Empirical and Molecular Formulas

How do you find an empirical formula?

●●○ Intermediate | Reactions & Stoichiometry | Last reviewed 3 October 2026

Before you start: it helps to understand The Mole Concept and Formula Mass and Percent Composition.

What is it?

An **empirical formula** shows the **simplest whole-number ratio** of the atoms in a compound.

A **molecular formula** shows the **actual number** of each kind of atom in one molecule.

Compound	Molecular formula	Empirical formula
Glucose	$C_6H_{12}O_6$	CH_2O
Hydrogen peroxide	H_2O_2	HO
Benzene	C_6H_6	CH
Water	H_2O	H_2O (already the simplest ratio)

KEY IDEA

The molecular formula is always a whole-number multiple of the empirical formula. Glucose, $C_6H_{12}O_6$, is $6 \times CH_2O$.

Why does it matter?

When chemists analyse an unknown compound, the experiment does not hand them a formula. It tells them **how much of each element** is present, usually as a percentage by mass.

Working out the empirical formula turns those measurements into a ratio of atoms. Add a measured molar mass and you get the molecular formula. This is one of the first steps in identifying a new or unknown substance.

How does it work?

From percent composition to empirical formula

1. **Assume a 100 g sample.** Each percentage then becomes a mass in grams (40.00% → 40.00 g).

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2. **Convert grams to moles** by dividing by each element's atomic mass.
3. **Divide every mole value by the smallest one.** This gives the mole ratio.
4. **Make whole numbers.** Values very close to whole numbers (such as 1.99 or 2.01) can be rounded. If a ratio ends in about .5, multiply every value by 2; about .33 or .67, multiply by 3; about .25 or .75, multiply by 4.
5. **Write the formula** using these whole numbers as subscripts.

From empirical formula to molecular formula

You need the compound's molar mass, which is measured separately. Then:

$$n = \frac{\text{molar mass}}{\text{empirical formula mass}}$$

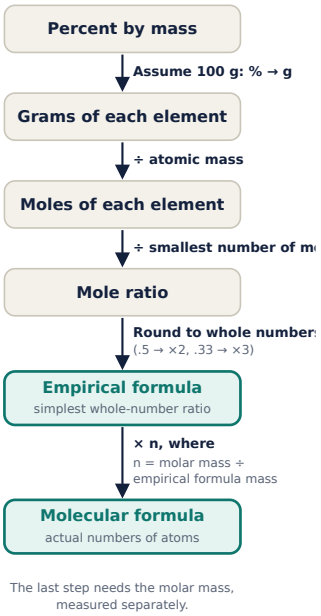
Multiply every subscript in the empirical formula by n (which should be a whole number).

> **THINK OF IT LIKE THIS**
>
> A recipe that uses 2 cups of flour for every 1 cup of sugar gives the *ratio*, 2 : 1. That's like the empirical formula. A baker who uses 6 cups of flour and 3 cups of sugar has the same ratio but a bigger batch. That's like the molecular formula. To know the batch size you need one more piece of information: for a compound, its molar mass.

> **MORE PRECISELY**
>
> Experimental percentages carry measurement error, so mole ratios rarely come out as exact whole numbers. A value such as 1.98 is safely rounded to 2, but 1.50 is not "nearly 2": it signals a ratio of 3 : 2. For compounds containing carbon and hydrogen, the percentages often come from **combustion analysis**, in which a sample is burned and the masses of $\mathrm{CO_2}$ and $\mathrm{H_2O}$ formed are measured.

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Visualise it



From percentages to a molecular formula. Every route goes through moles.

Worked example

WORKED EXAMPLE: Empirical and molecular formula of a sugar

Question: A compound is 40.00% C, 6.71% H and 53.29% O by mass. Its molar mass is 180.16 g/mol. Find its empirical and molecular formulas. (C = 12.01 g/mol, H = 1.008 g/mol, O = 16.00 g/mol)

Step 1 In 100 g: 40.00 g C, 6.71 g H, 53.29 g O.

