CHEM 2101

Chapter - 3

Lecture Notes

Stoichiometry

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Chapter-3

Stoichiometry

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IMPORTANT TERMS

Formula weight (FW)

It is the sum of the atomic weights of all atoms in a formula unit of the compound.

Avagadro number (N_A)

It is the number of atoms in a 12g sample of carbon-12. One mole of a substance contains Avogadro's number of particles. (It may be atoms, molecules, ions, electrons etc.). This value is equal to 6.023×10^{23}.

Mole

The amount of substance, that contains Avogadro number of particles.

Mole concept

Mole concept is defined as the amount of the substance that contains as many specified elementary particles as the number of atoms in 12 g of carbon-12 isotope. One mole of a substance consists of Avagadro number (6.023×10^{23}) of particles.

Molar mass

The mass of one molecular of the substance.

or

Molar mass is the mass of one mole of the substance.

$$\text{Molar mass} = \frac{Mass}{Mole}$$

Example: Carbon has a molar mass of exactly 12g/mol.

Empirical formula

It is a simplest formula of a compound which gives the ratio of all atoms present in it.

Molecular formula

It gives the exact number of atoms of all the elements present in a compound.

Stoichiometry

Stoichiometry is the calculation of quantities of reactants and products involved in the chemical reaction and it is the study of the relationship between the number of mole of the reactant and products in a reaction.

Stoichiometric equation

Stoichiometric equation is a short scientific representation of a chemical reaction.

Law of conservation of mass

In any chemical change, the total mass of the products formed is always equal to the total mass of the reactants.

Law of constant compositions

In any compound, the elements present in it are in definite fixed ratio by weight, whatever be its method of formation.

Law of multiple proportions

When an element A combines with another element B, to form more than one compound, the different weights of one of these elements which combine with the fixed weight of the other, will bear a simple integral ratio.

Law of reciprocal proportions

When two elements combine separately with a fixed mass of a third element, than the ratios of their masses in which they do so is either same (or) same whole number multiple of the ratio in which they combine with each other.

Balanced chemical equation

When in a chemical equation in which the numbers and kinds of atoms present on the reactant and product sides are equal, then the equation is referred to as balanced chemical equation.

Stoichiometry

Stichiometry is the branch of chemistry and chemical engineering that deals with the quantities of substances that enter into, and are produced by, chemical reactions.

Stoichiometry provides the quantitative relationship between reactants and products in a chemical reaction.

For example, when methane unites with oxygen in complete combustion, 16g of methane require 64g of oxygen. At the same time 44g of carbon dioxide and 36g of water are formed as reaction productions.

Every chemical reaction has its characteristic proportions. The method of obtaining these from chemical formulas, equations, atomic weights and molecular weights, and determination of what and how much is used and produced in chemical processes, is the major concern of Stoichiometry

3.1 Atomic Mass

The units in which the mass of an atom is expressed are atomic mass units. At one time, the lightest atom was assigned a mass of 1 amu and the mass of any other atom was expressed in terms of this standard. Today atomic mass units are defined in terms of the ^{12}C isotope, which is assigned a mass of exactly 12.000... amu.

Atomic mass and related units

1. **One *atomic mass unit* (amu) is 1/12 the mass of one atom of $^{12}_{6}C$.**

2. **6.022 x 10^{23} atomic mass units (amu) = 1.000 g.**

3. **The masses of all other isotopes are derived by comparison to $^{12}_{6}C$, one atom of which weighs 12 amu .**

4. **An *atomic mass* (average atomic mass or atomic weight) found on the periodic chart is the weighted average mass of all the isotopes of an element. The weighing is based on the percent distribution of isotopes on earth.**

5. **A *molecular mass* (molecular weight) is the sum of all the atomic masses of all the atoms in a molecule. For example the molecular weight of water is 2(1.00794 amu) + 15.9994 amu = 18.0153 amu/molecule.**

6. **A *formula mass* (formula weight) is the sum of all the atomic weight of all the atoms in a formula. The formula weight and molecular weight of water are one in the same thing. Since ionic substances such as salts do not consist of molecules, it is best to refer to their formula weights not molecular weights. The formula weight of $CaCl_2$ is (40.08 amu) + 2(35.45 amu) = 110.98 amu/formula unit.**

7. **One mol = 6.022 x 10^{23} just as 1 dozen = 12.**

8. **An *isotopic mass* is the mass of one atom of a specific isotope in atomic mass units. For example, the isotopic mass of $^{1}_{1}H$ = 1.0078 amu and that of $^{2}_{1}H$ = 2.0150 amu. Note: The atomic mass is the weighted average of naturally occurring isotopic masses. The weighting is done according to the (%) natural abundance on earth.**

Example 1

The Element magnesium (Mg) has three stable isotopes with the following masses and abundances:

Isotope	Mass (amu)	Abundance
^{24}Mg	23.9850	78.99%
^{25}Mg	24.9858	10.00%
^{26}Mg	25.9826	11.01%

Calculate the avearage atomic mass (atomic weight) of magnesium from these data.

Solution

A = atomic mass = 0.7899 (23.9850 amu) + 0.1000 (24.9858 amu) + 0.1101 (25.9826 amu)

A = 18.95 amu + 2.499 amu + 2.861 amu = 24.31 amu

Atomic Weight

The atomic weight of an element is the weighted average of the atomic masses of the different isotopes of an element.

Naturally occurring carbon, for example, is a mixture of two isotopes, ^{12}C (98.89%) and ^{13}C (1.11 %).

Individual carbon atoms therefore have a mass of either 12.000 or 13.03354 amu. But the average mass of the different isotopes of carbon is 12.011 amu.

$$\frac{98.89}{100} \times 12.000 \text{ amu} + \frac{1.11}{100} \times 13.003354 \text{ amu} = 12.011 \text{amu}$$

Molecular Weight

The molecular weight of a compound is the sum of the atomic weights of the atoms in the molecules that form these compounds.

Example:

The molecular weight of the sugar molecule found in cane sugar is the sum of the atomic weights of the 12 carbon atoms, 22 hydrogen atoms, and 11 oxygen atoms in a $C_{12}H_{22}O_{11}$ molecule.

$$\begin{aligned} 12 \text{ C atoms} &= 12(12.011) \text{ amu} &&= 144.132 \text{ amu} \\ 22 \text{ H atoms} &= 22(1.0079) \text{ amu} &&= 22.174 \text{ amu} \\ 11 \text{ O atoms} &= 11(15.9994) \text{ amu} &&= \underline{175.993 \text{ amu}} \\ & && 342.299 \text{ amu} \end{aligned}$$

$C_{12}H_{22}O_{11}$ has a molecular weight of 342.299 amu. A mole of $C_{12}H_{22}O_{11}$ would have a mass of 342.299 grams. This quantity is known as the molar mass, a term that is often used in place of the terms atomic weight or molecular weight.

Avogadro Number or Avogadro's Constant

Avogadro's number (or Avogadro's constant) is the number of elementary particles in a mole of any substance.

For most calculations, four significant figures for Avogadro's constant are enough: 6.022×10^{23}.

A mole of any substance contains Avogadro's number of elementary particles.

It doesn't matter whether we talk about a mole of atoms, a mole of molecules, a mole of electrons, or a mole of ions.

By definition, a mole always contains 6.022×10^{23} elementary particles.

