3. Chemical Calculations

Content

Introduction

Basic mathematical calculations used in chemistry and the knowledge required in respect of understanding chemistry principles are acquired in this unit.

3.1 Oxidation number

Oxidation number is used to determine the number of electrons transfer between atoms/ions in compounds and molecules. The oxidation number describes the loss or gain of electrons from an atom in a chemical compound. The oxidation number describes the charge that an atom would have if all bonds are considered to be ionic with no covalent component. The oxidation number of an atom in a covalent compound is found by assigning the electrons shared by atoms to the particular atom as follows:

(a) For **covalent bonds formed between similar atoms** – When there is no electronegativity difference between the two bonded atoms, the electrons are split equally between the atoms. For such bonds the oxidation number of atoms is zero.

(b) For **covalent bonds formed between different atoms** – When the covalent molecule is made up of different atoms the bonded electrons are not shared equally between the atoms. In these bonds, the bonded electrons are assigned to the atom that has the highest electronegativity. Accordingly, plus and minus oxidation numbers are introduced to explain the oxidation number.

The examples for different types of oxidation number exhibited by atoms/ ions are given in Table 3.1.

Table 3.1 The examples for various oxidation numbers exhibited by atoms/ ions

Type	Oxidation number	Example
Atoms in elemental state	Zero	Na(s), He(g), Hg(l), N_2(g)
Monoatomic ions	Equal to the charge	Na^+, O^{2-},Ca^{2+}
Fluorine	-1	NaF, OF_2
Oxygen	-2	H_2O, P_2O_5
	+2	OF_2 only
	-1	peroxides/ O_2^{2-}
	-1 and zero	superoxides/ O_2^-
Hydrogen	+1	H_2O, CH_4
	-1	Metal hydrides only (NaH)

3.1.1 Basic rules that applied in the determination of the oxidation number of an atom in a molecule/ polyatomic ion or in a compound

Two basic rules used to allocate oxidation numbers for atoms and ions in simple molecules, molecular ions and compounds are given below.

(a) The sum of the oxidation numbers of all the atoms in an compound is equal to zero.

(b) The sum of the oxidation numbers of all the atoms in an ion is equal to its charge.

Examples of the use of the above two rules are shown below.

The determination of oxidation number of an atom in molecules

Example 1: Phosphine (PH_3)

The oxidation number of P in PH_3

Total charge of PH_3 is zero,

3 [oxidation number of H] + [oxidation number of P] = 0

3 [+1] + [oxidation number of P] = 0

Oxidation number of P = -3

Example 2: Phosphoric acid (H_3PO_4)

The oxidation number of P in H_3PO_4

Total charge of H_3PO_4 is zero,

3 [oxidation number of H]+[oxidation number of P]+4[oxidation number of O] = 0

3 [+1] + [oxidation number of P] + 4[-2] = 0

Oxidation number of P = +5

The determination of oxidation number of an atom in polyatomic ions

Example 1: Sulphate ion (SO_4^{2-})

The oxidation number of S in SO_4^{2-}

Total charge of SO_4^{2-} is -2,

4 [oxidation number of O] + [oxidation number of S] = -2

4 [-2] + [oxidation number of S] = -2

Oxidation number of S = +6

The determination of oxidation number of an atom in compounds

Example 1: Calcium oxide (CaO)

The oxidation number of Ca in CaO

Total charge of CaO is zero,

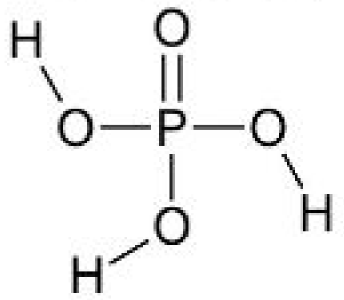
[oxidation number of Ca] + [oxidation number of O] = 0

[oxidation number of Ca] + [-2] = 0

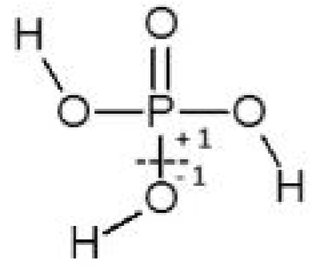
Oxidation number of Ca = +2

The structural formula of a molecule shows a graphic representation of its molecular structure and how the atoms are arranged. It also can be used to assign the oxidation number to each atom in the molecule using the electronegativity difference between the component atoms. This approach is mainly used to determine the oxidation number of atoms in covalent bonds. In this method, each pair of electrons in a covalent bond must be assigned to the most electronegative atom accordingly. The most electronegative atom gains the electron and it is marked with a (-1) charge. The atom that has less electronegativity loses an electron and it is marked with a (+1) charge. After assigning the electrons the final charge on the central atom is called as the oxidation number of the central atom. This is illustrated in the examples given below.

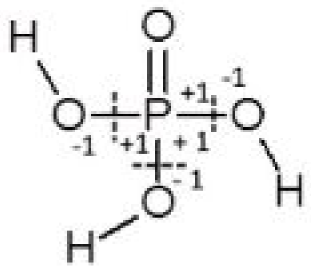
Example 1: Phosphoric acid (H_3PO_4)



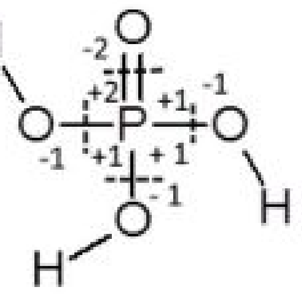
Step 1
Draw the bond structure of the compound.



Step 2
Based on the electronegativity difference assign +1 or -1 to atoms bonded together.



Step 3
Continue step 2 with all the bonds around the target element.

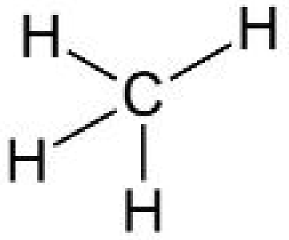


Step 4
Add all the assigned values around the target element.
Phosphorus = (+2)+(+1)+(+1)+(+1) = +5
Oxidation number of the central atom of phosphorus is +5.

Figure 3.1 Steps in determining oxidation number of P atom in H_3PO_4

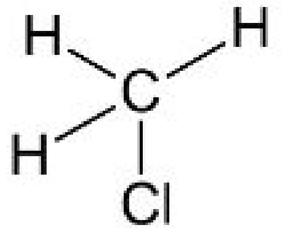
Oxidation number of carbon in compounds in which carbon at the center.

Example 1: Methane (CH_4)



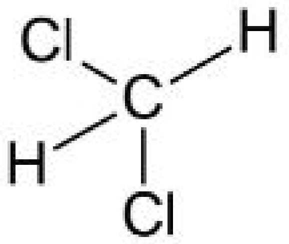
Oxidation number of C = -4

Example 2: Chloromethane (CH_3Cl)



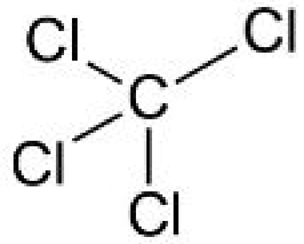
Oxidation number of C = -2

Eample 3: Dichloromethane (CH_2Cl_2)



Oxidation number of C = 0

Example 4: Tetrachloromethane (CCl_4)



Oxidation number of C = +4

3.1.2 Use of oxidation numbers to understand electron transfer between atoms in redox reactions

New products are formed by transfer of electrons from one atom to another when chemicals react. Consider the reaction between solid sodium and chlorine gas;

$$2Na(s) + Cl_2(g) \longrightarrow 2NaCl(s)$$

In this reaction, elemental sodium and chlorine become a positively charged sodium ion and negatively charged chloride ion respectively. (Na^+ and Cl^-).

In such reactions, one or more electrons are transferred from one atom to another atom. Reactions showing such electron transfers are called **oxidation-reduction reactions** or **redox reactions**.

- The loss of an electron/s from an atom/ ion is called **oxidation**.
- Conversely the gain of an electron/s by an atom/ ion is called **reduction**.

Oxidation (Loss of electrons) $$\underset{0}{Na(g)} \longrightarrow \underset{+1}{Na^+(g)} + e$$

In oxidation, oxidation number of an atom/ion increases. Therefore sodium is oxidized to sodium ion.

Reduction (Gain of electrons) $$\underset{0}{Cl_2(g)} + 2e \longrightarrow \underset{-1}{2Cl^-(g)}$$

In reduction, oxidation number of an atom/ion decreases. Therefore chlorine is reduced to chloride ions.

In the above example, chlorine is identified as the oxidizing agent and sodium is the reducing agent.

Further examples are given below to help to understand the electron transfer that occurs in redox reactions.

Example 1: Combustion of methane (CH_4)

This can be shown using the following balanced equation. In this reaction, oxidation numbers of C and O is changed when CO_2 and H_2O are formed as products.

Reaction	$CH_4(g)$	+	$2O_2(g)$	$\longrightarrow$	$CO_2(g)$	+	$2H_2O(l)$
Oxidation number	C = -4		O = 0		C = +4		H = +1
	H = +1				O = -2		O = -2

The oxidation number of hydrogen remains unchanged.

