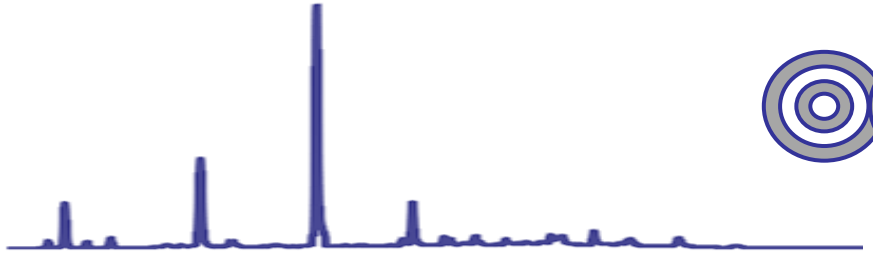
بسم الله الرحمن الرحيم

Stoichiometric Calculations



Ahmad Aqel Ifseisi
Professor of Analytical Chemistry
College of Science, Department of Chemistry
King Saud University
P.O. Box 2455 Riyadh 11451 Saudi Arabia
Building: 05, Office: 2A149, Lab: AA53
Tel. 014674198, Fax: 014675992
Web site: https://faculty.ksu.edu.sa/aifseisi
E-mail: aifseisi@ksu.edu.sa
ahmad3qel@gmail.com

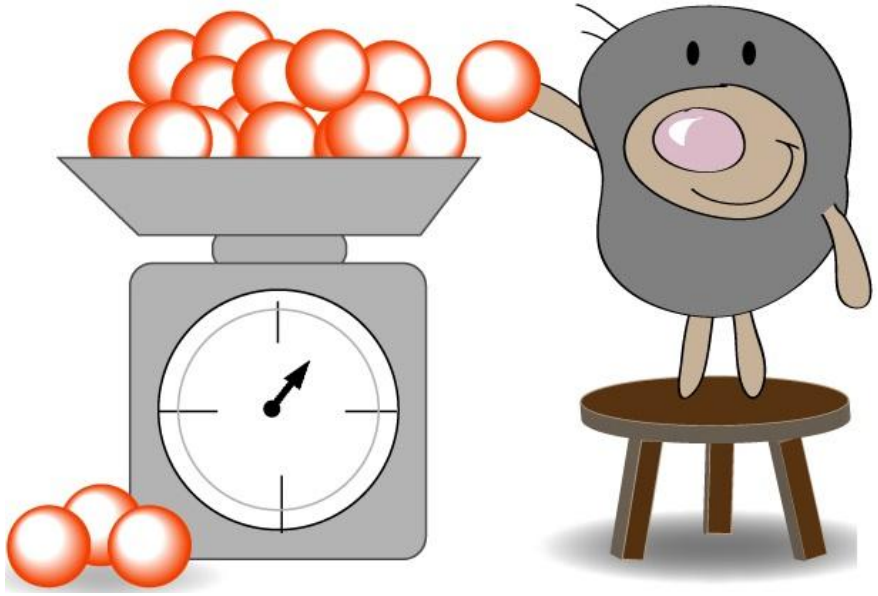
AMRC كرسي أبحاث المواد المتقدمة Advanced Materials Research Chair

جامعة الملك سعود King Saud University

Amount of Substance – The Mole

The mole is the **SI** unit for the amount of a chemical substance. It is always associated with specific microscopic entities such as atoms, molecules, ions, electrons, or other particles.

It is the amount of the specified substance that contains the same number of particles as the number of carbon atoms in exactly 12 grams of ^{12}C.



602,214,076,000,000,000,000,000 atoms

This important number is Avogadro's number:

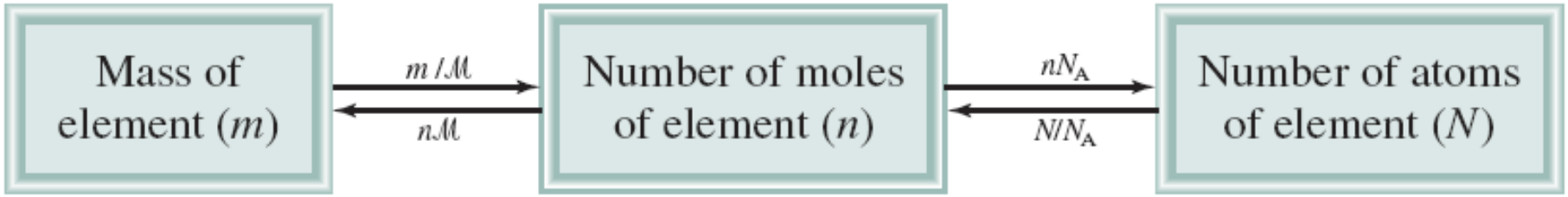
$$N_A = 6.022 \times 10^{23}$$

The definition was adopted in Nov 2018 as one of the seven SI base units; It is defined as exactly 6.022×10^{23} constitutive particles, which may be atoms, molecules, ions, or electrons.

One mole contains exactly $6.02214076 \times 10^{23}$ elementary entities

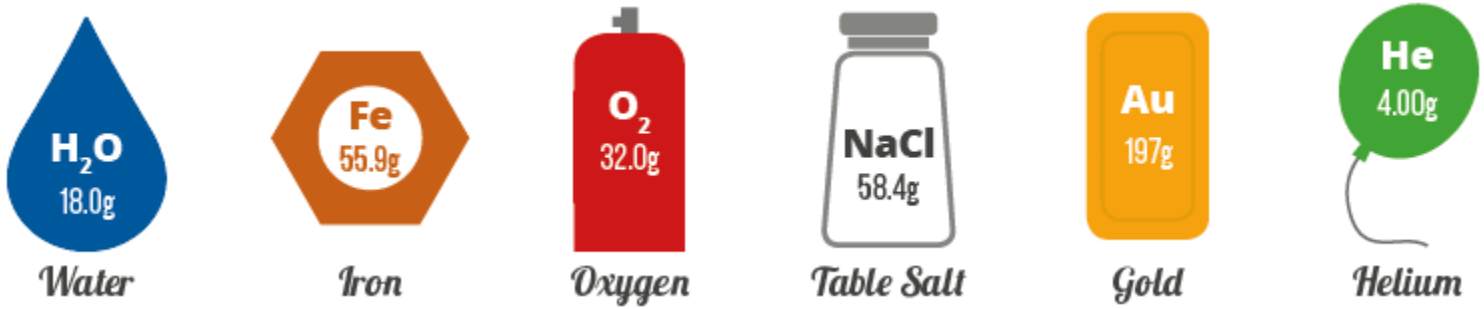
The molar mass $\mathcal{M}$ of a substance is the mass in grams of 1 mole of that substance.

The notions of Avogadro's number and molar mass enable us to carry out conversions between mass and moles of atoms and between moles and number of atoms



$$n = \frac{m}{\mathcal{M}} \qquad N_A = \frac{N}{n}$$

N_A : Avogadro's no. = 6.022×10^{23} mol^{-1}
n : no. of moles
N : no. of atoms, molecules, ions or particles
$\mathcal{M}$: molar mass (g/mol)
m : mass (g)



The Millimole

$$\text{Moles} = \frac{\text{grams}}{\text{formula weight (g/mol)}}$$

Since many experiments deal with very small quantities, a more convenient form of measurement is the millimole.

$$\text{Millimoles} = \frac{\text{milligrams}}{\text{formula weight (mg/mmol)}}$$

The millimole is 1/1000 of a mole

Note that…

g/mol is the same as mg/mmol

g/L is the same as mg/mL

mol/L is the same as mmol/mL

Example

Sulfur (S) is a nonmetallic element that is present in coal. When coal is burned, sulfur is converted to sulfur dioxide and eventually to sulfuric acid that gives rise to the acid rain phenomenon. How many atoms are in 16.3 g of S?

