

Chapter 10

How to do Calculations for Chemical Reactions I

When chemists plan to synthesize a chemical compound, they need to calculate what mass of each reactant that is needed. To do so, they need the principle of mole calculations together with a knowledge of the chemical equation. Here you will learn the necessary skills to do this.

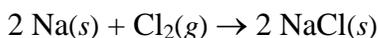
10.1 Background

Almost everything we utilize today has been produced by means of a chemical reaction. For example, the shells of electronic devices are usually made of plastic. The plastic was synthesized from a chemical compound which itself had been produced from oil. The silicon at the heart of most electronic devices is produced by converting silicon dioxide (the mineral quartz) to the element silicon using a chemical reaction and then purifying the silicon by means of another chemical reaction until it reaches the purity necessary to become a computer chip.

On the enormous scale of chemical factories, it is even more important to perform calculations to ensure that exactly the correct proportions of the reactants are mixed together so that there is no wastage with some of one reactant being left over. In many processes, in addition to the required product, some waste chemicals are produced. These not only contribute to pollution problems but they are also costly for the chemical company. For this reason, chemists are devising new chemical reactions which will enable our products to be manufactured in a more chemically-efficient process with less, or no, waste materials.

10.2 What Chemical Equations Tell Us

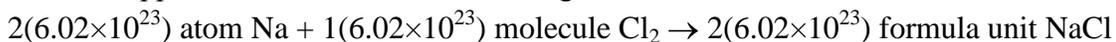
In Chapter 9, it was shown that a chemical reaction can be represented by a chemical equation. In fact, the chemical equation provides a large quantity of information. The reaction of sodium metal with chlorine gas to give solid sodium chloride can be used as an example.



In addition to telling us the formulas of the reactants and product, it provides the information as to how much of each is involved in the reaction. That is:



Unfortunately, in the laboratory it is impossible to work with individual atoms, molecules, and formula units. Suppose instead we work with Avogadro's numbers of each:



As (6.02×10^{23}) represents one mole of a substance, the statement above can be simplified to:



Thus a balanced chemical equation also indicates the number of moles of each of the chemicals involved in a chemical reaction.

Of course, there are no balances to measure moles but one can measure mass. Knowing the atomic masses of each of the elements, the quantities necessary can be calculated. This result is shown in the Figure below.

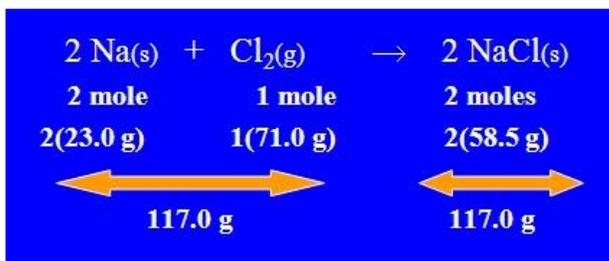


Figure 10.1 The moles and masses involved in the reaction of sodium metal with chlorine gas.

When the chemical reaction between two moles of sodium metal and one mole of chlorine gas has occurred, two moles of sodium chloride are formed. When the masses of the reactants are added together, this equals the mass of the product. This is known as the **Law of Conservation of Mass**: in any chemical reaction, there is no detectable difference between the total mass of the reactants and the total mass of the products.

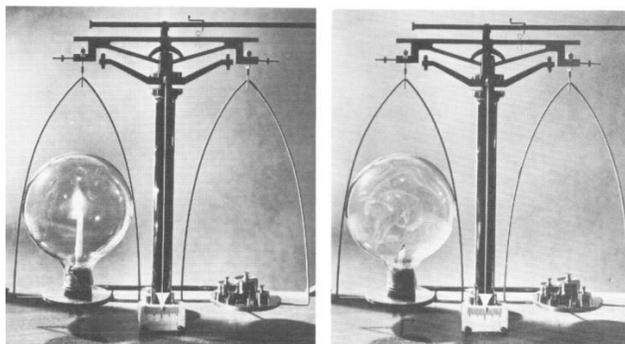


Figure 10.2 A simple experiment to illustrate the Law of Conservation of Mass. The mass of a candle and the surrounding atmosphere is the same before burning and after burning.

