Empirical and Molecular Formulae Notes | CIE | A-Level Chemistry

The formula of a compound provides essential information about the elements it contains and the ratio in which they are present. There are two main types of chemical formulae used to describe the composition of a molecule: the empirical formula and the molecular formula.

Defining Chemical Formulae

Understanding the distinction between an empirical and a molecular formula is crucial for interpreting chemical information and solving stoichiometric problems.

- An **empirical formula** represents the simplest whole-number ratio of atoms of each element present in a compound.
- A **molecular formula** shows the actual number of atoms of each element in one molecule of a compound.

For some compounds, like water (H_2O), the empirical and molecular formulae are the same. For many others, especially organic compounds, they are different.

Comparison of Empirical and Molecular Formulae

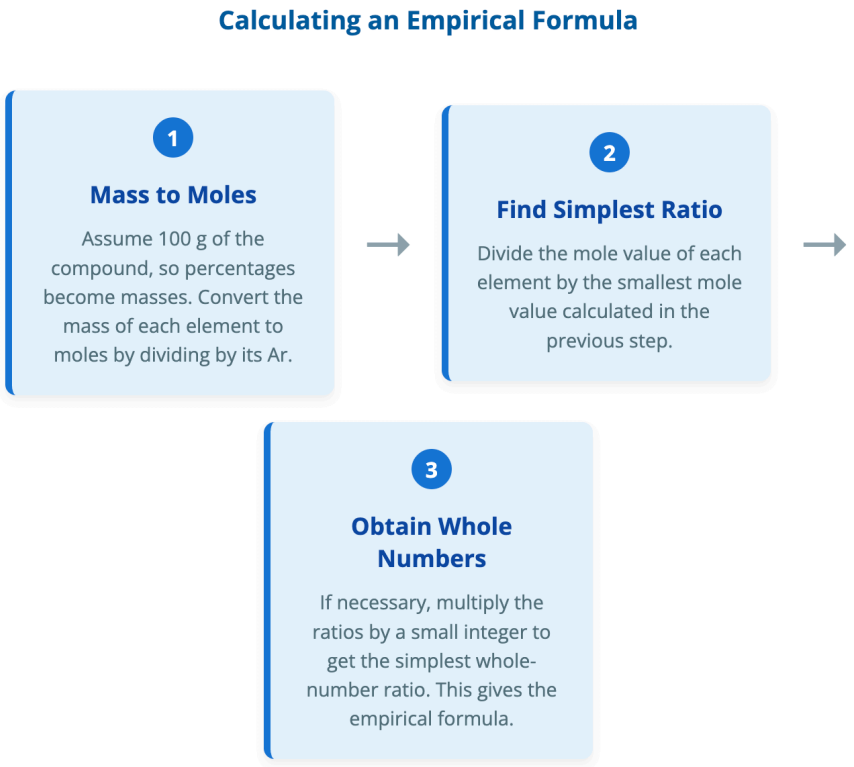
Feature	Empirical Formula	Molecular Formula
Information Provided	The simplest ratio of elements.	The actual number of atoms per molecule.
Uniqueness	Can be the same for different compounds (e.g., CH_2 is the empirical formula for ethene, propene, and butene).	Unique to a specific compound.
Example (Ethene)	CH_2	C_2H_4
Example (Glucose)	CH_2O	$C_6H_{12}O_6$
Example (Water)	H_2O	H_2O

Calculating the Empirical Formula

The empirical formula can be determined from experimental data, either from the percentage composition by mass of the elements in a compound or from the masses of elements in a known sample.

The calculation follows a clear, three-step process:

1. **Mass to Moles**: Convert the mass (or percentage) of each element into an amount in moles by dividing by its relative atomic mass (Ar).
2. **Find Simplest Ratio**: Divide the mole value for each element by the smallest mole value calculated in step 1.
3. **Obtain Whole Numbers**: If the results from step 2 are not whole numbers, multiply all the values by a small integer (usually 2 or 3) to obtain the simplest whole-number ratio.



Example Calculation from Percentage Composition

A compound contains 85.7% carbon and 14.3% hydrogen by mass. Determine its empirical formula.
(Ar values: C = 12.0, H = 1.0)

	Carbon (C)	**Hydrogen (H)**
Step 1: Moles	85.7 / 12.0 = 7.142	14.3 / 1.0 = 14.3

Step 2: Ratio	7.142 / 7.142 = 1	14.3 / 7.142 = 2

The simplest ratio of C:H is 1:2. The **empirical formula is CH_2.**

Example Calculation from Reacting Masses

When 1.55 g of phosphorus is completely combusted, 3.55 g of an oxide of phosphorus is produced. Deduce the empirical formula of the oxide.
(Ar values: P = 31.0, O = 16.0)

- Mass of Phosphorus = 1.55 g
- Mass of Oxygen = Total mass of oxide - Mass of phosphorus = 3.55 g - 1.55 g = 2.00 g

	Phosphorus (P)	**Oxygen (O)**
Step 1: Moles	1.55 / 31.0 = 0.0500	2.00 / 16.0 = 0.125
Step 2: Ratio	0.0500 / 0.0500 = 1	0.125 / 0.0500 = 2.5
Step 3: Whole Numbers	1 × 2 = 2	2.5 × 2 = 5

The simplest whole-number ratio of P:O is 2:5. The **empirical formula is P_2O_5.**

Determining the Molecular Formula

The molecular formula is always a whole-number multiple of the empirical formula. To determine the molecular formula, two pieces of information are required:

1. The empirical formula of the compound.
2. The relative molecular mass (Mr) of the compound.

Example Calculation

A compound has the empirical formula CH_2Br. Its relative molecular mass is 187.8. Deduce the molecular formula.
(Ar values: C = 12.0, H = 1.0, Br = 79.9)

1. Calculate the empirical formula mass:
   Mass of CH_2Br = 12.0 + (2 × 1.0) + 79.9 = 93.9
2. Find the multiplier:
   Multiplier (n) = Relative molecular mass / Empirical formula mass
   n = 187.8 / 93.9 = 2
3. Determine the molecular formula:
   Molecular Formula = (Empirical Formula)$_n$ = $(CH_2Br)_2$ = $C_2H_4Br_2$