1. The Mole

Early chemists discovered that substances combine in certain combinations to form new substances. For example, 32 g (grams) of oxygen combines with 4 g of hydrogen to form 36 g of water. Also, 32 g of oxygen combines with 12 g of carbon to form 44 g of carbon dioxide. Eventually people realized that substances are made of atoms, and that atoms combine in specific ratios. The various combinations of masses that were observed to react is explained when we account for different atoms having different masses.

The numbers of atoms encountered in everyday life is very large. Even a tiny quantity of a substance consists of a vast number of atoms. It is inconvenient to constantly talk about such large numbers of atoms when discussing chemical reactions – or substances in general. This approach to dealing with large numbers is actually quite common. For example, when discussing the national debt of the United States, we hear numbers like 14.3 trillion dollars. This number is expressed in units of trillions of dollars. This is much more convenient than writing the number as $14300000000000.

It turns out that there are typically a lot more atoms than there are dollars of national debt. Thus, the unit for numbers of particles used in chemistry is much bigger than 1 trillion. It is $N_A = 6.022\times10^{23}\ \text{mol}^{-1}$, the Avogadro constant. The unit itself is called the mole (or mol). If we have 1 mol of hydrogen atoms, we have 6.022×10^{23} hydrogen atoms. This number arises because chemists wanted 1 mol of hydrogen atoms (the lightest atoms) to have a mass of about 1 g. They achieve this by setting the mass of 1 mol of carbon-12 atoms to exactly 12 g (carbon-12 is the common isotope of carbon). This convention defines the value of the Avogadro constant.

1.1 How do we use the mole? Counting atoms and molecules

The masses of 1 mol of each type of atom[1] are given in the periodic table. With this data, we can determine how many atoms are in a sample by measuring the mass of the sample.

Example 1.1: If a sample of Helium has a mass of 6.600 g, then how many helium atoms are in the sample?

Approach: Find mol of He. Convert to number of atoms.

The molar mass of helium (i.e., the mass of 1 mol of helium atoms) is expressed as 4.003 g mol^{-1}. You find this in the periodic table. Therefore, 6.500 g of helium consists of

$$\frac{6.600\ \text{g}}{4.003\ \text{g mol}^{-1}} = 1.648_8\ \text{mol of helium}$$ [2]

To get the number of helium atoms *not* in units of mol, we simply multiply by $N_A = 6.022\times10^{23}$ atoms mol^{-1}. The Avogadro constant has units of "particles" per mole. Here, the particle is a helium atom. Thus, there are

$$1.648_8\ \text{mol} \times 6.022\times10^{23}\ \text{atoms mol}^{-1} = 9.929\times10^{23}\ \text{atoms}$$

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[1] Molar masses found in the periodic table are averages of isotope masses, weighted according to natural abundance.

[2] The final digit in 1.648_8 is written as a subscript to indicate that we are carrying the extra digit (the second 8) into the next step of the calculation. It is written as a subscript because it is *not a significant figure*. Carrying the extra figure reduces rounding errors during the steps of a calculation.

Observe how the units cancel out, leaving the desired unit of atoms:

$$1.648_8 \cancel{\text{mol}} \times 6.022\times10^{23} \text{ atoms } \cancel{\text{mol}}^{-1} = 9.929\times10^{23} \text{ atoms}$$

Dividing the mass of a sample of atoms by the molar mass of the atom gives the amount of the substance in mol.

$$\text{amount (in mol)} = \frac{\text{mass (in g)}}{\text{Molar mass (in g mol}^{-1}\text{)}} \qquad n = \frac{m}{M} \qquad 1.1$$

Multiplying by N_A then gives the number of atoms. We can use the same formula to count the number of molecules in a sample.

Example 1.2: How many water molecules are in 20.0 g of water?

Approach: Find number of moles of water. Convert to number of molecules.

$$\text{amount of water (mol)} = \frac{\text{mass of water}}{\text{Molar mass of water}}$$
$$= \frac{20.0 \text{ g}}{18.015 \text{ g mol}^{-1}} = 1.11_0 \text{ mol}$$

This is the amount of water. To answer the question, we must multiply by the Avogadro constant.

$$1.11_0 \text{ mol} \times 6.022\times10^{23} \text{ molecules mol}^{-1} = 6.68 \times10^{23} \text{ molecules}$$

The Avogadro constant has units of "particles" per mole. Here, the particle is a water molecule. The "particle" can be any unit we need.

