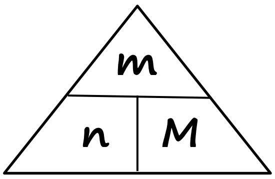
Achievement Standard Chemistry 91161: Carry out quantitative analysis

In addition to the titration (see other resources on No Brain Too Small), this AS also has a written component with calculations.

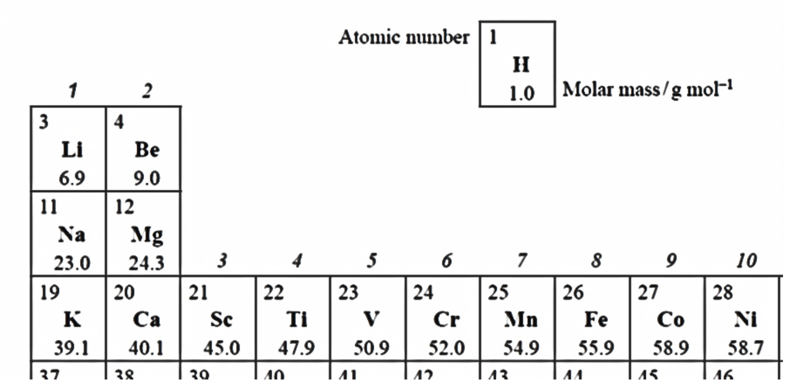
Important formula: n = m/M

n = m/M (which can be rearranged to m = n x M

where n is the amount of substance (mol)
m is the mass of substance (g)
and M is the molar mass of the substance (g mol^{-1})



The portion of the periodic table shown below shows the atomic number and molar mass of some elements. E.g. Na has a molar mass of 23.0 g mol^{-1}. This means 1 mol of Na has a mass of 23.0 g. This can be written M(Na) = 23.0 g mol^{-1} in questions.



Atomic number: 1 — H — 1.0 — Molar mass / g mol^{-1}

1	2	3	4	5	6	7	8	9	10
3 Li 6.9	4 Be 9.0								
11 Na 23.0	12 Mg 24.3								
19 K 39.1	20 Ca 40.1	21 Sc 45.0	22 Ti 47.9	23 V 50.9	24 Cr 52.0	25 Mn 54.9	26 Fe 55.9	27 Co 58.9	28 Ni 58.7
37	38	39	40	41	42	43	44	45	46

What is the mass of 1 mol of Mg? Answer: 24.3 g
What is the mass of 2 mol of Mg? Answer: m = n x M — m = 2 x 24.3 = 48.6 g
What is the mass of 0.75 mol of Mg? Answer: m = n x M — m = 0.75 x 24.3 = 18.225 g
How many mol of Mg are there is 56.0 g of Mg? Answer: n = m/M — n = 56.0/24.3 = 2.30 mol

<u>% Composition calculations</u>

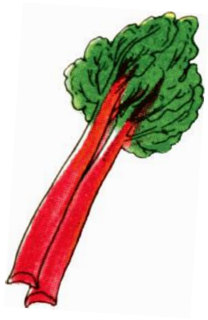
Citric acid, formula $C_6H_8O_7$, can be used to soften water which makes it useful in soaps and laundry detergents. It is also the acid found in citrus fruits. Calculate the percentage composition of citric acid.
M(C) = 12.0 g mol^{-1} M(H) = 1.00 g mol^{-1} M(O) = 16.0 g mol^{-1}

First calculate (M) $C_6H_8O_7$

- (M) $C_6H_8O_7$ = (12.0 x 6) + (1.00 x 8) + (16.0 x 7) = 192 g mol^{-1}

- %C = $\frac{(12.0 \times 6)}{192}$ x 100 = 37.5%
- %H = $\frac{(1.00 \times 8)}{192}$ x 100 = 4.17%
- %O = $\frac{(16.0 \times 7)}{192}$ x 100 = 58.3%

These will add up to 100% of course ☺



Rhubarb contains acids, one of which is malic acid, formula $C_4H_6O_5$. Calculate the percentage composition of malic acid.