The oxidation number of carbon changes from -4 to +4. Therefore, carbon is oxidized.

The oxidation number of oxygen changes from 0 to -2. Therefore, oxygen is reduced.

Oxidation reaction: Carbon in CH_4 is oxidized to produce CO_2.
Each carbon atom loses 8 electrons.
Reduction reaction: Oxygen is reduced to produce H_2O and CO_2.
Each oxygen atom gains 2 electrons.

Example 2: Combustion of propane (C_3H_8)
This is shown using the following balanced equation. In this reaction, oxidation numbers of C and O will change when CO_2 and H_2O are formed as products.

Reaction	$^{x}CH_3{}^{y}CH_2{}^{z}CH_3(g)$	+	$5O_2(g)$	$\longrightarrow$	$3CO_2(g)$	+	$4H_2O(l)$
Oxidation number	$^{x}C = -3$, $^{y}C = -2$, $^{z}C = -3$		$O = 0$		$C = +4$		$O = -2$
Cumulative oxidation number of carbon	$(-3)+(-2)+(-3) = -8$				$(+4)\times 3 = +12$		

The cumulative oxidation number of the three carbons changes from -8 to +12. Therefore, there is a total of 20 electrons **loss** when forming the product CO_2. Hence carbon is oxidized.

The oxidation number of oxygen changes from 0 to -2 in the product. Therefore, there is a total of 4 electrons **gain** when forming the product of two O^{2-}. Hence oxygen is reduced.

Oxidation reaction: Carbon in $CH_3CH_2CH_3(g)$ is oxidized to produce CO_2.
Reduction reaction: Oxygen is reduced to produce H_2O and CO_2.

Example 3: Formation of propane (C_3H_8) from propene (C_3H_6)
This is shown using the following balanced equation. In this reaction, oxidation numbers of C in C_3H_8 will change when C_3H_6 is produced and this can be shown as follows.

Reaction	$^{x}CH_3{}^{y}CH{}^{z}CH_2(g)$	+	$H_2(g)$	$\longrightarrow$	$^{x}CH_3{}^{y}CH_2{}^{z}CH_3(g)$
Oxidation number	$^{x}C= -3$, $^{y}C =-1$, $^{z}C= -2$		$H=0$		$^{x}C= -3$, $^{y}C= -2$, $^{z}C= -3$
Cumulative oxidation number of carbon	$(-3)+(-1)+(-2) = -6$		$H=0$		$(-3) + (-2) + (-3) = -8$

The cumulative oxidation number of the three carbons changes from -6 to -8. Therefore, there is a total of 2 electrons **gain** when forming the product. Hence carbon is reduced.

The oxidation number of hydrogen changes from 0 to +1in the product. Therefore, there is a 2 electrons **loss** in respect of hydrogen when forming the two H^+ in the product C_3H_8. Hence hydrogen is oxidized.

Reduction reaction: Carbon in $CH_3CHCH_2(g)$ is reduced to produce $CH_3CH_2CH_3(g)$
Oxidation reaction: Hydrogen is oxidized to produce $CH_3CH_2CH_3(g)$.

3.2 Nomenclature of inorganic compounds

IUPAC recommendations for nomenclature are used in the systematic way of naming compounds. IUPAC stands for *International Union of Pure and Applied Chemistry*. This section deals only with the inorganic nomenclature. With the aid of nomenclature chemical compounds can be specified with a unique name.

Trivial names (name used before the IUPAC nomenclature was introduced) are often still commonly used for some compounds in addition to the IUPAC names.

3.2.1 Names of ionic compounds derived from monoatomic ions

The way of writing the unmodified name for the monoatomic cation and then writing the modified name for the monoatomic anion with the suffix ***-ide*** at the end is shown in the Table 3.2.

Table 3.2 Names of common monoatomic ions

Cation	Name	Anion	Name
H^+	hydrogen	H^-	hydride
Na^+	sodium	Cl^-	chloride
K^+	potassium	Br^-	bromide
Ca^{2+}	calcium	O^{2-}	oxide
Al^{3+}	aluminium	S^{2-}	sulfide
Zn^{2+}	zinc	N^{3-}	nitride

Rules for writing the name of ionic compounds with an element that can only form one type of cation:

1. Name of the cation must always come first.
2. Name of the cation is the name of its element.
3. Name of the anion is the part of its element name and the suffix *–ide*.
4. Leave a space between the name of the cation and the anion.

Applications are shown in the examples below.

e.g.: NaCl - sodium chloride
MgO - magnesium oxide
CsBr - caesium bromide

3.2.2 Names of ionic compounds derived from elements that form more than one type of cations

The metal ions with variable oxidation numbers form more than one type of cations. In the trivial names, suffix *–ic* for the cation of higher charge (higher oxidation number) and *–ous* for the cation of lower charge (lower oxidation number) are used.

This can be seen in naming Fe^{2+} as ferrous and Fe^{3+} as ferric. Trivial and systematic names for common cations are given below in Table 3.3. However, in systematic names, the charge of the metal ion is shown using Roman numerals in parentheses after the name of the metal according to the oxidation number of the metal ions. It is also shown in Table 3.3 below.

Table 3.3 Names of cations that can form more than one positively charged ions

Cation	Trivial name	Systematic (IUPAC) name
Fe^{2+}	ferrous	iron(II)
Fe^{3+}	ferric	iron(III)
Cu^{+}	cuprous	copper(I)
Cu^{2+}	cupric	copper(II)
Co^{2+}	cobaltous	cobalt(II)
Co^{3+}	cobaltic	cobalt(III)
Sn^{2+}	stannous	tin(II)
Sn^{4+}	stannic	tin(IV)
Pb^{2+}	plumbous	lead(II)
Pb^{4+}	plumbic	lead(IV)
Hg_2^{2+}	mercurous	mercury(I)
Hg^{2+}	mercuric	mercury(II)

Rules for writing the name of ionic compounds composed of the elements showing variable oxidation numbers:

1. Name of the cation must always come first.
2. Name of the element is used as the name of the cation and the oxidation number (charge) is shown by capital Roman numerals in parentheses at the end of the cationic name.
3. Name of the anion is the part of its element's name which is written with the suffix –*ide* at the end of the anionic name.
4. Leave a space between the name of the cation and the anion.

e.g.: FeS - iron(II) sulfide**
Fe_2S_3 - iron(III) sulfide
CuCl - copper(I) chloride
$CuCl_2$ - copper(II) chloride

**Both sulfide and sulphide are correct and accepted, however for nomenclature only sulfide is accepted.

Trivial names for few of the above compounds are given below.

FeS - ferrous sulfide
Fe_2S_3 - ferric sulfide
CuCl - cuprous chloride
$CuCl_2$ - cupric chloride

3.2.3 Names of simple covalent compounds

Many elements form covalent compounds. When naming this type of compounds, the element with the positive oxidation number must be written first followed by the element with the negative oxidation number.

Rules for writing the name of simple covalent compounds:

1. First part of the name is written representing the less electronegative element and the second part of the name is written indicating the more electronegative element in the compound.
2. Write the name of the compound leaving a space between the first part and the second part.
3. Name the most electronegative atom by modifying its name with the suffix *–ide*.
4. Prefixes are used to represent the number of similar atoms in the compound. Based on the number of similar atoms prefixes are given as follows.
   1 = *mono*, 2 = *di*, 3 = *tri*, 4 = *tetra*, 5 = *penta*, 6 = *hexa*, 7 = *hepta*, 8 = *octa*
   However, the prefix *mono* is never used when naming the first element.
5. When the prefix ends in "*a*" or "*o*" and the second element name begins with "*a*" or "*o*", the final vowel of the prefix is dropped for ease of pronunciation.
   e.g.: mono + oxide = monoxide
   tetra + oxide = teroxide

e.g.: CO - carbon monoxide
H_2S - dihydrogen monosulfide
SO_3 - sulfur trioxide
N_2O_3 - dinitrogen trioxide
N_2O_4 - dinitrogen tetroxide
P_4O_6 - tetraphosphorus hexoxide
H_2O - dihydrogen monoxide
OF_2 - oxygen difluoride

3.2.4 Polyatomic ions

Some nonmetal atoms can bind covalently to form polyatomic ions. Polyatomic anions are more common than polyatomic cations.

Rules for writing the name of polyatomic ions.
The names of these ions are written using the following suffixes.

1. Names of polyatomic cations end with *-ium*.
2. Names of polyatomic anions end with suffixes *–ide*, *-ite* and *-ate*.

Names for common polyatomic ions are given in Table 3.4.

