

Chapter 4: Calculations Used in Analytical Chemistry

In this chapter, we describe several methods used to compute the results of a quantitative analysis.

- SI system of units and the distinction between mass and weight.
- the mole, a measure of the amount of a chemical substance.
- the various ways that concentrations of solutions are expressed.
- Finally, we treat chemical stoichiometry.

4A Some important units of measurement

4A-1 SI Units

SI is the acronym for the French “Système International d’Unités.”

- The International System of Units (SI) is based on 7 fundamental base units.
- Numerous other useful units, such as volts, hertz, coulombs, and joules, are derived from these base units.
- To express small or large measured quantities in terms of a few simple digits, pre-fixes are used with these base units and other derived 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

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}

The ångstrom unit Å is a non-SI unit of length widely used to express the wavelength of very short radiation such as X-rays ($1 \text{ Å} = 0.1 \text{ nm}$).

Thus, typical X-radiation lies in the range of 0.1 to 10 Å.

Metric units of kilograms (kg), grams (g), milligrams (mg), or micrograms (μg) are used in the SI system.

Volumes of liquids are measured in units of liters (L), milliliters (mL), microliters (μL), and sometimes nanoliters (nL).

The liter, the SI unit of volume, is defined as exactly 10^{-3} m^3 . The milliliter is defined as 10^{-6} m^3 , or 1 cm^3 .

4A-2 The Distinction Between Mass and Weight

Mass is an invariant measure of the quantity of matter in an object.

- Weight is the force of attraction between an object and its surroundings, principally the earth. Because gravitational attraction varies with geographical location, the weight of an object depend on where you weigh it.

For example, a crucible *weighs less in Denver than in Atlantic City* however, mass remains constant regardless of where you measure it.

- Weight and mass are related by the familiar expression

$$w = mg$$

w is the weight of an object,

m is its mass, and

g is the acceleration due to gravity.

Analytical data are based on mass rather than weight.

A balance is used to compare the mass of an object with the mass of one or more standard masses.

g affects both unknown and known equally, hence, the mass of the object is identical to the standard masses with which it is compared.

4A-3 The Mole

- The mole (abbreviated mol) 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, other particles, or specified groups of such particles as represented by a chemical formula.
- 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 .
- This is Avogadro's number $N_A = 6.022 \times 10^{23}$.
- The **molar mass M** of a substance is the mass in grams of 1 mole of that substance.

The number of moles n_x of a species X of molar mass M_x is given by

$$\text{amount } X = n_x = \frac{m_x}{M_x}$$

The molar mass of glucose is:

$$\begin{aligned} M_{\text{C}_6\text{H}_{12}\text{O}_6} &= \frac{6 \cancel{\text{ mol C}}}{\text{mol C}_6\text{H}_{12}\text{O}_6} \times \frac{12.0 \text{ g}}{\cancel{\text{ mol C}}} + \frac{12 \cancel{\text{ mol H}}}{\text{mol C}_6\text{H}_{12}\text{O}_6} \times \frac{1.0 \text{ g}}{\cancel{\text{ mol H}}} \\ &+ \frac{6 \cancel{\text{ mol O}}}{\text{mol C}_6\text{H}_{12}\text{O}_6} \times \frac{16.0 \text{ g}}{\cancel{\text{ mol O}}} = 180.0 \text{ g/mol C}_6\text{H}_{12}\text{O}_6 \end{aligned}$$

4A-4 The Millimole

1 millimole = 1/1000 of a mole 1 millimolar mass (mM) = 1/1000 of the molar mass.

