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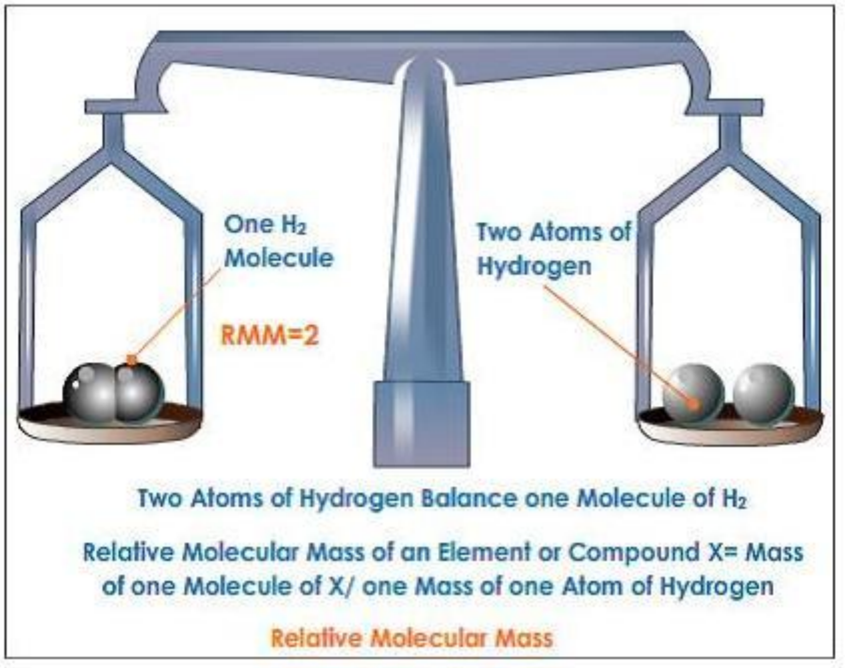
The Mole Concept (INCOMPLETE)



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THE MOLE CONCEPT

Amedeo Avogadro
(1776 – 1856)

3.1. AVOGADRO'S LAW

Avogadro's Law (also referred to as Avogadro's theory or Avogadro's hypothesis) is a principle stated in 1811 by the Italian chemist Amedeo Avogadro (1776-1856) that: **at the constant temperature and pressure, the volume of gas is directly proportional to the number of moles of gas present (Reger, S et al., 2009).** The law is represented mathematically as:

$$V \propto n$$

To remove the proportionality sign, we introduce a constant, k:

$$V = k \times n$$

Transposing the formula to make k the subject (dividing by n):

$$\frac{V}{n} = k$$

Where:

- k is a constant used to remove the proportionality sign.
- V is the volume of the gas
- n is the number of moles of the gas

This number (known as Avogadro's number) is 6.022×10^{23}. It is the number of molecules of any gas present in a volume of 22.41 L and is the same for all gases.

One mole of an ideal gas occupies **22.4** liters (dm^3) at STP, and occupies 24.45 litres at SATP (Standard Ambient Temperature and Pressure = 273K and 1 atm or 101.325 kPa). This volume is often referred to as the molar volume of an ideal gas. **Real gases (there is a distinction between 'real' gases and 'ideal' gases') may deviate from this value.** Ideal gases follow the ideal gas equation. (pV=nRT) but real gases don't follow the ideal gas equation instead there are other **virial** equations used to model their behaviour; one such equation is the van der Waals equation of state:

$$p = \frac{nRT}{V - nb} - a\left(\frac{n}{V}\right)^2$$

Where:

- a & b are van der Waals coeffiecient (these values are different for each gas)
- $\frac{n}{V}$ is known as the number volume, $\mathbb{N}$.

Avogadro's number is one of the fundamental constants of chemistry. It permits calculation of the amount of pure substance (mole) – the basis of stoichiometric relationships. It also makes possible determination of how much heavier a simple molecule of one gas is than that of another, as a result the relative molecular weights of gases can be ascertained by comparing the weights of equal volumes. Avogadro's number (conventionally represented by N_A in chemical calculations) is now considered to be the number of atoms present in *12 grams* of the carbon – 12 isotope (one mole of carbon 12) and can be applied to any type of chemical entity.

Problem

A 2.0 mole sample of a gas is known to occupy 30.0 L of volume. Calculate the V for 1.0 mole of the gas.

Solution

- $V_i/n_i = V_f/n_f$
- $\mathrm{V_f} = \mathrm{V_i} \times \mathrm{n_f}/\mathrm{n_i} = 30\ \mathrm{L} \times 1.0/2.0 = 15\ L$

Problem

$\mathbf{HCl_{(g)} + NH_{3(g)}}$ ==> $\mathbf{NH_4Cl_{(s)}}$

- 1 mole hydrogen chloride gas combines with 1 mole of ammonia gas to give 1 mole of ammonium chloride solid.
- 1 volume of hydrogen chloride will react with 1 volume of ammonia to form solid ammonium chloride
- e.g. 25cm^3 + 25cm^3 → solid product
- or 400dm^3 + 400 dm^3 → solid product (no gas formed)

Problem

$\mathbf{N_{2(g)} + 3H_{2(g)}}$ ==> $\mathbf{2NH_{3(g)}}$

- 1 mole of nitrogen gas combines with 3 mols of hydrogen gas to form 2 mol of a ammonia gas.
- 1 volume of nitrogen reacts with 3 volumes of hydrogen to produce 2 volumes of ammonia
- e.g. 50 cm^3 nitrogen reacts with 150 cm^3 hydrogen (3 x 50) ==> 100 cm^3 of ammonia (2 x 50)

Problem

$$C_3H_{8(g)} + 5O_{2(g)} \Longrightarrow 3CO_{2(g)} + 4H_2O_{(l)}$$

- 1 mole of propane gas reacts with 5 mols of oxygen gas to form 3 moles of carbon dioxide gas and 4 mols of liquid water.

- What volume of oxygen is required to burn 25cm^3 of propane, C_3H_8. Theoretical reactant volume ratio is **C_3H_8 : O_2** is **1 : 5** for burning the fuel propane. So actual ratio is **25** : **5x25**, so **125cm^3 oxygen** is needed.

- What volume of carbon dioxide is formed if 5dm^3 of propane is burned? Theoretical reactant-product volume ratio is **C_3H_8 : CO_2** is **1 : 3.** So actual ratio is **5** : **3x5**, so **15dm^3 carbon dioxide** is formed.

- What volume of air ($^1/_5$th oxygen) is required to burn propane at the rate of 2dm^3 per minute in a gas fire? Theoretical reactant volume ratio is **C_3H_8 : O_2** is **1 : 5.** So actual ratio is **2** : **5x2**, so **10dm^3 oxygen** per minute is needed, therefore, since air is only $^1/_5$th O_2, 5 x 10 = **50dm^3 of air** per minute is required

3.2. THE MOLE

John Dalton (1766 – 1844) published the first table of atomic weights in 1805. The system was based on the assumption of Hydrogen given an atomic weight of 1. The weights were based entirely on stoichiometry proportions of reactions and compounds and aided their acceptance **(Wikipedia, 2010)**.

Jöns Jacob Berzelius (1779–1848) was instrumental in the accurate determination of atomic weights. Unlike Dalton, Berzelius used Oxygen as the standard. Whilst oxygen was a better choice as the standard he chose to fix the atomic weight of oxygen as 100, an innovation which did not catch on **(Wikipedia, 2010)**.

Charles Frédéric Gerhardt (1816–56), Henri Victor Regnault (1810–78) and Stanislao Cannizzaro (1826–1910) expanded on Berzelius' work, resolving many of the problems of unknown stoichiometry of compounds, and the use of atomic weights attracted a large consensus by the time of the Karlsruhe Congress (1860). The convention had reverted to defining the atomic weight of hydrogen as 1 **(Wikipedia, 2010)**.

However the chemical convenience of having oxygen as the primary atomic weight standard became ever more evident with advances in analytical chemistry and the need for ever more accurate atomic weight determinations **(Wikipedia, 2010)**.

The mole (mol) is the SI base unit of amount of substance, one of a few units used to measure this physical quantity. The word 'mole' is derived from the latin word 'moles' which means 'a mass' **(Whitten, et al., 2009)**. The mole is commonly used in titration to determine the concentration of some substance in a solution. In this context, millimoles per litre (mmol/L), micromoles/litre (µmol/L), or nanomoles/L (nmol/L) are often used **(Wikipedia, 2010)**.

For pure substances the mole is defined as: the amount of substance that contains as many "elementary entities" (e.g. atoms, molecules, ions, electrons) as there are atoms in 12 gram of carbon – 12 (^{12}C) **(Rosenberg & Epstein, 1997).**

Thus, by definition, one mole of pure ^{12}C has a mass of *exactly* 12 g. The number of atoms or molecules contained in one mole of a pure substance is known as the Avogadro constant (or Avogadro's number). By convention it has dimension mol^{-1}, and its experimentally determined value is approximately 6.022142×10^{23} mol^{-1}. So a mole of any pure substance has mass in grams exactly equal to that substance's molecular or atomic mass; e.g., 1 mol of calcium-40 is equal to 40 g. In other words, the numerical value of a substance's molecular or atomic mass in atomic mass units is the same as that of its molar mass (the mass of one mole of that substance) in grams **(Wikipedia, 2010)**.