Table 3.4 Formulae and the name of the polyatomic ions

Ion	Name	Ion	Name
NH_4^+	ammonium	NO_3^-	nitrate
OH^-	hydroxide	ClO_3^-	chlorate
CN^-	cyanide	MnO_4^{2-}	manganate
HS^-	hydrogen sulfide	MnO_4^-	permanganate
O_2^{2-}	peroxide	CrO_4^{2-}	chromate
O_2^-	superoxide	$Cr_2O_7^{2-}$	dichromate
SO_3^{2-}	sulfite	$C_2O_4^{2-}$	oxalate
NO_2^-	nitrite	CO_3^{2-}	carbonate
ClO_2^-	chlorite	HCO_3^-	hydrogen carbonate
HSO_3^-	hydrogen sulfite	$S_2O_3^{2-}$	thiosulfate
SO_4^{2-}	sulfate	$S_4O_6^{2-}$	tetrathionate
HSO_4^-	hydrogen sulfate	PO_4^{3-}	phosphate
AlO_2^-	aluminate	HPO_4^{2-}	hydrogen phosphate
ZnO_2^{2-}	zincate	$H_2PO_4^-$	dihydrogen phosphate

Naming compounds with polyatomic ions

Several compounds are named below by referring to the rules discussed above.

$K_2Cr_2O_7$ has a simple cation and a polyatomic anion.
Name of the cationic part = potassium
Name of the anionic part = dichromate
Name of the compound = potassium dichromate

$(NH_4)_2Cr_2O_7$ has a polyatomic cation and a polyatomic anion.
Name of the cationic part = ammonium
Name of the anionic part = dichromate
Name of the compound = ammonium dichromate
Names of some common compounds with a polyatomic anion
KH_2PO_4 = potassium dihydrogen phosphate
FeC_2O_4 = iron(II) oxalate
$NaHCO_3$ = sodium hydrogen carbonate

3.2.5 Inorganic acids

Compounds with one or more ionizable protons in aqueous solutions and **an anion without oxygen** are named using the prefix *hydro-* followed by the name of the other nonmetal or group of non-metals modified with an *-ic* ending. The full name is composed of the term acid at the end.

HCl (hydrogen chloride) = hydrochloric acid
HBr (hydrogen bromide) = hydrobromic acid
HCN (hydrogen cyanide) = hydrocyanic acid
H_2S (dihydrogen sulfide) = hydrosulfuric acid

Compounds with one or more ionizable protons in aqueous solutions and **an anion with oxygen** are called oxoacids. The name of the anion is written with suffix and it is used as the name of the acid.

When the anion name ends in –ate, the suffix –ic is used.
H_2SO_4 (anion is SO_4^{2-} - sulfate) = sulfuric acid
When the anion name ends in –ite, the suffix –ous is used.
H_2SO_3 (anion is SO_3^{2-} - sulfite) = sulfurous acid

Naming different oxoanions (oxyanions) formed from the same central atom
An oxyanion or oxoanion is an ion with the generic formula $A_xO_y^{z-}$ where A represents a chemical element and O represents an oxygen atom. Some elements are able to form more than one oxoanion each containing different number of oxygen atoms. Series of oxoanions containing different numbers of oxygen atoms are generally named as follows.

The prefix *per–* is used for the anion with a higher number of oxygen atoms, and the prefix *hypo–* is used for the anion with a lower number of oxygen atoms.

According to the increasing order of oxidation number of the central atom of the oxoanion, their names can be derived as follows:

hypo____ite	*___ite*	*___ate*	*per___ate*
ClO^- = hypochlorite	ClO_2^- = chlorite	ClO_3^- = chlorate	ClO_4^- = perchlorate
(+1)	(+3)	(+5)	(+7)

These oxoanions are available in the form of oxoacids or salts. Chloro oxoacids and their sodium salts are given in Table 3.4.

Table 3.4 Formulae and names of chloro oxoacids and their sodium salts

Oxidation number of Cl	Formula of oxoacid	Name of oxoacid	Formula of salt	Name of salt
+1	$HClO$	hypochlorous acid	$NaClO$	sodium hypochlorite
+3	$HClO_2$	chlorous acid	$NaClO_2$	sodium chlorite
+5	$HClO_3$	chloric acid	$NaClO_3$	sodium chlorate
+7	$HClO_4$	perchloric acid	$NaClO_4$	sodium perchlorate

**Nomenclature considered in G. C. E. (A/L) Chemistry syllabus is referred to 2005 IUPAC red book*

3.3 Atomic mass, mole and Avogadro constant

3.3.1 The connection among atomic mass unit, mole and Avogadro constant

Since atoms are so small, the normal units of mass such as grams and kilograms are inconvenient to express their mass. Hence a smaller unit of mass called atomic mass unit (u) was introduced. Atomic mass is the mass of an atom of a chemical element expressed in atomic mass units. Different types of isotopes are found in elements. For an example, carbon has three isotopes namely ^{12}C, ^{13}C and ^{14}C. Therefore commonly average atomic mass of elements are used as the atomic mass.

3.3.2 Calculation of average atomic mass of elements

The average atomic mass of any atom can be calculated in the following way, illustrated for carbon and chlorine as typical elements.

Example 1:

The calculation of average atomic mass of natural carbon.

The mass percentage of the isotopes in a sample of carbon is 98.89% of ^{12}C, 1.11% of ^{13}C and the amount of ^{14}C is negligibly small.

Mass of a sample of 100 natural carbon atoms $= [(98.89 \times 12\ u) + (1.11 \times 13\ u)]$

The average atomic mass of natural carbon atom $= [(98.89 \times 12\ u) + (1.11 \times 13\ u)]/\ 100$

$= 12.01\ u$

Example 2:

The calculation of average atomic mass of chlorine.

The mass percentage of the isotopes in a sample of chlorine is 75.77% of ^{35}Cl and 24.23% of ^{37}Cl.

.

Mass of a sample of 100 natural chlorine atoms $= [(75.77 \times 35\ u) + (24.23 \times 37\ u)]$

The average atomic mass of natural chlorine atom $= [(75.77\times34.97\ u)+(24.23\times36.97\ u)]/\ 100$

$= 35.45\ u$

3.3.3 Mole

The amount of substance containing the same number of units/ entities equal to the number of atoms in exactly 12 g of ^{12}C or Avogadro's number is referred to as one mole.

Given below are examples for the number of entities contained in one mole of elements, molecules or ions.

1 mol of ^{12}C contains 6.022×10^{23} of ^{12}C atoms.

1 mol of $C_6H_{12}O_6$ contains 6.022×10^{23} of $C_6H_{12}O_6$ molecules.

1 mol of $CaCl_2$ contains 6.022×10^{23} of Ca^{2+} ions.

This concept can be used to understand further the relationship between the use of u and gram to count the number of atoms. Since 6.022×10^{23} atoms of ^{12}C have a mass of exactly 12 g, and each ^{12}C atom has a mass of 12 u, then,

$1\ u = 1.66 \times 10^{-24}\ g$

$6.022 \times 10^{23}\ u = 1\ g$

$(6.022 \times 10^{23}\ \text{atoms}) \times (12\ u/1\ \text{atom}) = 12.00\ g$

3.3.4 Molar mass

The molar mass is the mass of one mole of the substance. This is calculated as the mass of the given substance (chemical element or chemical compound) divided by the amount (moles) of that substance. The SI unit of molar mass is kg mol^{-1}. However usually molar mass is expressed in g mol^{-1}.

$$\text{molar mass of O} = 16.00 \text{ g mol}^{-1}$$
$$\text{molar mass of } H_2 = 2 \times 1.008 \text{ g mol}^{-1} = 2.016 \text{ g mol}^{-1}$$
$$\text{molar mass of } H_2O = (2 \times 1.008 \text{ g mol}^{-1}) + 16.00 \text{ g mol}^{-1} = 18.016 \text{ g mol}^{-1}$$

A mass of 18.016 g of water contains, Avogadro constant (one mol) of water molecules.

Example 3.1
Calculate the molar mass of NaCl.

Answer:

Molar mass of Na^+ = 22.99 g mol^{-1}
Molar mass of Cl^- = 35.45 g mol^{-1}
Molar mass of NaCl = 22.99 g mol^{-1} + 35.45 g mol^{-1}
= 58.44 g mol^{-1}

A mass of 58.44 g NaCl contains one mole of Na^+ ions and one mol of Cl^- ions. It also contains one mole of NaCl.

3.4 Types of chemical formulae

The chemical formula is used to represent the type of atoms and the number of atoms with the element symbols of each atom showing their exact numbers. More than one type of chemical formulae can be used to represent information of a compound. Two types of chemical formulae are discussed in this section which are used for chemical calculations.

(a) Empirical formula

This is the simplest type of formula derived from the composition of the atomic masses of the elements in a compound. The relative number of atoms of each element in a compound is shown using the empirical formula.

e.g.: For hydrogen peroxide (H_2O_2), the empirical formula is HO.
For ethane (C_2H_6), the empirical formula is CH_3.
For benzene (C_6H_6), the empirical formula is CH.
For ethyne (C_2H_2), the empirical formula is CH.