Solution

1 mol S = 32.07 g S

the conversion factor is $\frac{1 \text{ mol S}}{32.07 \text{ g S}}$

1 mol = 6.022 x 10^{23} particles (atoms)

the conversion factors are

$$\frac{6.022 \times 10^{23} \text{ S atoms}}{1 \text{ mol S}} \quad \text{and} \quad \frac{1 \text{ mol S}}{6.022 \times 10^{23} \text{ S atoms}}$$

$$16.3 \cancel{\text{g S}} \times \frac{1 \cancel{\text{mol S}}}{32.07 \cancel{\text{g S}}} \times \frac{6.022 \times 10^{23} \text{ S atoms}}{1 \cancel{\text{mol S}}} = 3.06 \times 10^{23} \text{ S atoms}$$

Example

How many hydrogen atoms are present in 25.6 g of urea [$(NH_2)_2CO$], which is used as a fertilizer, in animal feed, and in the manufacture of polymers? The molar mass of urea is 60.06 g/mol.

Solution

$$25.6 \text{ g } (NH_2)_2CO \times \frac{1 \text{ mol } (NH_2)_2CO}{60.06 \text{ g } (NH_2)_2CO} \times \frac{4 \text{ mol H}}{1 \text{ mol } (NH_2)_2CO} \times \frac{6.022 \times 10^{23} \text{ H atoms}}{1 \text{ mol H}}$$

$$= 1.03 \times 10^{24} \text{ H atoms}$$

Example

Find the number of moles and millimoles of benzoic acid (M = 122.1 g/mol) that are contained in 2.00 g of the pure acid.

Solution

$$\text{amount HBz} = n_{\text{HBz}} = 2.00 \text{ g HBz} \times \frac{1 \text{ mol HBz}}{122.1 \text{ g HBz}}$$

$$= 0.0164 \text{ mol HBz}$$

$$\text{amount HBz} = 2.00 \text{ g HBz} \times \frac{1 \text{ mmol HBz}}{0.1221 \text{ g HBz}} = 16.4 \text{ mmol HBz}$$

Example

What is the mass in grams of Na^+ (22.99 g/mol) in 25.0 g of Na_2SO_4 (142.0 g/mol)?

Solution

$$\text{amount } Na^+ = n_{Na^+} = \cancel{\text{mol } Na_2SO_4} \times \frac{2 \text{ mol } Na^+}{\cancel{\text{mol } Na_2SO_4}}$$

$$\text{amount } Na_2SO_4 = n_{Na_2SO_4} = 25.0 \cancel{\text{ g } Na_2SO_4} \times \frac{1 \text{ mol } Na_2SO_4}{142.0 \cancel{\text{ g } Na_2SO_4}}$$

$$\text{amount } Na^+ = n_{Na^+} = 25.0 \cancel{\text{ g } Na_2SO_4} \times \frac{1 \cancel{\text{ mol } Na_2SO_4}}{142.0 \cancel{\text{ g } Na_2SO_4}} \times \frac{2 \text{ mol } Na^+}{\cancel{\text{mol } Na_2SO_4}}$$

$$\text{mass } Na^+ = \cancel{\text{mol } Na^+} \times \frac{22.99 \text{ g } Na^+}{\cancel{\text{mol } Na^+}}$$

$$\text{mass } Na^+ = 25.0 \cancel{\text{ g } Na_2SO_4} \times \frac{1 \cancel{\text{ mol } Na_2SO_4}}{142.0 \cancel{\text{ g } Na_2SO_4}} \times \frac{2 \cancel{\text{ mol } Na^+}}{\cancel{\text{mol } Na_2SO_4}} \times \frac{22.99 \text{ g } Na^+}{\cancel{\text{mol } Na^+}}$$

$$= 8.10 \text{ g } Na^+$$

Example

Calculate the number of moles in 500 mg Na_2WO_4 (sodium tungstate).

Solution

$\mathcal{M}$ of the Na_2WO_4 = 293.8 g/mol
n = 1.7 x 10^{-3} mol

Example

What is the weight, in milligrams, of 0.250 mmol Fe_2O_3 (ferric oxide)?

Solution

$\mathcal{M}$ of the Fe_2O_3 = 159.7 g/mol
mass = 39.9 mg

How Do We Express Concentrations?

Solutions are **homogeneous** mixtures of two or more pure substances.

In a solution; the **solute** is dispersed uniformly throughout the **solvent**.

Component 1 (solute)	Component 2 (solvent)	State of Resulting solution	Examples
Gas	Gas	Gas	Air (N_2, O_2, Ar, CO_2…)
Gas	Liquid	Liquid	Soda water (CO_2 in water), O_2 in water
Gas	Solid	Solid	H_2 gas in palladium
Liquid	Liquid	Liquid	Ethanol in water
Liquid	Solid	Solid	Mercury in silver
Solid	Liquid	Liquid	Salt in water
Solid	Solid	Solid	Brass (Cu/Zn), Solder (Sn/Pb), Silver in gold

Solvent presents in the greater quantities and is used to dissolve the solute. All other substances are solutes. solutes present in smallest amount and is the substance dissolved in the solvent.

Ways of Expressing Concentration of Solutions

The **concentration** of a solution is the amount of solute present in a given amount of solvent, or a given amount of solution.

The concentration of a solution can be expressed either:
- **Qualitatively**
- **Quantitatively**

The terms **dilute** and **concentrated** are used to describe a solution qualitatively (unsaturated, saturated, and supersaturated solution).

Chemists use several different concentration units (different expressions), each of which has advantages as well as limitations;
- **Percent concentration**
- **Mole fraction**
- **Molar concentration (Molarity, *M*)**
- **Molal concentration (Molality, *m*)**
- **Normal concentration (Normality, *N*)**

Percent Concentration

Common Expressions (Mass vs. Volume)

- **Weight-to-Weight (wt/wt):** Mass of solute divided by mass of the total solution, multiplied by the scaling factor (e.g., 10^6 for ppm). Examples include mg/kg or µg/g.

$$\text{weight percent (w/w)} = \frac{\text{weight solute}}{\text{weight solution}} \times 100\%$$

- **Weight-to-Volume (wt/vol):** Mass of solute divided by the volume of the solution. Examples include mg/L (for ppm) or µg/L (for ppb).

$$\text{weight/volume percent (w/v)} = \frac{\text{weight solute, g}}{\text{volume solution, mL}} \times 100\%$$

- **Volume-to-Volume (vol/vol):** Volume of gaseous or liquid solute divided by the total volume of the sample, multiplied by the scaling factor. Examples include µL/L or nL/mL.

$$\text{volume percent (v/v)} = \frac{\text{volume solute}}{\text{volume solution}} \times 100\%$$

Weight percent is often used to express the concentration of commercial aqueous reagents. For example, nitric acid is sold as a 70% (w/w) solution, meaning that the reagent contains 70 g of HNO_3 per 100 g of solution.

Example: A solution of hydrochloric acid with 36% **HCl** by mass contains 36 g of **HCl** for each 100 g of solution.
Solute weight = 36 g
Solvent weight = 64 g
Total solution weight = 100 g

Volume percent is commonly used to specify the concentration of a solution prepared by diluting a pure liquid compound with another liquid. For example, a 5% (v/v) aqueous solution of methanol usually describes a solution prepared by diluting 5.0 mL of pure methanol with enough water to give 100 mL.