The most common method of determining the amount, expressed in moles, of pure substance the value of whose molar mass is known, is to measure its mass in grams and then to divide by its molar mass (expressed in g/mol). Molar masses may be easily calculated from tabulated values of atomic weights and the molar mass constant (which has a convenient defined value of 1 g/mol). Other methods include the use of the molar volume or the measurement of electric charge **(Wikipedia, 2010)**.

The current definition of the mole was approved during the 1960s. Earlier definitions had been based on the atomic mass of hydrogen (about one gram of hydrogen-1 gas, excluding its heavy isotopes), the atomic weight of oxygen, and the relative atomic mass of oxygen-16; the four different definitions were equivalent to within 1% **(Wikipedia, 2010)**.

3.3. THE MOLAR MASS

Molar mass, symbol *M*, is the mass of one mole of a substance (chemical element or chemical compound). It is a physical property which is characteristic of each pure substance. The base SI unit for mass is the kilogram but, for both practical and historical reasons, molar masses are almost always quoted in grams per mole (g/mol or g mol^{-1}).

3.4. MOLECULAR AND IONIC EQUATIONS

The **molecular equation** shows the overall reaction but not necessarily the actual forms of the reactants and products in solution **(Zumdahl, 2007)**. The **complete ionic equation** represents all reactants and products that are strong electrolytes as ions. All reactants and products are included **(Zumdahl, 2007)**. The **net ionic equation** includes only those components that undergo a change and spectator ions are not included **(Zumdahl, 2007)**.

3.4.1. NET IONIC EQUATIONS

Net ionic equations are useful in that they show only those chemical species directly participating in a chemical reaction. They are thus simpler than the overall equation.

The keys to being able to write net ionic equations are the ability to recognize monatomic and polyatomic ions, the solubility rules, and the rules for electrolyte behaviour.

3.4.2. ELECTROLYTE BEHAVIOUR

Materials dissociate into ions when in water because water is a polar solvent. The major experimental evidence is that these solutions are able to conduct an electrical current. Since an electrical current is a flow of charge and water molecules are neutral, the only explanation is that the flow of current is caused by the availability of these ions (positive and negative).

Any material whose aqueous solution will conduct an electrical current (i.e., which contains ions) is called an **electrolyte**.

Some materials are 100% dissociated into their ions in aqueous solution; these materials are termed **strong** electrolytes **(Atkins & de Paula, 2006)**. Materials which dissociate only partially into their ions are termed **weak** electrolytes **(Atkins & de Paula, 2006)**, and materials which do not dissociate at all are termed nonelectrolytes.

When writing chemical equations for reactions occurring in aqueous solution, it is often useful to write them showing the actual species in solution (i.e., as ions or molecules, as appropriate), rather than using the full “molecular” formula for all reactants and products. How can one tell whether a given material is a strong, weak, or nonelectrolyte when dissolved in water? The following list summarizes the “rules” for electrolyte behavior.

- All salts (ionic compounds) are strong electrolytes.

- Most acids are weak electrolytes (i.e., they are “weak acids”). This generalization includes both inorganic and organic (i.e., carbon-containing, whose formulas usually contain C, H, and O) acids. The only common exceptions to this generalization are HCl, HBr, HI, HNO_3, $HClO_4$ and H_2SO_4. These six are strong acids.

- Among <u>bases</u>, metal hydroxides are strong electrolytes (i.e., they are “strong bases”). Ammonia (NH_3) and organic bases (whose formulas usually contain C, H, and N, and which can be considered as being derived from ammonia by replacing one or more of the hydrogen atoms with carbon-containing groups) are weak.

- All other materials are nonelectrolytes.

Appropriate application of the above rules is crucial for writing chemical equations in net ionic form. Examples of this process are given below.

3.4.3. PRECIPITATION REACTIONS

Let's first start with a complete chemical equation and see how the net ionic equation is derived. For example, take the reaction of lead(II) nitrate with hydrochloric acid to form lead(II) chloride and nitric acid, shown below:

$$Pb(NO_3)_2\,(aq) + 2\,HCl\,(aq) \longrightarrow PbCl_2\,(s) + 2\,HNO_3\,(aq)$$

This complete equation may be rewritten in ionic form by using the solubility rules and rules for electrolyte behavior. All salts are strong electrolytes, therefore the lead(II) nitrate will be dissociated. Both hydrochloric acid and nitric acid are strong acids (they are on the list of exceptions) and will therefore be dissociated. The lead(II) chloride, however is insoluble—remember that all halides are soluble <u>except</u> the silver, lead, and mercury(I) halides. The above equation written in its dissociated (“ionic”) form is:

$$Pb^{2+}(aq) + 2\,NO_3^-\,(aq) + 2\,H^+(aq) + 2\,Cl^-\,(aq) \longrightarrow PbCl_2\,(s) + 2\,H^+(aq) + 2\,NO_3^-\,(aq)$$

Notice that the stoichiometry of the balanced equation must be maintained. $Pb(NO_3)_2$ is dissociated into Pb^{2+} and <u>**2**</u> NO_3^-, and the 2 HCl molecules shown in the reactants are dissociated into <u>**2**</u> H^+ and <u>**2**</u> Cl^-. At this point, one may cancel out those ions which have not participated in the reaction. Notice how the nitrate ions and hydrogen ions remain unchanged on both sides of the equation.

Ions which don't change during the chemical reaction are called **spectator ions** and can be removed from the equation without destroying the equality (as long as they are removed in *exactly the same number* from both sides!).

$$\mathrm{Pb^{2+}(aq) + \cancel{2\,NO_3}^{-}\,(aq) + \cancel{2\,H}^{+}(aq) + 2\,Cl^{-}\,(aq) \longrightarrow PbCl_2\,(s) + \cancel{2\,H}^{+}(aq) + \cancel{2\,NO_3}^{-}\,(aq)}$$

What remains is the <u>net</u> ionic equation, showing only those chemical species participating in the chemical process:

$$\mathrm{Pb^{2+}(aq) + 2\,Cl^{-}\,(aq) \longrightarrow PbCl_2\,(s)}$$

It is also possible to predict the net ionic equation given only the reactants. For example, suppose you had to determine the net ionic equation resulting from the mixing of solutions of barium bromide and sodium sulphate:

$$\mathrm{BaBr_2\,(aq) + Na_2SO_4\,(aq) \longrightarrow\ ?}$$

One way to approach this problem is to determine what ions are in solution. Since both reactants are salts, they will be fully dissociated into Ba^{2+}, Br^{-}, Na^{+}, and SO_4^{2-}. We know that barium bromide is soluble, but will sodium ions or sulphate ions combine with barium ions to form an insoluble compound? Barium ions and sodium ions, both being positive in charge, will repel each other, so no compound is expected to form between them. Similarly, since bromide and sulphate ions both have a negative charge, we would expect no compound to form from this combination. On the other hand, sulphate ions and barium ions could easily form barium sulphate. Now it is just a matter of consulting the solubility rules to see if barium sulphate is soluble or insoluble. The solubility rule for sulphates is that they are all soluble except for those of strontium, barium, and lead; silver sulphate and calcium sulphate are partially soluble. As you can see from these rules, barium sulphate will be insoluble. The sodium ions must therefore combine with bromide ions to form sodium bromide. According to the solubility rules, sodium bromide should be soluble—all sodium salts are soluble, as are most halides. Now we can write a complete balanced equation:

$$\mathrm{BaBr_2\,(aq) + Na_2SO_4\,(aq) \longrightarrow BaSO_4\,(s) + 2\,NaBr\,(aq)}$$

As before, the above equation can be rewritten in ionic form, showing the soluble species as ions in solution:

$$\mathrm{Ba^{2+}(aq) + 2\,Br^{-}\,(aq) + 2\,Na^{+}(aq) + SO_4^{2-}(aq) \longrightarrow BaSO_4\,(s) + 2\,Na^{+}(aq) + 2\,Br^{-}\,(aq)}$$

Next, cross out the spectator ions:

$$\mathrm{Ba^{2+}(aq) + \cancel{2\,Br}^{-}\,(aq) + \cancel{2\,Na}^{+}(aq) + SO_4^{2-}(aq) \longrightarrow BaSO_4\,(s) + \cancel{2\,Na}^{+}(aq) + \cancel{2\,Br}^{-}\,(aq)}$$

What remains is the balanced, net ionic equation:

$$\mathrm{Ba^{2+}(aq) + SO_4^{2-}(aq) \longrightarrow BaSO_4\,(s)}$$

Next, let's consider the case when a solution of magnesium chloride is mixed with one of copper(II) nitrate:

$$\mathrm{MgCl_2\,(aq) + Cu(NO_3)_2\,(aq) \longrightarrow\ ?}$$

As before, the most likely reaction is for the ions to "switch partners":

$$\mathrm{MgCl_2\,(aq) + Cu(NO_3)_2\,(aq) \longrightarrow Mg(NO_3)_2\,(?) + CuCl_2\,(?)}$$

According to the solubility rules, both $Mg(NO_3)_2$ and $CuCl_2$ are soluble in water (all nitrates are soluble; most halides are soluble):

$$\mathrm{MgCl_2\,(aq) + Cu(NO_3)_2\,(aq) \longrightarrow Mg(NO_3)_2\,(aq) + CuCl_2\,(aq)}$$

We now recognize that all four compounds are salts, and completely dissociated in water:

$$Mg^{2+}(aq) + 2\,Cl^{-}(aq) + Cu^{2+}(aq) + 2\,NO_3^{-}(aq) \longrightarrow Mg^{2+}(aq) + 2\,NO_3^{-}(aq) + Cu^{2+}(aq) + 2\,Cl^{-}(aq)$$

When we go to remove spectator ions, we notice that all the ions on the reactant side are exactly the same as those on the product side. This would mean that we would cross out all the ions as spectator ions, leaving nothing behind! In fact, that's exactly what happens in this "reaction." Because no precipitate or weak electrolyte has formed, our (correct) prediction in this case would be "no reaction."

