Al-Rasheed University College
Department of Medical Laboratory Technique

Chemistry
Lecture 1

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Qualitative and Quantitative Analysis

- The discipline of analytical chemistry consists of **qualitative analysis** and **quantitative analysis**.
- The **qualitative analysis** deals with the identification of elements, ions, or compounds present in a sample (we may be interested in whether only a given substance is present).
- The **quantitative analysis** deals with the determination of how much of one or more constituents is present.

Qualitative analysis tells us what chemicals are present.
Quantitative analysis tells us how much.

Analytes are the components of a sample that are determined.

MOLES: THE BASIC UNIT FOR EQUATING THINGS

- To simplify calculations, chemists have developed the concept of the **mole,** which is Avogadro's number (6.022×10^{23}) of atoms, molecules, ions, or other species. Numerically, it is the atomic, molecular, or formula weight of a substance expressed in **grams.**

The number of moles of a substance is calculated from

$$\text{Moles} = \frac{\text{grams}}{\text{formula weight (g/mol)}} \quad (5.1)$$

where formula weight represents the atomic or molecular weight of the substance. Thus,

$$\text{Moles } Na_2SO_4 = \frac{\text{g}}{\text{fw}} = \frac{\text{g}}{142.04 \text{ g/mol}}$$

$$\text{Moles } Ag^+ = \frac{\text{g}}{\text{fw}} = \frac{\text{g}}{107.870 \text{ g/mol}}$$

Since many experiments deal with very small quantities, a more convenient form of measurement is the **millimole**. The formula for calculating millimoles is

$$\text{Millimoles} = \frac{\text{milligrams}}{\text{formula weight (mg/mmol)}} \quad (5.2)$$

Just as we can calculate the number of moles from the grams of material, we can likewise calculate the grams of material from the number of moles:

$$\text{g } Na_2SO_4 = \text{moles} \times \text{fw} = \text{moles} \times 142.04 \text{ g/mol}$$

$$\text{g Ag} = \text{moles} \times \text{fw} = \text{moles} \times 107.870 \text{ g/mol}$$

Again, we usually work with millimole quantities, so

$$\boxed{\text{Milligrams} = \text{millimoles} \times \text{formula weight (mg/mmol)}} \qquad (5.3)$$

Note that g/mol is the same as mg/mmol, g/L the same as mg/mL, and mol/L the same as mmol/mL.

g/mol = mg/mmol = formula weight; g/L = mg/mL; mol/L = mmol/mL = molarity.

Example 5.2

(f.wt = 293.8 g/mol)

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

Solution moles = mmol x 0.001

$$\frac{500\ \text{mg}}{293.8\ \text{mg/mmol}} \times 0.001\ \text{mol/mmol} = 0.00170\ \text{mol}$$

moles = g / f.wt

= 0.5 / 293.8 = 0.00170 mol

Example 5.3

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

(f.wt=159.7 g/mol)

Solution mg Fe_2O_3 = mmol x f.wt

$$0.250\ \text{mmol} \times 159.7\ \text{mg/mmol} = 39.9\ \text{mg}$$

How Do We Express Concentrations of Solutions?

- Chemists express solution concentrations in a number of ways. We will review here the common concentration units that chemists use.

M, *N*, %, ppm, ppb, g/L, mg/dL, meq/L

- **Molarity (*M*)** of a solution is defined as the number of moles of solute per liter of solution or as the number of millimoles of solute per milliliter of solution.

M = mole / L	M = mmole / mL
mole = M x L	mmole = M x mL
mole = g / f.wt	mmole = mg / f.wt
M = g / f.wt / L	M = mg / f.wt / mL
g = M x L x f.wt	mg = M x mL x f.wt

Example 5.4

(169.9 g/mol)

A solution is prepared by dissolving 1.26 g $AgNO_3$ in a 250-mL volumetric flask and diluting to volume. Calculate the molarity of the silver nitrate solution. How many millimoles $AgNO_3$ were dissolved?

Solution $M = \text{g} / \text{f.wt} / \text{L}$

$$M = \frac{1.26 \text{ g}/169.9 \text{ g/mol}}{0.250 \text{ L}} = 0.0297 \text{ mol/L (or } 0.0297 \text{ mmol/mL)}$$

Then,

$$\text{Millimoles} = (0.0297 \text{ mmol/mL})(250 \text{ mL}) = 7.42 \text{ mmol}$$

$\text{mmole} = M \text{ x mL}$

Example 5.5

How many grams per milliliter of NaCl are contained in a 0.250 *M* solution?