Weight or volume percent is often used to indicate the composition of dilute aqueous solutions of solid reagents. For example, 5% (w/v) aqueous silver nitrate often refers to a solution prepared by dissolving 5 g of silver nitrate in sufficient water to give 100 mL of solution.

Trace Concentrations

The concentrations of very dilute solution (trace and ultra-trace analysis) is usually analytical methods used to detect and/or quantify trace (very small amounts) of substances.

Common Units for Expressing Trace Concentrations

Unit		Abbreviation	wt / wt	wt / vol	vol / vol
Milligram percent	1 part of solute per 10^5 parts of the total solution	mg%	mg/100g	mg/100mL	
Parts per Million	1 part of solute per 10^6 parts of the total solution (10^{-4}%)	ppm	mg/kg µg/g	mg/L µg/mL	µL/L nL/mL
Parts per Billion	1 part of solute per 10^9 parts of the total solution (10^{-7}%)	ppb	µg/kg ng/g	µg/L ng/mL	nL/L pL/mL
Parts per Trillion	1 part of solute per 10^{12} parts of the total solution	ppt	ng/kg	ng/L	pL/L

Sometimes for this reason, these concentrations are written as ppmv or ppbv, and so on, indicating “by volume”.

1 ppm = 1000 ppb
1 ppb = 1000 ppt

Parts per Million (ppm)

$$\text{ppm of component} = \frac{\text{mass of component in soln}}{\text{total mass of soln}} \times 10^6$$

A solution whose solute concentration is 1 ppm contains 1 g of solute for each million (10^6) grams of solution.

This equivalent 1 mg of solute per kilogram of solution (**mg / kg**).

For aqueous solutions, because the density of water is 1 g/mL, this equivalent 1 mg of solute per liter of solution (**mg / L**).

The acceptable maximum concentrations of toxic or carcinogenic substances in the environment are often expressed in ppm or ppb. e.g., the maximum allowable concentration of arsenic in drinking water in USA is 0.010 ppm; that is 0.010 mg of arsenic per liter of water, this corresponds to 10 ppb.

ppm, ppb, and ppt expressions are very useful in trace and ultra-trace analyses.

Mole Fraction

$$\text{Mole fraction of component} = \frac{\text{moles of component}}{\text{total moles of all components}}$$

The symbol ***X*** is commonly used for mole fraction, with a subscript to indicate the component of interest.

$$X_A = \frac{\text{moles of A}}{\text{total moles in solution}}$$

For example; a solution containing 1.00 mol of HCl (36.5 g) and 8.00 mol water (144 g) has a mole fraction of HCl and water:

X_{HCl} = (1.00 mol) / (1.00 mol + 8.00 mol) = 0.111

X_{H2O} = (8.00 mol) / (1.00 mol + 8.00 mol) = 0.889 or 1.00 – 0.111 = 0.889

Mole fraction has no unit (the units in the numerator and the denominator cancel).
The sum of the mole fractions of all components of a solution must equal 1.

Molarity and Molality

The Molarity ***M*** of a solute in a solution is defined as:

$$\text{Molarity} = \frac{\text{moles solute}}{\text{liters soln}}$$

Molarity is the most widely used

Since volume is temperature-dependent, molarity can change with temperature.

The Molality ***m*** of a solution, defined as:

$$\text{Molality} = \frac{\text{moles of solute}}{\text{kilograms of solvent}}$$

Since both moles and mass do not change with temperature, molality (unlike molarity) is *not* temperature-dependent. Thus, molality is often the concentration unit of choice when a solution is to be used over a range of temperatures.

Normality

Normality (*N*) expresses the concentration of a solution in terms of equivalents of reactive species per liter of solution. Unlike molarity, it depends on the specific chemical reaction.

$$N = \frac{\text{equivalents of solute}}{\text{volume of solution (L)}}$$

$$\boldsymbol{N = M \times n}$$

where *n*-factor is the number of equivalents per mole in the particular reaction.

For **H_2SO_4** in a complete acid–base neutralization:

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

One mole of H_2SO_4 provides **2 equivalents of H^+**.

Therefore:

$$N = M \times 2$$

A **0.50 M H_2SO_4** solution has:

N = 0.50×2 = 1.0 N

Example

A sample of 0.892 g of potassium chloride (KCl) is dissolved in 54.6 g of water. What is the percent by mass of KCl in the solution?

Solution

$$\text{percent by mass of KCl} = \frac{\text{mass of solute}}{\text{mass of soln}} \times 100\%$$

$$= \frac{0.892\ \text{g}}{0.892\ \text{g} + 54.6\ \text{g}} \times 100\%$$

$$= 1.61\%$$

Example

Calculate the molar concentration of ethanol in an aqueous solution that contains 2.30 g of C_2H_5OH (46.07 g/mol) in 3.50 L of solution.

Solution

$$\text{amount } C_2H_5OH = n_{C_2H_5OH} = 2.30 \text{ g } \cancel{C_2H_5OH} \times \frac{1 \text{ mol } C_2H_5OH}{46.07 \text{ g } \cancel{C_2H_5OH}}$$

$$= 0.04992 \text{ mol } C_2H_5OH$$

$$c_{C_2H_5OH} = \frac{2.30 \text{ g } \cancel{C_2H_5OH} \times \dfrac{1 \text{ mol } C_2H_5OH}{46.07 \text{ g } \cancel{C_2H_5OH}}}{3.50 \text{ L}}$$

$$= 0.0143 \text{ mol } C_2H_5OH/\text{L} = 0.0143 \text{ M}$$

Example

(a) A solution is made by dissolving 13.5 g of glucose ($C_6H_{12}O_6$) in 0.100 kg of water. What is the mass percentage of solute in this solution?

(b) A 2.5 g sample of groundwater was found to contain 5.4 μg of Zn^{2+}. What is the concentration of Zn^{2+} in ppm?

Solution

(a) The mass percentage of water in this solution is (100 – 11.9)% = 88.1%.

$$\textbf{Solve: } \text{Mass \% of glucose} = \frac{\text{mass glucose}}{\text{mass soln}} \times 100 = \frac{13.5\ \text{g}}{13.5\ \text{g} + 100\ \text{g}} \times 100 = 11.9\%$$

(b) In this case we are given the number of micrograms of solute. Because 1 μg is 1 x 10^{-6} g, 5.4 μg = 5.4 x 10^{-6} g.

$$\textbf{Solve: } \text{ppm} = \frac{\text{mass of solute}}{\text{mass of soln}} \times 10^6 = \frac{5.4 \times 10^{-6}\ \text{g}}{2.5\ \text{g}} \times 10^6 = 2.2\ \text{ppm}$$

Example

What is the molar concentration of K^+ in a solution that contains 63.3 ppm of $K_3Fe(CN)_6$ (329.3 g/mol)?

Solution

Because the solution is so dilute, it is reasonable to assume that its density is 1.00 g/mL.

$$63.3 \text{ ppm } K_3Fe(CN)_6 = 63.3 \text{ mg } K_3Fe(CN)_6/L$$

$$\frac{\text{no. mol } K_3Fe(CN)_6}{L} = \frac{63.3 \text{ mg } K_3Fe(CN)_6}{L} \times \frac{1 \text{ g } K_3Fe(CN)_6}{1000 \text{ mg } K_3Fe(CN)_6}$$

$$\times \frac{1 \text{ mol } K_3Fe(CN)_6}{329.3 \text{ g } K_3Fe(CN)_6} = 1.922 \times 10^{-4} \frac{\text{mol}}{L}$$

$$= 1.922 \times 10^{-4} \text{ M}$$

$$[K^+] = \frac{1.922 \times 10^{-4} \text{ mol } K_3Fe(CN)_6}{L} \times \frac{3 \text{ mol } K^+}{1 \text{ mol } K_3Fe(CN)_6}$$

$$= 5.77 \times 10^{-4} \frac{\text{mol } K^+}{L} = 5.77 \times 10^{-4} \text{ M}$$

Example

Calculate the molar concentrations of 1 ppm solutions each of Li^+ and Pb^{2+}.