3.4.4. ACID – BASE REACTIONS

Net ionic equations are often applied to acid-base reactions as well. The key to successfully writing the net ionic equation for acid-base reactions is to be able to distinguish between a strong and weak acid or base. The degree of dissociation for an acid is determined by the strength of the acid. For a strong acid, dissociation is complete (100%), thus we would show the acid dissociated into ions in the net ionic equation. In solution, weak acids dissociate to a small extent (usually < 5%). Since weak acids exist in solution predominantly as undissociated molecules, they are shown as neutral molecules (i.e., not shown to be dissociated into ions) in the net ionic equation. For the same reason, weak bases are also shown as undissociated in solution. Strong bases are shown dissociated into the metal cation and OH^{-}.

Organic acids usually contain C, H, and O in their molecular formula, and in particular, have a carboxylic acid functional group (COOH or CO_2H). All organic acids are weak. An example would be benzoic acid, $HC_6H_5CO_2$ or C_6H_5COOH. Ammonia (NH_3) and organic bases (usually derivatives of ammonia) are weak bases. For example methylamine, CH_3NH_2, is a weak base.

The products commonly produced by an acid-base reaction are a salt and water. To write the formula of the salt, it is helpful to know that the cation of the salt always comes from the base and the anion of the salt always comes from the acid. (One way to remember this is to keep the consonants together and the vowels together—**c**ation from the **b**ase and **a**nion from the **a**cid.)

Let's apply some of these rules to writing the net ionic equations for some acid-base reactions. What will be the complete, total ionic and net ionic equations for the reaction of an aqueous solution of nitric acid (HNO_3) with one of potassium hydroxide (KOH)?

$$HNO_3\,(aq) + KOH\,(aq) \longrightarrow ?$$

The cation of the base is potassium ion (K^+) and the anion of the acid is nitrate ion (NO_3^-), so the salt formed will be KNO_3 and the other product will be water. Since all nitrates are soluble, potassium nitrate will be aqueous, and the water will be in the liquid phase. The complete, balanced equation is:

$$HNO_3\,(aq) + KOH\,(aq) \longrightarrow KNO_3\,(aq) + H_2O\,(l)$$

According to the rules for electrolyte behavior given above, HNO_3, KOH, and KNO_3 are all strong electrolytes, and thus will dissociate completely. Water is in the "all other materials" category, so will be a nonelectrolyte and not shown dissociated. The total ionic equation will then be:

$$H^+\,(aq) + NO_3^-\,(aq) + K^+\,(aq) + OH^-\,(aq) \longrightarrow K^+\,(aq) + NO_3^-\,(aq) + H_2O\,(l)$$

We then eliminate the spectator ions (potassium and nitrate):

$$H^+\,(aq) + \cancel{NO_3}^-\,(aq) + \cancel{K}^+\,(aq) + OH^-\,(aq) \longrightarrow \cancel{K}^+\,(aq) + \cancel{NO_3}^-\,(aq) + H_2O\,(l)$$

What remains is the net ionic equation:

$$H^+ (aq) + OH^- (aq) \longrightarrow H_2O (l)$$

This same net ionic equation is the result for the reaction of <u>any</u> strong acid with <u>any</u> strong base.

Let's see what happens with the reaction of a weak acid with a strong base. What will be the complete, total ionic and net ionic equations for the reaction of benzoic acid ($HC_6H_5CO_2$) with sodium hydroxide?

The salt formed will be $NaC_6H_5CO_2$ (Na^+ from the base and $C_6H_5CO_2^-$ from the acid). This salt is soluble because all group IA compounds are soluble. Thus, the complete equation is:

$$HC_6H_5CO_2 (aq) + NaOH (aq) \longrightarrow NaC_6H_5CO_2 (aq) + H_2O (l)$$

Since benzoic acid is a weak acid (it contains carbon in its molecular formula, and is not one of the six common strong acids), it should <u>not</u> be shown dissociated in the total ionic or the net ionic equation. Both NaOH (metal hydroxide) and $NaC_6H_5CO_2$ (salt) are strong electrolytes. The total ionic equation therefore is:

$$HC_6H_5CO_2 (aq) + Na^+ (aq) + OH^- (aq) \longrightarrow Na^+ (aq) + C_6H_5CO_2^- (aq) + H_2O (l)$$

In this case, sodium ions are the only spectator ions:

$$HC_6H_5CO_2 (aq) + \cancel{Na}^+ (aq) + OH^- (aq) \longrightarrow \cancel{Na}^+ (aq) + C_6H_5CO_2^- (aq) + H_2O (l)$$

What remains is the net ionic equation:

$$HC_6H_5CO_2 (aq) + OH^- (aq) \longrightarrow C_6H_5CO_2^- (aq) + H_2O (l)$$

Finally, let's look at an acid-base reaction involving a weak base and a strong acid. What will be the complete, total ionic and net ionic equations for the reaction of HCl with methylamine (CH_3NH_2), a weak organic base? Since hydroxide is not a part of the formula of the weak base, water will not be a product in this case. The complete reaction will be:

$$HCl\ (aq) + CH_3NH_2\ (aq) \longrightarrow CH_3NH_3Cl\ (aq)$$

HCl will be dissociated since it is a strong acid. Since methylamine is a weak base, it will be shown undissociated in the equation. Salts of organic bases are soluble (similar to NH_4^+) and will be dissociated. The total ionic equation that results is:

$$H^+\ (aq) + Cl^-\ (aq) + CH_3NH_2\ (aq) \longrightarrow CH_3NH_3^+\ (aq) + Cl^-\ (aq)$$

The only spectator ion present is chloride:

$$H^+\ (aq) + \cancel{Cl^-\ (aq)} + CH_3NH_2\ (aq) \longrightarrow CH_3NH_3^+\ (aq) + \cancel{Cl}^-\ (aq)$$

What remains is the net ionic equation:

$$H^+\ (aq) + CH_3NH_2\ (aq) \longrightarrow CH_3NH_3^+\ (aq)$$

Problems & Solutions

Show the total ionic and net ionic forms of the following equations. If all species are spectator ions, please indicate that no reaction takes place. Note! You need to make sure the original equation is balanced before proceeding!

1. $AgNO_3\ (aq) + KCl\ (aq) \rightarrow AgCl\ (s) + KNO_3\ (aq)$

Molecular: $AgNO_3\ (aq) + KCl\ (aq) \rightarrow AgCl\ (s) + KNO_3\ (aq)$

Total Ionic: Ag^+ (aq) + $\cancel{NO_3}^-$ (aq) + $\cancel{K^+}$ (aq) + Cl^- (aq) → AgCl (s) + $\cancel{K^+}$ (aq) + $\cancel{NO_3}^-$ (aq)

Net Ionic: Ag^+ (aq) + Cl^- (aq) → AgCl (s)

2. $Mg(NO_3)_2$ (aq) + Na_2CO_3 (aq) → $MgCO_3$ (s) + $NaNO_3$ (aq)

Molecular: $Mg(NO_3)_2$ (aq) + Na_2CO_3 (aq) → $MgCO_3$ (s) + 2 $NaNO_3$ (aq)

Total Ionic: Mg^{2+} (aq) + $\cancel{2\ NO_3}^-$ (aq) + $\cancel{2\ Na}^+$ (aq) + CO_3^{2-} (aq) → $MgCO_3$ (s) + $\cancel{2\ Na}^+$ (aq) + 2 $\cancel{NO_3}^-$ (aq)

Net Ionic: Mg^{2+} (aq) + CO_3^{2-} (aq) → $MgCO_3$ (s)

3. Strontium bromide (aq) + potassium sulphate (aq) → strontium sulphate (s) + potassium bromide (aq)

Molecular: $SrBr_2$ (aq) + K_2SO_4 (aq) → $SrSO_4$ (s) + 2 KBr (aq)

