UNIT 04: Reactions & Stoichiometry

Symbols, relative atomic mass and the periodic table

Each element has a symbol, an atomic number and an atomic mass number listed on the periodic table. Some elements have a symbol made up of one letter, others have two. It is important when writing the two letter symbols to ensure that you use a lower case letter for the second letter. This may sound trivial but is very important, for example Co (Cobalt), a metal element, is not the same as CO (Carbon monoxide), a gaseous compound made from Carbon (C) and Oxygen (O).

Atomic numbers are printed above the symbol, atomic masses below.

	Group																	
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Period 1	1 H 1																	2 He 4
2	3 Li 7	4 Be 9											5 B 11	6 C 12	7 N 14	8 O 16	9 F 19	10 Ne 20
3	11 Na 23	12 Mg 24	T R A N S I T I O N M E T A L S										13 Al 27	14 Si 28	15 P 31	16 S 32	17 Cl 35.5	18 Ar 36
4	19 K 39	20 Ca 40	21 Sc 45	22 Ti 48	23 V 51	24 Cr 52	25 Mn 55	26 Fe 56	27 Co 59	28 Ni 59	29 Cu 64	30 Zn 65	31 Ga 70	32 Ge 73	33 As 75	34 Se 79	35 Br 80	36 Kr 84
5	37 Rb 86	38 Sr 88	39 Y 89	40 Zr 91	41 Nb 93	42 Mo 96	43 Tc 99	44 Ru 101	45 Rh 103	46 Pd 106	47 Ag 108	48 Cd 112	49 In 115	50 Sn 119	51 Sb 122	52 Te 128	53 I 127	54 Xe 131
6	55 Cs 133	56 Ba 137	57 La* 139	72 Hf 178	73 Ta 181	74 W 184	75 Re 186	76 Os 190	77 Ir 192	78 Pt 195	79 Au 197	80 Hg 201	81 Tl 204	82 Pb 207	83 Bi 209	84 Po 210	85 At 210	86 Rn 222
7	87 Fr 223	88 Ra 226	89 Ac† 226	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg							

*Lanthanides	58 Ce 140	59 Pr 141	60 Nd 144	61 Pm 147	62 Sm 150	63 Eu 152	64 Gd 157	65 Tb 159	66 Dy 163	67 Ho 165	68 Er 167	69 Tm 169	70 Yb 173	71 Lu 175
†Actinides	90 Th 232	91 Pa 231	92 U 238	93 Np 237	94 Pu 242	95 Am 243	96 Cm 247	97 Bk 251	98 Cf 251	99 Es 254	100 Fm 253	101 Md 256	102 No 254	103 Lr 257

Formulae of compounds

The chemical formula of a compound shows the exact ratio of the different elements that are present. The numbers of each element are recorded using a subscript to the right of the elements symbol. When only one atom is present, the subscript one is assumed (understood), and not written.

Percentage composition in chemical formula

To determine the % composition of an individual element within a compound, simply express the mass of each element as a % of the mass of the compound.

Empirical formulae

The empirical formula is the simplest whole number ratio of the atoms of each element in that compound and can be calculated from mass data. There is a simple method to follow.

① Take the percentage of each element present, assume a sample of 100 g, and divide that mass by the appropriate mass number. (This gives the number of moles - see later).

② Find the smallest number calculated in ① and divide all the results of the calculations in ① by that number. (This gives the molar ratio). <u>N.B. Avoid rounding up or down too much at this stage and be lenient with significant figures.</u>

③ The results from ② should be in a convenient ratio and give the empirical formula. <u>N.B. It may be that the ratio includes a decimal (fraction) such as .500, .250 or .333 etc. If so then multiply all numbers by 2, 4 or 3 as appropriate to remove the decimal.</u>

For example; calculate the empirical formula for the compound containing 40.1% carbon, 6.60% hydrogen and 53.3% oxygen.