Solution

1 ppm = 1 mg/L

$$M_{Li} = \frac{1.00 \text{ mg Li/L} \times 10^{-3} \text{g/mg}}{6.94 \text{ g Li/mol}} = 1.44 \times 10^{-4} \text{ mol/L Li}$$

$$M_{Pb} = \frac{1.00 \text{ mg Pb/L} \times 10^{-3} \text{g/mg}}{207 \text{ g Pb/mol}} = 4.83 \times 10^{-6} \text{ mol/L Pb}$$

Because lead is much heavier than lithium, a given weight contains a smaller number of moles and its molar concentration is less

Example

Calculate the molality of a sulfuric acid solution containing 24.4 g of sulfuric acid in 198 g of water. The molar mass of sulfuric acid is 98.09 g.

Solution

$$\text{moles of } H_2SO_4 = 24.4 \text{ g } H_2SO_4 \times \frac{1 \text{ mol } H_2SO_4}{98.09 \text{ g } H_2SO_4}$$
$$= 0.249 \text{ mol } H_2SO_4$$

$$m = \frac{0.249 \text{ mol } H_2SO_4}{0.198 \text{ kg } H_2O}$$
$$= 1.26\ m$$

Example

Calculate the molality of a 35.4 percent (by mass) aqueous solution of phosphoric acid (H_3PO_4). The molar mass of phosphoric acid is 97.99 g.

Solution

Suppose that you start with a 100.0 g of the solution, then the mass of phosphoric acid is 35.4 percent, or 35.4 g, and mass of water must be 100.0% – 35.4% = 64.6% or 64.6 g.

$$\text{moles of } H_3PO_4 = 35.4 \text{ g } H_3PO_4 \times \frac{1 \text{ mol } H_3PO_4}{97.99 \text{ g } H_3PO_4}$$
$$= 0.361 \text{ mol } H_3PO_4$$

The mass of water is 64.6 g, or 0.0646 kg.

$$\text{molality} = \frac{0.361 \text{ mol } H_3PO_4}{0.0646 \text{ kg } H_2O}$$
$$= 5.59\ m$$

Example

The density of a 2.45 *M* aqueous solution of methanol (CH_3OH) is 0.976 g/mL. What is the molality of the solution? The molar mass of methanol is 32.04 g.

Solution

The total mass of 1 L of a 2.45 *M* solution of methanol is

$$1 \text{ L soln} \times \frac{1000 \text{ mL soln}}{1 \text{ L soln}} \times \frac{0.976 \text{ g}}{1 \text{ mL soln}} = 976 \text{ g}$$

Because this solution contains 2.45 moles of methanol, the amount of water (solvent) in the solution is

$$\begin{aligned} \text{mass of } H_2O &= \text{mass of soln} - \text{mass of solute} \\ &= 976 \text{ g} - \left(2.45 \text{ mol } CH_3OH \times \frac{32.04 \text{ g } CH_3OH}{1 \text{ mol } CH_3OH}\right) \end{aligned} \quad = 898 \text{ g}$$

$$\begin{aligned} \text{molality} &= \frac{2.45 \text{ mol } CH_3OH}{0.898 \text{ kg } H_2O} \\ &= 2.73 \, m \end{aligned}$$

Example

An aqueous solution of hydrochloric acid contains 36% HCl by mass. **(a)** Calculate the mole fraction of HCl in the solution. **(b)** Calculate the molality of HCl in the solution.

Solution

(a) To calculate the mole fraction of HCl, we convert the masses of HCl and H_2O to moles:

$$\text{Moles HCl} = (36\text{ g HCl})\left(\frac{1\text{ mol HCl}}{36.5\text{ g HCl}}\right) = 0.99\text{ mol HCl}$$

$$\text{Moles } H_2O = (64\text{ g } H_2O)\left(\frac{1\text{ mol } H_2O}{18\text{ g } H_2O}\right) = 3.6\text{ mol } H_2O$$

$$X_{HCl} = \frac{\text{moles HCl}}{\text{moles } H_2O + \text{moles HCl}} = \frac{0.99}{3.6 + 0.99} = \frac{0.99}{4.6} = 0.22$$

(b) To calculate the molality of HCl in the solution, We use the calculated number of moles of HCl in part (a), and the mass of solvent is 64 g = 0.064 kg:

$$\text{Molality of HCl} = \frac{0.99\text{ mol HCl}}{0.064\text{ kg } H_2O} = 15\ m$$

Example

A solution with a density of 0.876 g/mL contains 5.0 g of toluene (C_7H_8) and 225 g of benzene. Calculate the molarity and the molality of the solution.

Solution

The volume of the solution is obtained from the mass of the solution (mass of solute + mass of solvent = 5.0 g + 225 g = 230 g) and its density.

$$\text{Moles } C_7H_8 = (5.0 \text{ g } C_7H_8)\left(\frac{1 \text{ mol } C_7H_8}{92 \text{ g } C_7H_8}\right) = 0.054 \text{ mol}$$

The density of the solution is used to convert the mass of the solution to its volume:

$$\text{Milliliters soln} = (230 \text{ g})\left(\frac{1 \text{ mL}}{0.876 \text{ g}}\right) = 263 \text{ mL}$$

$$\text{Molarity} = \left(\frac{\text{moles } C_7H_8}{\text{liter soln}}\right) = \left(\frac{0.054 \text{ mol } C_7H_8}{263 \text{ mL soln}}\right)\left(\frac{1000 \text{ mL soln}}{1 \text{ L soln}}\right) = 0.21 \, M$$

Molality:

$$(0.054 \text{ mol } C_7H_8)/(0.225 \text{ kg solvent}) = 0.24 \, m$$

Example

Calculate the normality of a solution prepared by dissolving 4.90 g of H_2SO_4 in water and making the final volume 500 mL.