Total Ionic: Sr^{2+} (aq) + $\cancel{2\ Br}^-$ (aq) + $\cancel{2\ K}^+$ (aq) + SO_4^{2-} (aq) → $SrSO_4$ (s) + $\cancel{2\ K}^+$ (aq) + $\cancel{2\ Br}^-$ (aq)

Net Ionic: Sr^{2+} (aq) + SO_4^{2-} (aq) → $SrSO_4$ (s)

4. Manganese(II) chloride (aq) + ammonium carbonate (aq) → manganese(II) carbonate (s) + ammonium chloride (aq)

Molecular: $MnCl_2$ (aq) + $(NH_4)_2CO_3$ (aq) → $MnCO_3$ (s) + 2 NH_4Cl (aq)

Total Ionic: Mn^{2+} (aq) + $\cancel{2\ Cl}^-$ (aq) + $\cancel{2\ NH_4}^+$ (aq) + CO_3^{2-} (aq) → $MnCO_3$ (s) + $\cancel{2\ NH_4}^+$ (aq) + $\cancel{2\ Cl}^-$ (aq)

Net Ionic: Mn^{2+} (aq) + CO_3^{2-} (aq) → $MnCO_3$ (s)

5. Chromium(III) nitrate (aq) + iron(II) sulphate (aq) → chromium(III) sulphate (aq) + iron(II) nitrate (aq)

Molecular: 2 $Cr(NO_3)_3$ (aq) + 3 $FeSO_4$ (aq) → 3 $Fe(NO_3)_2$ (aq) + $Cr_2(SO_4)_3$ (aq)

Total Ionic: $\cancel{2\,Cr}^{3+}$ (aq) + $\cancel{6\,NO_3}^{-}$ (aq) + $\cancel{3\,Fe}^{2+}$ (aq) + $\cancel{3\,SO_4}^{2-}$ (aq) → $\cancel{2\,Cr}^{3+}$ (aq) + $\cancel{6\,NO_3}^{-}$ (aq) + $\cancel{3\,Fe}^{2+}$ (aq) + $\cancel{3\,SO_4}^{2-}$ (aq)

Net Ionic: No Reaction

Please complete the following reactions, and show the total ionic and net ionic forms of the equation:

1. K_3PO_4 (aq) + $Al(NO_3)_3$ (aq) →

Molecular: K_3PO_4 (aq) + $Al(NO_3)_3$ (aq) → $AlPO_4$ (s) + 3 KNO_3 (aq)

Total Ionic: $\cancel{3\,K}^{+}$ (aq) + PO_4^{3-} (aq) + Al^{3+} (aq) + $\cancel{3\,NO_3}^{-}$ (aq) → $AlPO_4$ (s) + $\cancel{3\,K}^{+}$ (aq) + $\cancel{3\,NO_3}^{-}$ (aq)

Net Ionic: Al^{3+} (aq) + PO_4^{3-} (aq) → $AlPO_4$ (s)

2. BeI_2 (aq) + Cu_2SO_4 (aq) →

Molecular: BeI_2 (aq) + Cu_2SO_4 (aq) → $BeSO_4$ (aq) + 2 CuI (s)

Total Ionic: $\cancel{Be}^{2+}$ (aq) + 2 I^- (aq) 2 Cu^+ (aq) + $\cancel{SO_4}^{2-}$ (aq) → $\cancel{Be}^{2+}$ (aq) + $\cancel{SO_4}^{2-}$ (aq) + 2 CuI (s)

Net Ionic: $\cancel{2}$ Cu^{2+} (aq) + $\cancel{2}$ I^- (aq) → $\cancel{2}$ CuI (s)

3. $Ni(NO_3)_3$ (aq) + KBr (aq) →

Molecular: $Ni(NO_3)_3$ (aq) + 3 KBr (aq) → $NiBr_3$ (aq) + 3 KNO_3 (aq)

Total Ionic: $\cancel{Ni}^{3+}$ (aq) + $\cancel{3\,NO_3}^{-}$ (aq) + $\cancel{3\,K}^{+}$ (aq) + $\cancel{3\,Br}^{-}$ (aq) → $\cancel{Ni}^{3+}$ (aq) + $\cancel{3\,NO_3}^{-}$ (aq) + $\cancel{3\,K}^{+}$ (aq) + $\cancel{3\,Br}^{-}$ (aq)

Net Ionic: No Reaction

4. cobalt(III) bromide + potassium sulfide →

Molecular: 2 $CoBr_3$ (aq) + 3 K_2S(aq) → Co_2S_3 (s) + 6 KBr (aq)

Total Ionic: $2\,Co^{3+}\,(aq) + \cancel{6\,Br}^{-}\,(aq) + \cancel{6\,K}^{+}\,(aq) + 3\,S^{2-}\,(aq) \rightarrow Co_2S_3\,(s) + \cancel{6\,K}^{+}\,(aq) + \cancel{6\,Br}^{-}\,(aq)$

Net Ionic: $2\,Co^{3+}\,(aq) + 3\,S^{2-}\,(aq) \rightarrow Co_2S_3\,(s)$

5. barium nitrate + ammonium phosphate →

Molecular: $3\,Ba(NO_3)_2\,(aq) + 2\,(NH_4)_3PO_4\,(aq) \rightarrow Ba_3(PO_4)_2\,(s) + 6\,NH_4NO_3\,(aq)$

Total Ionic: $3\,Ba^{2+}\,(aq) + \cancel{6\,NO_3}^{-}\,(aq) + \cancel{6\,NH_4}^{+}\,(aq) + PO_4^{3-}\,(aq) \rightarrow Ba_3(PO_4)_2\,(s) + \cancel{6\,NH_4}^{+}\,(aq) + \cancel{6\,NO_3}^{-}\,(aq)$

Net Ionic: $3\,Ba^{2+}(aq) + 2\,PO_4^{3-}\,(aq) \rightarrow Ba_3(PO_4)_2\,(s)$

6. calcium hydroxide + iron(III) chloride →

Molecular: $3\,Ca(OH)_2\,(aq) + 2\,FeCl_3\,(aq) \rightarrow 3\,CaCl_2\,(aq) + 2\,Fe(OH)_3\,(s)$

Total Ionic: $\cancel{3\,Ca}^{2+}\,(aq) + 6\,OH^{-}\,(aq) + 2\,Fe^{3+}\,(aq) + \cancel{6\,Cl}^{-}\,(aq) \rightarrow \cancel{3\,Ca}^{2+}\,(aq) + \cancel{6\,Cl}^{-}\,(aq) + 2\,Fe(OH)_3\,(s)$

Net Ionic: $2\,Fe^{3+}\,(aq) + 6\,OH^{-}\,(aq) \rightarrow 2\,Fe(OH)_3\,(s)$ simplifies to:

$Fe^{3+}\,(aq) + 3\,OH^{-}\,(aq) \rightarrow Fe(OH)_3\,(s)$

7. rubidium fluoride + copper(II) sulphate →

Molecular: $2\,RbF\,(aq) + CuSO_4\,(aq) \rightarrow Rb_2SO_4\,(aq) + CuF_2\,(aq)$

Total Ionic: $\cancel{2\,Rb}^{+}(aq) + \cancel{2\,F}^{-}\,(aq) + \cancel{Cu}^{2+}\,(aq) + \cancel{SO_4}^{2-}\,(aq) \rightarrow \cancel{2\,Rb}^{+}\,(aq) + \cancel{SO_4}^{2-}\,(aq) + \cancel{Cu}^{2+}\,(aq) + \cancel{2\,F}^{-}\,(aq)$

Net Ionic: No Reaction

3.4.5. SOLUBILITY RULES

- All salts of Group IA, and ammonium are soluble.
- All salts of nitrates, chlorates and acetates are soluble.

- All salts of halides are soluble except those of silver(I), copper(I), lead(II), and mercury(I).
- All salts of sulphate are soluble except for barium sulphate, lead(II) sulphate, and strontium sulphate.
- All salts of carbonate, phosphate and sulphite are insoluble, except for those of group IA and ammonium.
- All oxides and hydroxides are insoluble except for those of group IA, calcium, strontium and barium.
- All salts of sulphides and insoluble except for those of Group IA and IIA elements and of ammonium.

3.5. CALCULATIONS BASED ON MOLE CONCEPT

STOICHIOMETRY PROBLEMS

Most stoichiometry problems follow a set strategy which revolves around the mole. This strategy is:

$$\text{Quantity A} \longrightarrow \text{Mols A} \longrightarrow \text{Mols B} \longrightarrow \text{Quantity B}$$

You will be using this strategy or some portion of it most of the time. We'll look at each step of this strategy and then combine these steps for more complicated problems.