3.2 Mole concept (Define moles)

The mole may be defined as the amount of substance that contains as the number of atoms in 12g of carbon – 12 isotope.

One mole of an atom or a molecule contains Avogadro number of particles (i.e. 6.022×10^{23})

One mole	=	**6.022×10^{23} particles.**
1 mole C	=	**6.022×10^{23} C atoms.**
1 mole H_2O	=	**6.022×10^{23} H_2O molecules.**
1 mole NaCl	=	**6.022×10^{23} Na^+ ions and 6.022×10^{23} Cl^- ions.**
One mole of oxygen molecule	=	**6.022×10^{23} oxygen molecule.**
One mole of oxygen atom	=	**6.022×10^{23} oxygen atoms**
One mole of ethanol	=	**6.022×10^{23} ethanol molecules**

More Examples of Moles

Moles of Element

1 mole Mg	=	**6.022×10^{23} Mg atoms**
1 mole Au	=	**6.022×10^{23} Au atoms**

Moles of Compounds

1 mole NH_3	=	**6.022×10^{23} NH_3 molecules**
1 mole $C_9H_8O_4$	=	**6.022×10^{23} Aspirin molecules.**

In using the term mole for ionic substances, we mean the number of formula units of the substance. For example, a mole of sodium carbonate, Na_2CO_3 is a quantity containing 6.023×10^{23} Na_2CO_3 units.

But each formula unit of Na_2CO_3 contains $2 \times 6.022 \times 10^{23}$ Na^+ ions and $1 \times 6.022 \times 10^{23}$ CO_3^{2-} ions.

When using the term mole, it is important to specify the formula of the unit to avoid any misunderstanding.

Example 1:

A mole of oxygen atom (with the formula O) contains 6.022×10^{23} Oxygen atoms.

A mole of oxygen molecule (formula O_2) contains 6.022×10^{23} O_2 molecules.

(i.e) $2 \times 6.022 \times 10^{23}$ oxygen atoms.

Example 2:

Consider the following reaction.

$$2H_2 + O_2 \rightarrow 2H_2O$$

In this reaction one molecule of oxygen reacts with two molecules of Hydrogen. So it would be desirable to take the molecules of H_2 and O_2 in the ratio 2 : 1, so that the reactants are completely consumed during the reaction. But atoms and molecules are so small in size that is not possible to count them individually.

In order to overcome these difficulties, the concept of mole was introduced. According to this concept number of particles of the substance is related to the mass of the substance.

Examples 3

Solved Problems

1. Calculate the mass of 500. atoms of iron (Fe).

$$500.\ \cancel{\text{atoms Fe}} \times \frac{1\ \cancel{\text{mol Fe}}}{6.022 \times 10^{23}\ \cancel{\text{atoms Fe}}} \times \frac{55.85\ \text{g Fe}}{1\ \cancel{\text{mol Fe}}} = 4.64 \times 10^{-20}\ \text{g Fe}$$

2. How many Fe atoms and how many moles of Fe atoms are in 500.0g of iron?

$$500.\ \cancel{\text{g Fe}} \times \frac{1\ \text{mol Fe}}{55.85\ \cancel{\text{g Fe}}} = 8.953\ \text{mol Fe}$$

$$8.953\ \cancel{\text{mol Fe}} \times \frac{6.022 \times 10^{23}\ \text{atoms Fe}}{1\ \cancel{\text{mol Fe}}} = 5.391 \times 10^{24}\ \text{atoms Fe}$$

3.3 Molar Mass

The molar mass (molecular weight) of a substance is the mass of one mole of the substance. The mass and moles can be related by means of the formula.

$$\text{Molar mass} = \frac{\text{Mass}}{\text{Mole}}$$

- **Number of grams in 1 mole**
- **Equal to the numerical value of the atomic mass**

1 mole of C atoms	=	**12.0 g**
1 mole of Mg atoms	=	**24.3 g**
1 mole of Cu atoms	=	**63.5 g**

Molar Mass of Compounds

Mass in grams of 1 mole equal numerically to the sum of the atomic masses.

1 mole of $CaCl_2$ = 110.92 g/mole

1 mole Ca	=			**40.08 g**
2 moles Cl	=	**2 x 35.45**	=	**70.84 g**
				110.92 g/mole

1 mole of N_2O_4 = 92.02 g/mole

2 moles N	=	**2 x 14.01**	=	**28.02 g**
4 moles O	=	**4 x 16.00**	=	**64.00 g**
				92.02 g/mole

Example: Carbon has a molar mass of exactly 12g/mol.

Example 1

Solved Problem:

Calculate the Molar mass of the following substances:

1. NH_3
2. N_2O_4
3. $(NH_4)_2Cr_2O_7$

Solution

1. NH_3

14.01 g/mol + 3 (1.008 g/mol) = 17.03 g/mol

2. N_2O_4

2 (14.01 g/mol) + 4 (1.008 g/mol) = 32.05 g/mol

3. $(NH_4)_2Cr_2O_7$

2 (14.01 g/mol) + 8(1.008 g/mol) + 2 (52.00 g/mol) + 7 (16.00 g/mol) = 141.96 g/mol

Examples for Some more Solved Problem:

A. **1 mole of K_2O is equal to how many grams?**

Solution

1 mole of K_2O = 94.2 g

[2 K x 39.1 g/mole + 1 O x 16.0 g/mole]

B. **1 mole of $Al(OH)_3$ is equal to how many grams?**

Solution

1 mole of Al(OH)3 = 78.0 g

[1 Al x 27.0 g/mole + 3 O x 16.0 g/mole + 3 H x 1.0 g/mole]

C. Prozac, $C_{17}H_{18}F_3NO$, is a widely used antidepressant that inhibits the uptake of serotonin by the brain. It has a molar mass of

1. **40.0 g/mole**
2. **262 g/mole**
3. **309 g/mole**

Solution

Prozac, $C_{17}H_{18}F_3NO$, is a widely used antidepressant that inhibits the uptake of serotonin by the brain. It has a molar mass of

3. **309.32 g/mole**

[17C (12.01) + 18H (1.0008) + 3 F (19.00) + 1 N (14.01) + 1 O (16.00)]

D. What is the percent carbon in $C_5H_8NO_4$ (MSG monosodium glutamate), a compound used to flavor foods and tenderize meats?

Molar mass = 146.12 g/mole

[5C (12.01) + 8H (1.0008) + 1 N (14.01) + 4 O (16.00)]

$$\text{Percentage of Carbon} = \frac{\text{Total g C}}{\text{Total g of Compound}} \times 100$$

$$= \frac{60.05 \text{ g C}}{146.12 \text{ g MSG}} \times 100 = 41.09 \text{ \% C}$$

E. Molar Mass Factors for CH_4

Methane CH_4 known as natural gas is used in gas cook tops and gas heaters. Express the molar mass of methane in the form of conversion factors.

Molar mass of CH_4 = 16.0g

$$\frac{16.0 \text{ g } CH_4}{1 \text{ mole } CH_4} \quad \text{and} \quad \frac{1 \text{ mole } CH_4}{16.0\text{g } CH_4}$$

Calculations with Molar Mass

$$\text{Grams} \xleftrightarrow{\text{Molar mass}} \text{Moles}$$

Moles and Grams

Aluminium is often used for the structure of light-weight bicycle frames. How many grams of Al are in 3.00 moles of Al?