Solution g/mL = M x f.wt x 0.001

$$0.250 \text{ mol/L} = 0.250 \text{ mmol/mL}$$

$$0.250 \text{ mmol/mL} \times 58.4 \text{ mg/mmol} \times 0.001 \text{ g/mg} = 0.0146 \text{ g/mL}$$

Example 5.6

How many grams Na_2SO_4 should be weighed out to prepare 500 mL of a 0.100 *M* solution?

Solution

$$g = M \times L \times f.wt$$

$$= 0.1 \times (500/1000) \times 142 = 7.10 \text{ g}$$

- **Normality (*N*)** of a solution is defined as the number of equivalents of solute per liter of solution or as the number of milliequivalents of solute per milliliter of solution.

N = eq / L

eq = N x L

eq = g / eq.wt

N = g / eq.wt / L

g = N x L x eq.wt

N = meq / mL

meq = N x mL

meq = mg / eq.wt

N = mg / eq.wt / mL

mg = N x mL x eq.wt

eq.wt = f.wt / n

n = number of reacting units

$$N = M \times n$$

- The **equivalent weight** is the formula weight divided by the number of reacting units. Table 5.1 lists the reacting units used for different types of reactions

- For acids and bases, the number of reacting units is based on the number of protons (i.e., hydrogen ions) an acid will furnish or a base will react with.

- For oxidation–reduction reactions it is based on the number of electrons an oxidizing or reducing agent will take on or supply.

Table 5.1

Reacting Units in Different Reactions

Reaction Type	Reacting Unit
Acid–base	H^+
Oxidation–reduction	Electron

- Thus, for example, sulfuric acid, H_2SO_4, has two reacting units of protons; that is, there are two equivalents of protons in each mole. Therefore,

$$\text{Equivalent weight} = \frac{98.08\ \text{g/mol}}{2\ \text{eq/mol}} = 49.04\ \text{g/eq}$$

$$\text{Number of equivalents (eq)} = \frac{\text{wt (g)}}{\text{eq wt (g/eq)}} = \text{normality (eq/L)} \times \text{volume (L)}$$

- We typically use milliequivalents (meq) instead of equivalents

$$\text{meq} = \frac{\text{mg}}{\text{eq wt (mg/meq)}} = \text{normality (meq/mL)} \times \text{mL}$$

Equivalent weight g/eq = mg/meq; eq/L = meq/mL = normality.

- In clinical chemistry, equivalents are frequently defined in terms of the number of charges on an ion rather than on the number of reacting units.
- Thus, for example, the equivalent weight of Ca^{+2} is one-half its atomic weight, and the number of equivalents is twice the number of moles.

DENSITY CALCULATIONS—HOW DO WE CONVERT TO MOLARITY?

- The concentration of many fairly concentrated commercial acids and bases are usually given in terms of percent by weight.
- It is frequently necessary to prepare solutions of a given approximate molarity from these substances.
- In order to do so, we must know the density in order to calculate the molarity. Sometimes substances list specific gravity rather than density.

$$M = \% \times d \times 1000 / f.wt$$

> **Density** expresses the mass of a substance per unit volume. In SI units, density is expressed in units of kg/L or, alternatively, g/mL.