Converting Quantity A to Mols A

The more ways you can find the mols of a substance, the easier stoichiometry problems will become. Many times the units will help you get to your goal. Take for instance converting the mass of a substance to moles of the substance. You will need a "conversion factor" which will contain both mass and mol units. If you think about it, the molar mass just happens to have these units. Now it's just a matter of getting the units to cancel to achieve the "conversion". Let's look at an example where you are given 25.0 g of $CaCO_3$ and want to find how many mols of $CaCO_3$ are present. First calculate the molar mass of $CaCO_3$:

1 Ca = 40.08 g/mol x 1 = 40.08 g/mol
1 C = 12.01 g/mol x 1 = 12.01 g/mol
3 O = 16.00 g/mol x 3 = 48.00 g/mol
40.08 g/mol + 12.01 g/mol + 48.00 g/mol = 100.09 g/mol $CaCO_3$

The molar mass should be calculated to at least the same number of significant figures as the quantity you need to convert. I generally like to go one significant figure beyond the number I need. Next, use the molar mass to convert the 25.0 g mass of $CaCO_3$ to mols $CaCO_3$. Let the units help you decide whether to multiply or divide by the molar mass:

$$25.0\ \mathrm{g\ CaCO_3}\ \mathrm{x}\ \frac{1\ \mathrm{mol\ CaCO_3}}{100.09\ \mathrm{g\ CaCO_3}} = 0.250\ \mathrm{mol\ CaCO_3}$$

Notice how the gram units cancel, leaving you with mols.

Converting mols into grams

This conversion may be accomplished by a similar calculation as the conversion of grams to mols. Intuitively, you should realize that the same conversion factor will be used--the molar mass. As before, let the units help you decide whether you need to multiply or divide by the molar mass. Given 0.750 mol $CaCO_3$, the number of grams of $CaCO_3$ would be calculated as:

$$0.750\ \mathrm{mol\ CaCO_3}\ \mathrm{x}\ \frac{100.09\ \mathrm{g\ CaCO_3}}{1\ \mathrm{mol\ CaCO_3}} = 75.1\ \mathrm{g\ CaCO_3}$$

Mol A to Mol B Conversions

Once the mol of a quantity is known, a valid stoichiometric comparison may be made. The mol quantity is a scaled up version of what is happening on the molecular level. From mols you may go to the number of grams of a substance (as you did on the previous page), go to number of molecules using Avogadro's number, or go to mols of another substance based on how these two substances relate in a balanced chemical equation. Let's first look at how you can convert from mols of one substance to mols of another substance.

Suppose you had 0.100 mol of sodium carbonate and wanted to know how many mols of sodium ions are present. The chemical formula for sodium carbonate is Na_2CO_3. This means one mole of sodium carbonate contains 2 mols of sodium, 1 mol of carbon and 3 mols of oxygen. In this case, we need to compare the mols of sodium carbonate and mols of sodium ions. Again, we will let the units help us set up the problem:

$$0.100\ \text{mol Na}_2\text{CO}_3 \text{ x } \frac{2\ \text{mol Na}^+}{1\ \text{mol Na}_2\text{CO}_3} = 0.200\ \text{mol Na}^+$$

Notice how the units cancel. Also, in this case, we were able to due a stoichiometric comparison within the same compound.

In other cases, a reaction may be involved and a comparison of two different compounds is necessary. Given a balanced chemical reaction, the stoichiometric coefficients relate the mols reactants and products. Let's look at a typical reaction:

$$2\ KClO_3 \rightarrow 2\ KCl + 3\ O_2$$

In this reaction, 2 mols of potassium chlorate ($KClO_3$) will decompose into 2 mols of potassium chloride (KCl) and 3s mols of oxygen (O_2). If you were given 0.400 mol of

$KClO_3$, and wanted to know how many mols of O_2 will form, use the stoichiometric coefficients to set up a mol ratio in which mols of $KClO_3$ will cancel and mols of O_2 remain:

$$0.400 \text{ mol KClO}_3 \text{ x } \frac{3 \text{ mol O}_2}{2 \text{ mol KClO}_3} = 0.600 \text{ mol O}_2$$

From mols you may also find the number of particles by using Avogadro's number. These particles may be atoms, ions, or molecules. The key word here is particles. That should tip you off that Avogadro's number will be used. Avogadro's number, 6.02×10^{23}, represents how many particles are found in 1 mol, so it may be used to convert mols of a substance to particles or the number of particles to mols. Using the above example, let's calculate how many molecules of oxygen were formed:

$$0.600 \text{ mol O}_2 \text{ x } \frac{6.02 \text{ x } 10^{23} \text{ molecules O}_2}{1 \text{ mol O}_2} = 3.61 \text{ x } 10^{23} \text{ O}_2 \text{ molecules}$$

Using the entire strategy

Now that you know how to convert grams to mols, mols A to mols B, and mols to grams, you can utilize the entire strategy, Quantity A → mols A → mols B → Quantity B to work a typical stoichiometry problem encountered in which the theoretical yield of a substance is calculated. The theoretical yield represents the maximum amount of a product that may be produced from a given set of reactants. Here's a typical problem:

If ammonia, NH3, is burned in air, the following reaction takes place:

$$4\ NH_3 + 3\ O_2 \rightarrow 2\ N_2 + 6H_2O$$

Given that you started with 51.0 g of NH_3, how many g of water will be produced?

You might want to write down what you know about any component of the reaction below that component and what you are trying to find. That will help you identify Quantity A and Quantity B and thus let you know where to start:

$4\ NH_3 + 3\ O_2 \rightarrow 2\ N_2 + 6H_2O$

51.0 g ? g

(Quantity A) (Quantity B)

Execute the strategy:

$$51.0\ \text{g NH}_3 \text{ x } \frac{1\ \text{mol NH}_3}{17.0\ \text{g NH}_3} \text{ x } \frac{6\ \text{mol H}_2\text{O}}{4\ \text{mol NH}_3} \text{ x } \frac{18.0\ \text{g H}_2\text{O}}{1\ \text{mol H}_2\text{O}} = 80.0\ \text{g H}_2\text{O}$$

Quantity A → mol A → mol B → Quantity B

The first step was to convert Quantity A to mols A -- grams of ammonia to mols of ammonia. Next the mols A was converted to mols B -- mols of ammonia was converted to mols water. Finally, mols B was converted to Quantity B -- mols water was converted to grams water. The 81.0 g H_2O produced represents the theoretical yield --the maximum amount of water which can be produced.

In the above problem, we assumed that we had more than enough oxygen to completely consume the ammonia. This assumption may be made when no information is given about the amount of oxygen present during the reaction. In a limiting reagent problem, initial quantities of both reactants are given, and it is not possible to tell which reactant will be used up first. If you need help with limiting reactant problems, please see the specific handout that deals with this topic.

3.6. EMPIRICAL FORMULA

The empirical formula is the simplest formula for a compound. A molecular formula is the same as or a multiple of the empirical formula, and is based on the actual number of atoms of each type in the compound. For example, if the empirical formula of a compound is C_3H_8 , its molecular formula may be C_3H_8 , C_6H_{16} , etc.

An empirical formula is often calculated from elemental composition data. The weight percentage of each of the elements present in the compound is given by this elemental composition.

Let's determine the empirical formula for a compound with the following elemental composition:

40.00% C, 6.72% H, 53.29% O.

The first step will be to assume exactly 100 g of this substance. This means in 100 g of this compound, 40.00 g will be due to carbon, 6.72 g will be due to hydrogen, and 53.29 g will be due to oxygen. We will need to compare these elements to each other stoichiometrically. In order to compare these quantities, they must be expressed in terms of moles. So the next task will be to convert each of these masses to moles, using their respective atomic weights:

$$40.00\,\mathrm{g\,C} \times \frac{1\,\mathrm{mol\,C}}{12.01\,\mathrm{g\,C}} = 3.331\,\mathrm{mol\,C}$$

$$6.72\,\mathrm{g\,H} \times \frac{1\,\mathrm{mol\,H}}{1.008\,\mathrm{g\,H}} = 6.667\,\mathrm{mol\,H}$$

$$53.29\,\mathrm{g\,O} \times \frac{1\,\mathrm{mol\,O}}{16.00\,\mathrm{g\,O}} = 3.331\,\mathrm{mol\,O}$$

Take notice that since the composition data was given to four significant figures, the atomic weights used in the calculation were to at least four significant figures. Using fewer significant figures may actually lead to an erroneous formula.

Now that the moles of each element are known, a stoichiometric comparison between the elements can be made to determine the empirical formula. This is achieved by dividing through each of the mole quantities by whichever mole quantity is the smallest number of moles. In this example, the smallest mole quantity is either the moles of carbon or moles of oxygen (3.331 mol):

$$\frac{3.331\,\text{mol C}}{3.331\,\text{mol}} = 1.000\ \text{C} = 1\,\text{C}$$

$$\frac{6.667\,\text{mol H}}{3.331\,\text{mol}} = 2.001\ \text{H} = 2\,\text{H}$$

$$\frac{3.331\,\text{mol O}}{3.331\,\text{mol}} = 1.000\,\text{O} = 1\,\text{O}$$

The ratio of C:H:O has been found to be 1:2:1, thus the empirical formula is: CH_2O. Again, as a reminder, this is the simplest formula for the compound, and not necessarily the molecular formula. Suppose we know that the molecular weight of this compound is 180 g/mol. With this information, the molecular formula may be determined. The formula weight of the empirical formula is 30 g/mol. Divide the molecular weight by the empirical formula weight to find a multiple:

$$\frac{180\,\text{g/mol}}{30\,\text{g/mol}} = 6$$

The molecular formula is a multiple of 6 times the empirical formula:

$C_{(1 \times 6)}\ H_{(2 \times 6)}\ O_{(1 \times 6)}$ which becomes $C_6H_{12}O_6$

Alternatively, the empirical and molecular formula may be determined from experimental data. Suppose we have a compound containing the elements, C, H and S. A 7.96 mg sample of this compound is burned in oxygen and found to form 16.65 mg of

CO_2. The sulfur in 4.31 mg of the compound is converted into sulphate by a series of reactions, and precipitated as $BaSO_4$. The $BaSO_4$ was found to have a mass of 11.96 mg. The molecular weight of the compound was found to be 168 g/mol. Using this data, what is the molecular formula of the compound?