(b) Molecular formula

The molecular formula is the formula that shows the actual number of atoms of each element in a molecule of a compound.

e.g.: The molecular formula of hydrogen peroxide is H_2O_2.
The molecular formula of ethane is C_2H_6.
The molecular formula of benzene is C_6H_6.
The molecular formula of ethyne is C_2H_2.

3.4.1 Chemical calculations using chemical formulae

Mass percentage of an element in the chemical formula

The mass percentage of a given element in a compound can be determined using the following equations.

$$\text{Mass \% of element A} = \frac{\text{moles of A in formula} \times \text{atomic mass of A (g mol}^{-1}\text{)}}{\text{molar mass of the compound (g mol}^{-1}\text{)}} \times 100$$

Always cumulative individual mass percentages of all elements in a compound adds up to 100%. As an example the calculation of mass percentage of carbon and hydrogen of ethane is given below.

Example 3.2

Calculate the mass percentage of carbon and hydrogen of ethane

Answer:

Molecular formula of ethane is C_2H_6.

Two moles of carbon and six moles of hydrogen are present in one mole of ethane.

$$\text{Mass percentage of carbon} = \frac{2\text{ mol} \times 12\text{ g mol}^{-1}}{(2\text{ mol} \times 12\text{ g mol}^{-1}) + (6\text{ mol} \times 1\text{ g mol}^{-1})} \times 100$$

$$= 80\%$$

$$\text{Mass percentage of hydrogen} = \frac{6\text{ mol} \times 1\text{ g mol}^{-1}}{(2\text{ mol} \times 12\text{ g mol}^{-1}) + (6\text{ mol} \times 1\text{ g mol}^{-1})} \times 100$$

$$= 20\%$$

3.4.2 Determination of the empirical and molecular formula of a compound

Basic steps to determine the empirical formula

1. Obtain the mass of each element present in the compound concerned in grams.
2. Divide each mass by the molar mass of the corresponding element to determine the number of moles of each type of element present.
3. Divide the number of moles of each element by the smallest number of moles obtained in step 2, to convert the smallest number to 1. If all numbers produced are integers or very close to integers, then these numbers represent the subscript values of each element in the empirical formula. However, if one or more numbers are not integers, then follow the step 4.

4. Multiply the numbers produced at the end of step 3 by the smallest possible integer that will convert all of them to whole numbers.
   (When the decimal value is less than 2 or more than 8, round off the number to the closest integer).
   These numbers represent the subscript values of each element in the empirical formula.

3.4.3 Determination of molecular formula using the empirical formula mass and molecular mass

1. Calculate the empirical formula mass from the empirical formula.
2. Divide the molecular mass by the empirical formula mass.
3. The division produces a whole number.
4. Multiply the subscripts in the empirical formula by this number to determine the molecular formula.

An example to understand the above process is given below.

Example 3.3

Determine the molecular formula of a compound with the elemental percentages of Cl = 71.65%, C =24.27% and H = 4.07% and the molar mass of the compound is 98 g mol^{-1}

Answer:

Step 01: Mass percentages: Cl = 71.65%, C = 24.27%, H = 4.07%

Step 02: In 100 g of the compound; Cl= 71.65 g, C=24.27 g and H=4.07 g
Atomic masses of Cl = 35.5, C = 12 and H = 1.
In 100 g of the compound, number of moles present;
Moles of Cl = 71.65 g/35.5 g mol^{-1} = 2.043 mol
Moles of C = 24.27 g/ 12 g mol^{-1} = 2.022 mol
Moles of H = 4.07 g/ 1 g mol^{-1} = 4.07 mol

Step 03: Cl = 2.043 ÷ 2.022 = 1.01 C = 2.022 ÷ 2.022 = 1 H = 4.07 ÷ 2.022 = 2.01

Step 04: Empirical formula = CH_2Cl
Empirical formula mass = 49 g mol^{-1}

If molar mass of the compound is known, then the chemical formula of the compound can be determined.

Step 05:
$$\frac{\text{Molecular formula mass}}{\text{Empirical formula mass}} = 98\ \text{g mol}^{-1} \div 49\ \text{g mol}^{-1} = 2$$
Molecular formula = (empirical formula) × 2
= $(CH_2Cl)_2 \times 2$ = $C_2H_4Cl_2$

3.5 Composition of a substance in a mixture

3.5.1 Composition given in fractions

Three common methods are used to express the composition of a substance in a mixture based on fraction values.

Equation		
Mass fraction of A (w/w)	=	$\frac{\text{mass of A}}{\text{total mass of each substance in the mixture}}$
Volume fraction of A (v/v)	=	$\frac{\text{volume of A}}{\text{total volume of the mixture}}$
Mole fraction of A (x_A)	=	$\frac{\text{amount of moles of A}}{\text{total number of moles in the mixture}}$

Explanation of fractions using mole fraction

The mole fraction (x), is the ratio between the amount of moles of a component and the total amount of moles of all the components present in the mixture.

e.g.: The mole fraction of solute (A) dissolved in a solution is the number of moles of that component (n_A) divided by the total number of moles of all the components in the mixture ($n_A + n_B + n_C + \ldots\ldots$).

$$\boxed{\text{Mole fraction on of A } (x_A) = \frac{n_A}{n_A + n_B + n_C + \ldots}}$$

3.5.2 Percentage composition in a solution (homogeneous mixture)

Equation		
Mass percent (w/w)	=	$\frac{\text{mass of the solute}}{\text{mass of the solution}} \times 100$
Volume percent (v/v)	=	$\frac{\text{volume of the solute}}{\text{volume of the solution}} \times 100$
Mole percentage	=	$\frac{\text{moles of the solute}}{\text{total number of moles of solute and solvent}} \times 100$

Since numerator and denominator are expressed with the same units, final expression do not have units.

The composition of a solution can be specified using the amount of solute present in a given quantity of the solution. One such common way to describe the composition of a solution in terms of the mass percentage is given below.

e.g.: using mass percentage

$$\text{Mass percent} = \frac{\text{mass of the solute}}{\text{mass of the solution}} \times 100\%$$

$$\text{Mass percent} = \frac{\text{mass of the solute}}{\text{mass of the solute + mass of the solvent}} \times 100\%$$

When the mass of the solute is very small compared to the mass of the solution (homogeneous mixture), the composition of the solute can be expressed as follows.

Equation			**Alternative expression of composition**
parts per thousand (ppt)	=	$\frac{\text{mass of the solute}}{\text{mass of the solution}} \times 10^3$	g kg^{-1} mg g^{-1}
parts per million (ppm)	=	$\frac{\text{mass of the solute}}{\text{mass of the solution}} \times 10^6$	mg kg^{-1} μg g^{-1}
parts per billion (ppb)	=	$\frac{\text{mass of the solute}}{\text{mass of the solution}} \times 10^9$	μg kg^{-1}

When volume of the solute is very small compared to the volume of the solution (homogeneous mixture), the composition of the solute can be expressed as follows.

Equation			**Alternative expression of composition**
parts per thousand (ppt)	=	$\frac{\text{volume of the solute}}{\text{volume of the mixture}} \times 10^3$	mL L^{-1}
parts per million (ppm)	=	$\frac{\text{volume of the solute}}{\text{volume of the mixture}} \times 10^6$	μL L^{-1}
parts per billion (ppb)	=	$\frac{\text{volume of the solute}}{\text{volume of the mixture}} \times 10^9$	nL L^{-1}

For dilute solutions composition can be expressed using weight/volume. It can be expressed in ppm and ppb. These can be given in alternative units of mg dm^{-3} and μg dm^{-3} respectively.

Metric prefixes are used to distinguish between units of different size and it is useful to describe quantities in a more scientific manner (see Table 3.6).

Table 3.6 Metric prefixes

Metric Prefix	Metric Symbol	Multiple	Metric Prefix	Metric Symbol	Multiple
tera-	T	10^{12}	deci-	d	10^{-1}
giga-	G	10^{9}	centi-	c	10^{-2}
mega-	M	10^{6}	milli-	m	10^{-3}
kilo-	k	10^{3}	micro-	μ	10^{-6}
hecto-	h	10^{2}	nano-	n	10^{-9}
deca-	da	10^{1}	pico-	p	10^{-12}

Example 3.4

Calculate the mole fraction and the mole percentage of a 20.0% hydrogen peroxide solution by mass.

Answer:

Mole fraction of H_2O_2 ($X_{H_2O_2}$) = $n_{H_2O_2}/n_{\text{total}} = \dfrac{(\text{moles of } H_2O_2)}{[(\text{moles of } H_2O_2 + (\text{moles of } H_2O)]}$

In the hydrogen peroxide solution, mass of H_2O_2 = 200.0 g, mass of H_2O = 800.0 g

moles of H_2O_2 = 200.0 g/ 34 g mol^{-1} = 5.88 mol

moles of H_2O = 800.0 g/ 18 g mol^{-1} = 44.44 mol

Mole fraction of H_2O_2 = 5.88 mol/ (5.88 + 44.44) mol = 0.116

Mole percentage of H_2O_2 = mole fraction ($X_{H_2O_2}$) × 100 = 11.6%

3.5.3 Molality *

The molality (m) of a solution is the amount of moles of the solute per kilogram of the solvent.