1 mmol = 10^{-3} mol, and 10^3 mmol = 1 mol

4A-5 Calculating the Amount of a Substance in Moles or Millimoles

EXAMPLE 4-1

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

Solution

If we use HBz to represent benzoic acid, we can write that 1 mole of HBz has a mass of 122.1 g. Therefore,

$$\begin{aligned}\text{amount HBz} = n_{\text{HBz}} &= 2.00 \text{ g HBz} \times \frac{1 \text{ mol HBz}}{122.1 \text{ g HBz}} && (4-1) \\ &= 0.0164 \text{ mol HBz}\end{aligned}$$

To obtain the number of millimoles, we divide by the millimolar mass (0.1221 g/mmol), that is,

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

EXAMPLE 4-2

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

The chemical formula tells us that 1 mole of Na_2SO_4 contains 2 moles of Na^+ , that is,

$$\text{amount Na}^+ = n_{\text{Na}^+} = \cancel{\text{mol Na}_2\text{SO}_4} \times \frac{2 \text{ mol Na}^+}{\cancel{\text{mol Na}_2\text{SO}_4}}$$

To find the number of moles of Na_2SO_4 , we proceed as in Example 4-1:

$$\text{amount Na}_2\text{SO}_4 = n_{\text{Na}_2\text{SO}_4} = 25.0 \text{ g Na}_2\text{SO}_4 \times \frac{1 \text{ mol Na}_2\text{SO}_4}{142.0 \text{ g Na}_2\text{SO}_4}$$

Combining this equation with the first leads to

$$\text{amount Na}^+ = n_{\text{Na}^+} = 25.0 \text{ g Na}_2\text{SO}_4 \times \frac{1 \text{ mol Na}_2\text{SO}_4}{142.0 \text{ g Na}_2\text{SO}_4} \times \frac{2 \text{ mol Na}^+}{\text{mol Na}_2\text{SO}_4}$$

To obtain the mass of sodium in 25.0 g of Na_2SO_4 , we multiply the number of moles of Na^+ by the molar mass of Na^+ , or 22.99 g. And so,

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

Substituting the previous equation gives the mass in grams of Na^+ :

$$\begin{aligned} \text{mass Na}^+ &= 25.0 \text{ g Na}_2\text{SO}_4 \times \frac{1 \text{ mol Na}_2\text{SO}_4}{142.0 \text{ g Na}_2\text{SO}_4} \times \frac{2 \text{ mol Na}^+}{\text{mol Na}_2\text{SO}_4} \times \frac{22.99 \text{ g Na}^+}{\text{mol Na}^+} \\ &= 8.10 \text{ g Na}^+ \end{aligned}$$

4B Solutions and their concentrations

4B-1 Concentration of Solutions

The molar concentration c_x of a solution of a solute species X is the number of moles of that species that is contained in 1 liter of the solution (not 1 L of the solvent).

$$c_x = \frac{n_x}{V} \quad \text{molar concentration} = \frac{\text{moles of solute}}{\text{volume in liters}}$$

n , number of moles of solute and V , the volume of solution

The unit of molar concentration is **molar**, symbolized by M, which has the dimensions of mol/L, or mol L⁻¹.

Molar concentration is also the number of millimoles of solute per milliliter of solution.

EXAMPLE 4-3

Calculate the molar concentration of ethanol in an aqueous solution that contains 2.30 g of $\text{C}_2\text{H}_5\text{OH}$ (46.07 g/mol) in 3.50 L of solution.

Solution

To calculate molar concentration, we must find both the amount of ethanol and the volume of the solution. The volume is given as 3.50 L, so all we need to do is convert the mass of ethanol to the corresponding amount of ethanol in moles.

$$\begin{aligned}\text{amount } \text{C}_2\text{H}_5\text{OH} = n_{\text{C}_2\text{H}_5\text{OH}} &= 2.30 \text{ g } \text{C}_2\text{H}_5\text{OH} \times \frac{1 \text{ mol } \text{C}_2\text{H}_5\text{OH}}{46.07 \text{ g } \text{C}_2\text{H}_5\text{OH}} \\ &= 0.04992 \text{ mol } \text{C}_2\text{H}_5\text{OH}\end{aligned}$$

To obtain the molar concentration, $c_{\text{C}_2\text{H}_5\text{OH}}$, we divide the amount by the volume. Thus,

$$\begin{aligned}c_{\text{C}_2\text{H}_5\text{OH}} &= \frac{2.30 \text{ g } \text{C}_2\text{H}_5\text{OH} \times \frac{1 \text{ mol } \text{C}_2\text{H}_5\text{OH}}{46.07 \text{ g } \text{C}_2\text{H}_5\text{OH}}}{3.50 \text{ L}} \\ &= 0.0143 \text{ mol } \text{C}_2\text{H}_5\text{OH}/\text{L} = 0.0143 \text{ M}\end{aligned}$$

There are two ways of expressing molar concentration:

Molar analytical concentration is the total number of moles of a solute, regardless of its chemical state, in 1 L of solution. The molar analytical concentration describes how a solution of a given concentration can be prepared.