The strategy will be to use stoichiometry to determine the mass percent of each of the elements in the compound, and then use the mass percentages to determine the empirical formula. Notice that since all the data is in milligrams, we may carry out the calculations using milli- units throughout.

The only source of carbon for the CO_2 formed came from the compound, thus, determine the milligrams of carbon found in 16.65 mg of CO_2 :

$$16.65\,\text{mg CO}_2 \text{ x } \frac{1\,\text{mmol CO}_2}{44.01\,\text{mg CO}_2} \text{ x } \frac{1\,\text{mmol C}}{1\,\text{mmol CO}_2} \text{ x } \frac{12.01\,\text{mg C}}{1\,\text{mmol C}} = 4.544\,\text{mg C}$$

Now that the "part" of the sample due to carbon is known, one may calculate the percent carbon in the compound, using the mass the sample as the "whole":

$$\frac{4.544\,\text{mg C}}{7.96\,\text{mg sample}} \text{ x } 100 = 57.1\%\text{C}$$

The only source of sulfur for the precipitate of $BaSO_4$, came from the compound, thus, determine the milligrams of sulfur in 11.96 mg of $BaSO_4$:

$$11.96\,\text{mg BaSO}_4 \text{ x } \frac{1\,\text{mmol BaSO}_4}{233.39\,\text{mg BaSO}_4} \text{ x } \frac{1\,\text{mmol S}}{1\,\text{mmol BaSO}_4} \text{ x } \frac{32.06\,\text{mg S}}{1\,\text{mmol S}} = 1.643\,\text{mg S}$$

Similarly, determine the percent sulfur in the compound, using the mass of sulfur as the "part" and the mass of compound as the "whole":

$$\frac{1.643\,\text{mg S}}{4.31\,\text{mg sample}} \text{ x } 100 = 38.1\,\%\text{S}$$

The percentage of hydrogen may determined by difference:

%H = 100.0% - 57.1 %C - 38.1 %S = 4.8 %H

From the elemental composition, we may determine the empirical formula, in the same manner as used in the first example. First, assume exactly 100 g of the compound. In 100 grams of the compound, 57.1 g would be due to carbon, 38.0 g would be due to sulfur and 4.9 g would be due to hydrogen. Convert each of these masses into moles using the corresponding atomic weight for each element:

$$57.1\,\text{g C x } \frac{1\,\text{mol C}}{12.01\,\text{g C}} = 4.75\,\text{mol C}$$

$$4.8\,\text{g H x } \frac{1\,\text{mol H}}{1.008\,\text{g H}} = 4.8\,\text{mol H}$$

$$38.0\,\text{g S x } \frac{1\,\text{mol S}}{32.06\,\text{g S}} = 1.19\,\text{mol S}$$

Now that the moles of each element are known, the empirical formula may be determined by dividing the moles of each element by the smallest number of moles. This yields a ratio of the number of each element in the empirical formula.

$$\frac{4.75\,\text{mol C}}{1.19\,\text{mol}} = 3.99\,\text{C} = 4\,\text{C}$$

$$\frac{1.19\,\text{mol S}}{1.19\,\text{mol}} = 1.00\,\text{S} = 1\,\text{S}$$

$$\frac{4.8\,\text{mol H}}{1.19\,\text{mol}} = 4.0\,\text{H} = 4\,\text{H}$$

The ratio of C:H:S has been found to be 4:4:1, thus the empirical formula is: C_4H_4S. The molar mass of the empirical formula is 84 g/mol. Since the molecular weight of the actual compound is 168 g/mol, and is double the molar mass of the empirical formula, the molecular formula must be twice the empirical formula:

$$C_{(4 \times 2)}\ H_{(4 \times 2)}\ S_{(1 \times 2)} \text{ which becomes } C_8H_8S_2$$

Problem

The analgesic, aspirin, has the following elemental percent composition: 60.00% C, 4.48% H, and 35.53% O.

a) Find the empirical formula of aspirin.
b) If the molar mass of aspirin is 180 g/mol, what is the molecular formula of aspirin?

Solution

Assume exactly 100 grams of aspirin. As a result, 60.00% C becomes 60.00 g C, 4.48% H becomes 4.48 g H and 35.53% O becomes 35.53 g O. Convert each of these masses to moles:

$$60.00 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 4.996 \text{ mol C}$$

$$4.48 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 4.44 \text{ mol H}$$

$$35.53 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 2.221 \text{ mol O}$$

Divide through by the smallest moles to find the ratio of C:H:O :

$$\frac{4.006 \text{ mol C}}{2.221 \text{ mol O}} : \frac{4.44 \text{ mol H}}{2.221 \text{ mol O}} : \frac{2.221 \text{ mol O}}{2.221 \text{ mol O}}$$

$$2.250 : 2.00 : 1.000$$

The ratio does not work out to a whole numbers, so since 2.25 is 2 ¼, which is 9/4, multiply the entire ratio by 4:

2.250 x 4 = 9 C 2.00 x 4 = 8 H 1.000 x 4 = 4 O

The empirical formula is thus: **$C_9H_8O_4$.** The empirical formula is the simplest possible formula for a compound.

1. Paradichlorobenzene is the active ingredient in the insecticide known as mothballs. The elemental percent composition of paradichlorobenzene is: 49.02% C, 2.74% H, and 48.24% Cl.

   (a) Find the empirical formula of paradichlorobenzene.
   (b) If the molar mass of paradichlorobenzene 147 g/mol, what is the molecular formula of this compound?

2. Many sunscreens contain the compound para-aminobenzoic acid (PABA). The elemental percent composition of PABA is: 61.31% C, 5.15% H, 10.21% N, and 23.33% O.

   (a) Find the empirical formula of PABA.
   (b) If the molar mass of PABA is 137 g/mol, what is the molecular formula of PABA?

3. Potassium Ferricyanide is a water soluble red dye used in products such as bingo dabbers. The elemental percent composition of potassium ferricyanide: 35.62% K, 21.89% C, 16.96% Fe, and 25.53% N.

   a) Find the empirical formula of potassium ferricyanide.
   b) If the molar mass of potassium ferricyanide is 329 g/mol, what is the molecular formula of potassium ferricyanide?

4. Lindane is an insecticide used to kill lice. The elemental percent composition of lindane is: 24.78% C, 2.08% H, and 73.14% Cl.

(a) Find the empirical formula of lindane.
(b) If the molar mass of lindane is 290 g/mol, what is the molecular formula of lindane?

Solutions

Always use at least the same number of significant figures for the molar masses of the elements as are given for the elemental composition. For example, if you are given 43.89% C, then use at least 12.01g/mol for the molar mass of carbon. Using fewer significant figures (12 g/mol or 12.0 g/mol, in this case) could actually lead to the incorrect formula. On the other hand, when determining the multiple for converting the empirical formula to a molecular formula, whole number molar masses are typically sufficient.

When given the elemental percent composition, it is convenient to assume 100 grams of the substance. Doing so allows you to have a reference point in that the percentage of the element becomes the mass. For example, if the elemental composition of a compound is 54.3 %A and 45.7 %B, assuming 100 grams allows you to start with 54.3 g of A and 45.7 g of B.

1 b. The molecular formula is either the same as, or a multiple of the empirical formula. To find the multiple, one must compare the molar mass (MM) of the actual compound to the empirical formula weight (EFW). It is not necessary to use many significant figures to find this multiple.

Calculate the EFW: 9(12 g C/mol C) + 8(1 g H/mol H) + 4(16 g O/mol O) = 180 g/mol
The molar mass of aspirin is given to be 180 g/mol
Determine the multiple:

$$\frac{\text{MM}}{\text{EFW}} = \frac{180\text{ g/mol}}{180\text{ g/mol}} = 1$$

Since the multiple is "1", the empirical formula is identical to the molecular formula: **$C_9H_8O_4$**.