Solution

3.00 moles Al → ? g Al

1. **Molar mass of Al**

   1 mole Al = 26.98 g Al

2. **Conversion factors for Al**

   $$\frac{26.98 \text{ g Al}}{1 \text{ mol Al}} \quad \text{or} \quad \frac{1 \text{ mol Al}}{26.98 \text{ g Al}}$$

3. **Set- up**

   $$3.00 \cancel{\text{ moles Al}} \times \frac{26.98 \text{ g Al}}{1 \cancel{\text{ mole Al}}}$$

   Answer = 80.94 g Al

3.4 Percent Composition of Compounds

Mass of one element in a compound compared to the total mass of the whole compound

There are two ways in describing the composition of a compound:

1. **In terms of the numbers of its constituent atoms.**
2. **In terms of the percentage (by mass) of its elements.**

We can obtain the mass percents of the elements from the formula of the compound by comparing the mass of each element present in 1 mole of the compound to the total mass of 1 mole of the compound.

- **Calculate the molar mass.**

- **Divide the total mass of each element in the formula by the molar mass and multiply by 100.**

Mass percent of an element:

$$\text{Mass \%} = \frac{\text{Mass of element in compound}}{\text{Mass of compound}} \times 100\%$$

The formula of a compound shows its composition in terms of what elements it contains and how many of each. It is often useful to know the composition of a compound in terms of the masses of its elements.

For example,

Mercury(II) oxide decomposes to its elements mercury and oxygen.

$$2HgO_{(s)} + \text{heat} \rightarrow 2Hg_{(l)} + O_{2(g)}$$

The mass of mercury obtained as product from the decomposition can be calculated from the mass percent of Hg in HgO.

The Mass percent of an element in a compound is calculated from the mass of element present in one mole of the compound divided by the mass of one mole of the compound and converted to percent.

For the hypothetical compound A_2B_3:

$$\text{Mass \% A} = \frac{2A}{A_2B_3} \times 100\%$$

$$\text{Mass \% B} = \frac{3B}{A_2B_3} \times 100\%$$

Example 1

Solved Problem

What is the mass percent of Hg in HgO?

$$\text{Mass \% Hg} = \frac{\text{Atomic weight of Hg}}{\text{Formula weight of HgO}} \times 100\%$$

$$= \frac{200.6}{216.6} \times 100\%$$

$$= 92.61\%$$

Example 2

Solved Problem

What is the mass percent of each element in Na_3PO_4?

Mass of sodium	=	**3 x 22.99**	=	**68.97 g Na / mole Na_3PO_4.**
Mass of phosphorus	=	**1 x 30.97**	=	**30.97 g P / mole Na_3PO_4.**
Mass of oxygen	=	**4 x 16.00**	=	**64.00 g O / mole Na_3PO_4.**

Total mass of Na_3PO_4 (Formula weight) = 68.97 + 30.97 + 64.00 = 163.9 g/mol.

$$\text{The mass \% of Na} = \frac{68.97}{163.9} \times 100\% = 42.08\ \%$$

$$\text{The mass \% of P} = \frac{30.97}{163.9} \times 100\% = 18.90\ \%$$

$$\text{The mass \% of O} = \frac{64.00}{163.9} \times 100\% = 39.05\ \%$$

Example

Solved Problem

Arrange the following substances in order of increasing mass percent of carbon.

a. **Caffeine, $C_8H_{10}N_4O_2$**
b. **Sucrose, $C_{12}H_{22}O_{11}$**
c. **Ethanol, C_2H_5OH**

Atomic weight of C = 12.01

Solution

a. Caffeine, $C_8H_{10}N_4O_2$

Molar Mass = 8 (12.01) + 10 (1.008) + 4(14.01) + 2 (16.00) = 194.20 g/mol

$$\%C = \frac{8\ (12.01)\ g\ C}{194.20\ g\ C_8H_{10}N_4O_2} \times 100 = \frac{96.08}{194.20} \times 100 = 49.47\ \%C$$

b. Sucrose, $C_{12}H_{22}O_{11}$

Molar Mass = 12 (12.01) + 22 (1.008) + 11 (16.00) = 342.30 g/mol

$$\%C = \frac{12\ (12.01)\ g\ C}{342.30\ g\ C_{12}H_{22}O_{11}} \times 100 = \frac{144.12}{342.30} \times 100 = 42.10\ \%C$$

c. Ethanol, C_2H_5OH

Molar Mass = 2 (12.01) + 5 (1.008) + 1 (16.00) + 1 (1.008) = 46.07 g/mol

$$\%C = \frac{2\ (12.01)\ g\ C}{46.07\ g\ C_2H_5OH} \times 100 = \frac{24.02}{46.07} \times 100 = 52.14\ \%C$$

The order from lowest to highest mass percentage of carbon is:

Sucrose, $C_{12}H_{22}O_{11}$ < Caffeine, $C_8H_{10}N_4O_2$ < Ethanol, C_2H_5OH

3.5 Determining the formula of a compound

Types of Formula

The formulas for compounds can be expressed as an empirical formula and as a molecular(true) formula.

Empirical	Molecular (true)	Name
CH	C_2H_2	acetylene
CH	C_6H_6	benzene
CO_2	CO_2	carbon dioxide
CH_2O	$C_5H_{10}O_5$	ribose

Molecular formula = (empirical formula)$_n$

[n = integer]

$$n = \frac{\text{Molar Mass}}{\text{Empirical formula mass}}$$

Molecular mass = Vapour density x 2

Molecular formula = C_6H_6 = $(CH)_6$

Empirical formula = CH

Empirical Formula

An empirical formula of a compound is the simplest formula with the smallest integer subscripts. It gives the simple ratio of number of atoms of various elements present in that compound.

Example: E.F of Benzene is CH.

For most ionic substances, the empirical formula is the formula of the compound. This is often not the case for molecular substances. For example, the formula of sodium peroxide, an ionic compound of Na^+ and O_2^{2-}, is Na_2O_2. Its empirical formula is NaO. Thus empirical formula tells you the ratio of number of atoms in the compound.

Determining the empirical formula

The percentage of the elements in the compound is determined by suitable methods and from the data collected, the empirical formula is determined by the following steps.

1. Determine the percentage of each element in your compound.

2. Treat % as grams, and convert grams of each element to moles of each element.

3. Find the smallest whole number ratio of atoms.

4. If the ratio is not all whole numbers, multiply each by an integer so that all elements are in whole number ratio.

5. Finally write down the symbols of the various elements side by side and put the above numbers as the subscripts to the lower right hand of each symbol. This will represent the empirical formula of the compound.

Molecular Formula

Molecular formula of a compound is a formula, which gives the exact number of various elements present in a molecule of that compound.

Example: **M.F of Benzene is C_6H_6.**

Molecular formula from Empirical formula

The molecular formula of a compound is a multiple of its empirical formula.

Determining the molecular formula

1. **Calculate the empirical formula.**
2. **Find out the empirical formula mass by adding the atomic mass of all the atoms present in the empirical formula of the compound.**
3. **Divide the molecular mass (determined experimentally by some suitable method) by the empirical formula mass and find out the value of n which is a whole number.**
4. **Multiply the empirical formula of the compound with n, so as to find out the molecular formula of the compound.**

Example:

Some solved problem:

1. **Determining the empirical and molecular formulas for a compound that gives the following percentages upon analysis (in mass percents):**

   71.65% Cl

   24.27% C

   4.07% H

   The molar mass is known to be 98.96 g/mol.