1.2 Balancing Chemical Reactions

Chemical reactions are happening all the time. Some are slow, and barely noticeable. Others are fast. Some of these involve the release of energy in the form of heat, light and/or sound. Chemical reactions are conversions of one set of compounds – the *reactants* – into another set of compounds – the *products*. They readily occur when there are stable products that can be reached through some rearrangement of the atoms of the reactants. A principal feature of any chemical reaction is that the total number of each type of atom, among reactants, must equal the same tally for the products. Atoms are neither created nor destroyed in a chemical reaction (this is the Law of Conservation of Mass). This allows us to balance chemical reactions and use the associated stoichiometric coefficients to determine the expected amounts of the various products.

Example 1.3: Balance the following chemical reactions:

(a) $Mg(s) + Cl_2(g) \rightarrow MgCl_2(s)$
(b) $Ca(s) + O_2(g) \rightarrow CaO(s)$
(c) $CH_4(g) + O_2(g) \rightarrow CO_2(g) + H_2O(g)$

(a) This chemical equation is already balanced. There are two chlorine atoms and one magnesium on each side of the equation.

(b) Calcium is already balanced – one Ca on each side. To balance oxygen, we need two mol of CaO on the right. This changes the calcium balance, which is fixed by having two mol of Ca on the left. The result is

$$2\ Ca(s) + O_2(g) \rightarrow 2\ CaO(s)$$

It is also acceptable to balance this reaction using ½ as the coefficient of $O_2(g)$ – i.e.

$$Ca(s) + \tfrac{1}{2}\ O_2(g) \rightarrow CaO(s)$$

(c) Carbon is already balanced. To balance H we need two mol H_2O on the right. Now we need two mol O_2 on the left two balance the four mol O on the right – two from CO_2 and two from 2 H_2O. The result is

$$CH_4(g) + 2\ O_2(g) \rightarrow CO_2(g) + 2\ H_2O(g)$$

This method is called balancing by *inspection*. There are reactions that are more challenging to balance. Often these are oxidation-reduction reactions, which are balanced with the half-reaction method. This method will be reviewed in class.

1.3 Stoichiometry and limiting reactant

Knowing the amounts of substances is important because the coefficients in a chemical reaction give the relative *amounts* of the substances that react and are produced. For example, the balanced chemical equation

$$2\ H_2(g) + O_2(g) \rightarrow 2\ H_2O(l)$$

tells us that the amount of hydrogen needed to completely consume a sample of oxygen is twice the amount of oxygen in the sample. It also tells us that the amount of water produced equals the amount of hydrogen consumed.

Sometimes the relative amounts of reactants *actually used* in a reaction are not the same as the stoichiometric coefficients. In such cases we must determine the reactant that is completely consumed (the *limiting* reactant). The other reactant(s) is(are) in excess.

Example 1.4: Suppose we carry out the above reaction with 30.0 g of O_2 and 4.00 g of H_2.

(a) Which reactant is the limiting reactant?
(b) How much of the other reactant remains at the end of the reaction?
(c) What mass of water is produced?

Approach: Find the number of moles of each reactant. Use reaction stoichiometry to determine the limiting reactant.

$$\text{amount of } O_2 = \frac{30.0\text{ g}}{31.9988\text{ g mol}^{-1}} = 0.937_5\text{ mol}$$

$$\text{amount of } H_2 = \frac{4.00\text{ g}}{2.01588\text{ g mol}^{-1}} = 1.98_4\text{ mol}$$

(a) To completely consume 1.98_4 mol of H_2 requires $1.98_4/2 = 0.992_0$ mol of O_2. However, there is not enough O_2 (only 0.938 mol). Therefore, O_2 is the *limiting reactant*. The 0.938 mol of O_2 is consumed completely, and some H_2 remains unreacted.

(b) The amount of H_2 consumed is twice the amount of O_2 consumed. 1.876 mol of H_2 is consumed, leaving $1.98_4 - 1.876 = 0.10_8$ or 0.11 mol of H_2 unreacted.

(c) Since the amount of H_2 consumed equals the amount of H_2O produced, 1.876 mol of H_2O is produced.

