



Pesticides and agricultural productivity calculations

Learning objectives

- 1 Calculate yields, percentage yields and atom economies and apply these to reactions involving alternatives to agrochemicals.
- 2 Describe that the actual yield of a reaction is usually less than the theoretical yield and this is due to incomplete reactions, practical losses and side reactions.
- 3 Handle data in a variety of chemistry contexts.

Introduction

With an ever-growing population, it is becoming more vital than ever to ensure there is enough food for everyone. Pesticides play an important role in boosting agricultural productivity but can have negative impacts on human health. In this task, you will look at some alternatives and link key mathematical skills to each one.

Moth mimics and plant factories

Each crop attracts different types of animals. One method of protecting crops is to release a chemical called a pheromone nearby. This pheromone attracts animals away from the crop, protecting them. However, producing these chemicals in a laboratory is often very expensive. An alternative method of producing these pheromones is to 'grow' them in plants.

This method involves adding copper sulfate (CuSO_4) to the plant to tune the genetic activity so the plant can still grow.

Yield

As is the case in all industrial chemical processes, it is important to understand whether a chemical reaction is both possible and able to be profitable. Chemists use a variety of calculations that allow them to predict these factors.

One of these calculations is the yield of a chemical reaction. The yield of a chemical reaction is the maximum possible mass of a product that can be made in a chemical reaction. This is often called the 'theoretical yield'. We can calculate this from the balanced symbol equation if we know the relative formula mass and mass of the limiting reagent. However, we often do not produce 100% of the theoretical yield. We form less, what we call the 'actual yield'.



1. Predict why a reaction will often produce less than the theoretical yield.

Percentage yield

Chemists, therefore, use the following equation to calculate the percentage of product formed. It ranges from 0% (no products formed) to 100% (all of the products formed). It is calculated using this equation:

$$\text{Percentage yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100$$

Example:

In a reaction to produce water, the theoretical yield was 10 g, however the actual yield was 6 g. To calculate the percentage yield:

$$\text{Percentage yield} = \frac{6}{10} \times 100 = 60\%$$

One method of producing the copper sulfate needed to treat the plants mentioned above is to react copper with sulfuric acid.

Word equation: copper + sulfuric acid → copper sulfate + water + sulfur dioxide

Symbol equation: $\text{Cu} + 2\text{H}_2\text{SO}_4 \rightarrow \text{CuSO}_4 + 2\text{H}_2\text{O} + \text{SO}_2$

2. In this reaction, the theoretical yield of copper sulfate was 14.5 g. However, only 8.6 g were produced. Calculate the percentage yield.



Atom economy

Another useful calculation that chemists use is called atom economy. This is a measure of the amount of starting materials that end up as useful products. A higher atom economy (closer to 100%) means that more of the products are useful. To calculate it you must know the relative molecular mass (Mr) of all the reactants and that of the desired product. It is therefore vital that the symbol equation is balanced.

You calculate it using:

$$\text{Atom economy} = \frac{\text{Total Mr of the desired product}}{\text{Total Mr of all reactants}} \times 100$$

Worked example – using the reaction above to produce copper sulfate (CuSO₄):



Mr of the desired product (CuSO₄) = 63.5 (Cu) + 32 (S) + (16 × 4) (O × 4) = 159.5

Mr of all reactants = 63.5 (Cu) + (1 × 4) (H × 4) + (32 × 2) (S) + (16 × 8) (O × 8) = 259.5

$$\text{Atom economy} = \frac{159.5}{259.5} \times 100 = \mathbf{61.46435\%}$$

3. State the above % to 1 decimal place. _____
4. State the above % to 2 decimal places. _____
5. State the above % to 2 significant figures. _____
6. State the above % to 3 significant figures. _____

Hexadecenoic acid (C₁₆H₃₀O₂) is one pheromone precursor that researchers have engineered *Camelina* plants to produce rather than synthesise it at a much higher cost. Once the pheromones are produced in the plant, they have been found to work as well as commercially made versions at a much lower cost.

One method of creating hexadecenoic acid commercially forms only the desired, useful product when the symbol equation is balanced.

7. Calculate the relative molecular mass (Mr) of hexadecenoic acid and state the atom economy for this reaction. Explain your answer.



Why are alternatives needed?

Many essential oils and plant extracts are potential alternatives to pesticides, however many of these are harmful too. Thymol (C₁₀H₁₄O) from thyme oil is particularly toxic to insects such as varroa mites which attack honeybees.

Thymol can be produced synthetically via the following reaction:



8. Prove, with a calculation, that the atom economy for this reaction is 100%.

9. Suggest three reasons why an atom economy of 100% is good for sustainable development.

Extension task

Create a science magazine article or leaflet to demonstrate the importance of chemical calculations to allow chemists to quantify yields and maximise efficiency in global contexts.