Equation			Unit
Molality	=	$\dfrac{\text{moles of the solute}}{\text{mass of the solvent}} = \dfrac{\text{mol}}{\text{kg}}$	mol kg^{-1}
Molality	=	$\dfrac{\text{milimoles of the solute}}{\text{mass of the solvent}} = \dfrac{\text{mmol}}{\text{kg}}$	mmol kg^{-1}

e.g.: Sucrose solution contains 1.25 mol of sucrose (solute) in every kilogram of water (solvent). Therefore the molality of the sucrose solution is 1.25 mol kg^{-1}.

**Not relevant to current G. C. E. (A/L) syllabus*

3.5.4 Molarity (Commonly used to express concentration)

The volume of a solution can be measured more conveniently than its mass. The concentration of a solution is defined as the number of moles of solute in a litre or one cubic decimetre volume of a solution. The SI unit of molarity (M) is mol m^{-3}. However more commonly used unit is mol dm^{-3} or mol L^{-1}.

e.g.: A 1.25 mol dm^{-3} or 1.25 M sucrose solution contains 1.25 moles of sucrose (solute) in 1 dm^3 of solution.

Equation			**Unit**
Molarity	=	$\frac{\text{moles of the solute}}{\text{volume of the solution}} = \frac{\text{mol}}{\text{dm}^3}$	mol dm^{-3}
Molarity	=	$\frac{\text{milimoles of the solute}}{\text{volume of the solution}} = \frac{\text{mmol}}{\text{dm}^3}$	mmol dm^{-3}

The amounts of water used to prepare 1.25 mol dm^{-3} and 1.25 mol kg^{-1}, sucrose solutions are not the same due to the density criteria. This means, for a given solution, the molarity and the molality are not the same, however the difference can be negligible for dilute solutions.

Examples 3.5

A solution of NaCl is prepared by mixing 10 mg of NaCl and 500 g of water. Calculate the molality and the composition (in ppm) of the solution.

Answer:

To calculate the molality of the solution,
Molality (m) = moles of the solute/ mass of the solvent
Amount of moles of NaCl = 0.01 g/ 58.5 g mol^{-1} = 1.71×10^{-4} mol
Molality (m) = moles of the solute/ mass of the solvent = 1.71×10^{-4} mol/ 0.5 kg
= 3.42×10^{-4} mol kg^{-1}

Composition of NaCl (ppm)
Composition = (mass of NaCl (in grams)/ mass of the solution (in grams)) $\times 10^6$
= (0.01 g/(500 + 0.01)g)$\times 10^6$ = 19.9 ppm

3.6 Balancing chemical reactions

The chemicals initially involved in a reaction are called reactants. Substances formed from a chemical reaction are called products. Chemical changes can yield one or more products. A chemical change such as carbon combining with oxygen to produce carbon dioxide is an example of a chemical reaction. This chemical reaction can be represented using the chemical equation given below.

$$\underset{\text{Reactants}}{C(s) + O_2(g)} \longrightarrow \underset{\text{Products}}{CO_2(g)}$$

During a chemical reaction, atoms are neither created nor destroyed. Hence, there is a mass balance between reactants and products. In other words the total number of atoms in the reaction molecules is equal to the total number of atoms in the product molecules. A chemical reaction which depicts the aforesaid material balance is known as a **balance chemical reaction**.

Any balanced chemical reaction must obey these rules.

Rules for balancing a chemical equation

(a) Number of atoms of the reactant side must be equal to the respective numbers of atoms of the product side.
(b) Formulae of reactants and products must never be changed to balance a given chemical equation.
(c) All parts of any balanced chemical equation can be divided or multiplied by any number to produce a new balanced equation.
(d) The best balanced (accepted) equation is the one that has the smallest whole number ratio between reactants and products. These integers are called **"coefficients"** of the balanced equation. These coefficient numbers are expressed as **stoichiometric numbers** in a balanced equation.

There are two methods of balancing chemical equations.

(a) Inspection method
(b) Redox method

3.6.1 Balancing a chemical reaction by inspection method

Step 1: Identify the reactants, products and their physical states. Write the appropriate formulae and the unbalanced chemical equation.

Step 2: Balance the equation by inspection, starting with the element/s which appears at the least number of places. Continue element by element to determine the coefficients to balance the atoms on both the reactants and products.

Step 3: Use coefficients to balance the atoms/ ions on both sides of the arrow. Also, check whether the coefficients used are the smallest integers that can be used to balance the equation.

Simple chemical equations can be balanced using the inspection method. Consider the examples given below.

Example 1:Reaction between sulfuric acid and sodium hydroxide to produce sodium sulphate and water.

Step 1: Reactants = sulfuric acid and sodium hydroxide
Products = sodium sulfate and water
Unbalanced chemical equation:

$H_2SO_4 + NaOH \longrightarrow Na_2SO_4 + H_2O$

Step 2: Balancing the chemical equation using sodium atoms on the product side. The total number of sodium atoms on the product side is two. Therefore the coefficient of the reaction with respect to sodium is 2.

Then the chemical equation is,

$H_2SO_4 + 2NaOH \longrightarrow Na_2SO_4 + H_2O$

Step 3: Balance the rest of the atoms/ ions on both sides of the arrow.

The balanced chemical equation:

$H_2SO_4 + 2NaOH \longrightarrow Na_2SO_4 + 2H_2O$

The balanced chemical equation with the physical states is given below.

$H_2SO_4(aq) + 2NaOH(aq) \longrightarrow Na_2SO_4(aq) + 2H_2O(l)$

Example 2: Reaction between nitrogen and hydrogen to produce ammonia.

Step 1: Reactants = nitrogen and hydrogen

Products = ammonia

Unbalanced chemical equation:

$N_2 + H_2 \longrightarrow NH_3$

Step 2: Balancing the chemical equation using nitrogen atoms on the reactant side. The total number of nitrogen atoms on the reactant side is two. Therefore the coefficient of the reaction with respect to nitrogen is 2.

Then the chemical equation is,

$N_2 + H_2 \longrightarrow 2NH_3$

Step 3: Using the coefficients balance the atoms/ions on both sides of the arrow.

The balanced chemical equation:

$N_2 + 3H_2 \longrightarrow 2NH_3$

The balanced chemical equation with the physical states is given below.

$N_2(g) + 3H_2(g) \longrightarrow 2NH_3(g)$

3.6.2 Balancing a chemical reaction by the redox method

Redox reactions are a type of chemical interactions that involve the change of oxidation number of atoms. The redox reactions are balanced using the following methods.

Method 01 - Oxidation number change method

This considers the change in oxidation number and uses them as coefficients of reactants.

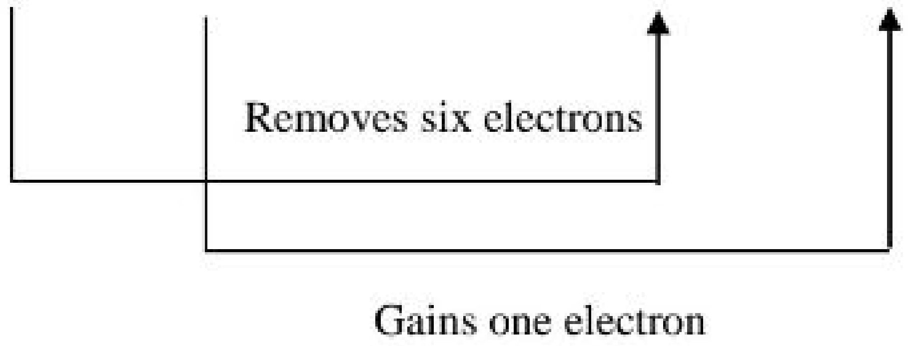
As an example, the reaction between S and HNO_3 is shown below. The following steps are applied to balance the equation.

Step 1: Correctly write the formulae for the reactants and the products of the chemical reaction.

$S(s) + HNO_3(aq) \longrightarrow H_2SO_4(aq) + NO_2(aq) + H_2O(aq)$

Step 2: Determine correctly the atoms that undergo oxidation and reduction and calculate the oxidation number change as shown below in the cited example.

$$\underset{0}{S(s)} + \underset{+5}{HNO_3(aq)} \longrightarrow \underset{+6}{H_2SO_4(aq)} + \underset{+4}{NO_2(aq)} + H_2O(aq)$$



Step 3: If the oxidation number change is not equal then multiply it to such a number, so that these numbers become equal as shown below. (The number of electrons exchange should be equal.)

$$S(s) + 6HNO_3(aq) \longrightarrow H_2SO_4(aq) + 6NO_2(aq) + H_2O(l)$$

Step 4: Balance the remaining atoms.

$$S(s) + 6HNO_3(aq) \longrightarrow H_2SO_4(aq) + 6NO_2(aq) + 2H_2O(l)$$

Method 02 - Half reaction method

In every oxidation-reduction reaction, one reactant is reduced and another reactant is oxidized. In some cases the same atom in the reactant is oxidized and reduced and such reactions are called disproportionation reactions. These two reactions (oxidation and reduction) are referred to as half reactions. The relevant steps to identify and balance the redox reaction using half reactions is given below.