	C	H	O
Assuming 100g sample, the % by mass	40.1	6.60	53.3
RAM (from periodic table)	12.011	1.0079	16.00
① % by mass ÷ RAM	3.34	6.55	3.33
② divide by smallest	1	2	1
③ Empirical formula	**$C_1H_2O_1$ or CH_2O**		

Task 04a

1. ***Calculate the empirical formulae of the three oxides of iron shown below.***

   (a) 77.78% Fe, 22.22% O
   (b) 70.00% Fe, 30.00% O
   (c) 72.40% Fe, 27.60% O

2. ***A hydrocarbon (a compound containing only hydrogen & carbon) is found to be 7.690% H and 92.31% C by mass. Calculate its empirical formula.***

Formulae of Molecules - Molecular formulae

Once the empirical formula has been established, and given further appropriate data, the molecular formula can be calculated. The molecular formula tells us exactly how many atoms of each element are present in the compound rather than just the simplest whole number ratio. It is a simple multiple of the empirical formula. Hence, in the example of an empirical formula of CH_2O, the molecular formula could be $C_2H_4O_2$ or $C_3H_6O_3$ etc. To find the molecular formula it is necessary to know the Molar mass or Relative Molecular Mass (RMM). Given the RMM to be 60 g mol^{-1} it is clear the molecular formula is $C_2H_4O_2$, i.e., twice the empirical.

Task 04b

The same compound as in question #2 in Task 4a has a molar mass of 78.00 g mol^{-1}. What is the molecular formula of the compound?

Chemical equations

Chemical equations are a shorthand method used to illustrate what happens during a chemical reaction. There are a number of steps to writing an equation.

1. Write down the equation in words.
2. Fill in the correct formulae for all the substances.
3. Balance the equation. Balancing the equation can be tricky and requires practice. It involves the following steps.

   I. Ensure the correct formulae are being used for all the reactants and products
   II. Balance each element in turn remembering to multiply brackets out carefully. This process in rather unscientific and is essentially a process of trial and error but can be helped by the following tips;

If an element appears in only one compound on each side of the equation, try balancing that first. Secondly, if one of the reactants or products appears as the free element, try balancing that last.

   III. When balancing, only place numbers in front of whole formulae. Do not change the (correct) formulae of any of the reactants or products, or add any extra formulae. The numbers that appear in front of each formula are called the stoichiometric coefficients. They have an extremely important role to play in calculations since they give the reacting ratio (i.e. the number of moles of one substance that react with, or are produced from, others).

4. Add state symbols, (s) for solid, (l) for liquid, (g) for gas and (aq) for aqueous meaning in solution with water.

Task 04c

1. ***Write balanced equations for the following reactions.***

   (a) ***Hydrogen + Copper (II) oxide ➔ Copper + Water***

   (b) ***Carbon + Oxygen ➔ Carbon monoxide***

   (c) ***Magnesium + Sulfuric acid ➔ Hydrogen + Magnesium Sulfate***

2. ***Balance the following equations.***

(a)	Ca	+	H_2O	➔	H_2	+	$Ca(OH)_2$		
(b)	Cu	+	O_2	➔	CuO				
(c)	Na	+	O_2	➔	Na_2O				
(d)	Fe	+	HCl	➔	$FeCl_2$	+	H_2		
(e)	Fe	+	Br_2	➔	$FeBr_3$				
(f)	C_4H_8	+	O_2	➔	CO_2	+	H_2O		
(g)	Na_2CO_3	+	HI	➔	NaI	+	CO_2	+	H_2O
(h)	$CuCO_3$			➔	CuO	+	CO_2		
(i)	$Pb(NO_3)_2$			➔	PbO	+	NO_2	+	O_2
(j)	H_2SO_4	+	KOH	➔	K_2SO_4	+	H_2O		
(k)	$NaHCO_3$			➔	Na_2CO_3	+	H_2O	+	CO_2
(l)	Al	+	O_2	➔	Al_2O_3				

The mole concept and calculations from equations

Atomic Mass Units

We have seen previously how atoms are comprised of protons, neutrons and electrons and how the protons and neutrons have masses of approx. 1 atomic mass unit (amu) respectively and that electrons do not contribute significantly to the mass. If we define the amu as having a mass of 1.66×10^{-24} g we can see that atoms are extremely small and have an extremely small mass.

