Chapter 2: Calculations Used in Analytical Chemistry

Quantitative Chemical Analysis
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Chapter 2
Calculation Used in Analytical Chemistry

- **Some Important Units of Measurement**

SI units: Scientists throughout the world have adopted a standardized system of units known as the **International System of Units** or **SI units**. The system is based on metric system (such as Mass: kg; Length: m; Time: s; Temperature: K; Amount of substance: mol; Electric current: A etc.). Other units are derived from the base units.

TABLE 4-1

SI Base Units

Physical Quantity	Name of Unit	Abbreviation
Mass	kilogram	kg
Length	meter	m
Time	second	s
Temperature	kelvin	K
Amount of substance	mole	mol
Electric current	ampere	A
Luminous intensity	candela	cd

Prefixes are used with the base units and other derived units to express small or large measured quantities in terms of a few simple digits (such as giga: 10^9; mega: 10^6; Kilo: 10^3; deci: 10^{-1}; centi: 10^{-2}: milli: 10^{-3}; micro: 10^{-6}; nano: 10^{-9}; pico: 10^{-12}; femto: 10^{-15}; atto: 10^{-18} etc.).

The Mole: The mole is the SI unit for the amount of chemical species. The mole is associated with a chemical formula and Avogadro's number (6.022×10^{23}) of particles. The molar mass (M) of a substance is the mass in grams of one mole of the substance. Molar masses are calculated by summing the atomic masses of all the elements appearing in a chemical formula.

TABLE 4-2

Prefixes for Units

Prefix	Abbreviation	Multiplier
yotta-	Y	10^{24}
zetta-	Z	10^{21}
exa-	E	10^{18}
peta-	P	10^{15}
tera-	T	10^{12}
giga-	G	10^{9}
mega-	M	10^{6}
kilo-	k	10^{3}
hecto-	h	10^{2}
deca-	da	10^{1}
deci-	d	10^{-1}
centi-	c	10^{-2}
milli-	m	10^{-3}
micro-	μ	10^{-6}
nano-	n	10^{-9}
pico-	p	10^{-12}
femto-	f	10^{-15}
atto-	a	10^{-18}
zepto-	z	10^{-21}
yocto-	y	10^{-24}

Molar Mass of **formaldehyde** CH_2O

$$M_{CH_2O}$$

$$= \frac{1 mol C}{mol CH_2O} \times \frac{12.0 g}{mol C} + \frac{2 mol H}{mol CH_2O} \times \frac{1.0 g}{mol H} + \frac{1 mol O}{mol CH_2O} \times \frac{16.0 g}{mol O}$$

$$= 30.0 g / mol CH_2O$$

Molar Mass of **glucose** $C_6H_{12}O_6$

$$M_{C_6H_{12}O_6}$$

$$= \frac{6 mol C}{mol C_6H_{12}O_6} \times \frac{12.0 g}{mol C} + \frac{12 mol H}{mol C_6H_{12}O_6} \times \frac{1.0 g}{mol H} + \frac{6 mol O}{mol C_6H_{12}O_6} \times \frac{16.0 g}{mol O}$$

$$= 180.0 g / mol C_6H_{12}O_6$$

Thus, 1mol of formaldehyde has a mass of 30.0 g and 1mol of glucose has a mass of 180.0 g.

Mass and Weight:

Mass : is an invariant measure of the amount of matter in an object.

Weight: is the force of attraction between an object and earth.

The weight of an object depends on the location because gravitational attraction varies with geographic location. The mass of an object remains constant regardless of locations.

A chemical analysis is always **based on mass** so that the results will not depend on locality.

The Millimole: The millimole (mmol) is 1/1000 of a mole. Sometimes it is more convenient to make calculations with millimoles (mmol) rather than mole. The mass in grams of a millimole of a substance is known as the millimolar mass which is 1/1000 of the molar mass

$$1 \text{ m mol} = 10^{-3} \text{ mol}$$

Example 1: Determine the number of moles and millimoles of benzoic acid (HBz) (Molar mass = 122.1 g/mol) in 2.00 g of the pure acid.

Amount of HBz = 2.00 g x (1 mol HBz)/(122.1 g HBz) = 0.0164 mol HBz.

millimolar mass = 0.1221 g/mmol

Amount of HBz = 2.00 g HBz x (1 mmol HBz)/(0.1221 g HBz) = 16.4 mmol HBz.

Example 2: Determine the mass in grams of Na^+ (22.99 g/mol) in 25.0 g of Na_2SO_4(142.0 g/mol).

$$\text{Amount fo } Na^+ = 25.0 \text{ g } Na_2SO_4 \times \frac{1 \text{ mol } Na_2SO_4}{142.0 \text{ g } Na_2SO_4}$$

$$\times \frac{2 \text{ mol } Na^+}{1 \text{ mol } Na_2SO_4} \times \frac{22.99 \text{ g } Na^+}{1 \text{ mol } Na^+}$$

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

SOLUTIONS AND THEIR CONCENTRATIONS

- Chemists express the concentration of species in solution in several ways. The most important ways are described in this section.