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

2.5 L **9535-03**

Hydrochloric Acid, 36.5-38.0%

Acide Hydrochlorique

'BAKER ANALYZED'® A.C.S. Reagent

HCl **FW 36.46**

LOT

Meets A.C.S. Specifications

Meets Reagent Specifications for testing USP/NF monographs

Appearance	Passes Test
Assay (as HCl) (by acid-base titrn)	36.5 - 38.0 %
Color (APHA)	10 max.
Extractable Organic Substances	5 ppm max.
Free Chlorine (as Cl)	1 ppm max.
Residue after Ignition	3 ppm max.
Specific Gravity at 60°/60°F	1.185 - 1.192
Bromide (Br)	0.005 % max.
Trace Impurities (in ppm)	
Phosphate (PO_4)	1 max.
Sulfate (SO_4)	0.5 max.
Sulfite (SO_3)	0.8 max.
Ammonium (NH_4)	3 max.
Trace Impurities (in ppb)	
Aluminum (Al)	100 max.
Arsenic and Antimony (as As)	5 max.
Boron (B)	50 max.
Calcium (Ca)	200 max.
Chromium (Cr)	100 max.
Copper (Cu)	100 max.
Gold (Au)	100 max.
Heavy Metals (as Pb)	100 max.
Iron (Fe)	100 max.
Lead (Pb)	50 max.
Magnesium (Mg)	300 max.
Manganese (Mn)	300 max.
Mercury (Hg)	5 max.
Nickel (Ni)	100 max.
Potassium (K)	300 max.
Sodium (Na)	300 max.
Tin (Sn)	300 max.
Titanium (Ti)	300 max.
Zinc (Zn)	100 max.

Water	CAS No: 7732-18-5
Hydrogen Chloride	CAS No: 7647-01-0

SAF-T-DATA™ System

HEALTH	FLAMMABILITY	REACTIVITY	CONTACT
3	0	2	3
SEVERE	NONE	MODERATE	SEVERE

LABORATORY PROTECTIVE EQUIPMENT

GOGGLES & SHIELD — LAB COAT & APRON — VENT HOOD — PROPER GLOVES

STORAGE COLOR: WHITE

DOT Name: HYDROCHLORIC ACID UN1789

CAS NO: 7647-01-0

J. T. Baker NEUTRASORB® or TEAM® 'Low Na+' acid neutralizers are recommended for spills of this product.

MADE IN USA

NFPA: 3 0 0

011021691

G34

$$M = \% \times d \times 1000 / f.wt$$

tyco Specialty Products

J.T.B

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).

$$M = \% \times d \times 1000 / f.wt$$

$$M = 0.705 \times 1.42 \times 1000 / 63 = 15.89$$

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).

$$M = \% \times d \times 1000 / f.wt$$

$$M = 0.37 \times 1.18 \times 1000 / 36.5 = 11.96$$

$$M_1V_1 = M_2V_2$$

$$11.96 \times V_1 = 6 \times 100$$

$$V_1 = 50.16$$

Thus, dilute 50.16 mL of the concentrated reagent to 100 mL

SOLID SAMPLES

$$\%(\text{wt/wt}) = \left[\frac{\text{wt solute (g)}}{\text{wt sample (g)}}\right] \times 10^2 \ (\%/\text{g solute/g sample})$$

$$\text{ppm (wt/wt)} = \left[\frac{\text{wt solute (g)}}{\text{wt sample (g)}}\right] \times 10^6 \ (\text{ppm/g solute/g sample})$$

$$\text{ppm} = \mu\text{g/g} = \text{mg/kg}$$

$$\text{ppb (wt/wt)} = \left[\frac{\text{wt solute (g)}}{\text{wt sample (g)}}\right] \times 10^9 \ (\text{ppb/g solute/g sample})$$

$$\text{ppb} = \text{ng/g} = \mu\text{g/kg}$$

Common Units for Expressing Trace Concentrations

Unit	Abbreviation	wt/wt	wt/vol	vol/vol
Parts per million	ppm	mg/kg	mg/L	μL/L
(1 ppm = 10^{-4}%)		μg/g	μg/mL	nL/mL
Parts per billion	ppb	μg/kg	μg/L	nL/L
(1 ppb = 10^{-7}% = 10^{-3} ppm)		ng/g	ng/mL	pL/mL[a]
Milligram percent	mg%	mg/100 g	mg/100 mL	

Example 5.14

A 2.6 g sample of plant tissue was analyzed and found to contain 3.6 μg zinc. What is the concentration of zinc in the plant in ppm? In ppb?

Solution $\text{ppm} = \mu\text{g/g}$ =

$$\frac{3.6\ \mu\text{g}}{2.6\ \text{g}} = 1.4\ \mu\text{g/g} \equiv 1.4\ \text{ppm}$$

$$\frac{3.6 \times 10^3\ \text{ng}}{2.6\ \text{g}} = 1.4 \times 10^3\ \text{ng/g} \equiv 1400\ \text{ppb}$$

One ppm is equal to 1000 ppb. One ppb is equal to 10^{-7}%.