2 a. Assume exactly 100 g of para-dichlorobenzene. As a result, 49.02% C becomes 29.02 g C, 2.74 % H becomes 2.74 g H and 48.24% Cl becomes 48.24 g Cl. Convert each of the masses to moles:

$$49.02 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 4.082 \text{ mol C}$$

$$2.74 \text{ g H} \ \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 2.72 \text{ mol H}$$

$$48.24 \text{ g Cl} \ \frac{1 \text{ mol Cl}}{35.45 \text{ g Cl}} = 1.361 \text{ mol Cl}$$

Divide through by the smallest moles to find the ratio of C:H:Cl :

$$\frac{4.082 \text{ mol C}}{1.361 \text{ mol Cl}} : \frac{2.72 \text{ mol H}}{1.361 \text{ mol Cl}} : \frac{1.361 \text{ mol Cl}}{1.361 \text{ mol Cl}}$$

$$3.00 : 2.00 : 1.00$$

The empirical formula of para-dichlorobenzene is **C_3H_2Cl**. This is the simplest formula for the compound.

2 b. The molecular formula is either the same as, or a multiple of the empirical formula. To find the multiple, one must compare the molar mass (MM) of the actual compound to the empirical formula weight (EFW). It is not necessary to use many significant figures to find this multiple.

Calculate the EFW: 3(12 g/mol) + 2(1 g/mol) + 1(35.5 g/mol) = 73.5 g/mol

The molar mass of para-dichlorobenzene is given to be 147 g/mol.

Determine the multiple:

$$\frac{147 \text{ g/mol}}{73.5 \text{ g/mol}} = 2$$

The molecular formula is found by multiplying the subscripts of the empirical formula by the multiple of 2:

$$C_{3 \times 2}H_{2 \times 2}Cl_{1 \times 2} = \mathbf{C_6H_4Cl_2}$$

3 a. Assume exactly 100 g of PABA. Thus, 61.31% C becomes 61.31 g C, 5.15% H becomes 5.15 g H, 10.21 g N becomes 10.21 g N and 23.33% O becomes 23.33 g O. Convert each of these masses to moles:

$$61.31 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 5.105 \text{ mol C}$$

$$5.15 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 5.109 \text{ mol H}$$

$$10.21 \text{ g N} \times \frac{1 \text{ mol N}}{14.01 \text{ g N}} = 0.7288 \text{ mol N}$$

$$23.33 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 1.458 \text{ mol O}$$

Divide through by the smallest moles to find the ratio of C:H:N:O :

$$\frac{5.105 \text{ mol C}}{0.7288 \text{ mol N}} : \frac{5.109 \text{ mol H}}{0.7288 \text{ mol N}} : \frac{0.7288 \text{ mol N}}{0.7288 \text{ mol N}} : \frac{1.458 \text{ mol O}}{0.7288 \text{ mol N}}$$

$$7.00 : 7.01 : 1.00 : 2.00$$

The empirical formula of PABA is **$C_7H_7NO_2$**. This is the simplest formula for the compound.

3 b. compound.

2 b. The molecular formula is either the same as, or a multiple of the empirical formula. To find the multiple, one must compare the molar mass (MM) of the actual compound to the empirical formula weight (EFW). It is not necessary to use many significant figures to find this multiple.

Calculate the EFW of PABA: 7(12 g/mol) + 7(1 g/mol) + 1(14 g/mol) + 2(16 g/mol) = 137 g/mol

The molar mass of PABA is given to be 137 g/mol.

Determine the multiple:

$$\frac{\text{MM}}{\text{EFW}} = \frac{137 \text{ g/mol}}{137 \text{ g/mol}} = 1$$

The molecular formula for PABA is the same as the empirical formula: **$C_7H_7NO_2$.**

4 a. Assume exactly 100 grams of potassium ferricyanide. As result, 35.62 % K becomes 35.62 g K, 16.96 %Fe becomes 16.96 g Fe, 21.89 %C becomes 21.89 g C and 25.53 %N becomes 25.53 g N. Convert each of these masses to moles:

$$35.62 \text{ g K} \times \frac{1 \text{ mol K}}{39.10 \text{ g K}} = 0.9110 \text{ mol K}$$

$$16.96 \text{ g Fe} \times \frac{1 \text{ mol Fe}}{55.85 \text{ g Fe}} = 0.3056 \text{ mol Fe}$$

$$21.89 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 1.823 \text{ mol C}$$

$$25.53 \text{ g N} \times \frac{1 \text{ mol N}}{14.01 \text{ g N}} = 1.823 \text{ mol N}$$

Divide through by the smallest moles to find the ratio of K:Fe:C:N :

$$\frac{0.9110 \text{ mol K}}{0.3056 \text{ mol Fe}} : \frac{.3056 \text{ mol Fe}}{.3056 \text{ mol Fe}} : \frac{1.823 \text{ mol C}}{.3056 \text{ mol Fe}} : \frac{1.823 \text{ mol N}}{.3056 \text{ mol Fe}}$$

$$3.000 : 1.000 : 6.000 : 6.000$$

The empirical formula for potassium ferricyanide is **$K_3FeC_6N_6$.** This is the simplest formula for this compound.

4 b. The molecular formula is either the same as, or a multiple of the empirical formula. To find the multiple, one must compare the molar mass (MM) of the actual compound to the empirical formula weight (EFW). It is not necessary to use many significant figures to find this multiple.

Calculate the EFW for potassium ferricyanide:

$$3(39 \text{ g/mol}) + 1(55.85 \text{ g/mol}) + 6(12 \text{ g/mol}) + 6(14 \text{ g/mol}) = 329 \text{ g/mol}$$

The molar mass of potassium ferricyanide is given to be 329 g/mol.

Determine the multiple:

$$\frac{\text{MM}}{\text{EFW}} = \frac{329 \text{ g/mol}}{329 \text{ g/mol}} = 1$$

The molecular formula is the same as the empirical formula: **$K_3FeC_6N_6$**

5 a. Assume exactly 100 g of lindane. As a result, 24.78 %C becomes 24.78 g C, 2.08 %H becomes 2.08 g H and 73.14% Cl becomes 73.14 g Cl. Convert each of these masses to moles:

$$24.78 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 2.063 \text{ mol C}$$

$$2.08 \text{ g H} \times \frac{1 \text{ mol H}}{1.08 \text{ g H}} = 2.063 \text{ mol H}$$

$$73.14 \text{ g Cl} \times \frac{1 \text{ mol Cl}}{35.45 \text{ g Cl}} = 2.063 \text{ mol Cl}$$

Divide through by the smallest moles to find the ratio of C:H:Cl :

$$\frac{2.063 \text{ mol C}}{2.063 \text{ mol C}} : \frac{2.063 \text{ mol H}}{2.063 \text{ mol C}} : \frac{2.063 \text{ mol Cl}}{2.063 \text{ mol C}}$$

$$1.000 \quad : \quad 1.000 \quad : \quad 1.000$$

The empirical formula for lindane is **CHCl**. This is the simplest formula for the compound.

5 b. The molecular formula is either the same as, or a multiple of the empirical formula. To find the multiple, one must compare the molar mass (MM) of the actual compound to the empirical formula weight (EFW). It is not necessary to use many significant figures to find this multiple.

Calculate the EFW: 1(12 g/mol) + 1(1 g/mol) + 1(35.5 g/mol) = 48.5 g/mol

The molar mass of lindane is given to be 290 g/mol.

Determine the multiple:

$$\frac{\text{MM}}{\text{EFW}} = \frac{290 \text{ g/mol}}{28.5 \text{ g/mol}} = 6$$

The molecular formula of lindane is found by multiplying the subscripts of the empirical formula by the multiple of 6:

$$C_{1\times6}H_{1\times6}Cl_{1\times6} = \mathbf{C_6H_6Cl_6}$$

3.7. TITRIMETRIC ANALYSIS

3.7.1. BASIC PRINCIPLES

In titrimetric analysis volumetrically measures the amount of reagent, often called a titrant, required to complete a chemical reaction with the analyte. A generic chemical reaction for titrimetric analysis is **(Bialkowski, 2005)**

$$aA + tT \rightarrow products$$

Where:

- a moles of analyte A contained in the sample reacts with t moles of the titrant T in the titrant solution.

The reaction is generally carried out in a flask containing the liquid or dissolved sample. Titrant solution is volumetrically delivered to the reaction flask using a burette. Delivery of the titrant is called a titration. The titration is complete when sufficient titrant has been added to react with all the analyte. This is called the *equivalence point.* **(Bialkowski, 2005)**

An indicator is often added to the reaction flask to signal when all of the analyte has reacted. The titrant volume where the signal is generated is called the *end point*. The equivalence and end points are rarely the same. **(Bialkowski, 2005)**

3.7.2. SUCCESSFUL TITRATIONS

A few rules of thumb for designing a successful titration are:

- The titrant should either be a standard or should be standardized.

- The reaction should proceed to a stable and well defined equivalence point.
- The equivalence point must be able to be detected.
- The titrant's and sample's volume or mass must be accurately known.
- The reaction must proceed by a definite chemistry. There should be complicating side reactions.
- The reaction should be nearly complete at the equivalence point. In other words, chemical equilibrium favors products.
- The reaction rate should be fast enough to be practical.