First calculate (M) $C_4H_6O_5$

- (M) $C_4H_6O_5$ = (12.0 x 4) + (1.00 x 6) + (16.0 x 5) = 134 g mol^{-1}

- $\%C = \frac{(12.0 \times 4)}{134} \times 100 = 35.8\%$
- $\%H = \frac{(1.00 \times 6)}{134} \times 100 = 4.48\%$
- $\%O = \frac{(16.0 \times 5)}{134} \times 100 = 59.7\%$

Empirical formula and the molecular formulae

Empirical formulas give the lowest whole number ratio of the atoms in a compound.
The molecular formula gives the exact composition of one molecule.

Examples:

molecular formula	empirical formula
C_2H_4	CH_2
$C_6H_{12}O_6$	CH_2O
H_2O	H_2O
C_4H_{10}	C_2H_5

Example 1:
Rhubarb plants contain oxalic acid.
Oxalic acid is 26.7% carbon, 2.22% hydrogen and 71.1% oxygen, and has a molar mass of 90.0 g mol^{-1}.
Use the following molar masses to calculate both the empirical formula and the molecular formula of oxalic acid: M(C) = 12.0 g mol^{-1} M(H) = 1.00 g mol^{-1} M(O) = 16.0 g mol^{-1}

- Assume that you have 100 g of the compound. Then 100 g of oxalic acid would contain 26.7 g of carbon, 2.22 g of hydrogen and 71.1 g of oxygen

	Carbon	Hydrogen	Oxygen
Mass (g)	26.7	2.22	71.1
Moles (mol) n = m/M	26.7 / 12.0 = 2.225	2.22/1.00 = 2.22	71.1/16.0 = 4.44375
divide each by the smallest # of moles	2.225/2.22 = 1.00	2.22/2.22 = 1.00	4.44375/2.22 = 2.00
Simplest whole number ratio	1	1	2

- Ratio is 1:1:2 so empirical formula is CHO_2

Oxalic acid has a molar mass of 90.0 g mol^{-1}.

- Empirical formula CHO_2 has a molar mass of 12.0 + 1.00 + (16.0 x 2) = 45.0 g mol^{-1}.
- # of CHO_2 units is 90.0/45.0 = 2
- Molecular formula is therefore 2 x CHO_2, that is $C_2H_2O_4$

Example 2:
Tile cleaners contain hydrogen peroxide. Hydrogen peroxide is 94.12% oxygen and 5.88% hydrogen. It has a molar mass of 34.0 g mol^{-1}. Use the following molar masses to calculate both the empirical formula and the molecular formula of hydrogen peroxide. M(H) = 1.00 g mol^{-1} M(O) = 16.0 g mol^{-1}

- Assume that you have 100.00 g of the compound. Then 100g of hydrogen peroxide would contain 94.12 g of oxygen and 5.88g of hydrogen.

	Hydrogen	Oxygen
Mass (g)	5.88	94.12
Moles (mol)	5.88/1.00 = 5.88	94.12/16.0 = 5.8825
divide each by the smallest # of moles	5.88/5.88 = 1.00	5.8825/5.88 = 1.00
Simplest whole number ratio	1	1

- Ratio is 1:1 so empirical formula is HO

Hydrogen peroxide has a molar mass of 34.0 g mol^{-1}.

- Empirical formula HO has a mass of 1.00 + 16.0 = 17.0 g mol^{-1}.
- # of HO units is 34.0/17.0 = 2
- Molecular formula is therefore 2 x HO, that is H_2O_2

Note: If you end up with a simplest ratio of, say, 1 Fe : 1.5 O, then simply multiply both x 2 to give Fe_2O_3.