The **molar equilibrium concentration**, or just equilibrium concentration, refers to the molar concentration of a particular species in a solution at equilibrium.

To specify the molar equilibrium concentration of a species, it is necessary to know how the solute behaves when it is dissolved in a solvent.

They are usually symbolized by placing square brackets around the chemical formula for the species. Ex., $[\text{H}_2\text{SO}_4] = 0.00 \text{ M}$; $[\text{H}^+] = 1.01 \text{ M}$.

-The IUPAC recommends the general term “concentration” to express the composition of a solution with respect to its volume, with four sub terms: amount concentration, mass concentration, volume concentration, and number concentration.

-- Molar concentration, molar analytical concentration, and molar equilibrium concentration are all amount concentrations by this definition.

For example, the molar equilibrium concentration of H_2SO_4 in a solution with a molar analytical concentration, $c_{\text{H}_2\text{SO}_4} = 1 \text{ M}$, is actually 0.0 M, because the sulfuric acid is completely dissociated into a mixture of H^+ , HSO_4^- , SO_4^{2-} ions.

There are essentially no H_2SO_4 molecules in this solution. The equilibrium concentrations of the ions are 1.01, 0.99, and 0.01 M, respectively.

because SO_4^{2-} and HSO_4^- are the only two sulfate-containing species in the solution.

The molar equilibrium concentrations are usually symbolized by placing square brackets around the chemical formula for the species.

Ex., $[\text{H}_2\text{SO}_4] = 0.00 \text{ M}$;

$[\text{H}^+] = 1.01 \text{ M}$.

$[\text{SO}_4^{2-}] = 0.01 \text{ M}$ and $[\text{HSO}_4^-] = 0.99 \text{ M}$

EXAMPLE 4-4

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

Solution

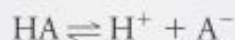
As in Example 4-3, we calculate the number of moles of Cl_3CCOOH , which we designate as HA, and divide by the volume of the solution, 10.0 mL, or 0.0100 L. Therefore,

$$\begin{aligned} \text{amount HA} = n_{\text{HA}} &= 285 \text{ mg HA} \times \frac{1 \text{ g HA}}{1000 \text{ mg HA}} \times \frac{1 \text{ mol HA}}{163.4 \text{ g HA}} \\ &= 1.744 \times 10^{-3} \text{ mol HA} \end{aligned}$$

The molar analytical concentration, c_{HA} , is then

$$c_{\text{HA}} = \frac{1.744 \times 10^{-3} \text{ mol HA}}{10.0 \text{ mL}} \times \frac{1000 \text{ mL}}{1 \text{ L}} = 0.174 \frac{\text{mol HA}}{\text{L}} = 0.174 \text{ M}$$

In this solution, 73% of the HA dissociates, giving H^+ and A^- :



The equilibrium concentration of HA is then 27% of c_{HA} . Thus,

$$\begin{aligned} [\text{HA}] &= c_{\text{HA}} \times (100 - 73)/100 = 0.174 \times 0.27 = 0.047 \text{ mol/L} \\ &= 0.047 \text{ M} \end{aligned}$$

The equilibrium concentration of A^- is equal to 73% of the analytical concentration of HA, that is,

$$[\text{A}^-] = \frac{73 \text{ mol A}^-}{100 \text{ mol HA}} \times 0.174 \frac{\text{mol HA}}{\text{L}} = 0.127 \text{ M}$$

Because 1 mole of H^+ is formed for each mole of A^- , we can also write

$$[\text{H}^+] = [\text{A}^-] = 0.127 \text{ M}$$

EXAMPLE 4-5

Describe the preparation of 2.00 L of 0.108 M BaCl_2 from $\text{BaCl}_2 \cdot 2\text{H}_2\text{O}$ (244.3 g/mol).