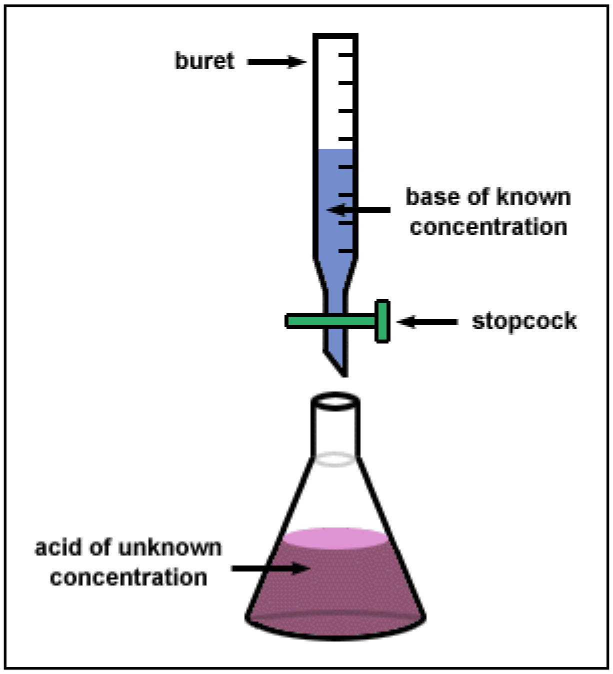

Figure 1 - Titration setup: the titrant drops from the burette into the analyte solution in the flask. An indicator present then changes colour permanently at the endpoint.

3.7.3. TYPES OF TITRATIONS

3.7.3.1. ACID-BASE TITRATION

These titrations are based on the neutralization reaction that occurs between an acid and a base, when mixed in solution. The acid (resp. base) is added to a burette which was rinsed with the same acid prior to this addition to prevent contamination or diluting of the acid being measured. The base (resp. acid) is added to a volumetric flask which had been rinsed with distilled water prior to the addition to prevent contamination or dilution of the base/alkali being measured. The solution in the volumetric flask is often a standard solution; one whose concentration is exactly known. The solution in the burette, however, is the solution whose concentration is to be determined by titration. The indicator used for such an acid-base titration often depends on the nature of the constituents as described in the above section. Common indicators, their colours, and the pH range in which they change colour, are given in the table above. When more precise results are required, or when the titration constituents are a weak acid and a weak base, a pH meter or a conductance meter are used. **(Wikipedia, 2010)**

3.7.3.2. REDOX TITRATION

These titrations are based on a redox reaction between an oxidizing agent and a reducing agent. The oxidizing agent (resp. reducing agent) is added to the burette which was rinsed with the same oxidizing agent. The reducing agent (resp. oxidizing agent) is added to the conical flask, which had been rinsed with distilled water. Like in an acid-base titration, the standard solution is often the one in the conical flask, and the solution whose concentration is to be determined is the one in the burette. The procedure for carrying out redox titrations is similar to that required for carrying out acid-base titrations. **(Wikipedia, 2010)**

Most commonly, a potentiometer or a redox indicator are used to determine the end point of the titration. For example, when one of constituents of the titration is the oxidizing agent potassium dichromate, the colour change of the solution from orange to green is not definite and thus an indicator such as sodium diphenylamine is used. The analysis of wines for their sulphur dioxide content requires the use of iodine as an oxidizing agent. In this case, starch is used as an indicator; a blue starch-iodine complex is formed once an excess of iodine is present, thus signalling the endpoint of the titration. **(Wikipedia, 2010)**

On the other hand, some redox titrations do not require an indicator, due to the intense colour of some of the constituents. For instance, in a titration where the oxidizing agent potassium permanganate (permanganometry) is present, a slight faint persisting pink colour signals the endpoint of the titration, and no particular indicator is therefore required. **(Wikipedia, 2010)**

Titration Calculations

A solution whose concentration is known is called a standard solution. Finding the concentration of the second solution is called standardising it.

Problem

25 cm^3 of 0.100 M NaOH solution required 23.5 cm^3 of dilute hydrochloric acid for neutralization. Calculate the concentration of the hydrochloric acid.

Solution

$$\mathrm{HCl\ (aq) + NaOH(aq) \rightarrow NaCl\ (s) + H_2O\ (l)}$$

So:

$$\frac{25\ \mathrm{cm}^3}{1000\ \mathrm{cm}^3/\mathrm{dm}^3} \times 0.100\ \mathrm{mol/dm}^3 = \frac{23.5\ \mathrm{cm}^3}{1000\ \mathrm{cm}^3/\mathrm{dm}^3} \times \mathrm{M_{HCl}}$$

Transposing to find the concentration of HCl:

$$\mathrm{M_{HCl}} = \frac{25\ \mathrm{cm}^3 \times 0.100\ \mathrm{mol/dm}^3}{1000\ \mathrm{cm}^3/\mathrm{dm}^3} \times \frac{1000\ \mathrm{cm}^3/\mathrm{dm}^3}{23.5\ \mathrm{cm}^3} = 0.106\ \mathrm{mol/dm}^3$$

Problem

25 cm^3 of sodium hydroxide solution of unknown concentration was titrated with dilute sulphuric acid of concentration 0.050 mol/dm^3. 20.0 cm^3 of the acid was required to neutralize the alkali. Find the concentration of the sodium hydroxide solution in mol/dm^3.

Solution

$$2\text{NaOH} + \text{H}_2\text{SO}_4 \rightarrow \text{Na}_2\text{SO}_4 + 2\text{H}_2\text{O}$$

- Number of moles of H_2SO_4 = $20/1000 \times 0.050 = 0.001\ mol$
- Number of moles of NaOH = $2 \times 0.001 = 0.002\ mol$

$$\text{M}_{\text{NaOH}} = \frac{\text{mol}}{\text{volume}} = \frac{0.002}{25/1000} \times \frac{\text{mol}}{\text{dm}^3} = 0.08\ \text{mol/dm}^3$$

Problem

2.10 g of sodium hydrogen carbonate was dissolved in water and the solution made up to 250 cm^3. 25.0 cm^3 of this solution was pipetted into a conical flask and some methyl orange indicator added. This solution was neutralised by 25.9 cm^3 of dilute hydrochloric acid added from a burette. Calculate the concentration of the acid in g/dm^3.

Solution

$$\text{NaHCO}_3 + \text{HCl} \rightarrow \text{NaCl} + \text{CO}_2 + \text{H}_2\text{O}$$

$$\text{Concentration of NaHCO}_3 = \frac{\text{mol}}{\text{vol}} = \frac{0.025\ \text{mol}}{250\ \text{cm}^3/1000\text{dm}^3} = 0.1\ \text{mol/dm}^3$$

$$\text{Number of moles of NaHCO}_3\ \text{used} = \text{conc}'\text{n} \times \text{vol} = 0.1 \times \frac{25}{1000} = 0.0025\ mol$$

$$\text{Number of moles of HCl} = 0.0025\ \text{mol}$$

$$\text{Concentraton of HCl} = \frac{\text{mol}}{\text{volume}} = \frac{0.0025\ \text{mol}}{25.9\ \text{cm}^3/1000\ \text{dm}^3} = 0.0965\ \text{mol/dm}^3$$

MORE COMPLEX PROBLEMS

Problem

25.0 cm^3 of iron (II) sulphate solution of concentration 0.100 mol dm^3 was acidified with an equal volume of dilute sulphuric acid (an excess), and then titrated with potassium manganate (VII) solution. It required 20.6 cm^3 of potassium manganate (VII) solution to react the end point of the titration. Find the concentration of the potassium manganate (VII) solution in mol/dm^3.

Solution

$$\mathrm{MnO_4^-(aq) + 8H^+(aq) + \ 5Fe^{2+}(aq) \rightarrow Mn^{2+}(aq) + 5Fe^{3+}(aq) + 4H_2O(l)}$$

Dividing by 5:

$$\frac{1}{5}\mathrm{MnO_4^-(aq)} + \frac{8}{5}\mathrm{H^+(aq) + \ Fe^{2+}(aq)} \rightarrow \frac{1}{5}\mathrm{Mn^{2+}(aq) + Fe^{3+}(aq)} + \frac{4}{5}\mathrm{H_2O(l)}$$

$$\text{Number of moles of FeSO}_4 \text{ used} = \text{conc}'\text{n} \times \text{vol} = 0.100\ \times \frac{25}{1000} = 0.0025 \text{ mol}$$

$$\text{Number of moles of KMnO}_4 = \frac{1}{5} \times 0.0025 = 0.0005 \text{ mol}$$

$$\text{Conc}'\text{n of KMnO}_4 = \frac{\text{mol}}{\text{vol}} = \frac{0.0005}{20.6/1000} = 0.024 \text{ mol/dm}^3$$

Problem

An excess of potassium iodide solution was added to 25.0 cm^3 of copper (II) sulphate solution and the iodide liberated was titrated with standard sodium thiosulphate solution. 15.7 cm^3 of 0.200 mol/dm^3 sodium thiosulphate solution, $Na_2S_2O_4$ was needed to react with all the iodine. Find the concentration of the copper (II) sulphate solution in grams of CuSO4 per dm^3.

Solution

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