Chapter 14

HOW TO DO CALCULATIONS FOR CHEMICAL REACTIONS II

This chapter shows how all the sections on mole calculations can be put together to provide quantitative information about a chemical reaction. The information can be provided in any of three ways: in terms of mass; of concentration and volume of a solution; or of pressure, volume and temperature of a gas.

14.1 Background

On a day-to-day basis, it is analytical chemistry that affects our lives the most. It is through chemical analysis that the chemical components of our drinking water can be monitored; that the composition of our foodstuffs can be determined; and that levels of airborne pollutants can be studied. **Analytical chemistry** is the study of the separation, identification, and quantification of the chemical components of natural and synthetic materials.

Analytical chemistry has two major parts: the identification of what compounds or elements are in a substance – **qualitative analysis**; and the determination of the quantity or concentration of specific compounds or elements in a substance – **quantitative analysis**. There are two ways in which quantitative analysis is performed: by **classical methods** or **instrumental methods**. This chapter will cover classical methods involving the careful measurements of volumes of solutions (**volumetric or titrimetric analysis**) or of masses of solids (**gravimetric analysis**). Instrumental methods require expensive and specialized electronic equipment – each piece of equipment designed to identify specific types of compounds, element composition, or certain properties, such as acidity.

Figure 14.1 A modern analytical chemistry laboratory

14.2 Reactions Involving Mass Measurements – A Review

In Chapter 10, How to do Calculations for Chemical Reactions I, it was shown how, given the mass of one substance, that using the mole principle and the appropriate chemical equation, it is

possible to calculate the mass of any other substance, either reactant or product. The flowchart for the process is shown in Figure 14.2.
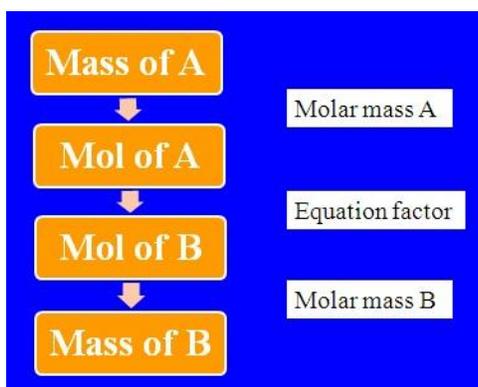

Figure 14.2 Flowchart for the calculation of mass of substance B from mass of substance A.

In the subsequent sections, it will be shown how such calculations can be undertaken using other types of measurements.

14.3 Reactions Involving Solution Measurements

In Chapter 13, Solutions are Everywhere!, the link between volume and concentration of a solution with the moles of solvent was introduced:

$$\text{Molar concentration} = \frac{\text{mole of solute (mol)}}{\text{volume of solution (L)}}$$

This relationship can be incorporated into stoichiometry calculations when either or both of the substances is present as a solution. The flowchart for this is shown in Figure 14.3.
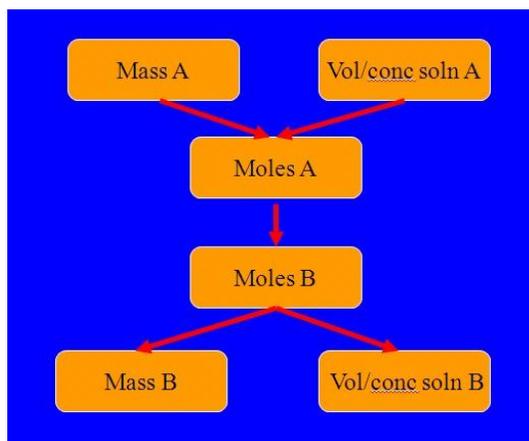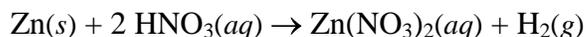

Figure 14.3 Flowchart showing the use of either masses or volumes and concentrations of solutions for stoichiometry calculations.