Solution

To determine the number of grams of solute to be dissolved and diluted to 2.00 L, we note that 1 mole of the dihydrate yields 1 mole of BaCl_2 . Therefore, to produce this solution we will need

$$2.00 \text{ L} \times \frac{0.108 \text{ mol BaCl}_2 \cdot 2\text{H}_2\text{O}}{\text{L}} = 0.216 \text{ mol BaCl}_2 \cdot 2\text{H}_2\text{O}$$

The mass of $\text{BaCl}_2 \cdot 2\text{H}_2\text{O}$ is then

$$0.216 \text{ mol BaCl}_2 \cdot 2\text{H}_2\text{O} \times \frac{244.3 \text{ g BaCl}_2 \cdot 2\text{H}_2\text{O}}{\text{mol BaCl}_2 \cdot 2\text{H}_2\text{O}} = 52.8 \text{ g BaCl}_2 \cdot 2\text{H}_2\text{O}$$

Dissolve 52.8 g of $\text{BaCl}_2 \cdot 2\text{H}_2\text{O}$ in water and dilute to 2.00 L.

EXAMPLE 4-6

Describe the preparation of 500 mL of 0.0740 M Cl^- solution from solid $\text{BaCl}_2 \cdot 2\text{H}_2\text{O}$ (244.3 g/mol).

Solution

$$\begin{aligned} \text{mass BaCl}_2 \cdot 2\text{H}_2\text{O} &= \frac{0.0740 \text{ mol Cl}^-}{\text{L}} \times 0.500 \text{ L} \times \frac{1 \text{ mol BaCl}_2 \cdot 2\text{H}_2\text{O}}{2 \text{ mol Cl}^-} \\ &\quad \times \frac{244.3 \text{ g BaCl}_2 \cdot 2\text{H}_2\text{O}}{\text{mol BaCl}_2 \cdot 2\text{H}_2\text{O}} = 4.52 \text{ g BaCl}_2 \cdot 2\text{H}_2\text{O} \end{aligned}$$

Dissolve 4.52 g of $\text{BaCl}_2 \cdot 2\text{H}_2\text{O}$ in water and dilute to 0.500 L or 500 mL.

Percent Concentration

$$\text{weightpercent}(w/w) = \frac{\text{weightsolute}}{\text{weightsolution}} \times 100\%$$

$$\text{volumepercent}(v/v) = \frac{\text{volumesolute}}{\text{volumesolution}} \times 100\%$$

$$\text{weight/volumepercent}(w/v) = \frac{\text{weightsolute, g}}{\text{volumesolution, mL}} \times 100\%$$

- In IUPAC terminology, weight percent is mass concentration and volume percent is volume concentration.
- Weight percent is often used to express the concentration of commercial aqueous reagents. Volume percent is commonly used to specify the concentration of a solution prepared by diluting a pure liquid compound with another liquid.
- Weight or volume percent is often used to indicate the composition of dilute aqueous solutions of solid reagents.

Parts per million and parts per billion

In IUPAC terminology, parts per billion, parts per million, and parts per thousand are mass concentrations.

For very dilute solutions, **parts per million (ppm)** is a convenient way to express concentration:

$$C_{ppm} = \frac{\text{mass of solute}}{\text{mass of solution}} \times 10^6 \text{ ppm}$$

For even more dilute solutions, 10^9 ppb rather than 10^6 ppm is used in the previous equation to give the results in **parts per billion (ppb)**.

The term **parts per thousand (ppt)** is also used, especially in oceanography.

EXAMPLE 4-7

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. Therefore, according to Equation 4-2,

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

$$\frac{\text{no. mol } K_3Fe(CN)_6}{L} = \frac{63.3 \text{ mg } K_3Fe(CN)_6}{L} \times \frac{1 \text{ g } K_3Fe(CN)_6}{1000 \text{ mg } K_3Fe(CN)_6}$$
$$\times \frac{1 \text{ mol } K_3Fe(CN)_6}{329.3 \text{ g } K_3Fe(CN)_6} = 1.922 \times 10^{-4} \frac{\text{mol}}{L}$$

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

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

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

Solution-Diluent Volume Ratios

The composition of a dilute solution is sometimes specified in terms of the volume of a more concentrated solution and the volume of solvent used in diluting it.