For example, 1 atom of Cl^{35} contains 17 protons and 18 neutrons. This is a total of 35 amu (ignoring the electrons) and has a mass of 5.81×10^{-23} g. This is a very small number so we use the concept of the mole (see below) to overcome the problem of handling such small quantities. As you will see 1 mole contains 6.022×10^{23} particles. So if we take 1 mole of Cl^{35} atoms they will have a mass of $(5.81 \times 10^{-23}\ \text{g})(6.022 \times 10^{23}) = 35.0$ g.

Relative Atomic Mass (RAM) or Molar Mass

RAM is defined as the weighted average of the masses of all the atoms in a normal isotopic sample of the element based upon the scale where 1 mole of atoms of the C^{12} isotope has a mass of exactly 12.00 g.

We have seen previously how elements occur in nature as a number of different isotopes an as a result they have a RAM that is not an integer. For example, chlorine occurs in nature as approx. 75% Cl^{35} and 25% Cl^{37}

Average Relative Atomic Mass of 1 mole of chlorine atoms = $\dfrac{(35 \times 75) + (37 \times 25)}{100}$ = 35.5 g

Average relative atomic masses are the mass numbers recorded on the periodic table. The relative masses of atoms shown on the periodic table can be used to determine the relative masses of molecules and ions by simple summation.

Relative Molecular Mass (RMM) or Molar Mass - Found by adding all of the individual RAM's together in one molecule of a compound.

Relative Formula Mass (RFM) or Molar Mass - Found by adding all of the individual RAM's together in one formula unit of an ionic compound.

Avogadro's number and the mole concept

In chemistry, amounts of substances are measured in moles (mols). The mole is a standard number of particles (atoms, ions or molecules) and can be defined as, the amount of any substance that contains the same number of particles, as there are C^{12} atoms in 12.00g of the C^{12} isotope. The actual number of particles in a mole, known as the Avogadro constant or number is found to be 6.022×10^{23} particles per mole and has the unit, mol^{-1}. For example, one mole of atoms = 6.02×10^{23} atoms.

The average Relative Atomic Mass (RAM) of each element is given on the periodic table. The figure shows the average mass of one mole of atoms of that particular element. This leads to the relationships below.

$$\text{Number of Moles of an Element} = \frac{\text{mass of sample}}{\text{RAM}} = \frac{\text{mass of sample}}{\text{Molar Mass}}$$

$$\text{Number of Moles of a Molecular compound} = \frac{\text{mass of sample}}{\text{RMM}} = \frac{\text{mass of sample}}{\text{Molar Mass}}$$

$$\text{Number of Moles of an Ionic compound} = \frac{\text{mass of sample}}{\text{RFM}} = \frac{\text{mass of sample}}{\text{Molar Mass}}$$

Task 04d

1. ***What is the mass of one mole of sodium chloride, NaCl***
2. ***How many moles of Ca atoms are there in 140. g of calcium?***
3. ***How many moles of $CuBr_2$ are there in 0.522 g of copper(II) bromide?***
4. ***How many moles of CO_2 molecules are there in 23.0 g of carbon dioxide?***
5. ***How many 'particles' are present in each of the chemicals in questions #1-4 above?***

If we know the number of moles of a substance that is present in a reaction and we know a balanced chemical equation, (i.e. we know the reacting ratio), it is possible to calculate the moles of another substance present in the equation. Use this method;

1. Write a correct and balanced equation.
2. Find the number of moles present by using a moles relationship for one substance.
3. Use the stoichiometric coefficients in the equation to find the reacting ratio of the moles. Use this relationship to find the number of moles of the unknown substance.
4. Re-apply a moles relationship for the unknown substance.