EXAMPLE 14.1

Zinc metal reacts with dilute nitric acid in a single replacement reaction to give zinc nitrate solution and hydrogen gas:

$$Zn(s) + 2\ HNO_3(aq) \rightarrow Zn(NO_3)_2(aq) + H_2(g)$$

What is the minimum volume of $0.200\ mol \cdot L^{-1}$ nitric acid necessary to completely react with 8.64 g of zinc metal?

Answer

The figure below shows that starting from the mass of zinc, using moles and the equation factor, the volume of nitric acid can be calculated:
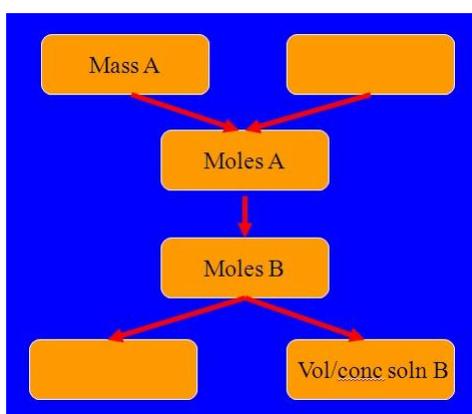
Strategy	Relationship
Mass of Zn $\rightarrow$ mol Zn	1 mol Zn $\equiv$ 65.4 g
Mol of Zn $\rightarrow$ mol of HNO_3	1 mol Zn $\equiv$ 2 mol HNO_3
Mol/conc HNO_3 $\rightarrow$ vol HNO_3	v = n/c

$$\text{mol Zn} = 8.64\ g\ Zn \times \left(\frac{1\ mol}{65.4\ g}\right) = 0.132\ mol\ Zn$$

$$\text{mol } HNO_3 = 0.132\ mol\ Zn \times \left(\frac{2\ mol\ HNO_3}{1\ mol\ Zn}\right) = 0.264\ mol\ HNO_3$$

$$\text{volume } HNO_3 = \frac{0.264\ mol}{0.200\ mol \cdot L^{-1}} = 1.32\ L$$

14.4 Volumetric Analysis

In analytical laboratories, stoichiometric calculations are often used to determine the concentration of one solution knowing the precise (and accurate) concentration and volume of another solution. Such solutions of very precise concentration are known as *standard solutions*.

To undertake a volumetric analysis, specialized and highly precise (and accurate) glassware is used. The reaction takes place in an *Erlenmeyer flask* (Figure 14.4).
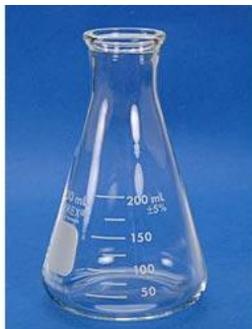

Figure 14.4 In volumetric analysis, the reaction is performed in an Erlenmeyer flask.

One of the reactants is measured out very precisely using a volumetric pipet as was discussed in Chapter 13 and placed in the flask. The other reactant is placed in a *buret* (Figure 14.5). A buret is a long glass cylinder with a tap at one end. Values of volume are etched along the barrel, with the numbers reading downwards.

Figure 14.5 In volumetric analysis, the other reactant is placed in a buret. On the left is a close-up of the tap.

The buret is filled using a *buret funnel* (Figure 14.6). Usually the buret is filled to slightly above the highest volume mark and then the tap opened briefly. In this way, any air trapped below the tap is ejected. The solution in the buret is called the *titrant* and the procedure is often called *titration*.

Figure 14.6 A buret funnel

It is most common to use volumetric analysis as a means of determining the concentration of an acid or a base using the neutralization type of double replacement reaction. In Chapter 9, Section 9.2, Chemical Change, it was noted that there are several ways of identifying when a chemical reaction has occurred, one of these being a colour change. As solutions of acids and of bases are usually colourless, this method cannot be directly used. However, a coloured dye called an *indicator* can be added to the solution in the flask. In Chapter 2, Section 2.6 Classification of Matter, the indicator called litmus was used on a qualitative basis to distinguish between an acid and a base. However, the colour change of litmus from dull blue in base to pink in acid (and the reverse) is too indistinct for quantitative measurements. Figure 14.7 shows the colour changes for the most commonly-used acid-base indicators.