Solution

[Atomic Mass - Cl=35.45; C=12.01; H=1.008]

Element	%	Relative No. of Moles	Quotient / Least number	Relative Number of Atoms
Chlorine	71.65	$71.65\ \cancel{g}\ Cl \times \dfrac{1\ mol\ Cl}{35.45\ \cancel{g}\ Cl} = 2.021\ mol Cl$	$\dfrac{2.021}{2.021} = 1$	1
Carbon	24.27	$24.27\ \cancel{g}\ C \times \dfrac{1\ mol\ C}{12.01\ \cancel{g}\ C} = 2.021\ mol C$	$\dfrac{2.021}{2.021} = 1$	1
Hydrogen	4.07	$4.07\ \cancel{g}\ H \times \dfrac{1\ mol\ H}{1.008\ \cancel{g}\ H} = 4.04\ mol\ H$	$\dfrac{4.04}{2.021} = 2$	2

Hence the empirical Formula is = $ClCH_2$

Calculation of Molecular Formula

Empirical Formula = $ClCH_2$

Empirical Formula Mass = 49.48 g /mol

$$n = \frac{\text{Molar mass}}{\text{Empirical formula mass}} = \frac{98.96\ \text{g/mol}}{49.48\ \text{g/mol}} = 2$$

Molecular Formula = (Empirical formula)$_n$

Molecular Formula = $(ClCH_2)_2$

Molecular Formula = $Cl_2C_2H_4$

The Name of the Compound is *dichloroethane*

Example 2:

Solved Problem:

A white powder is analysed and found to contain 43.64% phosphorus and 56.36% oxygen by mass. The compound has a molar mass of 283.88 g/mol. What are the compounds empirical formula and molecular formula?

Solution

[Atomic mass - P = 30.97; O = 16.00]

Element	%	Relative No. of Moles	Quotient / Least number	Relative Number of Atoms
Phosphorus	43.64	$43.64\cancel{g}P \times \frac{1 \text{ mol P}}{30.97\ \cancel{g}P} = 1.409$ mol P	$\frac{1.409}{1.409} = 1$	1
Oxygen	56.36	$56.36\ \cancel{g}O \times \frac{1 \text{ mol O}}{16.00\ \cancel{g}O} = 3.523$ mol O	$\frac{3.523}{1.409} = 2.5$	2.5

This yields the formula $PO_{2.5}$.

Since compounds must contain whole numbers of atoms, the empirical formula should contain only whole numbers.

To obtain the simplest set of whole numbers, we multiply both numbers by 2 to give the empirical formula P_2O_5.

Hence the empirical Formula is = P_2O_5

Calculation of Molecular Formula

Empirical Formula = P_2O_5

Empirical Formula Mass of P_2O_5 = 141.94 g /mol

$$n = \frac{\text{Molar mass}}{\text{Empirical formula mass}} = \frac{283.88 \text{ g/mol}}{141.94 \text{ g/mol}} = 2$$

Molecular Formula = (Empirical formula)$_n$

Molecular Formula = $(P_2O_5)_2$

Molecular Formula = $(P_2O_5)_2$ or P_4O_{10}

Example 3

Solved Problem

Caffeine, a stimulant found in coffee, tea, and chocolate, contains 49.48 % carbon, 5.15 % hydrogen, 28.87% nitrogen, and 16.49% oxygen by mass and has a molar mass of 194.2 g/mol. Determine the molecular formula of caffeine.

Solution

[Atomic mass - C = 12.01; H = 1.008; N = 14.01; O = 16.00]

Element	%	Relative No. of Moles	Quotient -------------- Least number	Relative Number of Atoms
Carbon	49.48	$49.48\ \cancel{g}\ C \times \frac{1\ mol\ C}{12.01\ \cancel{g}\ C} = 4.1199\ mol C$	$\frac{4.1199}{1.0306} = 4$	4
Hydrogen	5.15	$5.15\ \cancel{g}\ H \times \frac{1\ mol\ H}{1.008\ \cancel{g}\ H} = 5.109\ mol\ H$	$\frac{5.109}{1.0306} = 5$	5
Nitrogen	28.87	$28.87\ \cancel{g}\ N \times \frac{1\ mol\ N}{14.01\ \cancel{g}\ N} = 2.0606\ mol\ N$	$\frac{2.0606}{1.0306} = 2$	2
Oxygen	16.49	$16.49\ \cancel{g}\ O \times \frac{1\ mol\ O}{16.00\ \cancel{g}\ O} = 1.0306 mol\ O$	$\frac{1.0306}{1.0306} = 1$	1

Hence the empirical Formula is = $C_4H_5N_2O$

Calculation of Molecular Formula

Empirical Formula = $C_4H_5N_2O$

Empirical Formula Mass = 4 C (12.01)+ 5 H (1.008) + 2 N (14.01) + 1 O (16.00)

= 48.04 + 5.04 +28.02 + 16 = 97.1

$$n = \frac{\text{Molar mass}}{\text{Empirical formula mass}} = \frac{194.2\ \text{g/mol}}{97.1\ \text{g/mol}} = 2$$

Molecular Formula = (Empirical formula)$_n$

Molecular Formula = $(C_4H_5N_2O)_2$

The
Molecular Formula of Caffein is = $C_8H_{10}N_4O_2$

3.6 Chemical Equations

A chemical equation is the short scientific representation of a chemcical reaction. In order to write the chemical equation correctly, we must know the reacting substances, all the products formed and their chemical formulae.

$$\underset{\text{(Reactants)}}{CH_4 + 2O_2} \rightarrow \underset{\text{(Products)}}{CO_2 + 2H_2O}$$

Chemical Equations show

- The reactants which enter into a reaction.
- The products which are formed by the reaction.
- The amounts of each substance used and each substance produced.

Information conveyed by a chemical equation

1. A chemical equation is the stoichiometric equation, which is a short scientific representation of a chemical reaction.

2. The chemical equation explains the relationship between the number of mole of the reactants and products of a chemical reaction.

3. The chemical equation explains the conditions at which the reaction takes place such as temperature, pressure, catalyst, etc.

4. The physical states of products such as gas or precipitate is explained by ↑ or ↓ arrow mark.

Chemical equations give information in two major areas

- First, they tell us what substances are reacting (those being used up) and what substances are products (those being made).

- Second, the coefficients of a balanced equation tell us in what ratio the substances react or are produced.

Two important principles to remember:

- Every chemical compound has a formula, which cannot be altered.

- A chemical reaction must account for every atom that is used. This is an application of the Law of Conservation of Matter, which states that in a chemical reaction atoms are neither created nor destroyed.

Rules for writing equations.

