

2. Calculating Formulae

Calculating empirical formulae

There are two ways of calculating empirical formulae:

- Calculating from experimental data
- Calculating from percentage compositions.

Calculating empirical formulae from experimental data

- Work out empirical formulae from the masses of products formed in a reaction:
 1. How many moles of product made? [moles = mass ÷ M_r]
 2. Use moles of each product to find moles of atoms you started with
 3. Write down the ration of moles present at the start
 4. Divide by the smallest number of moles to get a whole number ratio
 5. This is the Empirical Formula!

$$M_r = \frac{\text{moles}}{\text{mass}} \quad \rightarrow \quad \text{moles} = \frac{\text{mass}}{M_r} \quad \text{mass (g)} \quad M_r (\text{g mol}^{-1})$$

2. Calculating Formulae

Example

When a hydrocarbon is burnt in excess oxygen, 4.4 g of carbon dioxide and 1.8 g of water are made. What is the empirical formula of the hydrocarbon?

1. Moles of CO₂ and H₂O produced:

$$\text{Moles } CO_2 = \frac{\text{mass}}{M_r} = \frac{4.4}{12+(16 \times 2)} = \frac{4.4}{44} = 0.10 \text{ moles}$$

$$\text{Moles } H_2O = \frac{\text{mass}}{M_r} = \frac{1.8}{(2 \times 1)+16} = \frac{1.8}{18} = 0.10 \text{ moles}$$

2. 1 mole of CO₂ contains 1 mole of C atoms - we started with 0.10 moles of C
1 mole of H₂O contains 2 moles of H atoms - we started with 2 × 0.10 moles of H
3. Starting with 0.10 moles of C and 0.20 moles of H
C : H ratio is 0.10 : 0.20
4. Dividing both sides by the smallest number (0.10) gives a whole number ratio of C : H = (0.10 ÷ 0.10) : (0.20 ÷ 0.10) = 1 : 2
5. Empirical Formula of hydrocarbon = CH₂

2. Calculating Formulae

Practice Questions:

1. When a hydrocarbon is burnt in excess oxygen, 17.6g of carbon dioxide and 10.8g of water are made. What is the empirical formula of the hydrocarbon?
2. When a hydrocarbon is burnt in excess oxygen, 3.52g of carbon dioxide and 2.88g of water are made. What is the empirical formula of the hydrocarbon?
3. 5.52g of sodium burns in air to produce 7.44g of sodium oxide. What is the empirical formula of sodium oxide?
4. 50.2g of iron reacts with air to produce 69.4g of an iron oxide. What is the empirical formula of this iron oxide?

2. Calculating Formulae

Calculating empirical formulae

Calculating empirical formulae from percentage compositions

- Work out empirical formulae from the percentages of different elements:
 1. Assume starting with 100g of the compound – turn % straight into masses!
 2. Work out how many moles of each element are in 100g of the compound
 3. Divide each number of moles by the smallest number of moles found in step 1.
This gives the ratio of the elements in the compound.
 4. Apply the numbers from the ratio to the Empirical Formula!

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Example

A compound is found to have percentage composition 56.5% potassium, 8.70% carbon and 34.8% oxygen by mass. Calculate the empirical formula.

1. If you had 100g of compound: 56.5g of K, 8.70g of C and 34.8g O
2. Use the formula $\text{moles} = \text{mass} \div M_r$ to work out moles of each element:

$$K: \frac{56.5}{39.1} = 1.445 \text{ moles} \quad C: \frac{8.70}{12} = 0.725 \text{ moles} \quad O: \frac{34.8}{16} = 2.175 \text{ moles}$$

3. Dividing each number of moles by the smallest number (0.725):

$$K: \frac{1.445}{0.725} = 2.0 \quad C: \frac{0.725}{0.725} = 1.0 \quad O: \frac{2.175}{0.725} = 3.0$$

This tells us the ratio of K : C : O in the compound is 2 : 1 : 3

4. Empirical Formula of compound = K_2CO_3

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Calculating molecular formulae

- Once the empirical formula is known – you just need the molar mass to work out the molecular formula.
- Dividing the molar mass by the mass of the empirical formula gives the factor needed to scale the empirical formula up to the molecular formula.

Example

When 4.6g of an alcohol with molar mass 92 g mol^{-1} , is burnt in excess oxygen, it produces 8.8g of carbon dioxide and 5.4g of water. Calculate the empirical formula for the alcohol and then its molecular formula.

1. Find the empirical formula first: Moles of CO_2 and H_2O produced:

$$\text{Moles } \text{CO}_2 = \frac{\text{mass}}{M_r} = \frac{8.8}{12+(16 \times 2)} = \frac{8.8}{44} = 0.20 \text{ moles}$$

$$\text{Moles } \text{H}_2\text{O} = \frac{\text{mass}}{M_r} = \frac{5.4}{(2 \times 1)+16} = \frac{5.4}{18} = 0.30 \text{ moles}$$

2. Calculating Formulae

Example

- 1 mole of CO_2 contains 1 mole of C atoms - we started with 0.20 moles of C
1 mole of H_2O contains 2 moles of H atoms - we started with 0.60 moles of H
- To find the moles of O from the alcohol, find the initial mass of O:
Use the moles of C and H to find starting mass of C and H
then subtract from mass of the alcohol
Mass of C = no of moles $\times M_r = 0.20 \times 12 = 2.4\text{g}$
Mass of H = no of moles $\times M_r = 0.60 \times 1 = 0.6\text{g}$
Mass of alcohol = mass of C + H + O
Mass of O = mass of alcohol – (mass of C + H)
Mass of O = $4.6 - (2.4 + 0.6) = 1.6\text{g}$
Moles of O in the alcohol = mass $\div M_r = 1.6 \div 16 = 0.10$ moles
- Ratio of C : H : O = 0.20 : 0.60 : 0.10
Divide through by smallest (0.1)
- Ratio = 2 : 6 : 1
- Empirical formula = $\text{C}_2\text{H}_6\text{O}$

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Example

7. Mass of the Empirical formula ($\text{C}_2\text{H}_6\text{O}$) =
 $(12 \times 2) + (1 \times 6) + 16 = 46 \text{ g}$
8. Divide the molar mass of the alcohol by this empirical formula mass:
 $92 \div 46 = 2$
9. So we need to scale the empirical formula by a factor of 2 to get the molecular formula:
10. Empirical formula = $\text{C}_2\text{H}_6\text{O}$
11. Molecular formula = $2 \times \text{C}_2\text{H}_6\text{O} = \text{C}_4\text{H}_{12}\text{O}_2$

2. Calculating Formulae

Practice Questions:

1. 3.1g of phosphorus burns in air to produce 7.1g of phosphorus oxide which has a molar mass of 284 g mol^{-1} . Calculate the empirical formula of phosphorus oxide and then its molecular formula.
2. A hydrocarbon is found to have a percentage composition of 85.7% carbon and 14.3% hydrogen by mass. Find the molecular formula of this hydrocarbon given that it has a molar mass of 56 g mol^{-1} .
3. An oxide of chlorine has a molar mass of 167 g mol^{-1} and contains 42.5% chlorine by mass. Find its molecular formula.
4. When 12.8 g of an alcohol, with a molar mass of 32 g mol^{-1} is burnt in excess oxygen, it produces 17.6g of carbon dioxide and 14.4g of water. Calculate the empirical and molecular formulae of the alcohol.
5. When 2.64 g of an alcohol, with a molar mass of 88 g mol^{-1} is burnt in excess oxygen, it produces 2.16g of water and 5.28 g of carbon dioxide. Calculate the empirical and molecular formulae of the alcohol.