Steps to balance redox reactions

Step A: Split the reaction into two half ionic reactions.
Step B: Balance both half ionic equations separately.
Step C: Combine the two half reactions to give a simplified balance equation and the final balanced chemical reaction.

example: Reaction of $K_2Cr_2O_7$ with SO_2 in the presence of $H_2SO_4(aq)$ giving Cr^{3+} ions and SO_4^{2-} ions as main products.

Step A: Split the reaction into two half reactions.

$$Cr_2O_7^{2-} + SO_2 \longrightarrow Cr^{3+} + SO_4^{2-}$$

Two half reactions are:

$$Cr_2O_7^{2-} \longrightarrow Cr^{3+}$$
$$SO_2 \longrightarrow SO_4^{2-}$$

Step B: Balance both half equations separately.

Methodology for step B.

Step 1: Assign oxidation numbers to each element on both sides of the reaction.
Step 2: Balance the atoms of each element being oxidized or reduced.
Step 3: Multiply the oxidation number by the number of atoms to obtain the "total" oxidation number on both sides.
Step 4: Balance the difference of oxidation number of half reaction by adding electrons to the other side.
Step 5: Balance the charge by adding H^+ ions in acidic solutions and OH^- ions in basic solutions.
Step 6: Balance the hydrogen/oxygen by adding H_2O molecules.
Step 7: Check the atoms on both sides.

Balance each half reaction using the methodology given in Step B as follows.
Reduction of $Cr_2O_7^{2-}$ to Cr^{3+} ions in acidic medium

Step 1: Assign oxidation number of chromium.

$$\underset{(+6)}{Cr_2O_7^{2-}(aq)} \longrightarrow \underset{(+3)}{Cr^{3+}(aq)}$$

Step 2: Balance the chromium atoms of both sides.

$$Cr_2O_7^{2-}(aq) \longrightarrow 2Cr^{3+}(aq)$$

Step 3: Multiply the oxidation number by the number of atoms to get the total oxidation number on both sides.

$$\underset{(+6) \times 2}{Cr_2O_7^{2-}(aq)} \longrightarrow \underset{(+3) \times 2}{2Cr^{3+}(aq)}$$

The difference of oxidation number is six.

(+12 to +6)

Step 4: Add electrons to balance the difference of oxidation number.

$$6e + Cr_2O_7^{2-}(aq) \longrightarrow 2Cr^{3+}(aq)$$

Calculate the total charge of both sides.

$$\underbrace{6e + Cr_2O_7^{2-}(aq)}_{\text{total charge is minus eight}} \longrightarrow \underbrace{2Cr^{3+}(aq)}_{\text{total charge is plus six}}$$

Step 5: Then add H^+ ions to balance the charge.

$$14H^+(aq) + 6e + Cr_2O_7^{2-}(aq) \longrightarrow 2Cr^{3+}(aq)$$

Step 6: Balance the hydrogen by adding H_2O molecules.

$$14H^+(aq) + 6e + Cr_2O_7^{2-}(aq) \longrightarrow 2Cr^{3+}(aq) + 7H_2O(aq)$$

Step 7: Check the atoms on both sides for balance.

$$14H^+(aq) + 6e + Cr_2O_7^{2-}(aq) \longrightarrow 2Cr^{3+}(aq) + 7H_2O(aq)$$

Oxidation of SO_2 to SO_4^{2-} ions in acidic medium

Steps 1, 2 and 3:

$$\underbrace{\underset{(+4)}{SO_2(g)} \longrightarrow \underset{(+6)}{SO_4^{2-}(aq)}}_{\text{The difference of oxidation number is two.}}$$

Step 4: Add electrons to balance the difference of oxidation number

$$SO_2(g) \longrightarrow SO_4^{2-}(aq) + 2e$$

Step 5: Calculate the total charge of both sides.

$$\underbrace{SO_2(g)}_{\text{total charge is zero}} \longrightarrow \underbrace{SO_4^{2-}(aq)}_{\text{total charge is minus four}} + 2e$$

Then add H^+ ions to balance the charge.

$$SO_2(g) \longrightarrow SO_4^{2-}(aq) + 2e + 4H^+(aq)$$

Steps 6 and 7: Add H_2O molecules to balance hydrogen.

$$2H_2O(aq) + SO_2(g) \longrightarrow SO_4^{2-}(aq) + 2e + 4H^+(aq)$$

Step C: Combine the two half reactions to give a simplified balanced equation and the final balanced chemical reaction.

Multiply the oxidation half equation by 3 to equalise the electrons on both sides. The combined equation is,

$$14H^+(aq) + Cr_2O_7^{2-}(aq) + 3SO_2(g) + 6H_2O(aq) + 6e \longrightarrow 2Cr^{3+}(aq) + 3SO_4^{2-}(aq) + 12H^+(aq) + 7H_2O(aq) + 6e$$

Simplified equation (balanced ionic equation) is,

$$2H^+(aq) + Cr_2O_7^{2-}(aq) + 3SO_2(g) \longrightarrow 2Cr^{3+}(aq) + 3SO_4^{2-}(aq) + H_2O(aq)$$

and the balanced chemical equation is,

$$H_2SO_4(aq) + K_2Cr_2O_7(aq) + 3SO_2(g) \longrightarrow Cr_2(SO_4)_3(aq) + K_2SO_4(aq) + H_2O(aq)$$

The information that can be obtained from balanced reactions

- The number of moles that react with each other in a reaction.
- The number of moles of products that are formed.
- The number of electrons that are involved in the redox reaction.

Thus in the reaction of $K_2Cr_2O_7$ with SO_2 in the presence of H_2SO_4(aq) discussed above,

1. $K_2Cr_2O_7$ is an ionic compound. One ion of $Cr_2O_7^{2-}$ reacts with three molecules of SO_2.
2. One mole of $K_2Cr_2O_7$ reacts with three moles of SO_2 to produce one mole of $Cr_2(SO_4)_3$, one mole of K_2SO_4 and one mole of H_2O.

Two other examples to illustrate the applications of balancing equations using the half reaction method are given below.

Example 3.6

Balance the redox ionic equation for the reaction between Fe^{2+}(aq) and NO_3^-(aq) in basic medium.

$Fe^{2+}(aq) + NO_3^-(aq) \longrightarrow Fe^{3+}(aq) + NO(g)$

Answer:

Balance half reactions:

Oxidation half reaction: $Fe^{2+}(aq) \longrightarrow Fe^{3+}(aq) + e$ ------ (1)

Reduction half reaction: $NO_3^-(aq) + 2H_2O(l) + 3e \longrightarrow NO(g) + 4OH^-(aq)$ ----- (2)

Multiply the oxidation half equation (1) by 3.

$3[Fe^{2+}(aq) \longrightarrow Fe^{3+}(aq) + e]$

$3Fe^{2+}(aq) \longrightarrow 3Fe^{3+}(aq) + 3e$ ----- (3)

Combine half equations (3) and (2).

$3Fe^{2+}(aq) + NO_3^-(aq) + 2H_2O(l)\ ) +3e \longrightarrow 3Fe^{3+}(aq) + NO(g) + 4OH^-(aq) + 3e$

Eliminate electrons.

$3Fe^{2+}(aq) + NO_3^-(aq) + 2H_2O(l) \longrightarrow 3Fe^{3+}(aq) + NO(g) + 4OH^-(aq)$

Example 3.7

Balance the redox ionic equation for the reaction between MnO_4^- and Fe under basic medium.

$MnO_4^- + Fe \longrightarrow MnO_2 + Fe^{2+}$

Answer:

Balance half reactions:

Oxidation half reaction: $Fe \longrightarrow Fe^{2+} + 2e$ ------ (1)

Reduction half reaction: $2H_2O + 3e + MnO_4^- \longrightarrow MnO_2 + 4OH^-$----- (2)

Multiply the oxidation half equation (1) by 3 and reduction half equation (2) by 2 and eliminate electrons while combining the two half equations.

$3Fe + 2MnO_4^- + 4H_2O \longrightarrow 3Fe^{2+} + 2MnO_2 + 8OH^-$

Limiting reagent/ reactant

In a reaction mixture, the reactant that is completely consumed is called the limiting reactant. Other reactants are called excess reactants. The following example shows the use of limiting reagent concept to calculate the amount of product produced by a given reaction.

Example: How many moles of NH_3 can be produced from 3 mol of N_2 and 6 mol of H_2?

Balanced chemical equation;

$$N_2(g) + 3H_2(g) \longrightarrow 2NH_3(g)$$

The number of moles of H_2 required to complete consumption of 3 moles of N_2
= number of moles of $N_2 \times 3 = 9$ mol
The required amount of moles is greater than the available amount of moles of H_2.
Therefore the limiting reagent is H_2.