- **Write down the formula(s) for any substance entering into the reaction. Place a plus (+) sign between the formulas as needed and put the yield arrow after the last one.**

- **Examine the formulas carefully and decide which of the four types of equations applies to the reaction you are considering. On the basis of your decision, write down the correct formulas for all products formed, placing them to the right of the arrow.**

Some Conventions for Writing Chemical Equations

Notation	Meaning	Example
Add (g) after formula	Substance is a gas	$HCl_{(g)}$
Add (l) after formula	Substance is a liquid	$H_2O_{(l)}$
Add (s) after formula	Substance is a solid	$NaCl_{(s)}$
Add (aq) after formula	Substance is dissolved in aqueous (water) solution	$C_{12}H_{22}O_{11(aq)}$
Above arrow	Substance is a catalyst	$C_2H_4\ (g) + H_2\ (g) \xrightarrow{Pt} C_2H_6(g)$
Above arrow	Substance is the solvent	$NaCl(s) \xrightarrow{H_2O} NaCl(aq)$
Above/below arrow	Conditions used for reaction	$C_2H_4\ (g) + H_2\ (g) \xrightarrow[1\ atm,\ 2000^oC]{Pt} C_2H_6(g)$

Some things to remember about writing equations:

1. **The diatomic elements when they stand alone are always written H_2, N_2, O_2, F_2, Cl_2, Br_2, I_2**
2. **The sign, →, means "yields" and shows the direction of the action.**
3. **A small delta, (Δ), above the arrow shows that heat has been added.**
4. **A double arrow, ↔, shows that the reaction is reversible and can go in both directions.**
5. **Before beginning to balance an equation, check each formula to see that it is correct. NEVER change a formula during the balancing of an equation.**
6. **Balancing is done by placing coefficients in front of the formulas to insure the same number of atoms of each element on both sides of the arrow.**
7. **Always consult the Activity Series of metals and nonmetals before attempting to write equations for replacement reactions.**
8. **If a reactant or product is a solid, (s) is placed after the formula.**
9. **If a reactant or product is a gas, (g) is placed after it.**
10. **If a reactant or product is in water solution, (aq) is placed after it.**
11. **Some products are unstable and break down (decompose) as they are produced during the reaction. You need to be able to recognize these products when they occur and write the decomposition products in their places.**

Examples

$H_2CO_{3(aq)} \rightarrow H_2O_{(l)} + CO_{2(g)}$
Carbonic acid, as in soft drinks, decomposes when it is formed.

$H_2SO_{3(aq)} \rightarrow H_2O_{(l)} + SO_{2(g)}$
Sulfurous acid also decomposes as it is formed.

$NH_4OH_{(aq)} \rightarrow NH_{3(g)} + H_2O_{(l)}$

You can definitely smell the odor of ammonia gas because whenever "ammonium hydroxide" is formed it decomposes into ammonia and water.

Chemical Reaction

A chemical reaction is a process that results in the inter conversion of chemical species. Chemical reactions may be elementary reactions or stepwise reactions. That is one substance is transformed into another.

Reactants and Products

$$\underset{\text{(Reactants)}}{CH_4 + O_2} \rightarrow \underset{\text{(Products)}}{CO_2 + H_2O}$$

Reactants (or 'substrates') are the starting materials for a reaction where as products are what we end up at the end of the reaction.

The reactants are on the left side of a chemical equation and the products are on the right side.

Reason for occurring chemical reaction

Chemical reactions occur because the products of the reaction have less energy than the reactants (drive toward less energy). These reactions release energy into the environment, like the burning of a match. Chemical reactions also occur because the products are more random (less ordered) than the reactant (drive toward greater entropy).

The Meaning of a Chemical Equation

1. Relative numbers of reactants and products.

   Coefficients give atomic / molecular / mole ratios.

2. The equation often gives the physical states of the reactants and products.

State	Symbol
Solid	*(s)*
Liquid	*(l)*
Gas	*(g)*
Dissolved in water (in aqueous solution)	*(aq)*

TABLE 3.2 Information Conveyed by the Balanced Equation for the Combustion of Methane

Reactants		Products
$CH_4(g) + 2O_2(g)$	$\longrightarrow$	$CO_2(g) + 2H_2O(g)$
1 molecule + 2 molecules	$\longrightarrow$	1 molecule + 2 molecules
1 mole + 2 moles	$\longrightarrow$	1 mole + 2 moles
6.022×10^{23} molecules + 2 (6.022×10^{23} molecules)	$\longrightarrow$	6.022×10^{23} molecules + 2 (6.022×10^{23} molecules)
16 g + 2 (32 g)		44 g + 2 (18 g)
80 g reactants	$\longrightarrow$	80 g products

Four basic types of chemical reactions

1. Synthesis (composition):

Two or more elements or compounds may combine to form a more complex compound.

Basic form: A+ X $\rightarrow$ AX

Examples of synthesis reactions:

Metal + oxygen $\rightarrow$ metal oxide

$2Mg_{(s)} + O_{2(g)} \rightarrow 2MgO_{(s)}$

2. Decomposition

A single compound breaks down into its component parts or simpler compounds.

Basic form: AX $\rightarrow$ A + X

Examples of decomposition reactions:

Metallic carbonates, when heated, form metallic oxides and $CO_{2(g)}$.
$CaCO_{3(s)} \rightarrow CaO_{(s)} + CO_{2(g)}$

3. Replacement

A more active element takes the place of another element in a compound and sets the less active one free.

Basic form: $A + BX \rightarrow AX + B$ **or** $AX + Y \rightarrow AY + X$

Examples of replacement reactions

Replacement of a metal in a compound by a more active metal.

$Fe_{(s)} + CuSO_{4(aq)} \rightarrow FeSO_{4(aq)} + Cu_{(s)}$

4. Ionic

Occurs between ions in aqueous solution. A reaction will occur when a pair of ions come together to produce at least one of the following:

- **a precipitate**
- **a gas**
- **water or some other non-ionized substance.**

Basic form: $AX + BY \rightarrow AY + BX$

Examples of ionic reactions

Formation of precipitate.

$NaCl_{(aq)} + AgNO_{3(aq)} \rightarrow NaNO_{3(aq)} + AgCl_{(s)}$

$BaCl_{2(aq)} + Na_2SO_{4(aq)} \rightarrow 2NaCl_{(aq)} + BaSO_{4(s)}$

3.7 Balancing chemical Equation

Balanced Chemical Equation

A chemical equation is called balanced equation only when the numbers and kinds of atoms present on both sides are equal.

Writing and balancing the Equations for a chemical reaction

1. **Determine what reaction is occurring. What are the reactants, products, and the physical states involved.**

2. **Write the unbalanced equation that summarizes the reaction described in step 1.**

3. **Balance the equation by inspection, starting with the most complicated molecule(s).**

4. **Determine what coefficients are necessary so that the same number of each type of atom appears on both reactant and product sides. Do not change the identies (formulas) of any of the reactants or products.**

Example for Balancing Chemical Equation

1. **Determine what reaction occurring. (It is sometimes helpful to write this in word form)**

$$\text{Hydrogen} + \text{Oxygen} \rightarrow \text{water}$$

2. **Write the unbalanced equation. (Focus on writing correctly atomic and compound formulas).**

$$H_2 + O_2 \rightarrow H_2O$$

3. **Balance the equation by inspection. (It is often helpful to work systematically from left to right).**

$$2H_2 + O_2 \rightarrow 2H_2O$$

4. **Include phase information.**

$$2H_{2(g)} + O_{2(g)} \rightarrow 2H_2O_{(l)}$$

Example 1

Hydrogen combines with bromine giving HBr.

$$H_2 + Br_2 \rightarrow HBr$$

This is the skeletal equation. The number of atoms of hydrogen on the left side is two but on the right side it is one. So the number of molecules of HBr is to be multiplied by two. Then the equation becomes.

$$H_2 + Br_2 \rightarrow 2HBr$$

This is the balanced (or) stoichiometric equation.