Task 04e

The combustion of methane (CH_4) can be summarized by the equation below.

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

1. ***Calculate the mass of O_2 required to produce 2.23 g of carbon dioxide.***
2. ***Calculate the mass of water produced when 34.0 g of CH_4 is burned.***

Volumetric analysis and moles

Chemical reactions are often carried out between substances that are in solution (dissolved in a solvent, usually water). The concentration of a solution can be measured in terms of the number of grams of the solute (solid) that has been dissolved in a particular volume of the solution (where water is usually the solvent), or more usually, in terms of the number of moles of the solute in a particular volume of the solution. Typical units are g dm^{-3} or g/dm^3 or mol dm^{-3} or mol/dm^3 or mol/L or mol L^{-1}.

The method of expressing the concentration of a solution in mol L^{-1} is the most common (and most useful) and is referred to as Molarity (M). So, for example, a solution that has a concentration of 0.250 mol L^{-1} can be referred to as 0.250 M solution, or a 0.250 "molar" solution. When concentration is measured in mol L^{-1}, or M, and volume in L, then, for solutions;

Moles = (concentration) (volume)

Task 04f

1. ***What mass of solute (solid sodium carbonate) must be used in order to prepare 275 mL of 1.20 mol L^{-1} sodium carbonate solution?***

2. ***A sample of copper (II) sulfate pentahydrate with a mass of 8.512 g is dissolved in 500.0 mL of water. A 25.00 mL portion completely reacts with 20.00 mL of a 0.1702 mol L^{-1} solution of iodide ions. In what molar ratio do Cu^{2+} and iodide ions react?***

<u>Questions #3-5 require balanced equations before they can be solved.</u>

3. ***Carbonates, in the form of antacid tablets, can be used to neutralize stomach acid. 25.0 mL of 0.100 mol L^{-1} sodium carbonate solution completely reacts with 35.3 mL of HCl in such a simulated neutralization. What is the concentration (molarity) of the acid?***

4. ***Some metals will react vigorously with acids to produce hydrogen gas. What mass of zinc metal, will react completely with 75.0 mL of 0.200 mol L^{-1} sulfuric acid?***

5. ***Hydroxides can be used to neutralize acids. What volume of 1.00 mol L^{-1} NaOH, would be required to completely neutralize 25.0 mL of 2.00 mol L^{-1} HCl?***

Dilution

Often, solutions are prepared by adding water to (diluting) more concentrated ones. For example, if 4.0 L of a 2.0 M solution was required, it could be made by diluting some 10. M solution. Calculations involving dilution problems involve three steps.

1. Calculate the number of moles present in the final, diluted solution, by applying moles = (concentration) (volume).
2. Calculate the volume of the starting, more concentrated solution that supplies this number of moles by applying moles = (concentration) (volume).
3. The volume of water that must be added to the concentrated solution is simply the difference between the volume of the final, diluted solution and the volume of the concentrated solution.

Worked Example

Calculate the volume of water that must be added to prepare 2.0 L of 3.0 M KOH from a stock solution that has a concentration of 8.0 mol L^{-1}.

1. Final solution must contain (2.0 L)(3 mol/L) mols = 6.0 mols of KOH.
2. Since moles = (concentration) (volume), the volume (in L) of the stock (concentrated) solution that contains 6.0 mols of KOH = $\frac{6.0 \text{ mol}}{8.0 \text{ mol/L}}$ = 0.75 L.
3. So, by taking 0.75 L of the stock solution and adding 1.25 L of water to make the solution up to 2.00 L, the final, diluted solution, will have a concentration (molarity) = $\frac{6.0 \text{ mol}}{2.0 \text{ L}}$ = 3.0 mol L^{-1} or 3.0 M.

Task 04g

1. ***Calculate the volume of 3.25 M nitric acid that must be diluted with water to produce 500. mL of 1.25 M nitric acid.***
2. ***Calculate the volume of 2.60 M KOH that must be diluted with water to produce 250. mL of 2.00 M KOH.***
3. ***What volume of water must be added to 4.0 M HCl in order to produce 2.0 L of 0.5 M HCl?***

Combustion Analysis

Compounds that contain carbon and hydrogen only, when burned completely in oxygen, will yield only carbon dioxide and water. Analysis of the mass of CO_2 and H_2O produced can be used to determine the empirical formula of the substance in question. This method assumes that all the carbon in CO_2 originated from the carbon in the original compound, and all the hydrogen in the water originated from the hydrogen in the original compound. The method is as follows.

1. Calculate the moles of CO_2 produced. Since there is one carbon atom in one molecule of CO_2 this is also the number of moles of C atoms present in the original compound.
2. Calculate the moles of H_2O produced. Since there are two hydrogen atoms in one molecule of H_2O multiply this number by two to calculate the number of moles of H atoms present in the original compound.
3. Calculate the mass of C and H present in the combusted sample by multiplying the moles of each by their RAM's.
4. If there is another element present (typically O) in the combusted substance then calculate its mass by subtracting the mass of C and H from the total mass of the combusted sample. Turn this mass into moles by dividing by the appropriate RAM. Find the smallest number of moles calculated and divide all the numbers of moles by that number. (This gives the molar ratio). <u>N.B. Avoid rounding up or down too much at this stage and be lenient with significant figures.</u>
5. The results from #4 should be in a convenient ratio and give the empirical formula. <u>N.B. It may be that the ratio includes a fraction such as .500, .250 or .333 etc. If so then multiply all numbers by 2, 4 or 3 as appropriate to remove the fraction.</u>
6. If necessary use the Molar Mass to turn the empirical formula into a molecular formula.

Task 04h

When 4-ketopentenoic acid is analyzed by combustion, it is found that a 0.3000 g sample produces 0.579 g of CO_2 and 0.142 g of H_2O. The acid contains only carbon, hydrogen, and oxygen. What is the empirical formula of the acid?

Analysis of hydrates

Hydrates are formula units with water associated with them. The water molecules are incorporated into the solid structure. For example, $CuSO_4.5H_2O$, copper(II) sulfate pentahydrate. Strong heating can evaporate the water. When water is removed the salts are called anhydrous (without water).

Task 04i

1. ***A sample of the hydrated salt $CoCl_2.xH_2O$, with a mass of 11.73 g is weighed, heated to drive off the water of crystallization, cooled and reweighed until constant mass (6.410 g) is achieved. Calculate the value of x.***
2. ***What is meant by the term, "constant mass" in question #1?***

Limiting Reactant

When all the reactants in a chemical reaction are completely consumed, i.e. they are all converted to products, then the reactants are said to be in stoichiometric proportions. On other occasions it may be necessary to ensure that only one particular reactant is completely used up. This is achieved by using an excess of all the other reactants. The reactant that is completely consumed is called the limiting reagent and it, is what determines the quantities of products that form.

Task 04j

The two non-metals, sulfur and chlorine, react according to the equation below.

$$S_{(s)} + 3Cl_{2(g)} \rightarrow SCl_{6(l)}$$

If 202 g of Sulfur are allowed to react with 303 g of Cl_2 in the reaction above, which is the limiting reactant, how much product will be produced and what mass of the excess reactant will be left over?

Percentage yield

In all chemical syntheses the yield of the product will be less than 100%. The % yield is given as

$$\% \text{ Yield } = \left(\frac{\text{actual yield of product}}{\text{theoretical yield of product}}\right) \text{X } 100$$

The yield is usually less than 100% since the reactants are often not pure, some of the product is lost during purification, the reaction may be reversible and/or side reactions may give by-products.

Task 04k

Aluminum will react with oxygen gas according to the equation below;

$$4Al + 3O_2 \rightarrow 2Al_2O_3$$

In one such reaction, 23.4 g of Al are allowed to burn in excess oxygen. 39.3 g of aluminum oxide are formed. What is the percentage yield?