Figure 14.7 Commonly-used acid-base indicators

In the titration, the Erlenmeyer flask is placed underneath the buret and a few drops of the indicator solution is added. A white tile or pad is placed underneath the flask so that, during the titration, any colour change is more apparent (Figure 14.8).
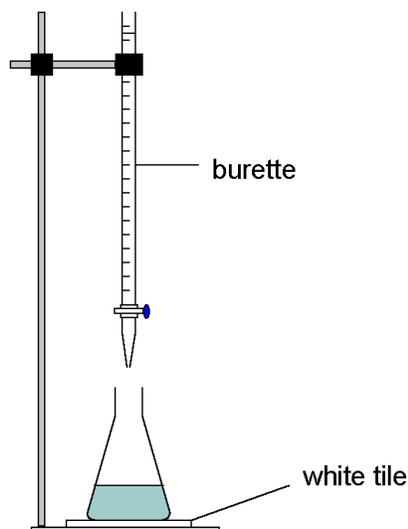
Figure 14.8 The arrangement of equipment for a titration.

The solution volume reading on the buret is recorded, the second decimal place being obtained by interpolation (see Chapter 3, Section 3.9, Volume). The titrant is then added slowly to the flask from the buret until there is the first permanent change in colour of the indicator. This change indicates that a miniscule excess of titrant, just over the stoichiometric value, has been added. The new reading of the volume of the buret is recorded and the difference gives the volume added.

The volume necessary to cause the colour change is called the ***end point***. The theoretical volume to reach the stoichiometric quantity of added titrant is called the ***equivalence point***. Thus the aim of a titration is to try to obtain an end point value as close as possible to the equivalence point. Two indicators that are particularly good for this purpose are phenolphthalein and bromthymol blue. If acid (in the flask) is titrated with base (in the buret), the end point with phenolphthalein is the first pinkish tinge to the colourless solution. With bromthymol blue, the colour change is yellow to blue and a green colour indicates the end point. To obtain better accuracy, several titrations are performed and the average value of titrant is used in the calculation.

The quantitative aspect of the titration is shown in the following calculation.


EXAMPLE 14.2
Barium hydroxide solution reacts with hydrochloric acid in a neutralization (double replacement) reaction to give a solution of barium chloride and water:

$$Ba(OH)_2(aq) + 2\ HCl(aq) \rightarrow BaCl_2(aq) + 2\ H_2O(l)$$
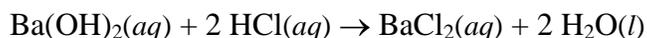
A volume of 25.00 mL of barium hydroxide solution is placed in an Erlenmeyer flask. It requires the addition of a volume of 17.64 mL of 0.1000 mol·L^{-1} hydrochloric acid to reach the end point. What is the concentration of the barium hydroxide solution?

Answer

The figure below shows that starting from the volume and concentration of the hydrochloric acid, using moles and the equation factor, the concentration of the barium hydroxide solution can be calculated:
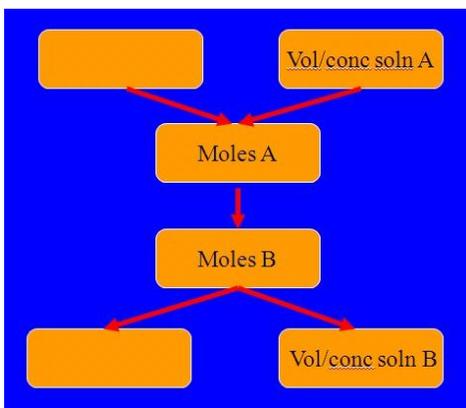
Strategy	Relationship
Vol/conc HCl $\rightarrow$ mol HCl	$n = v \times c$
Mol HCl $\rightarrow$ mol Ba(OH)$_2$	2 mol HCl $\equiv$ 1 mol Ba(OH)$_2$
Mol/vol Ba(OH)$_2$ $\rightarrow$ conc Ba(OH)$_2$	$v = n/c$