Solution

$$n = \frac{4.90}{98} = 0.050\ mol$$

$$M = \frac{0.050}{0.500} = 0.100\ M$$

$$N = M \times n\text{-factor}$$

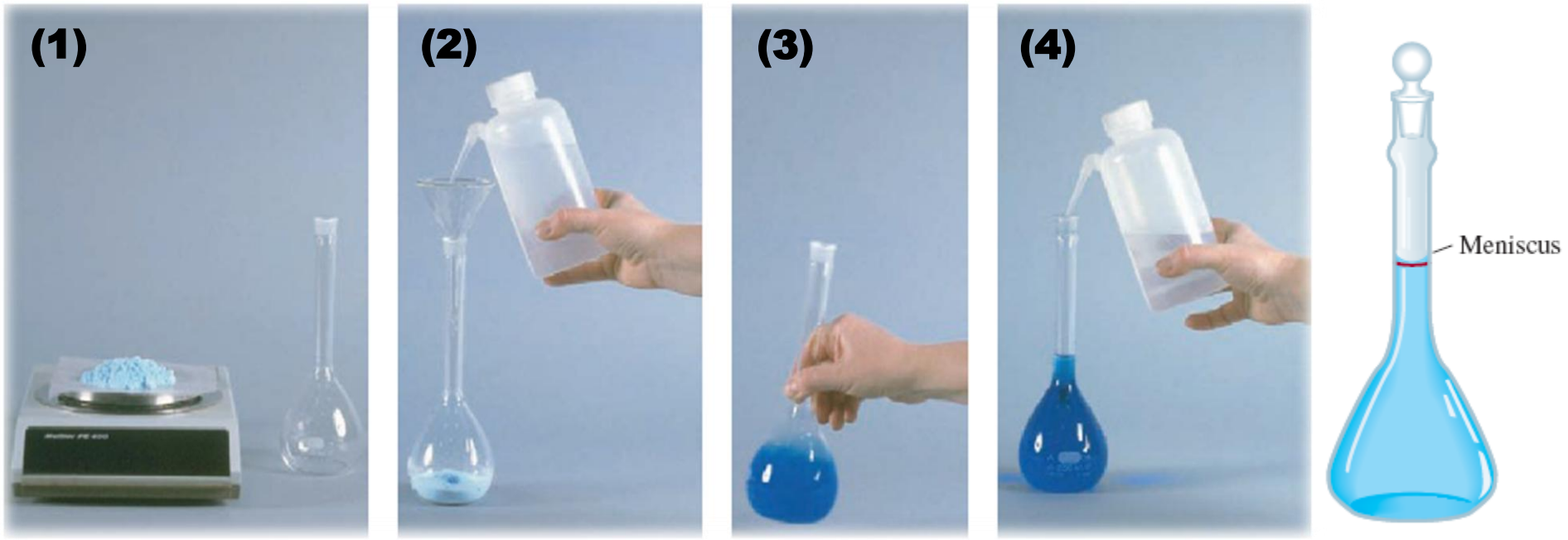
$$N = 0.100 \times 2 = \boxed{0.200\ N}$$

Alternative direct calculation

$$\text{Equivalent weight} = \frac{98}{2} = 49\ g/eq$$

$$N = \frac{4.90/49}{0.500} = \boxed{0.200\ N}$$

Preparation of Standard Solution



Procedure for preparation of 250 mL of 1.00 M solution of $CuSO_4$ ($\mathcal{M}$=159.5 g/mol).

0.25 mole of $CuSO_4$ (39.9 g) is weighed out and placed in the volumetric flask. Water is added to dissolve the salt, and the resultant solution is diluted to a total volume of 0.250 L. The molarity of the solution is:

M **= (0.250 mol $CuSO_4$) / (0.250 L soln) = 1.00 M**

Example

How many grams of potassium dichromate ($K_2Cr_2O_7$) are required to prepare a 250 mL solution whose concentration is 2.16 *M* ?

Solution

moles of solute = molarity x V soln. (L)

$$\text{moles of } K_2Cr_2O_7 = \frac{2.16 \text{ mol } K_2Cr_2O_7}{1 \cancel{\text{ L soln}}} \times 0.250 \cancel{\text{ L soln}}$$
$$= 0.540 \text{ mol } K_2Cr_2O_7$$

The molar mass of $K_2Cr_2O_7$ is 294.2 g, so

$$\text{grams of } K_2Cr_2O_7 \text{ needed} = 0.540 \cancel{\text{ mol } K_2Cr_2O_7} \times \frac{294.2 \text{ g } K_2Cr_2O_7}{1 \cancel{\text{ mol } K_2Cr_2O_7}}$$
$$= 159 \text{ g } K_2Cr_2O_7$$

Example

In a biochemical assay, a chemist needs to add 3.81 g of glucose to a reaction mixture. Calculate the volume in milliliters of a 2.53 *M* glucose solution that should be used for the addition.

Solution

The molar mass of $C_6H_{12}O_6$ is 180.2 g, so

$$3.81 \text{ g } \cancel{C_6H_{12}O_6} \times \frac{1 \text{ mol } C_6H_{12}O_6}{180.2 \text{ g } \cancel{C_6H_{12}O_6}} = 2.114 \times 10^{-2} \text{ mol } C_6H_{12}O_6$$

$$\begin{aligned} V &= \frac{n}{M} \\ &= \frac{2.114 \times 10^{-2} \text{ mol } C_6H_{12}O_6}{2.53 \text{ mol } C_6H_{12}O_6/\text{L soln}} \times \frac{1000 \text{ mL soln}}{1 \text{ L soln}} \\ &= 8.36 \text{ mL soln} \end{aligned}$$

Example

Describe the preparation of 2.00 L of 0.108 M $BaCl_2$ from $BaCl_2 \cdot 2H_2O$ (244.3 g/mol).

Solution

the mass of solute to be dissolved and diluted to 2.00 L,

$$2.00 \cancel{L} \times \frac{0.108 \text{ mol } BaCl_2 \cdot 2H_2O}{\cancel{L}} = 0.216 \text{ mol } BaCl_2 \cdot 2H_2O$$

The mass of $BaCl_2 \cdot 2H_2O$ is then

$$0.216 \cancel{\text{ mol } BaCl_2 \cdot 2H_2O} \times \frac{244.3 \text{ g } BaCl_2 \cdot 2H_2O}{\cancel{\text{mol } BaCl_2 \cdot 2H_2O}} = 52.8 \text{ g } BaCl_2 \cdot 2H_2O$$

Dissolve 52.8 g of $BaCl_2 \cdot 2H_2O$ in water and dilute to 2.00 L.

Example

Describe the preparation of 500 mL of 0.0740 M Cl^- solution from solid $BaCl_2 \cdot 2H_2O$ (244.3 g/mol).

Solution

$$\text{mass } BaCl_2 \cdot 2H_2O = \frac{0.0740 \text{ mol Cl}}{\text{L}} \times 0.500 \text{ L} \times \frac{1 \text{ mol } BaCl_2 \cdot 2H_2O}{2 \text{ mol Cl}}$$

$$\times \frac{244.3 \text{ g } BaCl_2 \cdot 2H_2O}{\text{mol } BaCl_2 \cdot 2H_2O} = 4.52 \text{ g } BaCl_2 \cdot 2H_2O$$

Dissolve 4.52 g of $BaCl_2 \cdot 2H_2O$ in water and dilute to 500 mL.

Dilution of Solutions

Concentrated solutions are often stored in the laboratory for use as needed; "**stock**" solutions are frequently diluted before working with them.

Dilution is the procedure for preparing a less concentrated solution from a more concentrated one.

Two potassium permanganate ($KMnO_4$) solutions of different concentrations

moles of solute before dilution = moles of solute after dilution

$$\underset{\text{moles of solute before dilution}}{M_i V_i} = \underset{\text{moles of solute after dilution}}{M_f V_f}$$

where M_i and M_f are the initial and final concentrations of the solution in molarity and V_i and V_f are the initial and final volumes of the solution, respectively.

The units of V_i and V_f must be the same (mL or L) for the calculation to work.

$M_i > M_f$ and $V_f > V_i$

Example

Describe how you would prepare 5.00 x 10^2 mL of a 1.75 *M* H_2SO_4 solution, starting with an 8.61 *M* stock solution of H_2SO_4.

Solution

$$M_i = 8.61\ M \qquad M_f = 1.75\ M$$
$$V_i = ? \qquad V_f = 5.00 \times 10^2\ \text{mL}$$

$$(8.61\ M)(V_i) = (1.75\ M)(5.00 \times 10^2\ \text{mL})$$
$$V_i = \frac{(1.75\ M)(5.00 \times 10^2\ \text{mL})}{8.61\ M}$$
$$= 102\ \text{mL}$$

Thus, we must dilute 102 mL of the 8.61 *M* H_2SO_4 solution with sufficient water to give a final volume of 5.00 x 10^2 mL in a 500 mL volumetric flask to obtain the desired concentration.