Example 2

Potassium permanganate reacts with HCl to give KCl and other products. The skeletal equation is

$$KMnO_4 + HCl \rightarrow KCl + MnCl_2 + H_2O + Cl_2$$

If an element is present only in one substance in the left hand side of the equation and if the same element is present only in one of the substances in the right side, it may be taken up first while balancing the equation.

According to the rule, the balancing of the equation may be started with respect to K, Mn, O (or) H but not with Cl.

There are

L.H.S.	R.H.S.
K = 1	1
Mn = 1	1
O = 4	1

So the equation becomes

$$KMnO_4 + HCl \rightarrow KCl + MnCl_2 + 4H_2O + Cl_2$$

Now there are eight hydrogen atoms on the right side of the equation we must write 8 HCl.

$$KMnO_4 + 8HCl \rightarrow KCl + MnCl_2 + 4H_2O + Cl_2$$

Of the eight chlorine atoms on the left, one is disposed of in KCl and two in $MnCl_2$ leaving five free chlorine atoms. Therefore, the above equation becomes

$$KMnO_4 + 8HCl \rightarrow KCl + MnCl_2 + 4H_2O + 5/2Cl_2$$

Equations are written with whole number coefficient and so the equation is multiplied through out by 2 to become.

$$2KMnO_4 + 16HCl \rightarrow 2KCl + 2\ MnCl_2 + 8H_2O\ 5Cl_2$$

Example 3

Balance Equations with Coefficients

Coefficients *in front* of formulas balance each type of atom

$$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$$

4 N	=	4 N
12 H	=	12 H
10 O	=	10 O

Example 4

Steps in Balancing An Equation

Fe_3O_4 +	H_2	$\rightarrow$	Fe	+	H_2O	
<u>Fe:</u>	Fe_3O_4 +	H_2	$\rightarrow$	3Fe	+	H_2O
<u>O:</u>	Fe_3O_4 +	H_2	$\rightarrow$	3Fe	+	$4H_2O$
<u>H:</u>	Fe_3O_4 +	$4H_2$	$\rightarrow$	Fe	+	$4H_2O$

Example 5

Write a balanced chemical equation that describes each of the following.

a). Iron metal reacts with oxygen to form rust, iron (III) oxide.

$$4Fe_{(s)} + 3O_{2(g)} \rightarrow 2Fe_2O_{3(s)}$$

b). Calcium metal reacts with water to produce aqueous calcium hydroxide and hydrogen gas.

$$Ca\ (s) + 2H_2O\ (l) \rightarrow Ca(OH)_2\ (aq) + H_{2(g)}$$

- **First Balance O**
- **Then balance H since it is on both products.**

c). Aqueous barium hydroxide reacts with aqueous sulfuric acid to produce solid barium sulfate and water.

$$Ba(OH)_{2(aq)} + H_2SO_{4(aq)} \rightarrow BaSO_{4(s)} + 2H_2O_{(l)}$$

- **Ba and S are already balanced.**
- **There are 6 O atoms on the reactant side and in order to get 6 O atoms on the product side, we will need $2H_2O$ molecules.**

3.8 Stoichiometric calculations: Amounts of Reactants and Products

- **Stoichiometry is the calculation of the quantities of reactants and products involved in the chemical reaction.**

- **It is the study of the relationship between the number of mole of the reactants and products of a chemical reaction.**

- **A stoichiometry equation is a short scientific representation of a chemical reaction.**

Rules for writing stoichiometric equations

1. In order to write the stoichiometric equation correctly, we must know the reacting substances, all the products formed and their chemical formula.

2. The formula of the reactants must be written on the left side of arrow with a positive sign between them.

3. The formula of the products formed are written on the right side of the arrow mark. If there is more than one product, a positive sign is placed between them.

4. The equation thus obtained are called skeleton equation. For example, the chemical reaction between Barium chloride and sodium sulphate producing BaSO4 and NaCl is represented by the equation as

$$BaCl_2 + Na_2SO_4 \rightarrow BaSO_4 + NaCl$$

This skeleton equation itself is not a balanced one. In many cases the skeleton equation is not a balanced one.

For example, the decomposition of lead nitrate giving lead oxide, NO_2 and oxygen. The skeletal equation for this reaction is

$$Pb(NO_3)_2 \rightarrow PbO + NO_2 + O_2$$

5. In the skeleton equation, the numbers and kinds of particles present on both sides of the arrow are not equal.

6. During balancing equation, the formula of substances should not be altered, but the number of molecules with it only be suitably changed.

7. Important conditions such as temperature, pressure, catalyst etc., may be noted above (or) below the arrow of the equation.

8. **An upward arrow (↑) is placed on the right side of the formula of a gaseous product and a downward arrow (↓) on the right side of the formula on a precipitated product.**

9. **All the reactants and products should be written as molecules including the elements like hydrogen, oxygen, nitrogen, fluorine, chlorine, bromine and iondine as H_2, O_2, N_2, F_2, Cl_2, Br_2 and I_2.**

Calculating Masses of Reactants and Products in chemical Reactions.

1. **Balance the equation for the reaction.**
2. **Convert the known mass of the reactant or product to moles of that substance.**
3. **Use the balanced equation to set up the appropriate mole ratios.**
4. **Use the appropriate mole ratios to calculate the number of moles of the desired reactant or product.**
5. **Convert from moles back to grams if required by the problem.**

Examples for writing mole factors

$$4Fe + 3O_2 \rightarrow 2\,Fe_2O_3$$

Mole factors for <u>Fe and O_2</u>

$$\frac{4 \text{ mole Fe}}{3 \text{ mole } O_2} \quad \text{and} \quad \frac{3 \text{ mole } O_2}{4 \text{ mole Fe}}$$

Mole factors for <u>Fe and Fe_2O_3</u>

$$\frac{4 \text{ mole Fe}}{2 \text{ mole } Fe_2O_3} \quad \text{and} \quad \frac{2 \text{ mole } Fe_2O_3}{4 \text{ mole Fe}}$$

Mole factors for <u>O_2 and Fe_2O_3</u>

$$\frac{3 \text{ mole } O_2}{2 \text{ mole } Fe_2O_3} \quad \text{and} \quad \frac{2 \text{ mole } Fe_2O_3}{3 \text{ mole } O_2}$$

Example 1

How many moles of Fe_2O_3 are produced when 6 moles O_2 react in the following reaction?

$$4Fe + 3O_2 \rightarrow 2Fe_2O_3$$

Solution:

$$6\ \cancel{\text{moles}\ O_2} \times \frac{2\ \text{moles}\ Fe_2O_3}{3\ \cancel{\text{moles}\ O_2}} = 4\ \text{mole}\ Fe_2O_3$$

Example 2

How many moles of Fe are needed to react 12.0 mole of O_2 in the following reaction?

$$4Fe + 3O_2 \rightarrow 2Fe_2O_3$$

Solution:

$$12.0\ \cancel{\text{mole}\ O_2} \times \frac{4\ \text{mole Fe}}{3\ \cancel{\text{mol}\ O_2}} = 16.0\ \text{mole Fe}$$

Example 3

The reaction between H_2 and O_2 produces 13.1 g of water. How many grams of O_2 reaction?