LIQUID SAMPLES

$$\%(\text{wt/vol}) = \left[\frac{\text{wt solute (g)}}{\text{vol sample (mL)}}\right] \times 10^2 \ (\%/\text{g solute/mL sample})$$

$$\text{ppm (wt/vol)} = \left[\frac{\text{wt solute (g)}}{\text{vol sample (mL)}}\right] \times 10^6 \ (\text{ppm/g solute/mL sample})$$

$$\text{ppb (wt/vol)} = \left[\frac{\text{wt solute (g)}}{\text{vol sample (mL)}}\right] \times 10^9 \ (\text{ppb/g solute/mL sample})$$

In dilute aqueous solution

$$\text{ppm} = \mu\text{g/mL} = \text{mg/L}$$

$$\text{ppb} = \text{ng/mL} = \mu\text{g/L}$$

A deciliter is 0.1 L or 100 mL.

Example 5.16

A 25.0-μL serum sample was analyzed for glucose content and found to contain 26.7 μg. Calculate the concentration of glucose in μg/mL and in mg/dL.

Solution

$$\text{ppm} = \mu\text{g/mL} :$$

µg/mL = 26.7 / 25 x 0.001 = 1070

mg/dL = ppm / 10

= 1070 / 10 = 107

[Note the relationship: 10 ppm (wt/vol) = 1 mg/dL]

- Clinical chemists frequently prefer to use a unit other than weight for expressing the amount of major electrolytes in biological fluids (Na^+, K^+, Ca^{2+}, Mg^{2+}, Cl^-, H_2PO4^-, etc.). This is the unit **milliequivalent** (meq).
- We can calculate the milliequivalents of a substance from its weight in milligrams simply as follows (similar to how we calculate millimoles):

$$\text{meq} = \frac{\text{mg}}{\text{eq wt (mg/meq)}} = \frac{\text{mg}}{\text{fw (mg/mmol)}/n\ \text{(meq/mmol)}}$$

n = charge on ion

mmole = mg/f.wt (mg/mmol)

Example 5.18

(f.wt = 65.4 g/mol)

The concentration of zinc ion in blood serum is about 1 mg/L. Express this as meq/L.

Solution

Convert from ppm → meq/L

meq/L = ppm / eq.wt

The equivalent weight of Zn^{2+} is 65.4 (mg/mmol)/2 (meq/mmol) = 32.7 mg/meq. Therefore,

eq.wt = f.wt / n

= 65.4/2=32.7

$$\frac{1\ \text{mg Zn/L}}{32.7\ \text{mg/meq}} = 3.06 \times 10^{-2}\ \text{meq/L Zn}$$

- The various ways that concentrations of solutions are expressed and the relationship between them

Convert from ppm → g/L	g/L = ppm x 10^{-3}
Convert from *M* → g/L	g/L = *M* x f.wt
Convert from ppm → *M*	*M* = ppm x 10^{-3} / f.wt
Convert from *M* → ppm	ppm = *M* x f.wt x 10^{3}
Convert from ppm → mg/dL	mg/dL = ppm/10
Convert from ppm → meq/L	meq/L = ppm/eq.wt
Convert from meq/L → ppm	ppm = meq/L x eq.wt
Convert from mg/dL → meq/L	meq/L = mg/dL x 10 / eq.wt
Convert from meq/L → mg/dL	mg/dL = meq x eq.wt / 10
Convert from meq/L → g/L	g/L = meq/L x eq.wt x 10^{-3}

A chloride concentration is reported as 300 mg/dL. What is the concentration in meq/L?

$$\text{meq/L} = \text{mg/dL} \times 10 / \text{eq.wt}$$

$$= 300 \times 10 / 35.5 = 84.5$$

A calcium concentration is reported as 5.00 meq/L. What is the concentration in mg/dL?

$$\text{eq.wt } Ca^{+2} = 40 / 2 = 20$$

$$\text{mg/dL} = \text{meq/L} \times \text{eq.wt} / 10$$

$$= 5 \times 20 / 10 = 10$$

A urine specimen has a chloride concentration of 150 meq/L. If we assume that the chloride is present in urine as sodium chloride, what is the concentration of NaCl in g/L?

$$\text{g/L} = \text{meq/L} \times \text{eq.wt} \times 10^{-3}$$

$$= 150 \times 58.5 \times 10^{-3} = 8.775$$