Example

How many milliliters of 3.0 *M* H_2SO_4 are needed to make 450 mL of 0.10 *M* H_2SO_4?

Solution

Calculating the moles of H_2SO_4 in the dilute solution:

$$\text{moles } H_2SO_4 \text{ in dilute solution} = (0.450 \text{ L soln})\left(\frac{0.10 \text{ mol } H_2SO_4}{1 \text{ L soln}}\right)$$

$$= 0.045 \text{ mol } H_2SO_4$$

Calculating the volume of the concentrated solution that contains 0.045 mol H_2SO_4:

$$\text{L conc soln} = (0.045 \text{ mol } H_2SO_4)\left(\frac{1 \text{ L soln}}{3.0 \text{ mol } H_2SO_4}\right) = 0.015 \text{ L soln}$$

Converting liters to milliliters gives 15 mL.
If we apply dilution low, we get the same result:

$$(3.0\ M)(V_{conc}) = (0.10\ M)(450 \text{ mL})$$

$$(V_{conc}) = \frac{(0.10\ M)(450 \text{ mL})}{3.0\ M} = 15 \text{ mL}$$

Either way, we see that if we start with 15 mL of 3.0 M H_2SO_4 and dilute it to a total volume of 450 mL, the desired 0.10 M solution will be obtained.

Example

You wish to prepare a calibration curve for the spectrophotometric determination of permanganate. You have a stock 0.100 M solution of $KMnO_4$ and a series of 100 mL volumetric flasks. What volumes of the stock solution will you have to pipet into the flasks to prepare standards of 1.00, 2.00, 5.00, and 10.0×10^{-3} M $KMnO_4$ solutions?

Solution

$\mathbf{C_1V_1 = C_2V_2}$

$0.100\ M \times V_1\ mL = 1.00 \times 10^{-3}\ M \times 100\ mL$

$V_1 = 1.00\ mL$

Similarly, for the other solutions we will need 2.00, 5.00, and 10.0 mL of the stock solution, which will be diluted to 100 mL

p-Functions

Scientists frequently express the concentration of a species in terms of its p-function, or p-value. The p-value is the negative logarithm (to the base 10) of the molar concentration of that species. Thus, for the species X,

$$\mathbf{pX = -\log [X]}$$

p-Values offer the advantage of allowing concentrations that vary over ten or more orders of magnitude to be expressed in terms of small positive numbers.

The best-known p-function is pH, which is the negative logarithm of $[H^+]$.

$pH = -\log [H^+]$

Example

Calculate the p-value for each ion in a solution that is 2.00×10^{-3} M in NaCl and 5.4×10^{-4} M in HCl.

Solution

$pH = -\log [H^+] = -\log (5.4 \times 10^{-4}) = 3.27$

To obtain pNa, we write
$pNa = -\log[Na^+] = -\log (2.00 \times 10^{-3}) = -\log (2.00 \times 10^{-3}) = 2.699$

The total Cl^- concentration is given by the sum of the concentrations of the two solutes:
$[Cl^-] = (2.00 \times 10^{-3}) + (5.4 \times 10^{-4})$
$= 2.54 \times 10^{-3}$ M
$pCl = -\log[Cl^-] = -\log (2.54 \times 10^{-3}) = 2.595$

Example

Calculate the molar concentration of Ag^+ in a solution that has a pAg of 6.372.

Solution

$pAg = -\log [Ag^+] = 6.372$

$\log [Ag^+] = -6.372$

anti-log
$[Ag^+] = 10^{-6.372}$
$[Ag^+] = 4.25 \times 10^{-7}$ M

Density and Specific Gravity of Solutions

Density expresses the mass of a substance per unit volume.

$$\text{Density} = \frac{\text{mass}}{\text{volume}}$$

The SI-derived unit for density is the kilogram per cubic meter (kg/m^3).

This unit is awkwardly large for most chemical applications. Therefore, grams per cubic centimeter (g/cm^3) and its equivalent, grams per milliliter (g/mL), are more commonly used for solid and liquid densities.

$$1\ g/cm^3 = 1\ g/mL = 1000\ kg/m^3$$

Because gas densities are often very low, we express them in units of grams per liter (g/L):

$$1\ g/L = 0.001\ g/mL$$

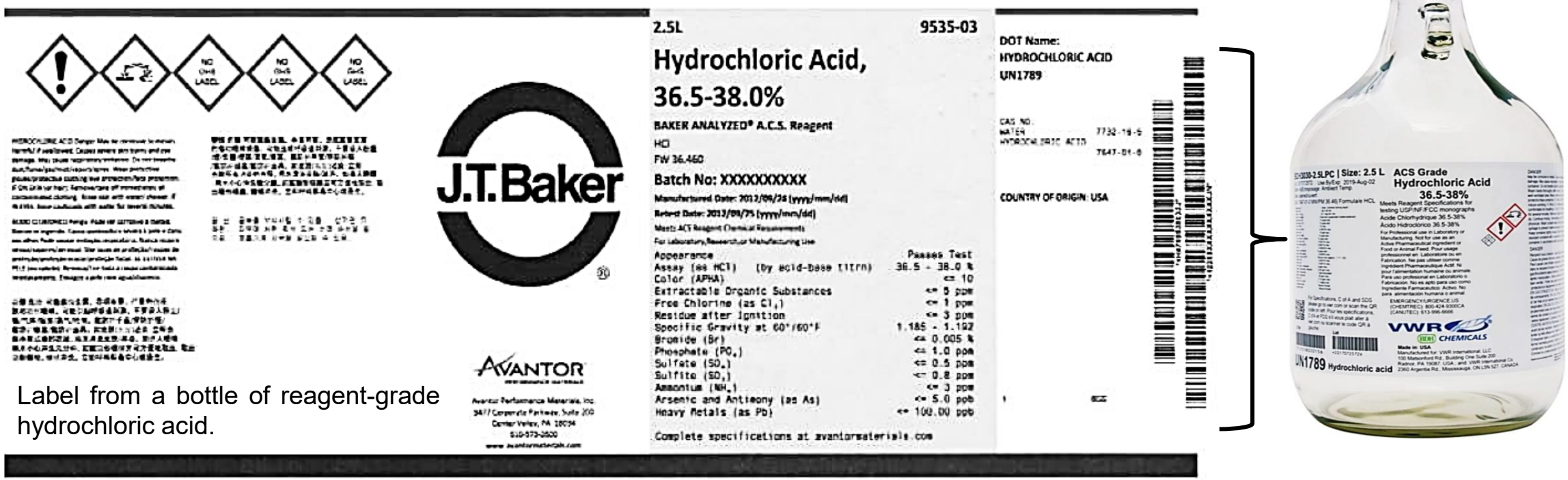
Specific gravity is the ratio of the mass of a substance to the mass of an equal volume of water.

Specific gravities of commercial concentrated acids and bases

Reagent	Concentration, % (w/w)	Specific Gravity
Acetic acid	99.7	1.05
Ammonia	29.0	0.90
Hydrochloric acid	37.2	1.19
Hydrofluoric acid	49.5	1.15
Nitric acid	70.5	1.42
Perchloric acid	71.0	1.67
Phosphoric acid	86.0	1.71
Sulfuric acid	96.5	1.84

Example

Describe the preparation of 100 mL of 6.0 M HCl from a concentrated solution that has a specific gravity of 1.18 and is 37% (w/w) HCl (36.5 g/mol).



Label from a bottle of reagent-grade hydrochloric acid.