$$\text{mol HCl} = 1.764 \times 10^{-2} \text{ L HCl} \times 0.1000 \text{ mol} \cdot \text{L}^{-1} = 1.764 \times 10^{-3} \text{ mol HCl}$$

$$\text{mol Ba(OH)}_2 = 1.764 \times 10^{-3} \text{ mol HCl} \times \left(\frac{1 \text{ mol Ba(OH)}_2}{2 \text{ mol HCl}} \right) = 8.820 \times 10^{-4} \text{ mol Ba(OH)}_2$$

$$\text{concentration Ba(OH)}_2 = \frac{8.820 \times 10^{-4} \text{ mol}}{2.500 \times 10^{-2} \text{ L}} = 3.528 \times 10^{-2} \text{ mol} \cdot \text{L}^{-1}$$

14.5 Gravimetric Analysis

An alternative to volumetric analysis is gravimetric analysis. *Gravimetric analysis* involves quantitative measurements using mass. For example, if there is a solution containing a compound or ion for which the concentration is needed to be found, a reagent can be added to cause one of the ions to precipitate. If this precipitate is filtered into a pre-weighed *filter crucible*, the filter can be dried and re-weighed to obtain the mass of the precipitate. A crucible is shown in Figure 14.9. The white pad in the bottom of the crucible consists of a glass mesh, with pores small enough to stop any precipitate passing through, but large enough for the solution to flow through.

Figure 14.9 A glass filter crucible

To speed up the filtration, the crucible is placed on a **filter flask** which has a rubber **filter crucible adapter** (Figure 14.10). A vacuum is applied through the rubber hose on the left so the solution is forced through the filter by the atmospheric pressure from above.
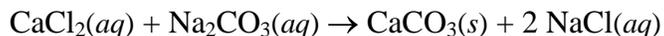

Figure 14.10 The equipment needed to perform a filtration

Here are two sample calculations.

EXAMPLE 14.3

A solution contains an unknown concentration of calcium chloride. When an excess of a sodium carbonate solution is added to 50.00 mL of calcium chloride solution, 6.213 g of a white precipitate of calcium carbonate is formed.

$$CaCl_2(aq) + Na_2CO_3(aq) \rightarrow CaCO_3(s) + 2\ NaCl(aq)$$

What is the concentration of the calcium chloride solution?

Answer

The figure below shows that starting from the mass of calcium carbonate, using moles and the equation factor, the concentration of the calcium chloride solution can be calculated:
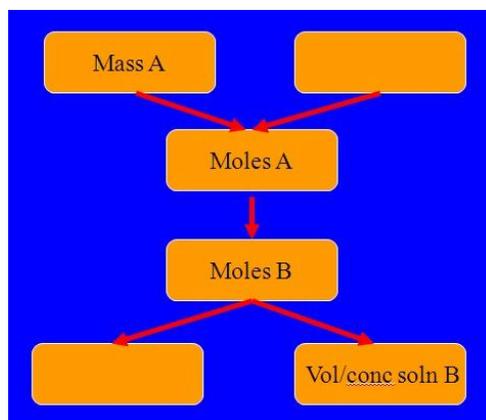
Strategy	Relationship
Mass of $CaCO_3 \rightarrow$ mol $CaCO_3$	1 mol $CaCO_3$ = 100.1 g
Mol of $CaCO_3 \rightarrow$ mol of $CaCl_2$	1 mol $CaCO_3 \equiv$ 1 mol $CaCl_2$
Mol/vol $CaCl_2 \rightarrow$ conc $CaCl_2$	$c = n/v$

