W3 REACTION STOICHIOMETRY

Amounts of Chemicals

Atoms and molecules are so small that we cannot directly measure the number in a sample or the number that change in a reaction. Instead, we use measurements such as the mass or volume to measure the amount. The volume can be converted to a mass using the density. The number of atoms or molecules present is related to the mass or volume through the atomic or molecular mass respectively.

For both cooks and chemists, it is most convenient to measure mass in grams and volume in litres (or millilitres).

A cook buying a large number of eggs will ask for them by the dozen, because it is less fiddly than dealing with the number of individual eggs. The chemist has the same problem with molecules, except that the number of molecules we deal with is huge. We count atoms and molecules not by the dozen but by the mole*. For the cook,

1 dozen eggs corresponds to 12 eggs.
2 dozen eggs corresponds to 24 eggs.
3 dozen eggplants corresponds to 36 eggplants.
2 dozen hydrogen atoms corresponds to 24 hydrogen atoms.

For the chemist,

1 mole of hydrogen atoms corresponds to $6.022 \times 10^{23}$ hydrogen atoms.
2 moles of water molecules corresponds to $2 \times 6.022 \times 10^{23}$ water molecules.
2 moles of eggs corresponds to $2 \times 6.022 \times 10^{23}$ eggs.

The principle is the same: a dozen always means 12 of a thing and a mole always means $6.022 \times 10^{23}$ of a thing. The only difference is the scale.

The molar mass is the mass, in grams, of one mole of a substance. The unit for the mole is "mol", just like the unit for the dozen is “doz”.

Example

The formula of carbon dioxide is CO$_2$.

One molecule of CO$_2$ contains one atom of carbon and two atoms of oxygen
One mole of CO$_2$ contains one mole of carbon atoms and two moles of oxygen atoms.

The mass of a mole of atoms of an element is called the atomic mass and is given in the periodic table, such as the one on the back cover of this manual and the one you will get on the data sheet in your exam.

The atomic masses of carbon and oxygen are 12.01 and 16.00 g respectively†.

* “mole” is not an abbreviation for “molecule”!
† Check that you can find these numbers on your periodic table.
The *molecular mass* of a compound is obtained by the summing the atomic weights of the constituent atoms multiplied by the number of those atoms present. For CO₂,

\[
\text{molar mass of CO}_2 = 12.01 \text{ (C)} + 2 \times 16.00 \text{ (O)} = 44.01 \text{ g mol}^{-1}
\]

One mole of CO₂ has a mass of 44.01 g and contains one mole of carbon atoms and two moles of oxygen atoms.

Ionic solids consist of an infinite array of ions rather than individual molecules. For these compounds, the *formula mass* is used. It is calculated from the formula in the same way as the molecular mass.

The formula mass is the mass, in grams, of one mole of an ionic compound.

**Example**
Magnesium chloride is an ionic solid with the formula MgCl₂. The atomic masses of magnesium and chlorine are 24.31 and 35.45 g respectively‡:

\[
\text{formula mass of MgCl}_2 = 24.31 \text{ (Mg)} + 2 \times 35.45 \text{ (Cl)} = 95.21 \text{ g mol}^{-1}
\]

Notice that is does not matter if you do not know whether something is ionic or not – the mass of a mole is the same.

<table>
<thead>
<tr>
<th>Molar mass is referred to as:</th>
</tr>
</thead>
<tbody>
<tr>
<td>atomic mass if the substance is an element,</td>
</tr>
<tr>
<td>molecular mass if the substance is a molecule</td>
</tr>
<tr>
<td>formula mass if the substance is an ionic compound.</td>
</tr>
</tbody>
</table>

Some elements, like helium and argon, exist as separate gaseous atoms. Others like iron and carbon exist as very large collections of atoms, joined together. In both of these cases, they are written with just the atomic symbol in chemical equations, such as He, Ar, Fe and C and the molar mass is referred to as atomic mass. Other elements, like hydrogen, oxygen and nitrogen, exist as small molecules like H₂, O₂ and N₂. Most commonly these molecules are made up of two atoms, in which case they are called *diatomics*. For these elements, the molar mass refers to the mass of the diatomic and the atomic mass refers to the mass of the atom.