Thus, a 1:4 HCl solution contains four volumes of water for each volume of concentrated hydrochloric acid.

This method of notation is frequently ambiguous.

p-Functions

The concentration of a species is expressed as its p-function, or p-value. The best-known p-function is pH, which is the negative logarithm of $[H^+]$.

The p-value is the negative logarithm (to the base 10) of the molar concentration of that species. Thus, for the species X,

$$pX = -\log [X]$$

EXAMPLE 4-8

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

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

To obtain pNa, we write

$$\text{pNa} = -\log[\text{Na}^+] = -\log (2.00 \times 10^{-3}) = -\log (2.00 \times 10^{-3}) = 2.699$$

The total Cl^- concentration is given by the sum of the concentrations of the two solutes:

$$\begin{aligned} [\text{Cl}^-] &= 2.00 \times 10^{-3} \text{ M} + 5.4 \times 10^{-4} \text{ M} \\ &= 2.00 \times 10^{-3} \text{ M} + 0.54 \times 10^{-3} \text{ M} = 2.54 \times 10^{-3} \text{ M} \\ \text{pCl} &= -\log[\text{Cl}^-] = -\log 2.54 \times 10^{-3} = 2.595 \end{aligned}$$

EXAMPLE 4-9

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

Solution

$$\begin{aligned} \text{pAg} &= -\log [\text{Ag}^+] = 6.372 \\ \log [\text{Ag}^+] &= -6.372 \\ [\text{Ag}^+] &= 4.246 \times 10^{-7} \approx 4.25 \times 10^{-7} \text{ M} \end{aligned}$$

Density and Specific Gravity of Solutions

- 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.
- Specific gravity is dimensionless and so is not tied to any particular system of unit
- Since the density of water is approximately 1.00 g/mL, we use density and specific gravity interchangeably.

TABLE 4-3

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 4-10

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

Solution

Let us first calculate the mass of acid per liter of concentrated solution


$$\frac{\text{g HNO}_3}{\text{L reagent}} = \frac{1.42 \text{ kg reagent}}{\text{L reagent}} \times \frac{10^3 \text{ g reagent}}{\text{kg reagent}} \times \frac{70.5 \text{ g HNO}_3}{100 \text{ g reagent}} = \frac{1001 \text{ g HNO}_3}{\text{L reagent}}$$

Then,

$$c_{\text{HNO}_3} = \frac{1001 \text{ g HNO}_3}{\text{L reagent}} \times \frac{1 \text{ mol HNO}_3}{63.0 \text{ g HNO}_3} = \frac{15.9 \text{ mol HNO}_3}{\text{L reagent}} \approx 16 \text{ M}$$

Figure 4-1 Label from a bottle of reagent-grade hydrochloric acid.


The specific gravity of the acid over the temperature range of 60° to 80°F is specified on the label.



HYDROCHLORIC ACID Danger May be corrosive to metals. Harmful if swallowed. Causes severe skin burns and eye damage. May cause respiratory irritation. Do not breathe dust/fume/gas/mist/vapors/spray. Wear protective gloves/protective clothing/eye protection/face protection. IF ON SKIN (or hair): Remove/take off immediately all contaminated clothing. Rinse skin with water/shower. IF IN EYES: Rinse cautiously with water for several minutes.

ÁCIDO CLORÍDRICO Perigo Pode ser corrosivo a metais. Nocivo se ingerido. Causa queimadura severa à pele e dano aos olhos. Pode causar irritação respiratória. Nunca respire névoas/vapores/aerossol. Use luvas de proteção/roupas de proteção/proteção ocular/proteção facial. SE ESTIVER NA PELE (ou cabelo): Remova/Tire toda a roupa contaminada imediatamente. Enxágue a pele com água/chuveiro.