$$\text{mol } CaCO_3 = 6.213 \text{ g } CaCO_3 \times \left(\frac{1 \text{ mol}}{100.1 \text{ g}}\right) = 6.207 \times 10^{-2} \text{ mol } CaCO_3$$

$$\text{mol } CaCl_2 = 6.207 \times 10^{-2} \text{ mol } CaCO_3 \times \left(\frac{1 \text{ mol } CaCl_2}{1 \text{ mol } CaCO_3}\right) = 6.207 \times 10^{-2} \text{ mol } CaCl_2$$

$$\text{concentration } CaCl_2 = \frac{6.207 \times 10^{-2} \text{ mol}}{5.000 \times 10^{-2} \text{ L}} = 1.241 \text{ mol} \cdot L^{-1}$$


EXAMPLE 14.4

2.778 g of a metal sulfate, M_2SO_4, where 'M' is an unknown metal, is dissolved in water and an excess of barium nitrate solution is added. 3.720 g of a precipitate of barium sulfate, $BaSO_4$ is formed:

$$Ba(NO_3)_2(aq) + M_2SO_4(aq) \rightarrow BaSO_4(s) + 2 \text{ } MNO_3(aq)$$
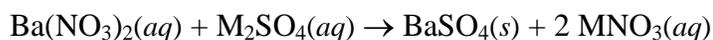
Determine the molar mass of the compound M_2SO_4 and then identify the metal 'M'.

Answer

The figure below shows that starting from the mass of barium sulfate, using moles and the equation factor, the molar mass of M_2SO_4 can be calculated, from that, the molar mass of 'M' can be found and then a Periodic Table will give the identity of the element.
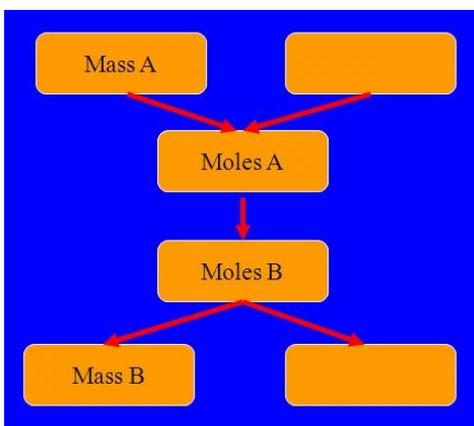
Strategy | Relationship
Mass of $BaSO_4 \rightarrow$ mol $BaSO_4$ | 1 mol $BaSO_4$ = 233.4 g
Mol of $BaSO_4 \rightarrow$ mol of M_2SO_4 | 1 mol $BaSO_4 \equiv$ 1 mol M_2SO_4
mol/mass of $M_2SO_4 \rightarrow$ molar mass M_2SO_4 | molar mass = m/n

$$\text{mol } BaSO_4 = 3.720 \text{ g } BaSO_4 \times \left(\frac{1 \text{ mol}}{233.4 \text{ g}}\right) = 1.594 \times 10^{-2} \text{ mol } BaSO_4$$

$$\text{mol } M_2SO_4 = 1.594 \times 10^{-2} \text{ mol } BaSO_4 \times \left(\frac{1 \text{ mol } M_2SO_4}{1 \text{ mol } BaSO_4}\right) = 1.594 \times 10^{-2} \text{ mol } M_2SO_4$$

$$\text{molar mass } M_2SO_4 = \frac{2.778 \text{ g}}{1.594 \times 10^{-2} \text{ mol}} = 174.3 \text{ g} \cdot \text{mol}^{-1}$$

$$\text{molar mass M} = \frac{(174.3 - 32.1 - [4 \times 16.0])}{2} \text{ g} \cdot \text{mol}^{-1} = 39.09 \text{ g} \cdot \text{mol}^{-1}$$

The element with a molar mass closest to 39.09 g·mol^{-1} is potassium. As potassium forms an ion with a +1 charge, then its sulfate would have the formula K_2SO_4.