**Example**
Oxygen in the atmosphere is present as either O₂ or O₃. The diatomic O₂ is the substance that we need to breathe and is what we almost always mean when we talk about oxygen. O₃ is ozone, which is nasty if we breathe it but is needed in the upper atmosphere.

\[
\text{atomic mass of oxygen} = 16.00 \text{ g} \\
\text{molar mass of oxygen} = \text{molecular mass of O}_2 = 2 \times 16.00 = 32.00 \text{ g mol}^{-1} \\
\text{molar mass of ozone} = \text{molecular mass of O}_3 = 3 \times 16.00 = 48.00 \text{ g mol}^{-1}
\]

‡ Check that you can find these numbers on your periodic table.
Q1. What is the molar mass of (a) water, H₂O, and (b) glucose, C₆H₁₂O₆?

(a)  

(b)  

Q2. What is the formula mass of ammonium chloride, NH₄Cl?


Q3. What is (a) the atomic mass and (b) the molar mass of chlorine? (Hint: chlorine exists as diatomic Cl₂.)

(a)  

(b)  

When chemicals react, it is the number of molecules (and hence the number of moles) which is important. As we generally measure the mass, we convert this into the number of moles. This is achieved using the molar mass (atomic, molecular or formula) using the relationships:

\[
\text{number of moles} = \frac{\text{mass}}{\text{molar mass}} \quad \text{and} \quad \text{mass} = \text{number of moles} \times \text{molar mass}
\]

**Example**

The number of moles in 10.0 g of CO₂ is given by:

\[
\text{number of moles} = \frac{\text{mass}}{\text{molar mass}} = \frac{10.0 \text{ g}}{44.01 \text{ g mol}^{-1}} = 0.227 \text{ mol}
\]

**Example**

The mass of 0.25 mol of MgCl₂ is given by:

\[
\text{mass} = \text{number of moles} \times \text{formula mass} = 0.25 \times 95.21 = 24 \text{ g}
\]

Q4. How many moles are there in (a) 120 g of water and (b) 0.5 g of glucose, C₆H₁₂O₆?

(a)  

(b)  

Q5. What is the mass of 0.33 mol of NH₄Cl?


Demonstrator's Initials
Amounts and Reactions

Chemistry is all about how and why substances react to form new substances. The symbols in a chemical equation show the substances that react (the reactants) on the left and the substances that are formed (the products) on the right. The physical state of the various species is indicated by (s) for a solid, (l) for a liquid or (g) for a gas. An arrow is used to show the transformation:

\[ \text{reactants} \rightarrow \text{products} \]

When carbon burns in air, it combines with oxygen to make carbon dioxide:

\[ \text{C(s)} + \text{O}_2(g) \rightarrow \text{CO}_2(g) \]

*One* atom of carbon reacts with *one* molecule of oxygen to make *one* molecule of carbon dioxide.

*One* mole of carbon reacts with *one* mole of oxygen to make *one* mole of carbon dioxide.

In this example, one C reacts with one O\(_2\): a 1:1 ratio. Not all chemical reactions are this simple and most involve more complicated ratios. For example, nitrogen and hydrogen react in a 1:3 ratio to produce ammonia, NH\(_3\). This is shown in the chemical equation:

\[ \text{N}_2(g) + 3\text{H}_2(g) \rightarrow 2\text{NH}_3(g) \]

*One* molecule of nitrogen reacts with *three* molecules of hydrogen to make *two* molecules of ammonia.

*One* mole of nitrogen reacts with *three* moles of hydrogen to make *two* moles of ammonia.

The numbers in front of the chemical formulae in the chemical equation are called the *reaction coefficients*: they tell us the ratios in which the substances react. Notice that if there is no number in front of the formula, the coefficient is just one.

**Example**

The chemical equation for the combustion of glucose is:

\[ \text{C}_6\text{H}_12\text{O}_6(s) + 6\text{O}_2(g) \rightarrow 6\text{CO}_2(g) + 6\text{H}_2\text{O}(l) \]

*One* mole of glucose reacts with *six* moles of oxygen to produce *six* moles of carbon dioxide and *six* moles of water.

Q6. What are the reaction coefficients for the following reactions? (The first one has been completed as an example.)