Solution

The concentration of the reagent,

$$c_{HCl} = \frac{1.18 \times 10^3 \text{ g reagent}}{\text{L reagent}} \times \frac{37 \text{ g HCl}}{100 \text{ g reagent}} \times \frac{1 \text{ mol HCl}}{36.5 \text{ g HCl}} = 12.0 \text{ M}$$

The volume of concentrated reagent,

$M_1V_1 = M_2V_2$

$12 \times V_1 = 6 \times 100$

$V_1 = 50$ mL

Example

Calculate the molar concentration of HNO_3 (63.0 g/mol) in a solution that has a specific gravity of 1.42 and is 70.5% HNO_3 (w/w).

Solution

70.5% HNO_3 mass by mass
Suppose the mass of solution = 100 g

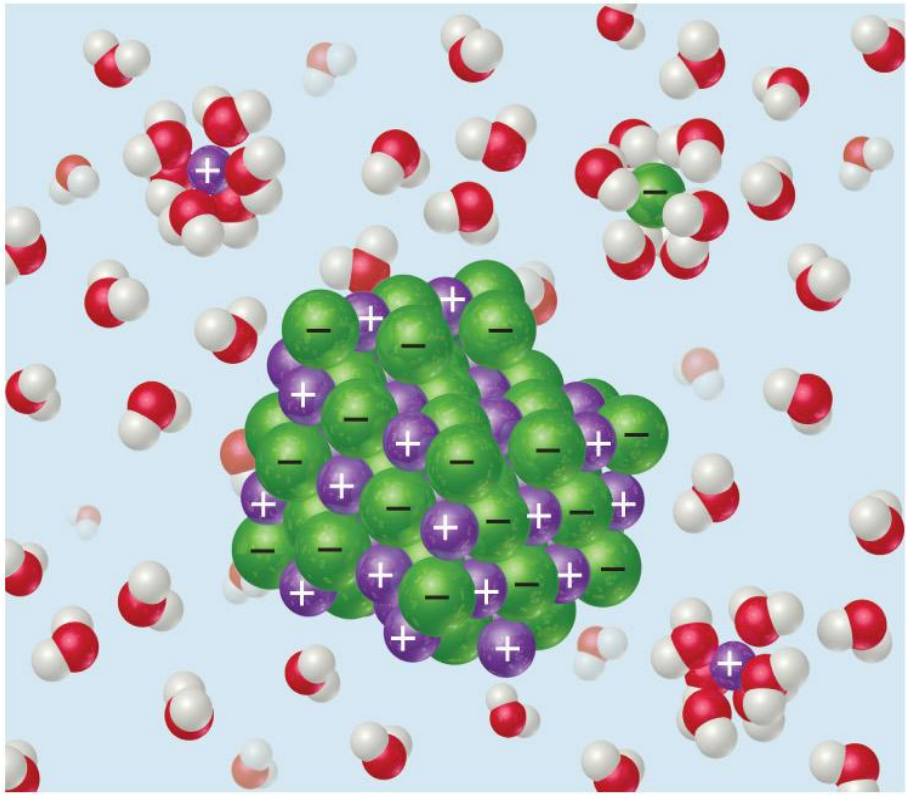
Mass HNO_3 = 70.5 g,
mole HNO_3 = 70.5 / 63.0 = 1.119 mole

To calculate M
Mass of solution = 100 g
d = m / v then, v = 100 / 1.42 = 70.42 mL

M = n (solute) / v (soln, L) = 1.119 / 0.07042 = 15.89 M

Or directly,,,
M = (assay x density x 10) / molar mass = (70.5 x 1.42 x 10) / 63.0 = 15.89 mol/L

Expressing the Concentration of an Electrolyte



-When an ionic substance dissolves in water, the solvent pulls the individual ions from the crystal and solvates them.

-This process is called **dissociation**.

-An **electrolyte** is a substances that dissociates into ions when dissolved in water.

-A **nonelectrolyte** may dissolve in water, but it does not dissociate into ions when it does so.

Strong and Weak Electrolytes

A **strong electrolyte** dissociates completely when dissolved in water (soluble ionic salts, strong acids and strong bases).
For example:

A **weak electrolyte** only dissociates partially when dissolved in water (produce a small concentration of ions when they dissolve, these ions exist in *equilibrium* with the unionized substance).
For example:

When an ionic compound dissolves, the relative concentrations of the ions introduced into the solution depend on the chemical formula of the compound.

For example, a 1.0 M solution of NaCl is 1.0 M in Na^+ ions and 1.0 M in Cl^- ions. Similarly, a 1.0 M solution of Na_2SO_4 is 2.0 M in Na^+ ions and 1.0 M in SO_4^{-2} ions

Molarity refers only to the amount of solute originally dissolved in water and does not take into account any **subsequent processes**, such as the **dissociation** of a salt or the ionization of an acid.

Consider what happens when a sample of potassium chloride (KCl) is dissolved in enough water to make a 1 *M* solution:

$$KCl(s) \xrightarrow{H_2O} K^+(aq) + Cl^-(aq)$$

Because KCl is a **strong electrolyte**, it undergoes complete dissociation in solution. Thus, a 1 *M* KCl solution contains 1 mole of K^+ ions and 1 mole of Cl^- ions, and no KCl units are present.

The concentrations of the ions can be expressed as $[K^+] = 1\ M$ and $[Cl^-] = 1\ M$.

Similarly, in a 1 *M* barium nitrate [$Ba(NO_3)_2$] solution

$$Ba(NO_3)_2(s) \xrightarrow{H_2O} Ba^{2+}(aq) + 2NO_3^-(aq)$$

we have $[Ba^{2+}] = 1\ M$ and $[NO_3^-] = 2\ M$ and no $Ba(NO_3)_2$ units at all.

Example

What are the molar concentrations of each of the ions present in a 0.025 *M* aqueous solution of calcium nitrate? ($Ca(NO_3)_2$)

Solution

$Ca(NO_3)_2$ composed of two NO_3^- ions for each Ca^{2+} ion in the compound, each mole of $Ca(NO_3)_2$ that dissolves dissociates into 1 mol of Ca^{2+} and 2 mol of NO_3^-.

Thus, a solution that is 0.025 *M* in $Ca(NO_3)_2$ is 0.025 *M* in Ca^{2+} and $2 \times 0.025\ M = 0.050\ M$ in NO_3^-:

$$\frac{\text{mol } NO_3^-}{\text{L}} = \left(\frac{0.025\ \text{mol } Ca(NO_3)_2}{\text{L}}\right)\left(\frac{2\ \text{mol } NO_3^-}{1\ \text{mol } Ca(NO_3)_2}\right) = 0.050\ M$$

The concentration of NO^{3-} ions is twice that of Ca^{2+} ions, as the subscript 2 after the NO^{3-} in the chemical formula $Ca(NO_3)_2$ suggests it should be.

Chemical Stoichiometry

How much product will be formed from specific amounts of starting materials (reactants)?

How much starting material must be used to obtain a specific amount of product?

Stoichiometry is the quantitative study of reactants and products in a chemical reaction.

To interpret a reaction quantitatively, we need to apply our knowledge of molar masses and the mole concept.

Mole method means that the stoichiometric coefficients in a chemical equation can be interpreted as the number of moles of each substance.

Stoichiometry deals with the ratios in which chemicals reacts

Law of Conservation of Mass

"We may lay it down as an incontestable axiom that, in all the operations of art and nature, nothing is created; an equal amount of matter exists both before and after the experiment. Upon this principle, the whole art of performing chemical experiments depends."
-- **Antoine Lavoisier**.

Atoms are neither created nor destroyed during any chemical reaction. The changes that occur during any reaction merely rearrange the atoms. The same collection of atoms is present both before and after the reaction.
-- **Dalton's atomic theory**.