Step 1 : **Write the equation**

$$H_2\,(g) + O_2\,(g) \rightarrow H_2O\,(g)$$

Step 2: **Balance the equation**

$$2H_2\,(g) + O_2\,(g) \rightarrow 2H_2O\,(g)$$

Step 3: **Organize data**

Mole Bridge

$$2H_2\,(g) + \underset{?\ g}{O_2\,(g)} \rightarrow \underset{13.1\ g}{2H_2O\,(g)}$$

Step 4: **Plan set-up**

g H_2O → mole H_2O → (<u>Use proper desired mole factor</u>) mole O_2 → g O_2

$$13.1\ \cancel{g\ H_2O} \times \frac{1\ \cancel{mole\ H_2O}}{18.0\ \cancel{g\ H_2O}} \times \frac{1\ \cancel{mole\ O_2}}{2\ \cancel{mole\ H_2O}} \times \frac{32.0\ g\ O_2}{1\ \cancel{mole\ O_2}} = 11.6\ g\ O_2$$

POINTS TO REMEMBER

1. **Read and equation in moles.**
2. **Convert given amount to moles.**
3. **Use mole factor to give desired moles.**
4. **Convert moles to grams**

Grams (given) → moles (given) → moles (desired) → grams (desired)

Example 4

How many grams of O_2 are needed to react 50.0 g of Na in the following reaction:

$$4Na + O_2 \rightarrow 2Na_2O$$

Solution:

Step 1 : **Write the equation**

$$4Na + O_2 \rightarrow 2Na_2O$$

Step 2: **Balance the equation**

Already balanced

$$4Na + O_2 \rightarrow 2Na_2O$$

Step 3: **Organize data**

Mole Bridge

4 Na	+	**O_2**	$\rightarrow$	**2 Na_2O**
50.0g		**? g**		

Step 4: **Plan set-up**

g Na $\rightarrow$ mole Na $\rightarrow$ (Use proper desired mole factor) mole O_2 $\rightarrow$ g O_2

$$50.0\ \cancel{g\ Na} \times \frac{1\ \cancel{mole\ Na}}{23.0\ \cancel{g\ Na}} \times \frac{1\ \cancel{mole\ O_2}}{4\ \cancel{mole\ Na}} \times \frac{32.0\ g\ O_2}{1\ \cancel{mole\ O_2}} = 17.4\ g\ O_2$$

Example 5

Acetylene gas C_2H_2 burns in the oxyacetylene torch for welding. How many grams of C_2H_2 are burned if the reaction produces 75.0 g of CO_2?

Solution:

Step 1 : **Write the equation**

$$C_2H_2 + O_2 \rightarrow CO_2 + H_2O$$

Step 2: **Balance the equation**

$$2C_2H_2\ (g) + 5O_2\ (g) \rightarrow 4CO_2\ (g) + 2H_2O\ (g)$$

Step 3: **Organize data**

Mole Bridge

$$2C_2H_2\ (g) + 5O_2\ (g) \rightarrow 4CO_2\ (g) + 2H_2O\ (g)$$

? g (under $2C_2H_2$) **75.0 g** (under $4CO_2$)

Step 4: **Plan set-up**

g CO_2 → mole CO_2 → (<u>Use proper desired mole factor</u>) mole C_2H_2 → g C_2H_2

$$75.0\ \cancel{g\ CO_2} \times \frac{1\ \cancel{mole\ CO_2}}{44.0\ \cancel{g\ CO_2}} \times \frac{2\ \cancel{mole}\ C_2H_2}{4\ \cancel{mole\ CO_2}} \times \frac{26.0\ g\ C_2H_2}{1\ \cancel{mole}\ C_2H_2} = 22.2\ g\ C_2H_2$$

Example 6

Propane reacts with oxygen to produce CO_2 and water. What mass of oxygen will react with 96.1g of propane?

Solution:

Step 1 : **Write the equation**

$$C_3H_8 + O_2 \rightarrow CO_2 + H_2O$$

Step 2: **Balance the equation**

$$C_3H_8\ (g) + 5O_2\ (g) \rightarrow 3CO_2\ (g) + 4H_2O\ (g)$$

Step 3: **Organize data**

Mole Bridge

$$C_3H_8\ (g) \quad + \quad 5O_2\ (g) \rightarrow \quad 3CO_2\ (g) + 4H_2O\ (g)$$

96.1 g ? g

Step 4: **Plan set-up**

g C_3H_8 → mole C_3H_8 → (<u>Use proper desired mole factor</u>) mole O2 → g O_2

[molar mass of C_3H_8 = 44.1 g/mol]

$$96.1\ \cancel{g\,C_3H_8} \times \frac{1\ \cancel{mole\ C_3H_8}}{44.1\ \cancel{g\ C_3H_8}} \times \frac{5\ \cancel{mole\ O_2}}{1\ \cancel{mole\ C_3H_8}} \times \frac{32.0\ g\ O_2}{1\ \cancel{mole\ O_2}} = 349\ g\ O_2$$

Example 7

Propane reacts with oxygen to produce CO_2 and water. What mass of CO_2 is produced when 96.1 g of propane is combusted with oxygen?

Solution:

Step 1 : **Write the equation**

$$C_3H_8 + O_2 \rightarrow CO_2 + H_2O$$

Step 2: **Balance the equation**

$$C_3H_8\ (g) + 5O_2\ (g) \rightarrow 3CO_2\ (g) + 4H_2O\ (g)$$

Step 3: **Organize data**

$$\overbrace{C_3H_8\ (g) \quad + \quad 5O_2\ (g) \rightarrow \quad 3CO_2}^{\text{Mole Bridge}}\ (g) + 4H_2O\ (g)$$

96.1 g ? g

Step 4: **Plan set-up**

g C_3H_8 $\rightarrow$ mole C_3H_8 $\rightarrow$ (<u>Use proper desired mole factor</u>) mole CO_2 $\rightarrow$ g CO_2

[molar mass of C_3H_8 = 44.1 g/mol]

$$96.1\ \cancel{g\,C_3H_8} \times \frac{1\ \cancel{mole\ C_3H_8}}{44.1\ \cancel{g\ C_3H_8}} \times \frac{3\ \cancel{mole\ CO_2}}{1\ \cancel{mole\ C_3H_8}} \times \frac{44.0\ g\ CO_2}{1\ \cancel{mole}\ O_2} = 288\ g\ CO_2$$

3.9 Limiting reactant

Limiting Reactant

Limiting reactant is the reactant in a chemical reaction that limits the amount of product that can be formed.

The reaction will stop when all the limiting reactant is consumed.

Excess Reactant

Excess reactant is the reactant in a chemical reaction that remains when a reaction stops when the limiting reactant is completely consumed.

The excess reactant remains because there is nothing with which it can react.

Solving limiting reactant problems

1. **Convert grams of reactants to moles.**
2. **Use stoichiometric ratios to determine the limiting reactant.**
3. **Solve as before, beginning the stoichiometric calculation with the grams of the limiting reactant.**

Example 1

Nitrogen gas can be prepared by passing gaseous ammonia over solid copper(II) oxide at high temperatures. The products of the reaction are solid copper and water vapour. If a sample containing <u>18.1 g of NH_3</u> is reacted with <u>90.4 g of CuO</u>, which is the limiting reactant? How many grams of N_2 will be formed.