14.6 Reactions Involving Gas Measurements

So far in this chapter, quantities in chemical reactions have been determined by means of:

$$\text{Molar mass} = \frac{\text{mass}}{\text{moles}} \quad \left(\text{or m.m.} = \frac{m}{n}\right)$$

$$\text{Concentration of a solution} = \frac{\text{mol solute}}{\text{volume solution}} \quad \left(\text{or c} = \frac{n}{V}\right)$$

As was discussed in Chapter 12, Section 12.6, The Ideal Gas Equation enables the measurable values for a gas to be related together:

$$\textbf{Pressure} \times \textbf{Volume} = \textbf{mol} \times \textbf{Gas Constant} \times \textbf{Temperature} \quad (\textbf{or PV} = \textbf{nRT})$$

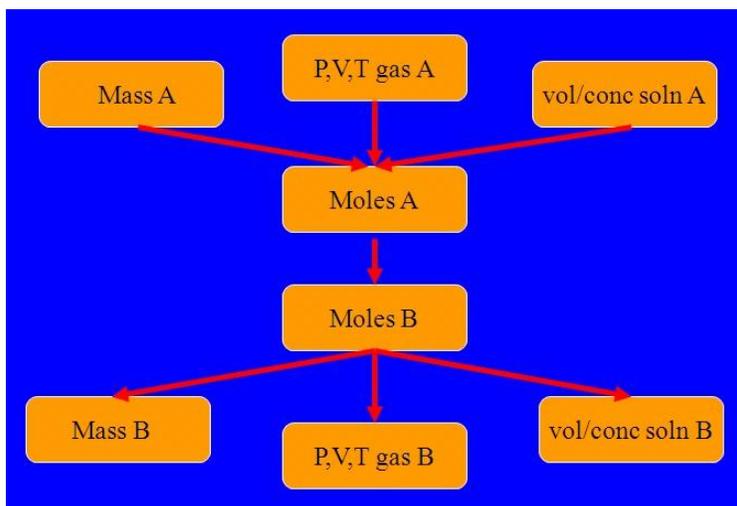Thus stoichiometry calculations can also incorporate gas values (Figure 14.11).

Figure 14.11 Flowchart showing the use of masses; or volumes and concentrations of solutions; or pressure, volume, and temperature of gases; for stoichiometry calculations.

The following two examples show how such calculations can be solved.

EXAMPLE 14.5
Solid phosphorus reacts with chlorine gas to form gaseous phosphorus pentachloride:

$2\ P(s) + 5\ Cl_2(g) \rightarrow 2\ PCl_5(g)$
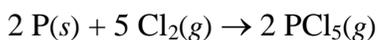
If 7.42 g of phosphorus are used, what is the minimum volume of chlorine gas required at a pressure of 102.1 kPa pressure and a temperature of 21°C?

Answer
The figure below shows that starting from the mass of phosphorus, using moles and the equation factor, the volume of chlorine gas can be calculated:
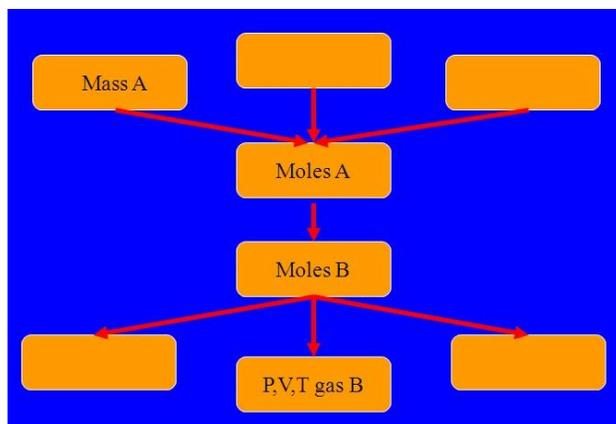
Strategy