What happens when hydrogen gas (H_2) burns in air (which contains oxygen, O_2) to form water (H_2O). This reaction can be represented by the chemical equation

$$H_2 + O_2 \longrightarrow H_2O$$

To conform with the **law of conservation of mass**, there must be the same number of each type of atom on both sides of the arrow (we should balance the equation).

$2H_2$	+ O_2	$\longrightarrow$	$2H_2O$
Two molecules	+ one molecule	$\longrightarrow$	two molecules
2 moles	+ 1 mole	$\longrightarrow$	2 moles
$2(2.02\ g) = 4.04\ g + 32.00\ g$		$\longrightarrow$	$2(18.02\ g) = 36.04\ g$
36.04 g reactants			36.04 g product

Stoichiometric Calculations

For the following general reaction:

$$A + 2\,B \rightarrow 3\,C + \tfrac{1}{2}\,D$$

$$\text{mol A} = \frac{\text{mol B}}{2} = \frac{\text{mol C}}{3} = 2\ \text{mol D}$$

Note…
Limiting and excess reactants criteria should be applied

Example

The food we eat is degraded, or broken down, in our bodies to provide energy for growth and function. A general overall equation for this very complex process represents the degradation of glucose ($C_6H_{12}O_6$) to carbon dioxide (CO_2) and water (H_2O):

$$C_6H_{12}O_6 + 6O_2 \longrightarrow 6CO_2 + 6H_2O$$

If 856 g of $C_6H_{12}O_6$ is consumed by a person over a certain period, what is the mass of CO_2 produced?

grams of $C_6H_{12}O_6$ $\longrightarrow$ moles of $C_6H_{12}O_6$ $\longrightarrow$ moles of CO_2 $\longrightarrow$ grams of CO_2

$$856 \text{ g } C_6H_{12}O_6 \times \frac{1 \text{ mol } C_6H_{12}O_6}{180.2 \text{ g } C_6H_{12}O_6} = 4.750 \text{ mol } C_6H_{12}O_6$$

$$4.750 \text{ mol } C_6H_{12}O_6 \times \frac{6 \text{ mol } CO_2}{1 \text{ mol } C_6H_{12}O_6} = 28.50 \text{ mol } CO_2$$

$$28.50 \text{ mol } CO_2 \times \frac{44.01 \text{ g } CO_2}{1 \text{ mol } CO_2} = 1.25 \times 10^3 \text{ g } CO_2$$

$$\text{mass of } CO_2 = 856 \text{ g } C_6H_{12}O_6 \times \frac{1 \text{ mol } C_6H_{12}O_6}{180.2 \text{ g } C_6H_{12}O_6} \times \frac{6 \text{ mol } CO_2}{1 \text{ mol } C_6H_{12}O_6} \times \frac{44.01 \text{ g } CO_2}{1 \text{ mol } CO_2}$$

$$= 1.25 \times 10^3 \text{ g } CO_2$$

Example

All alkali metals react with water to produce hydrogen gas and the corresponding alkali metal hydroxide. A typical reaction is that between lithium and water:

$$2\text{Li}(s) + 2\text{H}_2\text{O}(l) \longrightarrow 2\text{LiOH}(aq) + \text{H}_2(g)$$

How many grams of Li are needed to produce 9.89 g of H_2?

$$\text{grams of } \text{H}_2 \longrightarrow \text{moles of } \text{H}_2 \longrightarrow \text{moles of Li} \longrightarrow \text{grams of Li}$$

$$9.89 \text{ g } \text{H}_2 \times \frac{1 \text{ mol } \text{H}_2}{2.016 \text{ g } \text{H}_2} \times \frac{2 \text{ mol Li}}{1 \text{ mol } \text{H}_2} \times \frac{6.941 \text{ g Li}}{1 \text{ mol Li}} = 68.1 \text{ g Li}$$

Example

(a) What mass of $AgNO_3$ (169.9 g/mol) is needed to convert 2.33 g of Na_2CO_3 (106.0 g/mol) to Ag_2CO_3?
(b) What mass of Ag_2CO_3 (275.7 g/mol) will be formed?

Solution

$$Na_2CO_3(aq) + 2AgNO_3(aq) \rightarrow Ag_2CO_3(s) + 2NaNO_3(aq)$$

(a)

$$\text{amount } Na_2CO_3 = n_{Na_2CO_3} = 2.33 \text{ g } \cancel{Na_2CO_3} \times \frac{1 \text{ mol } Na_2CO_3}{106.0 \text{ g } \cancel{Na_2CO_3}}$$
$$= 0.02198 \text{ mol } Na_2CO_3$$

$$\text{amount } AgNO_3 = n_{AgNO_3} = 0.02198 \text{ } \cancel{\text{mol } Na_2CO_3} \times \frac{2 \text{ mol } AgNO_3}{1 \text{ } \cancel{\text{mol } Na_2CO_3}}$$
$$= 0.04396 \text{ mol } AgNO_3$$

$$\text{mass } AgNO_3 = 0.04396 \text{ } \cancel{\text{mol } AgNO_3} \times \frac{169.9 \text{ g } AgNO_3}{\cancel{\text{mol } AgNO_3}} = 7.47 \text{ g } AgNO_3$$

(b)

$$\text{amount } Ag_2CO_3 = \text{amount } Na_2CO_3 = 0.02198 \text{ mol}$$

$$\text{mass } Ag_2CO_3 = 0.02198 \text{ } \cancel{\text{mol } Ag_2CO_3} \times \frac{275.7 \text{ g } Ag_2CO_3}{\cancel{\text{mol } Ag_2CO_3}} = 6.06 \text{ g } Ag_2CO_3$$

Example

What mass of Ag_2CO_3 (275.7 g/mol) is formed when 25.0 mL of 0.200 M $AgNO_3$ are mixed with 50.0 mL of 0.0800 M Na_2CO_3?

Solution

$Na_2CO_3(aq) + 2AgNO_3(aq) \rightarrow Ag_2CO_3(s) + 2NaNO_3(aq)$

The initial amounts of reactants are:

$$\text{amount } AgNO_3 = n_{AgNO_3} = 25.0 \text{ mL } \cancel{AgNO_3} \times \frac{1 \text{ L } \cancel{AgNO_3}}{1000 \text{ mL } \cancel{AgNO_3}} \times \frac{0.200 \text{ mol } AgNO_3}{\text{L } \cancel{AgNO_3}} = 5.00 \times 10^{-3} \text{ mol } AgNO_3$$

$$\text{amount } Na_2CO_3 = n_{Na_2CO_3} = 50.0 \text{ mL } \cancel{Na_2CO_3 \text{ soln}} \times \frac{1 \text{ L } \cancel{Na_2CO_3}}{1000 \text{ mL } \cancel{Na_2CO_3}} \times \frac{0.0800 \text{ mol } Na_2CO_3}{\text{L } \cancel{Na_2CO_3}} = 4.00 \times 10^{-3} \text{ mol } Na_2CO_3$$

Because 1 mole of Na_2CO_3 is only needed to react with 2 mole $AgNO_3$
$AgNO_3$ is the **limiting reactant**

$$\text{mass } Ag_2CO_3 = 5.00 \times 10^{-3} \text{ } \cancel{\text{mol } AgNO_3} \times \frac{1 \text{ } \cancel{\text{mol } Ag_2CO_3}}{2 \text{ } \cancel{\text{mol } AgNO_3}} \times \frac{275.7 \text{ g } Ag_2CO_3}{\cancel{\text{mol } Ag_2CO_3}} = 0.689 \text{ g } Ag_2CO_3$$


Thank You!