10.3 Moles and Chemical Reactions

In Section 10.2, it was shown that 46.0 g of sodium were needed to exactly react with 71.0 g of chlorine gas. Supposing, instead, only 10.0 g of sodium were available, what mass of chlorine would be necessary to use up the 10.0 g of sodium? This is where the application of mole calculations becomes crucial. The calculations here use a different relationship, the equation factor. In a chemical reaction, the **equation factor** relates the number of moles of one species and the number of moles of another.

To illustrate, in the problem above, the relationship between the moles of sodium and the moles of chlorine would be:

$$\frac{2 \text{ mol Na}}{1 \text{ mol Cl}_2} \text{ or } \frac{1 \text{ mol Cl}_2}{2 \text{ mol Na}}$$

To see how the equation factor is used, the question above will be solved, to find what mass of chlorine gas is needed to use up 10.0 g of sodium metal. The equation factor is used like any other factor, so that the 'new' unit will be on top and the unit to be 'cancelled' will be on the bottom.

Strategy

Mass of Na → mol Na
 Mol of Na → mol of Cl₂
 Mol of Cl₂ → mass of Cl

Relationship

1 mol Na ≡ 23.0 g
 2 mol Na ≡ 1 mol Cl₂
 1 mole Cl₂ ≡ 71.0 g

$$\text{Mol Na} = 10.0 \text{ g Na} \times \left(\frac{1 \text{ mol}}{23.0 \text{ g}} \right) = 0.435 \text{ mol Na}$$

$$\text{Mol Cl}_2 = 0.435 \text{ mol Na} \times \left(\frac{1 \text{ mol Cl}_2}{2 \text{ mol Na}} \right) = 0.218 \text{ mol Cl}_2$$

$$\text{Mass Cl}_2 = 0.218 \text{ mol Cl}_2 \times \left(\frac{71.0 \text{ g}}{1 \text{ mol}} \right) = 15.5 \text{ g Cl}_2$$

The procedure is shown schematically below in Figure 10.3.

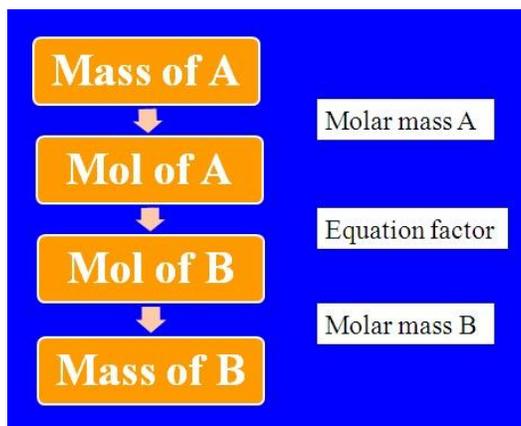


Figure 10.3 The procedure to find the mass of one element or compound (B) from the given mass of an element or compound (A)

EXAMPLE 10.1

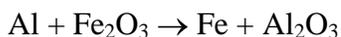
Iron metal can be produced by reacting aluminum metal with iron(III) oxide in a very exothermic reaction to give liquid iron metal and solid aluminum oxide. If 50.0 g of iron(III) oxide are used, what mass of iron metal will be produced?

Answer

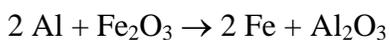
First, a balanced chemical equation is needed. To begin, a word equation is constructed:



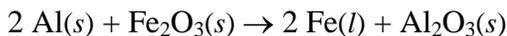
Iron(III) oxide has the formula Fe_2O_3 ; aluminum oxide has the formula Al_2O_3 . The unbalanced formula equation will be:



The equation can then be balanced:



And finally the phases added:



The calculation part of the question can now be performed:

Strategy

Mass of $\text{Fe}_2\text{O}_3 \rightarrow$ mol Fe_2O_3

Mol of $\text{Fe}_2\text{O}_3 \rightarrow$ mol of Fe

Mol of Fe \rightarrow mass of Fe

Relationship

1 mol $\text{Fe}_2\text{O}_3 \equiv 159.6$ g

2 mol Fe $\equiv 1$ mol Fe_2O_3

1 mole Fe $\equiv 55.8$ g

$$\text{Mol Fe}_2\text{O}_3 = 50.0 \text{ g Fe}_2\text{O}_3 \times \left(\frac{1 \text{ mol}}{159.6 \text{ g}} \right) = 0.313 \text{ mol Fe}_2\text{O}_3$$

$$\text{Mol Fe} = 0.313 \text{ mol Fe}_2\text{O}_3 \times \left(\frac{2 \text{ mol Fe}}{1 \text{ mol Fe}_2\text{O}_3} \right) = 0.626 \text{ mol Fe}$$

$$\text{Mass Fe} = 0.626 \text{ mol Fe} \times \left(\frac{55.8 \text{ g}}{1 \text{ mol}} \right) = 35.0 \text{ g Fe}$$



Figure 10.3 When aluminum metal and iron(III) oxide are heated together, the reaction is extremely exothermic.

10.4 How Much Reactant is Needed?

In the last problem, it was assumed that there was enough aluminum metal to react with the 50.0 g of iron(III) oxide. In the real world, where each reactant has to be purchased, it is usual to work out exactly how much of each reactant is needed to synthesize the product required. If it is the exact matching mass, then it is said that the reaction is performed using the *stoichiometric quantities*.

More often, one reactant is more expensive than the other and so it is important to use all of that reactant. In this case, an additional quantity of the other reagent is needed. The reactant which is totally consumed is called the *limiting reactant*. The reactant of which some is left over is called the *reactant in excess*. To ensure at least the stoichiometric quantity is used, the same type of calculation can be used.

EXAMPLE 10.2

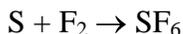
Calculate the minimum mass of fluorine gas needed to completely react with 68.0 g of sulfur to produce gaseous sulfur hexafluoride in a combination reaction.

Answer

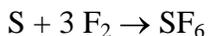
First, a word equation is constructed:

sulfur + fluorine \rightarrow sulfur hexafluoride gas

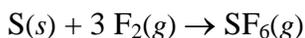
Sulfur is written as S (even though its common allotrope is S₈); fluorine gas as F₂ (one of the diatomic gases); and sulfur hexafluoride as SF₆. Thus the unbalanced molecular equation becomes:



The equation is then balanced:



And then the phases are added:



The calculation part of the question can now be performed:

Strategy

Mass of S → mol S

Mol of S → mol of F₂

Mol of F₂ → mass of F₂

Relationship

1 mol S ≡ 32.1 g

1 mol S ≡ 3 mol F₂

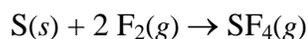
1 mole F₂ ≡ 38.0 g

$$\text{Mol S} = 68.0 \text{ g S} \times \left(\frac{1 \text{ mol}}{32.1 \text{ g}} \right) = 2.12 \text{ mol S}$$

$$\text{Mol F}_2 = 2.12 \text{ mol S} \times \left(\frac{3 \text{ mol F}_2}{1 \text{ mol S}} \right) = 6.36 \text{ mol F}_2$$

$$\text{Mass F}_2 = 6.36 \text{ mol F}_2 \times \left(\frac{38.0 \text{ g}}{1 \text{ mol}} \right) = 242 \text{ g F}_2$$

Though 242 g is the stoichiometric mass of fluorine gas need to react with all the sulfur, in the real laboratory, an excess of fluorine gas would be used. The reason for doing so is that if there is not quite enough fluorine, sulfur tetrafluoride is formed. As can be seen from the equation below, to form sulfur tetrafluoride, only two moles of fluorine are needed for each mole of sulfur:



10.5 Where Next?

The next Chapter builds upon Chapter 9, describing the properties of some interesting and unusual chemical elements, together with some of their chemical reactions.