	$2\ H_2(g)$	+ $O_2(g)$	→ $2\ H_2O(l)$
Before	1.984 mol	**0.938 mol** limiting reactant	0 mol
After	0.108 mol	0	1.876 mol

We are asked for the mass of H_2O produced. This is the theoretical yield, determined by calculation based on amount of limiting reagent used.

$$\text{mass of water} = \text{amount of water} \times \text{Molar mass of water}$$
$$= 1.876 \text{ mol} \times 18.015 \text{ g mol}^{-1} = 33.80 \text{ g}$$

1.4 Density

Sometimes we are given the volume of a substance and not its mass. To determine the amount of the substance, we need to know the density of the substance. The density of a substance is the mass per unit volume. For example, the density of water under ordinary conditions is about 1.00 g mL^{-1}. If we know the volume of a substance, then we can determine its mass from its density.

$$\text{mass} = \text{volume} \times \text{density} \qquad \text{or} \qquad m = V \times d \qquad 1.2$$

Example 1.5: The density of copper is 8.94 g mL^{-1}. What is the mass of a cube of copper 1.00 cm × 1.00 cm × 1.00 cm ? Note that 1 mL = 1 cm^3.

Approach: Find cube volume. Use density and volume to solve for mass.

First, we need the volume of the cube in mL

$$1.00 \text{ cm} \times 1.00 \text{ cm} \times 1.00 \text{ cm} = 1.00 \text{ cm}^3 = 1.00 \text{ mL}$$

The mass of the copper cube is $m = V \times d$,

$$1.00 \text{ mL} \times 8.94 \text{ g mL}^{-1} = 8.94 \text{ g}$$

Sometimes more elaborate unit conversions are required.

Example 1.6: What is the mass of a cube of copper 1.00 m × 1.00 m × 1.00 m ?

Again, we need the volume of the cube in mL.[3] This time, we will use the definition of the litre, 1 L = 1 dm^3 = 10^3 mL. [Note that 1 dm = 10^{-2} m].

$$V = (1.00 \text{ m})^3 = (10.0 \text{ dm})^3 = 10.0^3 \text{ dm}^3 = 1.00 \times 10^3 \text{ dm}^3 = 1.00 \times 10^3 \text{ L}$$
$$= 1.00 \times 10^3 \text{ L} \times 10^3 \text{ mL/L} = 10^6 \text{ mL}$$

The mass of the copper cube is

$$10^6 \text{ mL} \times 8.94 \text{ g mL}^{-1} = 8.94 \times 10^6 \text{ g} = 8.94 \times 10^3 \text{ kg}$$

[3] Alternatively, we could convert the density to units of g m^{-3}.

1.5 Solutions

Sometimes we are given a volume of a solution. We can determine the amount of a dissolved substance, if we know the concentration.

$$\text{amount} = \text{volume} \times \text{concentration} \quad \text{or, } n = c\,V \qquad 1.3$$

Example 1.7: How much HCl (mol) is in 250. mL of a solution with HCl concentration, [HCl], equal to 2.00 mol L^{-1}?

Approach: Use concentration and volume to find mol.

$$\text{amount of HCl (mol)} = 0.250 \text{ L} \times 2.00 \text{ mol L}^{-1} = 0.500 \text{ mol}$$

Note the conversion of volume in mL to volume in L because the concentration is given in mol L^{-1}.

The concentration of a substance is the number of moles per unit volume. Dissolved species can be very dilute (low concentration) or highly concentrated (high concentration).

A dilute solution can be prepared from a concentrated solution by adding pure water. This is called dilution.

Example 1.8: What volume of pure water (in mL) must be added to 100. mL of a [NaOH] = 2.00 mol L^{-1} sodium hydroxide solution to make a solution with [NaOH] = 0.500 mol L^{-1}?

Approach: Find mol NaOH. Use final concentration to find final volume. Take difference between final and initial volumes.

The amount of NaOH (mol) in the initial and final solutions is the same – only pure water is added. Therefore, since $n = cV$,

Amount of NaOH (mol) = amount initial = c_iV_i = amount final = c_fV_f
(You may recognize this as $c_1V_1 = c_2V_2$)

$$\text{amount of NaOH} = 0.100 \text{ L} \times 2.00 \text{ mol L}^{-1} = V_f \times 0.500 \text{ mol L}^{-1}$$

where V_f is the final solution volume.

$$V_f = \frac{0.100 \text{ L} \times 2.00 \text{ mol L}^{-1}}{0.500 \text{ mol L}^{-1}} = 0.400 \text{ L}$$

The volume of water added is the change between the final and the initial volumes:

$$\Delta V = V_f - V_i = 0.400 - 0.100 \text{ L} = 0.300 \text{ L}$$

Therefore, 300. mL of pure water must be added to perform the dilution.