Solution:

Step 1 : **Write the equation**

$$NH_3 + CuO \rightarrow N_2 + Cu + H_2O$$

Step 2: **Balance the equation**

$$2NH_3\,(g) + 3CuO\,(s) \rightarrow N_2\,(g) + 3Cu\,(s) + 3H_2O\,(g)$$

Step 3: **Organize data**

Mole Bridge

$$2NH_3\,(g) \quad + \quad 3CuO\,(s) \rightarrow N_2\,(g) + 3Cu\,(s) + 3H_2O\,(g)$$

Step 4: **Convert gram to mole of the given reactant.**

Molar mass of NH_3 = 17.03 g/mol
Molar mass of CuO = 79.55g/mol

$$18.1\ \cancel{g\ NH_3} \times \frac{1\ \text{mole}\ NH_3}{17.03\ \cancel{g\ NH_3}} = 1.06\ \text{mol}\ NH_3$$

$$90.4\ \cancel{g\ NH_3} \times \frac{1\ \text{mole}\ CuO}{79.55\ \cancel{g\ CuO}} = 1.14\ \text{mol}\ CuO$$

Step 5: To determine the limiting reactant, we use the mole ratio for CuO and NH_3.

$$1.06 \cancel{\text{mol}}\ NH_3 \times \frac{3 \text{ mole CuO}}{2 \cancel{\text{mol NH}_3}} = 1.59 \text{ mol CuO}$$

That is 1.59 mol CuO is required to react with 1.06 mol NH_3.

Since 1.14 mol CuO is actually present, the amount of CuO is limiting the reaction. So CuO is limiting reactant here.

Step 6: We can also verify this conclusion by comparing the mole ratio of CuO and NH_3 required by the balanced equation.

$$2NH_3\ (g) + 3CuO\ (s) \rightarrow N_2\ (g) + 3Cu\ (s) + 3H_2O\ (g)$$

mole bridge

$$\frac{\text{mol CuO}}{\text{mol NH}_3}\ (\text{required}) = \frac{3}{2} = 1.5$$

with the mole ratio actually present

$$\frac{\text{mol CuO}}{\text{mol NH}_3}\ (\text{actual}) = \frac{1.14}{1.06} = 1.08$$

Since the actual ratio is too small (<1.5) CuO is the limiting reactant.

Step 7: **Since CuO is the limiting reactant, we must use the amount of CuO to calculate the amount of N_2 formed.**

From the balanced equation, the mole ratio between CuO and N_2 is

$$\frac{1 \text{ mol } N_2}{3 \text{ mol CuO}}$$

Therefore,

$$1.14 \cancel{\text{mol}} \text{ CuO} \times \frac{1 \text{ mol } N_2}{3 \cancel{\text{mol}} \text{ CuO}} = 0.380 \text{ mol } N_2$$

Step 8:

Using molar mass of N_2 (28.0 g/mol) we can calculate the mass of N_2 produced.

$$0.380 \cancel{\text{mol}} \ N_2 \times \frac{28.0 \text{ g } N_2}{1 \cancel{\text{mol}} \ N_2} = 10.6 \text{ g } N_2$$

Percent yield

A comparison of the amount actually obtained to the amount it was possible to make.

$$\frac{\text{Actual yield}}{\text{Theoretical Yield}} \times 100\% = \text{Percent Yield}$$

Actual Yield

What you got by actually performing the reaction.

Theoretical yield

The theoretical yield is the amount of product that can be made - In other words it's the amount of product possible as calculated through the stoichiometry problem.

This is different from the actual yield, the amount one actually produces and measures.

Solving a stoichiometry problem involving Masses of Reactants and Products:

1. **Write and balance the equation for the reaction.**
2. **Convert the known masses of substances of moles.**
3. **Determine which reactant is limiting.**
4. **Using amount of the limiting reactant and the appropriate mole ratios, compute the number of moles of the desired product.**
5. **Convert from moles to grams, using the molar mass.**

Example for calculating Percent Yield:

Example 1:

If the reaction actually gave 6.63 grams of nitrogen instead of the predicted 10.6 g, calculate the percent yield.

$$\frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100\%$$

The percent yield of nitrogen would be

$$\frac{6.63 \text{ g } N_2}{10.6 \text{ g } N_2} \times 100\% = 62.5\%$$

Example 2:

Methanol can be manufactured by combination of gaseous carbon monoxide and hydrogen. Suppose 68.5 kg CO(g) is reacted with 8.60 Kg H_2 (g).

Calculate the theoretical yield of the CH_3OH. If 3.57×10^4 g CH_3OH is actually produced. What is the percent yiled of methanol.

Solution:

Step 1: Write the balanced equation

$$2H_2\,(g) + CO(g) \rightarrow CH_3OH\,(l)$$

Step 2: We have to calculate the moles of reactant.

$$68.5\ \cancel{kg\ CO} \times \frac{1000\cancel{g\ CO}}{1\ \cancel{kg\ CO}} \times \frac{1\ \text{mole CO}}{28.02\ \cancel{g\ CO}} = 2.44 \times 10^3\ \text{mol CO}$$

$$8.60\ \cancel{kg\ H_2} \times \frac{1000\cancel{g\ H_2}}{1\ \cancel{kg}\ H_2} \times \frac{1\ \text{mole}\ H_2}{2.016\cancel{g\ H_2}} = 4.27 \times 10^3\ \text{mol}\ H_2$$

Step 3: Determine limiting reactant.

To determine limiting reactant, we have to compare the mole ratio of H_2 and CO required by the balanced equation.

$$2H_2\,(g) + CO(g) \rightarrow CH_3OH\,(l)$$

Mole Bridge

$$\frac{\text{mol } H_2}{\text{mol CO}}\ \text{(required)} = \frac{2}{1} = 2$$

with the actual mole ratio

$$\frac{\text{mol } H_2}{\text{mol CO}}\ \text{(actual)} = \frac{4.27 \times 10^3}{2.44 \times 10^3} = 1.75$$

Since the actual mole ratio of H_2 to CO is smaller than the required ratio, H_2 is limiting reactant.

Step 4:

Since H_2 is limiting reactant, we must use the amount of H_2 and the mole ratio between H_2 and CH_3OH to determine the maximum amount of methanol that can be produced.

$$4.27 \times 10^3 \text{ mol } H_2 \times \frac{1 \text{ mol } CH_3OH}{2 \text{ mol } H_2} = 2.14 \times 10^3 \text{ mol } CH_3OH.$$

Step 5:

Now we have to calculate the theoretical yield in grams.

$$2.14 \times 10^3 \cancel{\text{mol CH}_3\text{OH}} \times \frac{32.04 \text{ g CH}_3\text{OH}}{1 \cancel{\text{mol CH}_3\text{OH}}} = 6.86 \times 10^4 \text{ g CH}_3\text{OH}$$

This is the theoretical yield.

Step 6:

Therefore the percent yield

$$\frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100\%$$

The percent yield of CH_3OH would be

$$\frac{3.57 \times 10^4 \text{g CH}_3\text{OH}}{6.86 \times 10^4 \text{ g CH}_3\text{OH}} \times 100\% = 52.0\ \%$$

Solving a stoichiometry problem involving Masses of Reactants and Products:

1. **Write and balance the equation for the reaction.**
2. **Convert the known masses of substances of moles.**
3. **Determine which reactant is limiting.**
4. **Using amount of the limiting reactant and the appropriate mole ratios, compute the number of moles of the desired product.**
5. **Convert from moles to grams, using the molar mass.**

The process is summarized in the diagram below: