# Chemical Calculations

## Introduction

### Rules for calculations

(a) **Always** work from first principles - formulas (unless stated) often confuse.

(b) **Always** show all the steps in your working, this reduces the chance of error. In examinations you get marks for knowing how to do a calculation even if your answer is wrong.

(c) **Never** round-up or round-down a figure during a calculation - wait until you have the final answer.

(d) **Always** give mole calculation answers to 3 decimal places.

(e) **Never** simply write down an answer with no indication of where it came from. (If you do this in an examination you will get no marks even if the answer is correct.)

(f) **Never** trust a calculator - try to do a rough approximation to check your answer. E.g. $17 \times 0.279 = 4.743$, to check multiply $17 \times 0.3$ = about 5 (you should be able to do this in your head, **NO CALCULATORS**) this gives you a rough idea of the range in which the answer lies. So, if your calculator says 474.3 you know that something is wrong.

### Quantities of chemicals

| Quantity | Common units | Meaning |
|---|---|---|
| Mass | gram (g)<br>kilogram (kg)<br>1kg = 1000g | Samples with the same mass give the same readings on a balance |
| Volume | cubic centimetre ($cm^3$)<br>litre (l or $dm^3$)<br>1 litre = $1dm^3$ = $1000cm^3$ | Samples with the same volume take up the same amount of space. Two liquids with the same volume for example, fill a measuring cylinder to the same level |
| Amount | mole (mol) | Samples with the same amount of a chemical contain the same number of atoms, molecules or ions. There are as many atoms in one mole of carbon as there are molecules in one mole of water. |

### Re-arranging formula

To re-arrange formula there is a simple rule: you can change any equation as much as you like as long as you always do the same thing to both sides.

For example, **Moles** = $\frac{\text{Mass}}{\text{R.M.M.}}$ is very useful if you want to find moles but what if you want to find R.M.M.?

You need to re-arrange the formula so that R.M.M. is standing alone on the left-hand side of the equation.

Multiply both sides by R.M.M. $\quad \text{Moles} \times \text{R.M.M.} = \frac{\text{Mass} \times \text{R.M.M.}}{\text{R.M.M.}}$

Cancel out R.M.M. on the right-hand side $\quad$ **Moles × R.M.M. = Mass**

Divide each side by Moles $\quad \frac{\text{Moles} \times \text{R.M.M.}}{\text{Moles}} = \frac{\text{Mass}}{\text{Moles}}$

Cancel out Moles on the left-hand side $\quad \text{R.M.M.} = \frac{\text{Mass}}{\text{Moles}}$

Note that during this process we have shown how to work out Mass.

**Powers of 10**

A lot of scientific work deals with numbers that are very large or very small. It is convenient to have a quick way of writing large numbers and small numbers. Powers of 10 do this job.

**Positive powers**

$10^1 = 10$
$10^2 = 10 \times 10 = 100$
$10^3 = 10 \times 10 \times 10 = 1000$
and so on

Note that
$10^2 + 10^2 = 2 \times 10^2 = 200$

but that
$10^3 \times 10^3 = 10^6 = 1\ 000\ 000$

Note also that
$10^0 = 1$

**Negative powers**

$10^{-1} = 1 \div 10 = 0.1$
$10^{-2} = 1 \div (10 \times 10) = 0.01$
$10^{-3} = 1 \div (10 \times 10 \times 10) = 0.001$
and so on

Note that
$10^{-1} + 10^{-1} = 2 \times 10^{-1} = 0.2$

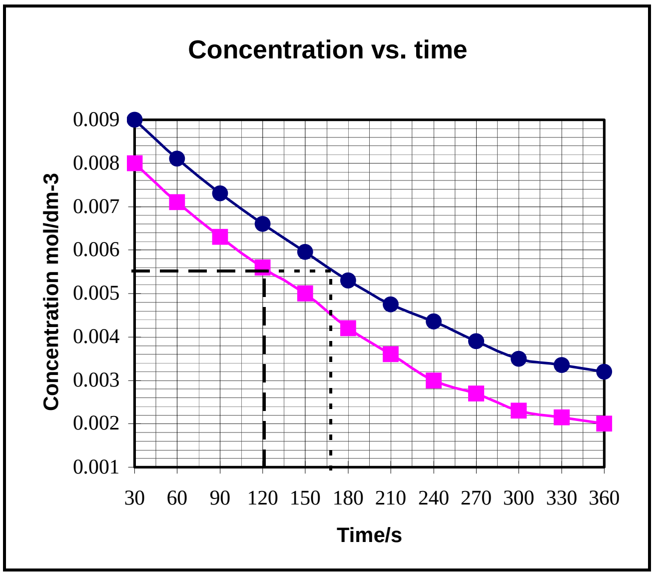
but that
$10^{-2} \times 10^{-3} = 10^{-5} = 0.00001$

**Calculations involving graphs**

When drawing graphs there are **five** points to remember:

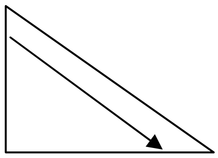
1. Draw axes and label them carefully.
2. Use a suitable scale to give you the largest possible graph on the grid provided.
3. Unless it is stated or observed, (i.e. from the information given it is obvious that both initial readings are zero), that the graph passes through the origin, scales ***do not*** have to start at zero.
4. Draw the best straight line or curve through the points, i.e. that on which the most number of points lie. If you have to draw more than one graph on the same axes make sure that each graph is clearly labelled and that they are easily distinguishable from each other. Use different coloured pens or mark one set of points with crosses (+) and the other set with circles (o).
5. Mark clearly on your graph the information that you are required to find by drawing in lines to the x and y axes where appropriate or by drawing in gradient lines, etc.

When you are working out the gradient of a graph use the formula: $\dfrac{y_2 - y_1}{x_2 - x_1}$ where $x_1$ and $y_1$ are the co-ordinates of the point with the **lowest** x value and $x_2$ and $y_2$ are the co-ordinates of the **higher** x value.

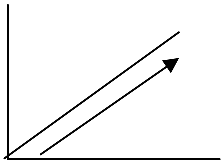



**Remember**

A graph going from top left to bottom right has a **negative** gradient.



A graph going from bottom left to top right has a **positive** gradient.



**1. Calculation of the relative molecular mass of a compound.**

**Worked examples**

(a) Work out the ***relative molecular mass*** (R.M.M.) of sodium chloride, NaCl.

In 1 molecule of this compound there is 1 atom of sodium, Na, and 1 atom of chlorine, Cl.

From your data book: the ***relative atomic mass*** (R.A.M.) of Na = 23.0, Cl = 35.45.

**So, R.M.M. of NaCl = 23.0 + 35.45 + 58.45**

(b) Work out the R.M.M. of hydrated magnesium sulphate, $MgSO_4.7H_2O$

In 1 molecule of this compound there is 1 mole of magnesium sulphate, containing 1 atom of magnesium, Mg, 1 atom of sulphur, S, and 4 atoms of oxygen, O, and also 7 moles of water, containing 14 atoms of hydrogen, H, and 7 atoms of oxygen, O.

From your data book: R.M.M. Mg = 24.31; S = 32.06; O = 16.00; H = 1.008.

**So, R.M.M. $MgSO_4.7H_2O$ = 24.31 + 32.06 + (4 × 16.00) + (14 × 1.008) + (7 × 16.00) =246.5**

**Questions**

Using your data book work out the relative molecular masses of the following compounds:

(a) KBr

(b) $Na_2CO_3.10H_2O$

**2. Calculation of the percentage by mass of elements in a compound.**

**Worked examples**

(a) Calculate the percentage by mass of carbon, C, and oxygen, O, in carbon dioxide, $CO_2$.

In 1 molecule of carbon dioxide there is 1 atom of carbon, C, and 2 atoms of oxygen, O.

From you data book: R.A.M. C = 12.01; O = 16.00. ∴R.M.M. $CO_2$ = 12.01 + (2 × 16.00) = 44.01

$$\%C \text{ in } CO_2 = \frac{\text{RAM C}}{\text{RAM CO}_2} \times 100 = \frac{12}{44} \times 100 = 27.3\%$$

$$\%O \text{ in } CO_2 = \frac{\text{RAM O}}{\text{RAMCO}_2} \times 100 = \frac{2 \times 16.00}{44} \times 100 = 72.7\%$$

(b) Calculate the percentage by mass of water in hydrated aluminium chloride, $AlCl_3.6H_2O$.

In 1 molecule of hydrated aluminium chloride there is 1 molecule of aluminium chloride and 6 molecules of water..

From your data book: R.M.M. $AlCl_3$ = 133.3; $H_2O$ = 18.0.

∴ R.M.M. $AlCl_3.6H_2O$ = 133.3 + (6 × 18) = 241.3

$$\%H_2O \text{ in } AlCl_3.6H_2O = \frac{6 \times \text{RMM water}}{\text{RMM AlCl}_3\text{.6H}_2\text{O}} \times 100 = \frac{6 \times 18}{241.3} \times 100 = 44.76\%$$

**Questions**

Calculate the percentage by mass of

(a) sulphur and oxygen in $SO_3$

(b) magnesium and nitrogen in $Mg_3N_2$

**3. Calculation of the number of moles in a given mass of a compound.**

**Worked examples**

(a) Calculate the number of moles in 5.61g of potassium hydroxide, KOH.

R.A.M. K = 39.1; H = 1.008; O = 16.00. $\therefore$ R.M.M. = 39.1 + 16.00 + 1.008 = 56.1

$$\boxed{\textbf{Number of moles} = \frac{\textbf{mass}}{\textbf{RMM}} = \frac{\textbf{5.61}}{\textbf{56.1}} = \textbf{0.100}}$$

(b) Calculate the number of moles in 305.38g of hydrated barium chloride, $BaCl_2.2H_2O$.

R.A.M. Ba = 137.34; Cl = 35.45; H = 1.008; O = 16.00.

$\therefore$ R.M.M. = 137.34 + (2 $\times$ 35.45) + (4 $\times$ 1.008) + (2 $\times$ 16.00) = 244.3

$$\boxed{\textbf{Number of moles} = \frac{\textbf{mass}}{\textbf{RMM}} = \frac{\textbf{305.38}}{\textbf{244.30}} = \textbf{1.250}}$$

**Questions**

Calculate the number of moles in

(a) 58.5g of sodium chloride.

(b) 50.0g of calcium carbonate

**4. Calculation of the formula of a compound.**

**Worked examples**

(a) What is the formula of the oxide formed when 2.30g of sodium combine with 0.80g of oxygen?

R.A.M. Na = 23.00; O = 16.00

Moles of Na = $\frac{2.30}{23.0} = 0.100$ ; Moles of O = $\frac{0.80}{16.0} = 0.050$

Mole ratio must be a whole number so divide both answers by the smallest number of moles.

Moles of Na = $\frac{0.100}{0.050} = 2$ ; Moles of O = $\frac{0.050}{0.050} = 1$

**Formula is $Na_2O$**

(b) Calculate the ***empirical*** (lowest mole ratio) formula of a compound containing 20.00% magnesium, 26.70% sulphur and 53.30% oxygen.

Assume 100g of compound, mass of Mg = 20.00g, S = 26.70g, O = 53.30g

R.A.M. Mg = 24.30; O = 16.00; S = 32.10

Moles Mg = $\frac{20.00}{24.30} = 0.823$; Moles O = $\frac{53.30}{16.0} = 3.331$; Moles S = $\frac{26.70}{32.10} = 0.831$;

Divide by the smallest number of moles

Ratio moles Mg = $\frac{0.823}{0.823} = 1$ : Moles O = $\frac{3.331}{0.823} = 4$ : Moles S = $\frac{0.831}{0.823} = 1$

**Formula is $MgSO_4$**

(c) A hydrocarbon (a compound containing carbon and hydrogen only) contains 80.00% carbon. Its relative molecular mass is 30.00. Calculate (i) its empirical formula, (ii) its molecular formula.

Assume 100g; Mass of C = 80.00g; Mass of H = 100.00 - 80.00 = 20.00g

R.A.M. C = 12.00; H = 1.00

(i) Moles of H = $\frac{20.00}{1.00} = 20.000$; Moles of C = $\frac{80.00}{12.00} = 6.666$

Divide by the smallest number of moles

Ratio moles H = $\frac{20.000}{6.666} = 3$ : Moles C = $\frac{6.666}{6.666} = 1$

**Empirical formula is $CH_3$**

(ii) RMM of empirical formula $CH_3$ = 12.00 + (3 $\times$ 1.00) = 15.0 but actual RMM is 30

Therefore multiplication factor = $\frac{\text{Actual RMM}}{\text{Empirical formula RMM}} = \frac{30}{15} = 2$

**Molecular formula is $C_2H_6$**

**Questions**

(a) What is the formula of the compound formed when

(i) 7.77g of iron, Fe, combine with 2.23g of oxygen, O?

(ii)18.46g of carbon combine with 1.52g of hydrogen?

(b) What is the formulae of the compounds formed in the following reactions

(i) 3.400g of calcium form 9.435g of a chloride?

(ii)4.662g of lithium form 5.328g of a hydride?

(c) Calculate the empirical formulae of the compounds with the following compositions

(i) 35.00% nitrogen, 5.00% hydrogen, 60.00% oxygen

(iii) a carbohydrate containing 6.70% hydrogen and 53.30% oxygen.

(d) Calculate the empirical formula and deduce the molecular formula of

(i) a liquid of RMM 44, containing 54.50% carbon, 36.40% oxygen and 9.10% hydrogen

**5. Calculations involving equations**

**Worked examples**

(a) How many moles of iodine can be obtained from 0.2 moles of potassium iodate(V)?

First write the equation: $KIO_3(aq) + 5KI(aq) + 6HCl(aq) \longrightarrow 3I_2(aq) + 6KCl(aq) + 3H_2O(l)$

This tells us that 1 mole of $KIO_3$ gives 3 moles of $I_2$.

Therefore 0.2 mole of $KIO_3$ gives 0.2 × 3 moles of $I_2$ = **0.6 moles of $I_2$**

(b) What is the maximum mass of ethyl ethanoate that can be obtained from 13.20g of ethanol?

First write the equation: $C_2H_5OH(l) + CH_3COOH(l) \longrightarrow CH_3COOC_2H_5(l) + H_2O(l)$

RMM $C_2H_5OH$ = 46.10; $CH_3COOC_2H_5$ = 88.10

Two methods can be used to calculate the answer.

**EITHER**

1 mole of $C_2H_5OH$ gives 1 mole of $CH_3COOC_2H_5$

Moles of ethanol = $\frac{13.20}{46.10} = 0.286 = \text{moles of ethyl ethanoate}$

**Mass of ethyl ethanoate = 0.286 × 88.10 = 25.22g**

**OR**

46.10g of ethanol gives 88.10g of ethyl ethanoate

So 1.00g of ethanol gives $\frac{88.10}{46.10}$ g of ethyl ethanoate = 1.911g

**13.20g of ethanol gives 13.20 × 1.911 = 25.22g of ethyl ethanoate**

**One mole of any gas occupies 22.4dm$^3$ at standard temperature and pressure (s.t.p)**
**OR**
**One mole of any gas occupies 24.0dm$^3$ at room temperature and pressure (r.t.p)**

(c) What volume of oxygen is needed for the complete combustion of 2dm$^3$ of propane?