1.6 Titration and solution stoichiometry

A strong acid such as HCl will react completely with a base. The acid is said to *neutralize* the base. We can detect when the base is completely consumed by adding a small amount of an acid-base indicator such as phenolphthalein to the base solution. Phenolphthalein makes the solution pink until all the base is consumed, at which point the solution turns colorless.

An HCl solution with known concentration can be used to determine the unknown concentration of a base solution.

Example 1.9: Suppose 221.6 mL of a standard HCl solution with [HCl] = 1.007 mol L^{-1} are required to completely neutralize the NaOH in 100.0 mL of a sample solution of unknown NaOH concentration. NaOH and HCl react according to

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

What is the NaOH concentration of the sample solution?

Approach: Find mol NaOH. Use NaOH volume and mol to determine concentration.

Since the reaction is 1:1, for complete reaction, the amount of HCl (mol) added must equal the amount of NaOH (mol) in the sample solution. Therefore,

$$\text{amount of NaOH} = \text{amount of HCl} = 0.2216\ \mathrm{L} \times 1.007\ \mathrm{mol\ L^{-1}} = 0.2231_5\ \mathrm{mol}$$

This amount of NaOH was present in 100.0 mL of the sample solution. Therefore, the NaOH concentration of the sample solution was $c = n / V$,

$$[\mathrm{NaOH}] = \frac{0.2231_5\ \mathrm{mol}}{0.1000\ \mathrm{L}} = 2.232\ \mathrm{mol\ L^{-1}}$$

Example 1.10: Suppose 178.1 mL of a standard HCl solution with [HCl] = 1.007 mol L^{-1} are required to completely neutralize the Na_2CO_3 in 100.0 mL of a sample solution of unknown Na_2CO_3 concentration. Na_2CO_3 and HCl react according to

$$\mathrm{Na_2CO_3(aq)} + 2\ \mathrm{HCl(aq)} \rightarrow 2\ \mathrm{NaCl(aq)} + \mathrm{H_2O(l)} + \mathrm{CO_2(g)}$$

What is the Na_2CO_3 concentration of the sample solution?

Approach: Find mol Na_2CO_3. Use volume and mol to find concentration.

Take note of the stoichiometry of the *balanced* equation. The amount of HCl added must be twice the amount of Na_2CO_3 in the sample solution. Therefore,

$$\text{amount of } \mathrm{Na_2CO_3} = \frac{1}{2} \times \text{amount of HCl}$$

$$= \frac{1}{2} \times \left(0.1781\ \mathrm{L} \times 1.007\ \mathrm{mol\ L^{-1}}\right) = 0.08967_3\ \mathrm{mol}$$

and

$$[\mathrm{Na_2CO_3}] = \frac{0.08967_3\ \mathrm{mol}}{0.1000\ \mathrm{L}} = 0.8967\ \mathrm{mol\ L^{-1}}$$

Problems:

1.1 How many grams of calcium oxide, CaO, can be produced from the reaction of 4.20 g of calcium metal and 1.60 g of oxygen gas?

1.2 (a) How many water molecules are in an Olympic-sized swimming pool (volume 2500 m^3)? The density of water is 1.00 g/mL. (b) If each water molecule were replaced by a solid cube with volume 1.00 cm^3, what volume swimming pool (in km^3) would be required to hold all the cubes?

1.3 What mass of hydrogen is required to produce 40.0 mL of water (density = 1.00 g mL^{-1}) in the hydrogen fuel cell reaction:

$$2\,H_2(g) + O_2(g) \rightarrow 2\,H_2O(l)$$

1.4 What is the concentration of a KOH solution, if 107 mL are required to neutralize 250 mL of 1.09 mol L^{-1} nitric acid (HNO_3) solution?

1.5 What volume of 1.21 mol L^{-1} LiOH solution is required to neutralize 305 mL of 0.511 mol L^{-1} H_2SO_4 solution?