The amount of N_2 moles required for complete consumption of 6 moles of H_2.
= amount of H_2 moles $\times 1/3 = 2$ mol
The required number of moles of N_2 is less than the available number of moles of N_2.
Therefore the excess reagent is N_2.
Based on the amount of limiting reagent (H_2), the amount of product (NH_3) formed
= amount of H_2 moles $\times 2/3 = 6$ mol $\times 2/3 = 4$ moles of NH_3

3.6.3 Balancing simple nuclear reactions

Radioactive nuclide can undergo radioactive decay by ejecting nuclear particles/electrons or producing energy in the form of gamma (γ) radiation. General characteristics of such emissions are given in Table 3.7.

Table 3.7 Characteristics of α, β and γ emissions

Name	Symbol	Charge	Mass
Alpha	${}^{4}_{2}He^{2+}$, ${}^{4}_{2}\alpha$	+2	Equal to the mass of a helium atom
Beta	${}^{0}_{-1}e$, ${}^{0}_{-1}\beta$	-1	Equal to the mass of an electron
Gamma	${}^{0}_{0}\gamma$, γ	0	No mass

The spontaneous change of a radioactive isotope of one element into an isotope of a different or same element is known as **radioactivity**. Such changes are called nuclear reactions or transmutations.

For example, radioactive decay of ${}^{226}_{88}Ra$ to ${}^{222}_{86}Rn$ can be written as follows.

$$\underset{\text{Parent nucleus}}{{}^{226}_{88}Ra} \longrightarrow \underset{\text{Daughter nucleus}}{{}^{222}_{86}Rn} + {}^{4}_{2}He$$

Rules for balancing nuclear reactions

Rule 01 The sum of the mass numbers of reacting nuclei must be equal to the sum of the mass numbers of the nuclei produced.

Rule 02 The sum of the atomic numbers of reacting nuclei must be equal to the sum of the atomic numbers of the nuclei produced.

Application of these rules are illustrated in the two examples given below.

Example 1:

	$^{226}_{88}Ra$	$\longrightarrow$	$^{4}_{2}He$	+	$^{222}_{86}Rn$
	Parent nucleus (Radium 226)		Alpha particle		Daughter nucleus (Radon 222)
Mass number :	226	$\longrightarrow$	4	+	222
Atomic number:	88	$\longrightarrow$	2	+	86

Example 2:

	$^{7}_{4}Be$	+	$^{0}_{-1}e$	$\longrightarrow$	$^{7}_{3}Li$
	Parent nucleus (Beryllium 7)		Beta particle		Daughter nucleus (Lithium 7)
Mass number :	7	+	0	$\longrightarrow$	7
Atomic number:	4	+	-1	$\longrightarrow$	3

In some nuclear reactions protons ($^{1}_{1}p$) and neutrons ($^{1}_{0}n$) are also involved.

3.7 Preparation of solutions

When a solute is dissolved in a solvent to form a homogeneous mixture it is known as a solution.

The solutions prepared with exactly known concentrations are called **standard solutions**. These standard solutions are standardized against primary standards. If a standard solution is prepared by using extremely pure, stable, not hydrated and highly water soluble compounds with higher molecular weights are considered as primary standards. Few examples for such compounds are anhydrous Na_2CO_3, $K_2Cr_2O_7$, and KIO_3.

A secondary standard is a chemical that has been standardized against a primary standard for use in specific analysis.

Solutions with known concentration can be prepared using the following methods and the exemplary procedures are given below.

Methods:

1. Dissolving a carefully measured mass or volume of a pure compound in a suitable solvent
2. Diluting a stock (concentrated) solution

Different ways of preparing solutions using the two methods indicated above are given below.

1. Preparation of 500.00 cm^3 of 1.0 mol dm^{-3} Na_2CO_3 solution

a. Calculate the required number of moles and then the required mass of Na_2CO_3.
b. Accurately weigh the required amount of Na_2CO_3 using a balance.
c. Place the Na_2CO_3 weighed in a 500.00 cm^3 volumetric flask and dissolve well with distilled water (The solute should be dissolved completely by using a minimum amount of water).
d. Dilute the solution up to 500.00 cm^3 mark, using distilled water and mix well to make a homogeneous solution.

2. Preparation of 250.00 cm^3 of 1.0 mol dm^{-3} HCl solution from conc. HCl solution (36% (w/w) with a density of 1.17 g ml^{-1} (1.17 g cm^{-3})

a. First calculate the concentration of the conc. HCl as follows.

Mass of HCl in 1 dm^3 of conc. HCl acid $= 1.17\ g\ cm^{-3} \times 1000\ cm^3 \times 36\%$

$= 421.2\ g$

Number of HCl moles in 1 dm^3 of conc. HCl $= 421.2\ g \div 36.5\ g\ mol^{-1}$

Concentration of the conc. HCl acid solution $= 11.5\ mol\ dm^{-3}$

b. Calculate the number of moles require to prepare the desired solution.

Amount of HCl moles in 250.00 cm^3 of 1.0 mol dm^{-3} HCl solution

$= (1.0\ mol \times 250\ cm^3) \div 1000\ cm^3$

$= 0.25\ mol$

The required volume of the concentrated HCl solution is v cm^3 (mL).

The calculation of volume v:

$0.25\ mol = (11.5\ mol \times v) \div 1000\ cm^3$

$v = 21.7\ cm^3$

c. Preparation of the solution

Accurately measured volume of 21.7 cm^3 of concentrated HCl is diluted up to the mark of the volumetric flask to prepare the solution of 250.00 cm^3 of 1.0 mol dm^{-3} HCl.

3. **Preparation of 100.00 cm^3 of 0.2 mol dm^{-3} Na_2CO_3 solution using 1.0 mol dm^{-3} Na_2CO_3 as the stock solution**
    a. Calculate the number of moles in 100.00 cm^3 of 0.2 mol dm^{-3} Na_2CO_3 solution.
    b. Calculate the volume of 1.0 mol dm^{-3} Na_2CO_3 needed to prepare 100.00 cm^3 of 0.2 mol dm^{-3} Na_2CO_3 solution.
    c. Accurately measure the calculated volume from 1.0 mol dm^{-3} Na_2CO_3 solution and place the solution in a 100.00 cm^3 volumetric flask.
    d. Dilute the solution up to 100.00 cm^3 mark using distilled water.

4. **Preparation of 250.00 cm^3 of 1 mol dm^{-3} HCl solution from 6 mol dm^{-3} stock solution of HCl.**

Assume the volume required from 6 mol dm^{-3} HCl solution is v cm^3.

The calculation for volume v is:

$0.25 \text{ mol} = 6 \text{ mol} \times v/1000 \text{ cm}^3$

$v = 41.6 \text{ cm}^3$

Then accurately measure the volume of 41.60 cm^3 of the 6 mol dm^{-3} HCl solution and add into a 250.00 cm^3 volumetric flask. Dialute up to the mark with distilled water to prepare the required solution.

5. **Preparation of 250.00 cm^3 of 1 mol dm^{-3} HCl solution by mixing of two stock solutions (example: 3 mol dm^{-3} and 0.5 mol dm^{-3} HCl solutions)**

Assume the volume required from the 3 mol dm^{-3} HCl be v cm^3.
Therefore the volume required from the 0.5 mol dm^{-3} HCl be (250.00 - v) cm^3.
Then the required number of moles of HCl in the solution to be prepared is 0.25 mol.

The calculation for volume v is:

$(v \times 3 \text{ mol dm}^{-3}/1000) + ((250.00 - v) \times 0.5 \text{ mol dm}^{-3}/1000) = 0.25 \text{ mol}$

$v = 50.00 \text{ cm}^3$

The volume required from 3 mol dm^{-3} HCl = 50.00 cm^3
The volume required from 0.5 mol dm^{-3} HCl = (250.00 - 50.00) cm^3

Mix 50.00 cm^3 of 3 mol dm^{-3} HCl and 200.00 cm^3 of 0.5 mol dm^{-3} HCl to prepare the solution of 250.00 cm^3 of 1 mol dm^{-3} HCl.

3.8 Calculations based on chemical reactions

Chemical reactions can be used to determine the concentration of an aqueous solution with an unknown amount of a substance using a solution with a known concentration. The solution with the known concentration (standard solution) reacts with the solution of an unknown concentration at a known stoichiometry. At the point in which the solution with an unknown amount of substance completely reacts with the standard, the concentration of the unknown solution can be calculated using concentration of the standard solution and the stoichiometry of the reaction.

example 1: Acid-base reaction

Calculate the concentration of $Ba(OH)_2$ solution which is reacted with a standard solution of 0.1 mol dm^{-3} HNO_3. A volume required from 0.1 mol dm^{-3} HNO_3 to react completely with 25.00 cm^3 of $Ba(OH)_2$ is 34.00 cm^3.