<table>
<thead>
<tr>
<th>C(_2)H(_4)O(_6)(s) + 6O(_2)(g) → 6CO(_2)(g) + 6H(_2)O(l)</th>
<th>C(_2)H(_4)O(_6): 1</th>
<th>O(_2): 6</th>
<th>CO(_2): 6</th>
<th>H(_2)O: 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) 2H(_2)(g) + O(_2)(g) → 2H(_2)O(l)</td>
<td>H(_2):</td>
<td>O(_2):</td>
<td>H(_2)O:</td>
<td></td>
</tr>
<tr>
<td>(b) 4Fe(s) + 3O(_2)(g) → 2Fe(_2)O(_3)(s)</td>
<td>Fe:</td>
<td>O(_2):</td>
<td>Fe(_2)O(_3):</td>
<td></td>
</tr>
<tr>
<td>(c) AgNO(_3) + NaCl → AgCl + NaNO(_3)</td>
<td>AgNO(_3):</td>
<td>NaCl:</td>
<td>AgCl:</td>
<td>NaNO(_3):</td>
</tr>
</tbody>
</table>
If we react one mole of glucose with six moles of oxygen, we can expect to get six moles of carbon dioxide and six moles of water. By multiplying each coefficient in the reaction by 0.5, it can be seen that if we react 0.5 mol of glucose with 3 mol of oxygen, we can expect to get 3 mol of carbon dioxide and 3 mol of water.

In the laboratory, we usually begin by weighing our reactants and end by weighing our products. This means we will need to convert these masses to moles, and vice versa using the method outlined previously.

**Example**
If 10.0 g of glucose is burnt in a vessel which is open to the air, how many grams of water will be produced?

The calculation follows the sequence:

mass of glucose we start with \(\rightarrow\) moles of glucose we start with \(\rightarrow\) moles of water we expect to make \(\rightarrow\) mass of water we expect to make

From Q1(b), the molar mass of \(\text{C}_6\text{H}_12\text{O}_6\) is 180.16 g mol\(^{-1}\). This corresponds to,

\[
\text{moles of glucose} = \frac{\text{mass}}{\text{molar mass}} = \frac{10.0}{180.16} = 0.0555 \text{ mol}
\]

The chemical equation, \(\text{C}_6\text{H}_12\text{O}_6(\text{s}) + 6\text{O}_2(\text{g}) \rightarrow 6\text{CO}_2(\text{g}) + 6\text{H}_2\text{O}(\text{l})\), shows that:

1 mol of \(\text{C}_6\text{H}_12\text{O}_6\) produces 6 mol of \(\text{H}_2\text{O}\).

0.0555 mol of \(\text{C}_6\text{H}_12\text{O}_6\) produces \(6 \times 0.0555\) mol of \(\text{H}_2\text{O}\).

Therefore 0.333 mol of water will be produced. From Q1(a), the molar mass of \(\text{H}_2\text{O}\) is 18.02 g mol\(^{-1}\), so the mass of water produced in the reaction is,

\[
\text{mass of water} = \text{number of moles} \times \text{molar mass} = 0.333 \text{ mol} \times 18.02 \text{ g mol}^{-1} = 6.00 \text{ g}
\]

Q7. What mass of \(\text{Fe}_2\text{O}_3\) is produced when 25.0 g of iron filings is burnt in air?

<table>
<thead>
<tr>
<th>chemical equation:</th>
</tr>
</thead>
<tbody>
<tr>
<td>moles of Fe at the start =</td>
</tr>
<tr>
<td>moles of (\text{Fe}_2\text{O}_3) expected at the end =</td>
</tr>
<tr>
<td>formula mass of (\text{Fe}_2\text{O}_3) =</td>
</tr>
<tr>
<td>mass of (\text{Fe}_2\text{O}_3) expected at the end =</td>
</tr>
</tbody>
</table>
Limiting Reactants

When glucose is burnt in the open air, there is enough oxygen in the air to ensure that all of the glucose reacts. The oxygen is said to be in excess meaning that there is more than enough of it. The reaction stops when the glucose runs out. When this happens, there is still oxygen left. Glucose is the limiting reactant as the amount of water and carbon dioxide is controlled by how much glucose there is at the start.

If we mix the exact number of moles of each reactant that is needed, they are said to be stoichiometric amounts.

More commonly, there is a limiting reactant. In the glucose example, it was easy to spot that glucose is the limiting reactant since the amount of oxygen in the air is effectively unlimited. In other cases, it may not be so obvious. If there is still some reactant left at the end of a reaction then it is present in excess. In many reactions, such as when there are many reactants or they are colourless gases or solutions, determining the limiting reagent is much more difficult. We then need to work out the number of moles of each reactant.

The limiting reactant is the one that produces the least amount of product.

Example
If solutions containing 2.0 mol of AgNO₃ and 3.0 mol of NaCl are mixed, how much AgCl will be produced? From above, the chemical reaction is:

$$\text{AgNO}_3 + \text{NaCl} \rightarrow \text{AgCl} + \text{NaNO}_3$$

- 2.0 mol of AgNO₃ can produce, at most, 2.0 mol of AgCl
- 3.0 mol of NaCl can produce, at most, 3.0 mol of AgCl

AgNO₃ is the limiting reactant. The reaction will produce 2.0 mol of AgCl and 1.0 mol of NaCl will be left over.

Example
If 3 mol of hydrogen and 2 mol of oxygen react, how much water is produced? The chemical equation is:

$$2\text{H}_2(g) + \text{O}_2(g) \rightarrow 2\text{H}_2\text{O}(l)$$

- 3 mol of H₂ can produce, at most, 3 mol of H₂O.
- 2 mol of O₂ can produce, at most, 4 mol of H₂O.
  (from the equation: 1 mol of O₂ produces 2 mol of H₂O)

H₂ is the limiting reactant: even though there is more H₂ than O₂ at the start!

From the chemical equation,

$$2 \text{mol of H}_2 \text{ will react with 1 mol of O}_2 \text{ to produce 2 mol of H}_2\text{O.}$$

Therefore,

$$3 \text{ mol of H}_2 \text{ will react with 1½ mol of O}_2 \text{ to produce 3 mol of H}_2\text{O.}$$

As the reaction started with 2 mol of O₂, there is still ½ mol left at the end.
Q8. N\textsubscript{2} and H\textsubscript{2} react to produce ammonia, NH\textsubscript{3}, according to the following chemical equation.

\[ \text{N}_2(g) + 3\text{H}_2(g) \rightarrow 2\text{NH}_3(g) \]

What amounts of N\textsubscript{2} and H\textsubscript{2} will remain at the end of the reaction if you start with 5.0 mol of H\textsubscript{2} and 2.0 mol of N\textsubscript{2} and react these to form NH\textsubscript{3}?

Limiting reactant is

Moles of NH\textsubscript{3} that could be produced =

Moles of N\textsubscript{2} and H\textsubscript{2} left at the end of the reaction =

Q9. When solutions of copper(II) sulfate and barium chloride are mixed they react to produce solid barium sulfate according to the chemical equation:

\[ \text{CuSO}_4 + \text{BaCl}_2 \rightarrow \text{CuCl}_2 + \text{BaSO}_4 \]

If the solutions contain 5.3 g of CuSO\textsubscript{4} and 8.2 g of BaCl\textsubscript{2}, which is the limiting reactant and what mass of BaSO\textsubscript{4} will be produced?

Hint: for each reactant, your calculation should follow the steps:

mass of reactant \rightarrow moles of reactant \rightarrow moles of product \rightarrow mass of product
Reaction Yield

As shown in the examples above, working out the limiting reactant enables us to calculate the mass of product we should obtain. This amount is called the theoretical yield. It is unlikely that this will be the actual yield. There are many reasons why the amount that we obtain is less than the theoretical yield. One limiting factor will always be the skill of the chemist. Sometimes the nature of the reaction means that even the best chemist cannot achieve a perfect yield. Many reactions lead to by-products that inevitably lower the yield. By working out the theoretical yield and measuring the actual yield, we can work out the percentage yield:

\[
\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%
\]

Example

In Q9, solutions containing 5.8 g of CuSO₄ and 8.2 g of BaCl₂ are mixed to produce a theoretical yield of 7.7 g of BaSO₄. If, in a real experiment, only 5.2 g of BaCl₂ is made:

\[
\text{percentage yield} = \frac{5.2 \text{ g}}{7.7 \text{ g}} \times 100\% = 68\%
\]

In this example, the actual and theoretical masses were used. The yields in moles can also be used as the units cancel.

Example

In the example on page W3-6, solutions containing 2.0 mol of AgNO₃ and 3.0 mol of NaCl are mixed to produce a theoretical yield of 2.0 mol of AgCl. If in an experiment, only 1.7 mol of AgCl is made,

\[
\text{percentage yield} = \frac{1.5 \text{ mol}}{2.0 \text{ mol}} \times 100\% = 75\%
\]

Q10. If the reaction discussed in Q8 produces 60 g of ammonia, what is the percentage yield?

The actual yield must be less than or equal to the theoretical yield. If the actual yield is higher, it can mean that measurements or calculations are wrong. However, it is actually quite common for yields to be higher than is theoretically possible without any measurement or calculation errors having been made. It is important to consider why this might occur.

Q11. Suggest a reason why the yield might be higher than the theoretical yield.