Step 2 Moles: C: $\frac{40.00\ \text{g}}{12.01\ \text{g/mol}} = 3.331\ \text{mol}$; H: $\frac{6.71\ \text{g}}{1.008\ \text{g/mol}} = 6.657\ \text{mol}$; O: $\frac{53.29\ \text{g}}{16.00\ \text{g/mol}} = 3.331\ \text{mol}$

Step 3 Divide by the smallest (3.331 mol): C = 1.000, H = 1.999, O = 1.000 (the units of mol cancel, leaving a ratio)

Step 4 Whole numbers: C : H : O = 1 : 2 : 1, so the empirical formula is CH_2O.

Step 5 Empirical formula mass: 12.01 g/mol + 2(1.008 g/mol) + 16.00 g/mol = 30.03 g/mol

Step 6 $n = \frac{180.16\ \text{g/mol}}{30.03\ \text{g/mol}} = 6.00$, so multiply every subscript by 6.

Answer: empirical formula CH_2O; molecular formula $\text{C}_6\text{H}_{12}\text{O}_6$ (glucose).

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WORKED EXAMPLE: When the ratio isn't a whole number

Question: An oxide of iron is 69.94% Fe and 30.06% O by mass. Find its empirical formula. (Fe = 55.85 g/mol, O = 16.00 g/mol)

Step 1 In 100 g: Fe: $\frac{69.94\ \text{g}}{55.85\ \text{g/mol}} = 1.252\ \text{mol}$; O: $\frac{30.06\ \text{g}}{16.00\ \text{g/mol}} = 1.879\ \text{mol}$

Step 2 Divide by the smallest (1.252 mol): Fe = 1.000, O = 1.500

Step 3 1.500 ends in .5, so multiply both by 2: Fe = 2, O = 3

Answer: the empirical formula is Fe_2O_3.

WORKED EXAMPLE: A hydrocarbon, all the way through

Question: A hydrocarbon is 85.6% C and 14.4% H by mass. Its molar mass is 56.1 g/mol. Find its empirical and molecular formulas. (C = 12.01 g/mol, H = 1.008 g/mol)

Step 1 In 100 g: $n(\text{C}) = \frac{85.6\ \text{g}}{12.01\ \text{g/mol}} = 7.127\ \text{mol}$ and $n(\text{H}) = \frac{14.4\ \text{g}}{1.008\ \text{g/mol}} = 14.29\ \text{mol}$

Step 2 Divide by the smallest (7.127 mol): C 1.000, H 2.004, which rounds safely to 2. Empirical formula: CH_2.

Step 3 Empirical formula mass: 12.01 g/mol + 2(1.008 g/mol) = 14.03 g/mol

Step 4 $n = \frac{56.1\ \text{g/mol}}{14.03\ \text{g/mol}} = 4.00$

Answer: empirical formula CH_2; molecular formula C_4H_8.

Common mistake

COMMON MISTAKE: Rounding 1.5 up to 2

A ratio of 1 : 1.5 is **not** "about 1 : 2". Rounding it would give FeO_2, which is wrong. Multiply every value by 2 instead to get 2 : 3. Only round values that are within a few hundredths of a whole number.

COMMON MISTAKE: Using the percentages as the ratio

The percentages are a ratio of **masses**, not of atoms. In the sugar example, 40.00 : 6.71 : 53.29 says nothing directly about the number of atoms. Always convert to moles first.

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⚠ **COMMON MISTAKE: Dividing by the wrong number**

Divide by the **smallest** number of moles, not the largest. Dividing by the smallest makes the smallest value exactly 1 and the others 1 or more.

NOTATION NOTE

- The empirical formula is also called the **simplest formula**.
- Formulas of ionic compounds such as NaCl and $\mathrm{Fe_2O_3}$ are empirical formulas, because ionic compounds are not made of separate molecules.
- A molecular formula shows *how many* atoms there are, but not how they are connected. That is shown by a **structural formula**.

Remember this

REMEMBER THIS

- **Empirical formula = simplest whole-number ratio; molecular formula = actual numbers of atoms.**
- **Percent → grams (assume 100 g) → moles → divide by the smallest → whole numbers.**
- **A ratio ending in .5 means multiply by 2; don't round it.**
- **Molecular formula = empirical formula × (molar mass ÷ empirical formula mass).**

References

1. Brown, T. L.; LeMay, H. E., Jr.; Bursten, B. E.; Murphy, C. J.; Woodward, P. M.; Stoltzfus, M. W. Chemistry: The Central Science, 15th ed.; Pearson, 2022.

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