The balanced chemical equation for the reaction between nitric acid and barium hydroxide is,

$$2HNO_3(aq) + Ba(OH)_2(aq) \longrightarrow Ba(NO_3)_2(aq) + 2H_2O(l)$$

Based on the balanced equation, two moles of HNO_3 react with one mole of $Ba(OH)_2$. Hence, the stoichiometry between HNO_3: $Ba(OH)_2$ is 2:1.

The calculation of the number of moles of HNO_3 consumed :

Amount of HNO_3 consumed = $0.1 \text{ mol} \times \frac{34.00 \text{ cm}^3}{1000 \text{ cm}^3} = 0.0034 \text{ mol}$

Amount of HNO_3 consumed = Amount of $Ba(OH)_2$ in 25.00 cm^3 × 2

0.0034 mol = Concentration of $(Ba(OH)_2 \times 0.025 \text{ dm}^3 \times 2$

Concentration of $Ba(OH)_2$ = 0.068 mol dm^{-3}

example 2: Redox reaction

Calculate the volume of 0.6 mol dm^{-3} $KMnO_4$ required to react completely with 27.00 cm^3 of 0.25 mol dm^{-3} $Fe(NO_3)_2$.

The balanced chemical reaction between MnO_4^- and Fe^{2+} is,

$$MnO_4^-(aq) + 5Fe^{2+}(aq) + 8H^+(aq) \longrightarrow 5Fe^{3+}(aq) + Mn^{2+}(aq) + 4H_2O(l)$$

The stoichiometry between MnO_4^-: $Fe^{2+}$is 1:5.

Amount of Fe^{2+} consumed = $0.25 \text{ mol} \times 27.00 \text{ cm}^3/1000 \text{ cm}^3$

= 6.75×10^{-3} mol

The amount of MnO_4^- required = $6.75 \times 10^{-3} \text{ mol} \div 5$

The volume of $KMnO_4$ solution required is v cm^3.

The calculation of volume v:

$$6.75 \times 10^{-3} \text{ mol} \div 5 = 0.6 \text{ mol dm}^{-3} \times v$$
$$v = 0.00225 \text{ dm}^3 = 2.25 \text{ cm}^3$$

example 3: Gravimetry

Calculate the mass of $BaSO_4$ that gets precipitated when a solution of 0.1 mol dm^{-3} $Ba(OH)_2$ completely reacts with 30.00 cm^3 of 0.2 mol dm^{-3} H_2SO_4 acid

The balanced chemical equation is,

$$H_2SO_4(aq) + Ba(OH)_2(aq) \longrightarrow BaSO_4(s) + 2H_2O(l)$$

Based on the balanced equation,

Calculation of the mass of $BaSO_4(s)$ formed

Amount of H_2SO_4 consumed = $0.2 \text{ mol dm}^{-3} \times \frac{30.00 \text{ cm}^3}{1000 \text{ cm}^3} = 0.006 \text{ mol}$

Amount of $BaSO_4$ precipitated = 0.006 mol

Molar mass of $BaSO_4$ = 233 g mol^{-1}

Mass of $BaSO_4$ precipitated = $0.006 \text{ mol} \times 233 \text{ g mol}^{-1}$

= 1.4 g

Solved Problems

Question 1:

A soil sample contains hematite (iron(III) oxide) as the main compound.

(a) Calculate the mass percentages of iron and oxygen in iron(III) oxide?

(b) Calculate the number of grams of iron that can be extracted from one kilogram of Fe_2O_3?

(c) How many kilograms of hematite ore, whch contains 66.4% Fe_2O_3, should be processed to produce one kilogram of iron?

Answer:

(a) Mass % of Fe

$$\frac{\text{mass of two moles of Fe}}{\text{mass of one mole of } Fe_2O_3} \times 100 = \frac{112\text{ g}}{160\text{ g}} \times 100 = 70\%$$

Mass % of O

Mass % O = 100% - mass % Fe = 100% - 70 % = 30 %

(b) The mass of Fe extracted from one kilogram of Fe_2O_3

Mass of Fe_2O_3 $= 1.0 \times 10^3\text{g}$

Percentage of Fe in Fe_2O_3 = 70%

Mass of Fe $= 1.0 \times 10^3\text{g} \times \frac{70\text{ g}}{100\text{ g}}$

$= 700\text{ g}$

(c) Mass of hematite needed

Mass of Fe_2O_3 $= 1\text{ kg} \times \frac{100\text{ g}}{66.4\text{ g}}$

Mass of hematite ore processed $= 1\text{kg} \times \frac{100\text{ g}}{66.4\text{ g}} \times \frac{100\text{ g}}{70\text{ g}}$

$= 2.151\text{ kg}$

Question 2

A student prepares a solution by mixing 4.0 mg of sodium ions (in the form of NaCl), 4.00 g of glucose ($C_6H_{12}O_6$), and 96 g of water.

(a) What is the molality of the glucose in solution?

(b) How many ppm of Na^+ does this solution contain?

Answer:

(a) molality $= \frac{\text{moles of solute}}{\text{mass of solvent (kg)}}$

moles of glucose $= \frac{4.0\text{ g}}{180\text{ g mol}^{-1}} = 0.022\text{ mol}$

mass of solvent (water) in kg = 0.096 kg

molality $= \frac{0.022 \text{ mol}}{0.096 \text{ kg}} = 0.23 \text{ mol kg}^{-1}$

(b) Mass of the solution = 0.004 g + 4.00 g + 96 g = 100.004 g

$$\text{ppm of Na}^+ = \frac{\text{mass of Na}^+}{\text{mass of the solution}} \times 10^6$$

$$= \frac{0.004 \text{ g}}{100.004 \text{ g}} \times 10^6 = 39.99 \text{ ppm}$$

Question 3

A mixture of NaCl and KCl weighed 5.48 g. The sample was dissolved in water and treated with excess of silver nitrate ($AgNO_3$). The resulting AgCl weighed 12.70 g. Calculate the mass percentage of NaCl in the mixture?

$$AgNO_3(aq) + Cl^-(aq) \longrightarrow AgCl(s) + NO_3^-(aq)$$

Answer:

$$\text{Moles of AgNO}_3 = \frac{12.70 \text{ g}}{143.32 \text{ g mol}^{-1}} = 0.088 \text{ mol}$$

Number of moles of NaCl + Number of moles of KCl = 0.088 mol

$$0.088 \text{ mol} = \frac{\text{mass of NaCl}}{58.44 \text{ g mol}^{-1}} + \frac{\text{mass of KCl}}{75.55 \text{ g mol}^{-1}}$$

Also, mass of NaCl + mass of KCl = 5.48 g

Assuming the mass of NaCl is x.

The mass of KCl = $(5.48 \text{ g} - x)$

Calculation of x using the total number of moles of Cl^- ions:

$$0.088 \text{ mol} = \frac{x}{58.44 \text{ g mol}^{-1}} + \frac{(5.48 \text{ g} - x)}{75.55 \text{ g mol}^{-1}}$$

Mass of NaCl = x = 4.06 g

Mass percentage of NaCl $= \frac{4.06 \text{ g}}{5.48 \text{ g}} \times 100 = 74.01\%$

Table 3.8 A summary of equations

Equation	Units
$\textbf{Mass fraction of A (w/w)} = \dfrac{\text{mass of A}}{\text{mass of substance or mixture}}$	-
$\textbf{Volume fraction of A (v/v)} = \dfrac{\text{volume of A}}{\text{volume of mixture}}$	-
$\textbf{Mole fraction of A } (x\text{A}) = \dfrac{\text{moles of A}}{\text{total moles of mixture}}$	-
$\text{Mass \% of element } x = \dfrac{\text{moles of } \boldsymbol{x} \text{ in formula} \times \text{molar mass of } \boldsymbol{x}\ (\text{g mol}^{-1})}{\text{molar mass of compound}} \times \mathbf{100}$	-
$\textbf{Mass Percent (w/w)} = \dfrac{\text{mass of the substance}}{\text{mass of the mixture}} \times \mathbf{100\%}$	-
$\textbf{Volume Percent (v/v)} = \dfrac{\text{volume of substance}}{\text{volume of mixture}} \times \mathbf{100\%}$	-
$\textbf{Parts per thousand (ppt)} = \dfrac{\text{mass of substance}}{\text{mass of mixture}} \times \mathbf{10^3}$	-
$\textbf{Parts per million (ppm)} \dfrac{\text{mass of substance}}{\text{mass of mixture}} \times \mathbf{10^6}$	-
$\textbf{Parts per billion (ppb)} = \dfrac{\text{mass of substance}}{\text{mass of mixture}} \times \mathbf{10^9}$	-
$\textbf{Molality (m)} = \dfrac{\text{moles of solute}}{\text{mass of solvent}}$	mol kg^{-1}
$\textbf{Molarity (M)} = \dfrac{\text{moles of solute}}{\text{volume of solution}}$	mol dm^{-3}
$\textbf{Mole fraction of A } (\mathbf{x_A}) = \dfrac{n_A}{n_A+n_B+n_C+\ldots}$	-