注意 危险 可能腐蚀金属。吞食有害。严重的皮肤灼伤和眼睛损伤。可能引起呼吸刺激。不要吸入粉尘/烟/气雾/蒸气/蒸汽/烟雾。戴防护手套/穿防护服/戴防护眼镜/戴防护面具。如皮肤(头发)沾染:立即去除所有沾染的衣服。用水清洗皮肤/淋浴。如进入眼睛:用水小心冲洗几分钟。如戴隐形眼镜并可方便地取出,取出隐形眼镜,继续冲洗。立即呼叫解毒中心或医生。



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Meets ACS Reagent Chemical Requirements
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Appearance	Passes Test
Assay (as HCl) (by acid-base titrn)	36.5 - 38.0 %
Color (APHA)	<= 10
Extractable Organic Substances	<= 5 ppm
Free Chlorine (as Cl ₂)	<= 1 ppm
Residue after Ignition	<= 3 ppm
Specific Gravity at 60°/60°F	1.185 - 1.192
Bromide (Br)	<= 0.005 %
Phosphate (PO ₄)	<= 1.0 ppm
Sulfate (SO ₄)	<= 0.5 ppm
Sulfite (SO ₃)	<= 0.8 ppm
Ammonium (NH ₄)	<= 3 ppm
Arsenic and Antimony (as As)	<= 5.0 ppb
Heavy Metals (as Pb)	<= 100.0 ppb


1 BGG


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COUNTRY OF ORIGIN: USA







(Label provided by Mallinckrodt Baker, Inc., Phillipsburg, NJ 08865)

EXAMPLE 4-11

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).

Solution

Proceeding as in Example 4-10, we first calculate the molar concentration of the concentrated reagent. We then calculate the number of moles of acid that we need for the diluted solution. Finally, we divide the second figure by the first to obtain the volume of concentrated acid required. Thus, to obtain the concentration of the reagent, we write

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

The number of moles HCl required is given by

$$\text{no. mol HCl} = 100 \text{ mL} \times \frac{1 \text{ L}}{1000 \text{ mL}} \times \frac{6.0 \text{ mol HCl}}{\text{L}} = 0.600 \text{ mol HCl}$$

Finally, to obtain the volume of concentrated reagent, we write

$$\text{vol concd reagent} = 0.600 \text{ mol HCl} \times \frac{1 \text{ L reagent}}{12.0 \text{ mol HCl}} = 0.0500 \text{ L or } 50.0 \text{ mL}$$

Therefore, dilute 50 mL of the concentrated reagent to 600 mL.

$$V_{concd} \times C_{concd} = V_{dil} \times C_{dil}$$

The two terms on the left are the volume and molar concentration of a concentrated solution that is being used to prepare a diluted solution having the volume and concentration given by the corresponding terms on the right.

This equation is based on the fact that the number of moles of solute in the diluted solution must equal the number of moles in the concentrated reagent.

This equation can be used with L and mol/L or mL and mmol/mL.

4C Chemical stoichiometry

Stoichiometry is the quantitative relationship among the amounts of reacting chemical species.

The stoichiometry of a reaction is the relationship among the number of moles of reactants and products as represented by a balanced chemical equation.

Empirical Formulas and Molecular Formulas

An empirical formula gives the simplest whole number ratio of atoms in a chemical compound.

A molecular formula specifies the number of atoms in a molecule.

One or more substances may have the same empirical formula but different molecular formulas. A structural formula provides additional information.

Ex., the chemically different ethanol and dimethyl ether share the same molecular formula C_2H_6O . Their structural formulas, C_2H_5OH and CH_3OCH_3 , reveal structural differences between these compounds that are not shown in their common molecular formula.