Write the equation: $C_3H_8(g) + 5O_2(g) \longrightarrow 3CO_2(g) + 4H_2O(l)$

1 mole of propane requires 5 moles of oxygen for combustion, therefore

1 volume of propane requires 5 volumes of oxygen for combustion

**2dm$^3$ of propane require 5 × 2dm$^3$ = 10dm$^3$ of oxygen for combustion.**

(d) What volume of hydrogen is obtained when 3.00g of zinc reacts with an excess of sulphuric acid at s.t.p.?

Write the equation: $Zn(s) + H_2SO_4(aq) \longrightarrow H_2(g) + ZnSO_4(aq)$

RAM: Zn = 65.4; Moles of Zn = $\frac{\mathbf{3.00}}{\mathbf{65.40}}$ = **0.04587**

1 mole of hydrogen occupies 22.4dm$^3$ at s.t.p.

1 mole of zinc form 1 mole of hydrogen, therefore

**0.04587 mole of Zn forms 0.04587 × 22.4dm$^3$ = 1.028dm$^3$ of hydrogen**

(e) 20cm$^3$ of ammonia are burned in an excess of oxygen at 110°C. 10cm$^3$ of nitrogen and 30cm$^3$ of steam are formed. Deduce the formula for ammonia.

Let the formula of ammonia be $N_aH_b$.

The equation for combustion is: $N_aH_b(g) + \frac{b}{4}O_2(g) \longrightarrow \frac{a}{2}N_2(g) + \frac{b}{2}H_2O(g)$

Volume of $N_aH_b$ = 20cm$^3$

Volume of $N_2(g)$ = $\frac{a}{2} \times 20$ = 10acm$^3$ = 10cm$^3$ formed, so a = 1

Volume of $H_2O(g)$ = $\frac{b}{2} \times 20$ = 10bcm$^3$ = 30cm$^3$ formed, so b = 3

**The formula of ammonia is $NH_3$**

(f) From 23.05g of ethanol are obtained 33.04g of ethyl ethanoate by esterification with ethanoic acid in the presence of concentrated sulphuric acid. What is the percentage yield of the reaction?

Write the equation: $C_2H_5OH(l) + CH_3COOH(l) \longrightarrow CH_3COOC_2H_5(l) + H_2O(l)$

RMM $C_2H_5OH$ = 46.10; $CH_3COOC_2H_5$ = 88.10

So 46.01g of ethanol should form 88.10g of ethyl ethanoate

23.05g of ethanol should form $\frac{23.05}{46.10} \times 88.10$ = 44.05g of ethyl ethanoate

Actual mass obtained = 33.04g

**Percentage yield** = $\frac{\textbf{Actual mass of product}}{\textbf{Calculated mass of product}} \times \mathbf{100}$

$$\textbf{Percentage yield} = \frac{33.04}{44.05} \times 100 = \textbf{74.93\%}$$

**Questions**

(a) The pollutant, sulphur dioxide, can be removed from the air by the reaction

$$2CaCO_3(s) + 2SO_2(g) + O_2(g) \longrightarrow 2CaSO_4(s) + 2CO_2(g)$$

What mass of calcium carbonate is needed to remove 10.0kg of sulphur dioxide?

(b) In the Solway process

$$NaCl(s) + NH_3(g) + H_2O(l) + CO_2(g) \longrightarrow NaHCO_3(s) + NH_4Cl(aq)$$

what volume of carbon dioxide, at r.t.p., is required to produce 1.00kg of sodium hydrogencarbonate?

(c) Phenol, $C_6H_5OH$, is converted to trichlorophenol, $C_6H_2Cl_3OH$. If 488g of product are obtained from 250g of phenol, calculate the percentage yield.