Mass of P → mol P

Mol of P → mol of Cl_2

Mol/P/T Cl_2 → vol Cl_2

Relationship

1 mol P = 31.0 g

2 mol P ≡ 5 mol Cl_2

V = nRT/P

$$\text{mol P} = 7.42 \text{ g P} \times \left(\frac{1 \text{ mol}}{31.0 \text{ g}}\right) = 0.239 \text{ mol P}$$

$$\text{mol } Cl_2 = 0.239 \text{ mol P} \times \left(\frac{5 \text{ mol } Cl_2}{2 \text{ mol P}}\right) = 0.598 \text{ mol } Cl_2$$
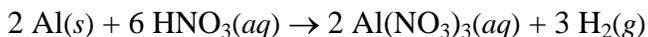
$$\text{volume } Cl_2 = \frac{0.598 \text{ mol} \times 8.31 \text{ kPa} \cdot \text{L} \cdot \text{mol}^{-1} \cdot \text{K}^{-1} \times 294 \text{ K}}{102.1 \text{ kPa}} = 14.3 \text{ L}$$

Figure 14.11 When a chlorine gas is squirted from a pipet onto red phosphorus, a violent exothermic reaction occurs.

EXAMPLE 14.6

Aluminum metal reacts with nitric acid in a single replacement reaction:

$$2\ Al(s) + 6\ HNO_3(aq) \rightarrow 2\ Al(NO_3)_3(aq) + 3\ H_2(g)$$

An excess of aluminum metal is added to 125 mL of 0.500 mol·L^{-1} nitric acid. What volume of hydrogen gas is produced at a pressure of 100.7 kPa and a temperature of 22°C?

Answer

The figure below shows that starting from the volume and concentration of nitric acid, using moles and the equation factor, the volume of hydrogen gas can be calculated:
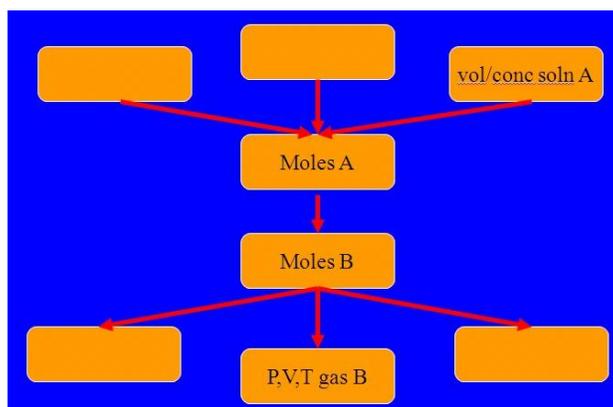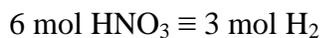

Strategy	Relationship
Vol/conc of $HNO_3 \rightarrow$ mol HNO_3	$n = c \times v$
Mol of $HNO_3 \rightarrow$ mol of H_2	6 mol $HNO_3 \equiv 3$ mol H_2
Mol/P/T $Cl_2 \rightarrow$ vol Cl_2	$V = nRT/P$

$$\text{mol } HNO_3 = 0.125\ \text{L } HNO_3 \times 0.500\ \text{mol} \cdot L^{-1} = 6.25 \times 10^{-2}\ \text{mol } HNO_3$$

$$\text{mol } H_2 = 6.25 \times 10^{-2}\ \text{mol } HNO_3 \times \left(\frac{3\ \text{mol } H_2}{6\ \text{mol } HNO_3} \right) = 3.13 \times 10^{-2}\ \text{mol } H_2$$

$$\text{volume } H_2 = \frac{3.13 \times 10^{-2}\ \text{mol} \times 8.31\ \text{kPa} \cdot L \cdot \text{mol}^{-1} \cdot K^{-1} \times 295\ K}{101.7\ \text{kPa}} = 0.754\ \text{L}$$

14.7 Where Next?

In Chapter 7, Section 7.2, An Overview, the categories of compounds were noted as inorganic compounds and organic compounds. Up to this point, discussion has focused upon the inorganic

compounds. In the last two chapters, you will be introduced to the very different world of organic compounds.