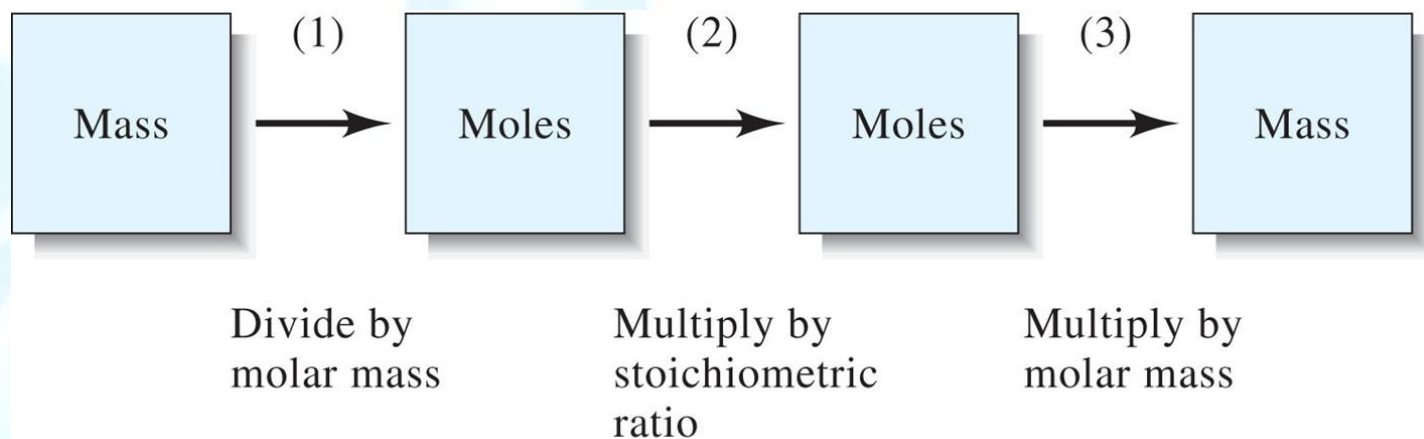
4C-2 Stoichiometric Calculations

A balanced chemical equation gives the combining ratios, or stoichiometry—in units of moles—of reacting substances and their products. Therefore, the equation



indicates that 2 moles of aqueous sodium iodide combine with 1 mole of aqueous lead nitrate to produce 1 mole of solid lead iodide and 2 moles of aqueous sodium nitrate.

Figure 4-2 Flow diagram for making stoichiometric calculations.



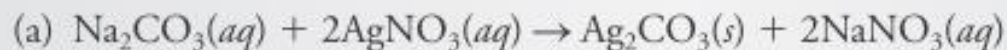
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- (1) When the mass of a reactant or product is given, the mass is first converted to the number of moles, using the molar mass.
- (2) The stoichiometric ratio given by the chemical equation for the reaction is then used to find the number of moles of another reactant that combines with the original substance or the number of moles of product that forms.
- (1) Finally, the mass of the other reactant or the product is computed from its molar mass.

EXAMPLE 4-12

(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



Step 1.

$$\begin{aligned} \text{amount Na}_2\text{CO}_3 = n_{\text{Na}_2\text{CO}_3} &= 2.33 \text{ g Na}_2\text{CO}_3 \times \frac{1 \text{ mol Na}_2\text{CO}_3}{106.0 \text{ g Na}_2\text{CO}_3} \\ &= 0.02198 \text{ mol Na}_2\text{CO}_3 \end{aligned}$$

Step 2. The balanced equation reveals that

$$\begin{aligned} \text{amount AgNO}_3 = n_{\text{AgNO}_3} &= 0.02198 \text{ mol Na}_2\text{CO}_3 \times \frac{2 \text{ mol AgNO}_3}{1 \text{ mol Na}_2\text{CO}_3} \\ &= 0.04396 \text{ mol AgNO}_3 \end{aligned}$$

In this instance, the stoichiometric factor is $(2 \text{ mol AgNO}_3)/(1 \text{ mol Na}_2\text{CO}_3)$.

Step 3.

$$\text{mass AgNO}_3 = 0.04396 \text{ mol AgNO}_3 \times \frac{169.9 \text{ g AgNO}_3}{\text{mol AgNO}_3} = 7.47 \text{ g AgNO}_3$$

(b) amount $\text{Ag}_2\text{CO}_3 = \text{amount Na}_2\text{CO}_3 = 0.02198 \text{ mol}$

$$\text{mass Ag}_2\text{CO}_3 = 0.02198 \text{ mol Ag}_2\text{CO}_3 \times \frac{275.7 \text{ g Ag}_2\text{CO}_3}{\text{mol Ag}_2\text{CO}_3} = 6.06 \text{ g Ag}_2\text{CO}_3$$

EXAMPLE 4-13

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

Mixing these two solutions will result in one (and only one) of three possible outcomes:

- An excess of AgNO_3 will remain after the reaction is complete.
- An excess of Na_2CO_3 will remain after the reaction is complete.
- There will be no excess of either reagent (that is, the number of moles of Na_2CO_3 is exactly equal to twice the number of moles of AgNO_3).