(d) In the blast furnace, the overall reaction is

$$2Fe_2O_3(s) + 3C(s) \longrightarrow 3CO_2(g) + 4Fe(s)$$

What is the maximum mass of iron that can be obtained from 700 tonnes of iron(III) oxide and 70 tonnes of coke? (1 tonne = 1000kg)

**Answers**

1. (a) ***39.1 + 79.9 = 119.0*** (b) ***(2 x 22.99) + 12 + (3 x 16.0) + [((2 x 1) + 16) x 10) = 286.1***

2. (a) ***S = (32/80) x 100 = 40%*** (b) ***Mg = [(3 x 24)/101] x 100 = 72.3%***

***O = [(3 x 16)/80] x 100 = 60%*** ***N = [(14 x 2)/101] x 100 = 27.7%***

3.(a) ***Moles = 58.5/58.5 = 1.000 mole*** (b) ***Moles = 50.00/100 = 0.500 moles***

4.(a) (i) ***Moles Fe = 7.77/56 = 0.138;*** ***Moles O = 2.23/16 = 0.139***

***Ratio Fe:O = 1:1;*** ***Formula = FeO***

(ii) ***Moles C = 18.46/12 = 1.53;*** ***Moles H = 1.52/1 = 1.52***

***Ratio C:H = 1:1;*** ***Formula = CH***

(b) (i) ***Mass Cl = 9.435 - 3.400 = 6.035g***

***Moles Ca = 3.400/40 = 0.085;*** ***Moles Cl = 6.035/35.5 = 0.170***

***Ratio Ca:Cl = 0.085/0.085:0.170/0.085 = 1:2; Formula =*** $CaCl_2$

(ii) ***Mass H = 5.328 - 4.662 = 0.666g***

***Moles Li = 4.662/7 = 0.666;*** ***Moles H = 0.666/1 = 0.666***

***Ratio Li:H = 1:1*** ***Formula = LiH***

(c) (i) ***Ratio N:H:O = 35/14:5/1:60/16 = 2.5:5.0:3.75 = 2.5/2.5:5.0/2.5:3.75/2.5 = 1:2:1.5***

***Multiply by 2 to give whole numbers; = 2:4:3*** ***Formula =*** $N_2H_4O_3$ ($NH_4NO_3$)

(ii) ***%C = 100 - (6.70+53.30) = 40.0;*** ***Ratio C:H:O = 40/12:6.7/1:53.3/16 = 3.33:6.67:3.33 = 1:2:1*** ***Formula =*** $CH_2O$

(d) (i) ***Ratio C:H:O = 54.5/12:36.4/16:9.1/1 = 4.54:2.275:9.1 = 2:1:4***

***Empirical formula =*** $C_2OH_4$ ($C_2H_4O$) ***Empirical mass = (12 x 2) + 16 + (4 x 1) = 44***

***Molecular formula =*** $C_2H_4O$

5. (a) ***Ratio*** $CaCO_3$:$SO_2$ ***= 1:1;*** ***Moles*** $SO_2$ ***= 10 000/64 = 156.25 = moles*** $CaCO_3$

***Mass*** $CaCO_3$ ***= 156.25 x 100 = 15625g = 15.625Kg***

(b) ***Ratio*** $CO_2$:$NaHCO_3$ ***= 1:1;*** ***Moles*** $NaHCO_3$ ***= 1000/84 = 11.9***

***Volume of*** $CO_2$ ***= 11.9 x 24 = 285.6 (286)***$dm^3$

(c) ***Ratio phenol:trip = 1:1; Moles phenol = 250/94 = 2.66; Expected yield = 2.66 x 197.5 = 525.35***

***Percentage yield = (488/525.35) x 100 = 92.9%***

(d) ***Moles*** $Fe_2O_3$ ***= 700/160 = 4.375; moles C = 70/12 = 5.883; Limiting factor = moles of coke. Maximum moles of Fe = (5.883 x 4)/3 = 7.778***

***Mass of Fe = 7.778 x 56 = 435.57 tonnes.***