gas in the laboratory. Calculate how many grams of solid zinc and how many mL of 1 M HCl is needed fro preparation of 5 L of hydrogen gas. Take into account that about 8% of the product is lost in your apparatus.
(AW of Zn: 65.4, Cl: 35.5, molar volume 24.5L/mol)

equation: $Zn(s) + 2HCl \rightarrow H_2(g) + ZnCl_2$

5 L H_2: 5/24.5 = 0.204 mol

+ 8% loss: 0.204/92 × 100 = 0.222 mol

Amount of 1 M HCl needed: 0.444 mol, present in **444 mL**

Amount of solid Zn needed: 0.222 × 65.4 = **14.5 g**

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?

Equation: $H_2SO_4 + 2\,KOH \rightarrow K_2SO_4 + 2\,H_2O$

Calculation: H_2SO_4 KOH

$$c_1 \cdot v_1 = c_2 \cdot v_2$$

$$c_1 = c_2 \cdot v_2 / v_1$$

$$c_1 = 0.1 \cdot 12 / 10 = 0.12$$

Including stoichiometry : $c(H_2SO_4)$ = 0.12/2 = **0.06 mol/L**

Further reading and practice

- Hand-outs on http://che1.lf1.cuni.cz
- Stoker: General, Organic and Biological Chemistry, 4th edition:
  - Chapter 6 (p.125-147) … mole, stoichiometry
  - [Chapter 7 (p.148-175) … gas laws]
  - Chapter 8 (p.176-203) … solutions (covers also osmotic pressure and osmolarity needed later)