As a first step, we must establish which of these situations applies by calculating the amounts of reactants (in moles) available before the solutions are mixed.

The initial amounts are

$$\begin{aligned}\text{amount AgNO}_3 &= n_{\text{AgNO}_3} = 25.0 \text{ mL AgNO}_3 \times \frac{1 \text{ L AgNO}_3}{1000 \text{ mL AgNO}_3} \\ &\times \frac{0.200 \text{ mol AgNO}_3}{1 \text{ L AgNO}_3} = 5.00 \times 10^{-3} \text{ mol AgNO}_3\end{aligned}$$

$$\begin{aligned}\text{amount Na}_2\text{CO}_3 &= n_{\text{Na}_2\text{CO}_3} = 50.0 \text{ mL Na}_2\text{CO}_3 \text{ soln} \times \frac{1 \text{ L Na}_2\text{CO}_3}{1000 \text{ mL Na}_2\text{CO}_3} \\ &\times \frac{0.0800 \text{ mol Na}_2\text{CO}_3}{1 \text{ L Na}_2\text{CO}_3} = 4.00 \times 10^{-3} \text{ mol Na}_2\text{CO}_3\end{aligned}$$

Because each CO_3^{2-} ion reacts with two Ag^+ ions, $2 \times 4.00 \times 10^{-3} = 8.00 \times 10^{-3}$ mol AgNO_3 is required to react with the Na_2CO_3 . Since we have insufficient AgNO_3 , situation (b) prevails, and the number of moles of Ag_2CO_3 produced will be limited by the amount of AgNO_3 available. Thus,

$$\begin{aligned}\text{mass Ag}_2\text{CO}_3 &= 5.00 \times 10^{-3} \text{ mol AgNO}_3 \times \frac{1 \text{ mol Ag}_2\text{CO}_3}{2 \text{ mol AgNO}_3} \times \frac{275.7 \text{ g Ag}_2\text{CO}_3}{1 \text{ mol Ag}_2\text{CO}_3} \\ &= 0.689 \text{ g Ag}_2\text{CO}_3\end{aligned}$$

EXAMPLE 4-14

What will be the molar analytical concentration of Na_2CO_3 in the solution produced when 25.0 mL of 0.200 M AgNO_3 is mixed with 50.0 mL of 0.0800 M Na_2CO_3 ?

Solution

We have seen in the previous example that formation of 5.00×10^{-3} mol of AgNO_3 requires 2.50×10^{-3} mol of Na_2CO_3 . The number of moles of unreacted Na_2CO_3 is then given by

$$\begin{aligned}n_{\text{Na}_2\text{CO}_3} &= 4.00 \times 10^{-3} \text{ mol Na}_2\text{CO}_3 - 5.00 \times 10^{-3} \text{ mol AgNO}_3 \times \frac{1 \text{ mol Na}_2\text{CO}_3}{2 \text{ mol AgNO}_3} \\ &= 1.50 \times 10^{-3} \text{ mol Na}_2\text{CO}_3\end{aligned}$$

By definition, the molar concentration is the number of moles of $\text{Na}_2\text{CO}_3/\text{L}$. Therefore,

$$c_{\text{Na}_2\text{CO}_3} = \frac{1.50 \times 10^{-3} \text{ mol Na}_2\text{CO}_3}{(50.0 + 25.0) \text{ mL}} \times \frac{1000 \text{ mL}}{1 \text{ L}} = 0.0200 \text{ M Na}_2\text{CO}_3$$

Suggested Problems

- 4.1, 4.4, 4.7-4.15 (odd)
- 4.17 (odd), 4.20 (odd), 4.23, 4.31, 4.35, 4-39