Molar Concentration: The molar concentration of a solution is the number of moles of the solute species that is contained in one liter of the solution. Molar concentration or molarity M, has the dimensions of **mol L^{-}.** Molarity is also equal to the number of millimoles of a solute per milliliter of solution.

Molarity = M = (no. mol solute)/(no. L solution)

= (no. mmol solute)/(no. mL solution)

= n/v

Example 3: 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.

Moles of ethanol = amount of C_2H_5OH

= 2.30 g x (1 mol)/(46.07 g)

= 0.04992 mol C_2H_5OH

Molar concentration (M) = (moles ethanol)/(volume)

= (0.04992 mol)/(3.50 L)

= 0.0143 mol C_2H_5OH/L

= 0.0143 M

Analytical Molarity: The analytical molarity of a solution gives the total number of moles of a solute in 1L of the solution (or total number of millimoles in 1 mL). A 1.0 M H_2SO_4 can be prepared by dissolving 1.0 mol or 98 g of H_2SO_4 in water and diluting to exactly 1.0 L.

Equilibrium Molarity: The equilibrium molarity or species molarity express the molar concentration of a particular species in a solution at equilibrium. The equilibrium molarity of H_2SO_4 in a solution with an analytical concentration of 1.0 M is 0.0 M because H_2SO_4 is entirely dissociated, there are no H_2SO_4 molecules as such in this solution.

Example 4: Calculate the analytical and equilibrium molar concentrations of the solute species in an aqueous solution that contains 285 mg of trichloroacetic acid (HA), Cl_3CCOOH (163.4 g/mol) in 10.0 mL. Trichloroacetic acid (HA) is 73% ionized in water.

Amount of HA = 285 mg HA x (1g HA)/(1000 mg HA) x (1 mol HA)/163.4 g HA)

= 1.744×10^{-3} mol HA

Molar analytical concentration

= (1.744×10^{-3} mol)/(10.0 mL) x (1000 mL)/1L

= 0.174 mol/L = 0.174 M

…Continued…

73% of HA dissociates giving H^+ and A^-

$$HA \rightleftharpoons H^+ + A^-$$

[HA] = 0.174 M x (100-73)/100

= 0.174 x 0.27 M = 0.047 M

[A-] = 0.174 M x 73/100 = 0.127 M

One mol H^+ is formed for each mol A^-.

Therefore, $[H^+]=[A^-]$ = 0.127 M

Percent concentration % : Concentration can be expressed in terms of percent (parts per hundred). Percent composition can be expressed in three different methods:

Weight percent (w/w)

= (weight solute)/(weight solution) x 100 %

Volume percent (v/v)

= (volume solute)/(volume solution) x 100%

Weight/Volume percent (w/v)

=(weight solute, g)/(volume solution, mL) x 100%

Parts Per Million and Parts Per Billion: For very dilute solutions, parts per million (ppm) is a convenient way to express concentration.

C_{ppm} = (mass of solute)/(mass of solution) x 10^6 ppm

where, C_{ppm} is the concentration in parts per million.

For even more dilute solution parts per billion is used

C_{ppb} =(mass of solute)/(mass of solution) x 10^9 ppb

Table 2.4 Common Units for Reporting Concentration

Name	Units	Symbol
molarity	$\frac{\text{moles solute}}{\text{liters solution}}$	M
formality	$\frac{\text{moles solute}}{\text{liters solution}}$	F
normality	$\frac{\text{equivalents solute}}{\text{liters solution}}$	N
molality	$\frac{\text{moles solute}}{\text{kilograms solvent}}$	m
weight percent	$\frac{\text{grams solute}}{\text{100 grams solution}}$	% w/w
volume percent	$\frac{\text{mL solute}}{\text{100 mL solution}}$	% v/v
weight-to-volume percent	$\frac{\text{grams solute}}{\text{100 mL solution}}$	% w/v
parts per million	$\frac{\text{grams solute}}{10^6 \text{ grams solution}}$	ppm
parts per billion	$\frac{\text{grams solute}}{10^9 \text{ grams solution}}$	ppb

Density

The density of a substance is its mass per unit volume. Density is expressed in units of kg/L or g/mL.

Density = mass / volume

Specific Gravity

Specific gravity is the ratio of its mass to the mass of an equal volume of water at $4^{o}C$. Specific gravity is dimensionless.