Calculations from equations

Example 1:
Malic acid reacts with sodium hydroxide. The equation for the reaction is:

$$C_4H_6O_5 + 2NaOH \rightarrow C_4H_4O_5Na_2 + 2H_2O$$

Calculate the maximum mass of sodium malate, $C_4H_4O_5Na_2$, which could be made from 15.0g of sodium hydroxide. M(C) = 12.0 g mol^{-1} M(H) = 1.00 g mol^{-1} M(O) = 16.0 g mol^{-1} M(Na) = 23.0 g mol^{-1}

- Write the equation: $C_4H_6O_5 + 2NaOH \rightarrow C_4H_4O_5Na_2 + 2H_2O$
- Identify the species you are interested in……. calculate the maximum mass of **sodium malate, $C_4H_4O_5Na_2$**, which could be made from 15.0g of **sodium hydroxide.**

- Calculate the mass of these; 2 mol of NaOH and 1 mol of $C_4H_4O_5Na_2$

$C_4H_6O_5$	+	**2NaOH**	→	**$C_4H_4O_5Na_2$**	+	$2H_2O$
		2 mol		1 mol		
		2 x (23.0 + 16.0 + 1.00)		(12.0 x 4) + (1.00 x 4) + (16.0 x 5) + (23.0 x 2)		
		80.0 g		178 g		

- By proportion 15.0 g $\frac{15.0}{80.0} \times 178 = 33.4$ g (3 s.f.)

Example 2:
Citric acid reacts with sodium hydroxide. The equation for the reaction is:

$$C_6H_8O_7 + 3NaOH \rightarrow C_6H_5O_7Na_3 + 3H_2O$$

Calculate the mass of sodium citrate, $C_6H_5O_7Na_3$, which is formed when 10.0g of sodium hydroxide reacts with citric acid. M(C) = 12.0 g mol^{-1} M(H) = 1.00 g mol^{-1} M(O) = 16.0 g mol^{-1} M(Na) = 23.0 g mol^{-1}

This can be calculated as in example 1. Alternatively you could use the method below.

- Write the equation: $C_6H_8O_7 + 3NaOH \rightarrow C_6H_5O_7Na_3 + 3H_2O$
- Identify the species you are interested in……. calculate the mass of sodium citrate, $C_6H_5O_7Na_3$, which is formed when 10.0g of sodium hydroxide reacts with citric acid

$$C_6H_8O_7 + \underset{3\text{ mol}}{3NaOH} \rightarrow \underset{1\text{ mol}}{C_6H_5O_7Na_3} + 3H_2O$$

- M(NaOH) = 23.0 + 16.0 + 1.00 = 40 g mol^{-1}.
- M($C_6H_5O_7Na_3$) = (12.0 x 6) + (1.00 x 5) + (16.0 x 7) + (23.0 x 3) = 258 40 g mol^{-1}.
- n(NaOH) = m/M = 10/40 = 0.250 mol
- n(NaOH) : n($C_6H_5O_7Na_3$) = 3:1 (This means 3 mol of NaOH react to form 1 mol of sodium citrate).
- n($C_6H_5O_7Na_3$) = 0.250/3 = 0.0833 mol
- m = nM   m($C_6H_5O_7Na_3$) = 0.0833 x 258 = 21.5g

Significant figures & correct units

Consistent use of significant figures and correct units are needed for excellence.

The questions will invariably be given to you with data given to 3 s.f. e.g. 24.0 g of Mg rather than 24 g (2 s.f.) or 24.00 g (4 s.f.)
Your final answer should therefore also be given to 3 s.f.

If you are given two pieces of data in a question, one to 3 s.f. and the other to 2 s.f. then the final answer should be given to 2 s.f. However NCEA Chemistry has a long history of obsession with 3 s.f. – just ask your Chemistry teacher!

Correct units are:

- Amount (n) – mol
- Mass (m) – g
- Molar mass (M) – g mol^{-1}
- Concentration (C) – mol L^{-1}
- Volume (V) – mL and L

C & V will be needed in titration calculations when using the formula n = CV and C = n/V.