**3 A Synthesis - Calculations**

The theoretical yield is the amount of product that can be, in theory, produced from the reactants. It is based on the assumption that the reactants react with 100 per cent efficiency. In reality, many factors affect how much product is produced. Some of these factors are difficult to predict, but one of the more obvious ones is the amount of each reactant. As soon as one reactant runs out, the reaction can no longer proceed and no more product can be made. The reactant which "runs out" is known as the limiting reagent, because it limits the progress of the reaction. Any other reactants are referred to as excess reagents, or reagents in excess.

There are many different methods for determining which chemical is the limiting reactant. In each case, the number of moles of each reactant is compared to the stoichiometric ratios needed in the reaction. One method is demonstrated in Worked example 20.2.1.

Once the limiting reactant has been determined, it is used to calculate the number of moles, and then the mass, volume or concentration of the product.

**WORKED EXAMPLE**

The synthesis of paracetamol (C8H9NO2)is a three-step process, with the final step being the reaction between 4-aminophenol (C6H7NO) and ethanoic anhydride (C4H603):

# C6H7NO + C4H6O3 **→** C8H9NO2 + C2H4O2

If 0.5 g of 4-aminophenol reacts with 0.4 g of ethanoic anhydride, what is the mass of paracetamol that can be produced?

# **ANSWER**

**1.** Calculate the number of moles of each reactant. $n= \frac{m}{M}$

*n(C6H7NO) =* $\frac{0.5}{109.1}$ = 0.00458 moles

*n(*C4H6O3) = $\frac{0.4}{102.1}$ = 0.003 92 moles

**2.** Determine the stoichiometric ratio (**SR**), using the coefficients from the equation, and the actual ratio (**AR**), using the moles calculated. Make sure that the same reactant is on top for both ratios.

**SR** = $\frac{1}{1}$ = 1

**AR** = $\frac{0.00458}{0.00392}$ = 1.168

**3.** Determine which reactant is limiting. If AR> SR, the reactant on the denominator is limiting. If SR> AR, the reactant on the top in limiting. In this case AR > SR, so the reactant in the denominator is limiting. Therefore, C4H6O3 is limiting.

**4.** Use the moles of the limiting reactant to calculate the number of moles of the product that can be produced.

n(C**8**H**9**N0**2**) = n(C4H60**3**)*n(*C8H9N02) = 0.003 92 moles

**5.** Use the number of moles of the product to calculate the mass of the product that can be produced.

*m = n x M*

m(C8H9N02) = 0.00392 x 151.163 = 0.593 g

The mass of paracetamol is 0.593 g.

# **TRY THESE YOURSELF**

**12½.** What mass of ammonia can be produced from 5.0 L of hydrogen gas and 3.0 L of nitrogen gas at standard temperature and pressure?

**13½.** What mass of sulphur trioxide can be produced from 1 kg of sulfur dioxide and 1 kg of oxygen gas?

2 SO(g) + O2(g)  → 2S0(g)

**YIELD CALCULATIONS**

The yield is usually given as a percentage of the possible yield. A yield of 90% means that only 90% of the amount of products that can be theoretically produced from the reactants, is actually produced. To calculate this percentage we need to:

* use stoichiometry to calculate the amount of product that can theoretically be produced from the reactants
* know the amount of product actually produced. Then calculate the percentage yield:

Percentage yield = $\frac{Actual Yield}{Theoretical yield}$ x 100

## WORKED EXAMPLE

If 5.0 g of sulphur reacts with excess oxygen to produce 7.5077g of sulphur dioxide, what is the percentage yield for the reaction?

**ANSWER**

1. Write a balanced equation . S + 02  → S02

2. Calculate the amount of product that can theoretically be produced from the reactants. $n= \frac{m}{M}$

$n\left(S\right)= \frac{5.0 g}{32.06 g}$ = 0.156 moles

*n(S)* ***:*** *n(S0****2****)*= 1 : 1 *n(S0****2****) =*  0.156 moles

$m(SO\_{2})= n ×M $ m(S02) =0 .156 x (32.06 + 2 x 16)

m(S02) = 9.99g (This is the theoretical yield or mass.)

3. Calculate the percentage yield using the theoretical yield or mass that you have calculated and the actual yield or mass given in the question.

$\% yield= \frac{actual yield}{Theoretical yield}$ x 100

$\% yield= \frac{7.50}{9.99}$ x 100 = 75.1%

Percentage yield is 75.1%

## TRY THESE YOURSELF

13¾. The synthesis of aspirin (acetylsalicylic acid) involves the reaction:

 C7H603 + C4H603 → C9H804 + C2H402

 salicylic acid ethanoic anhydride acetylsalicylic acid acetic acid

If 25.0 g of acetylsalicylic acid is produced when 30.0 g of salicylic acid reacts, calculate the percentage yield for the reaction.

14½. Producing ammonia in the Haber process is typically carried out at approximately 450°C and 200 atm. At this temperature and pressure, 35.0 L of nitrogen gas produces 1.50 kg of ammonia.

Calculate the percentage yield for the reaction.