Example 10: 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% HNO_3 (w/w).

$$\frac{\text{g } HNO_3}{\text{L - reagent}} = \frac{1.42 \text{ kg reagent}}{\text{L reagent}} \times \frac{10^3 \text{ g reagent}}{\text{kg reagent}} \times \frac{70 \text{ g } HNO_3}{100 \text{ g reagent}}$$

$$= \frac{994 \text{ g} HNO_3}{\text{L reagent}}$$

$$\text{Molar concentration} = \frac{994 \text{ g } HNO_3}{\text{L reagent}} \times \frac{1 \text{ mol } HNO_3}{63.0 \text{ g } HNO_3}$$

$$= 15.8 \text{ M}$$

Dilutions: Explanations and Examples of Common Methods

There are many ways of expressing concentrations and dilution. The following is a brief explanation of some ways of calculating dilutions that are common in biological science and often used at Biosciences.

Using $C_1V_1 = C_2V_2$

To make a fixed amount of a dilute solution from a stock solution, you can use the formula: $C_1V_1 = C_2V_2$ where:

V_1 = Volume of stock solution needed to make the new solution
C_1 = Concentration of stock solution
V_2 = Final volume of new solution
C_2 = Final concentration of new solution

Example: Make 5 mL of a 0.25 M solution from a 1 M solution.
Formula: $C_1V_1 = C_2V_2$
Plug values in: (V_1)(1 M) = (5 mL)(0.25 M)
Rearrange: V_1 = [(5 mL)(0.25 M)] / (1 M)V_1 = 1.25 mL

Q1: Find the weight of Na2C2O4 (FW = 134.00 g/mol) required to prepare 250 mL of 0.1000 M $Na_2C_2O_4$ solution.

Q2: Find the number of mmol of NaBr (FW = 102.89 g/mol) present in 1.2664 g of NaBr.

Q3 How many mg of NaCl (FW = 58.44 g/mol) are contained in 2.35 mmol of the compound ?

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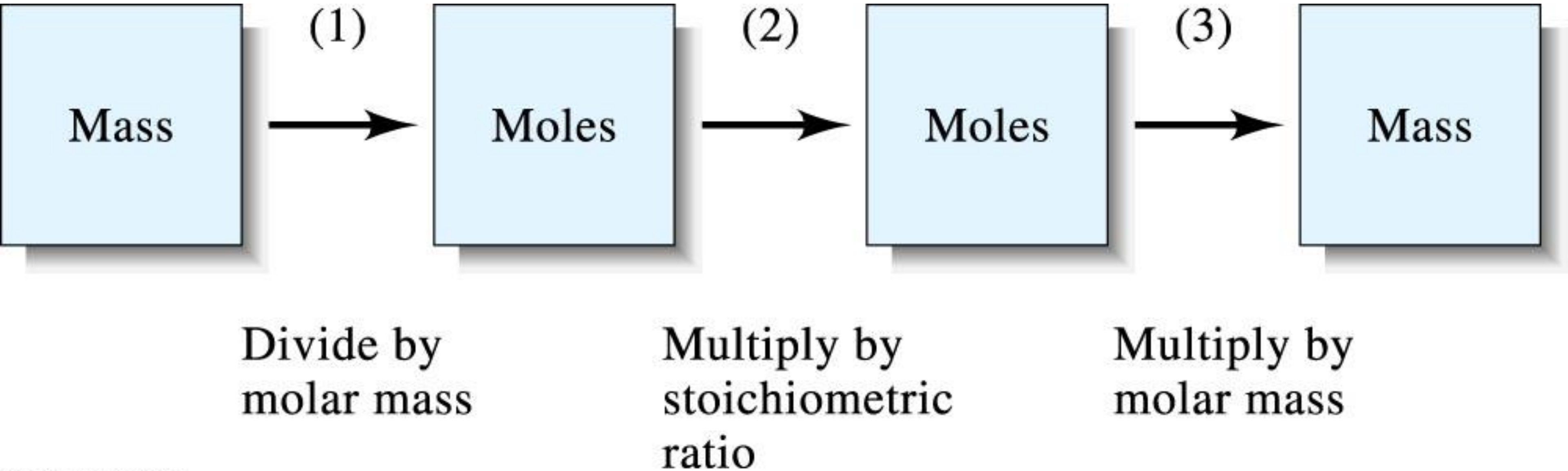
Chemical Stoichiomtry: The stoichiometry of a reaction is the relationship among the number of moles of reactants and products as shown by a balanced equation.

A balanced chemical equation is a statement of the combining ratios or stoichiometry in units of moles among the reacting substances and their products.

- Transformation of the known mass of a substance in grams to a corresponding number of moles
- Multiplication by a factor that accounts for the stoichiometry
- Reconversion of the data in moles back to the SI units called for in the answer


(1)
(2)
(3)
Mass
Moles
Moles
Mass
Divide by molar mass
Multiply by stoichiometric ratio
Multiply by molar mass

HOMEWORK QUESTIONS

1. If 30 grams of NaOH are dissolved and then diluted to 2.0 L with water,what is the molar concentration (molarity) of the solution?

2. Two grams (2.0 g) of salt are mixed with 50 grams of water. Find the weight % of the solution.

3. How many grams of salt must be added to 10 grams of water to create a 10% solution?