

Moles, formulae, gas volumes and atom economy

Chemistry grades 11-12 (A Level · IB · Class 11-12) · Lesson

Quick answer: The amount of substance, in mol, links mass, particle number, solution volume and gas volume. Use $n = m/M$, $n = cV$ and $pV = nRT$ with SI units, find empirical formulae from mole ratios, and judge a reaction's efficiency with atom economy, which compares the useful product's mass with all products.

Level: Chemistry grades 11-12 (A Level · IB · Class 11-12) · **Curriculum:** A Level 3.1.2

How do you calculate the amount of substance?

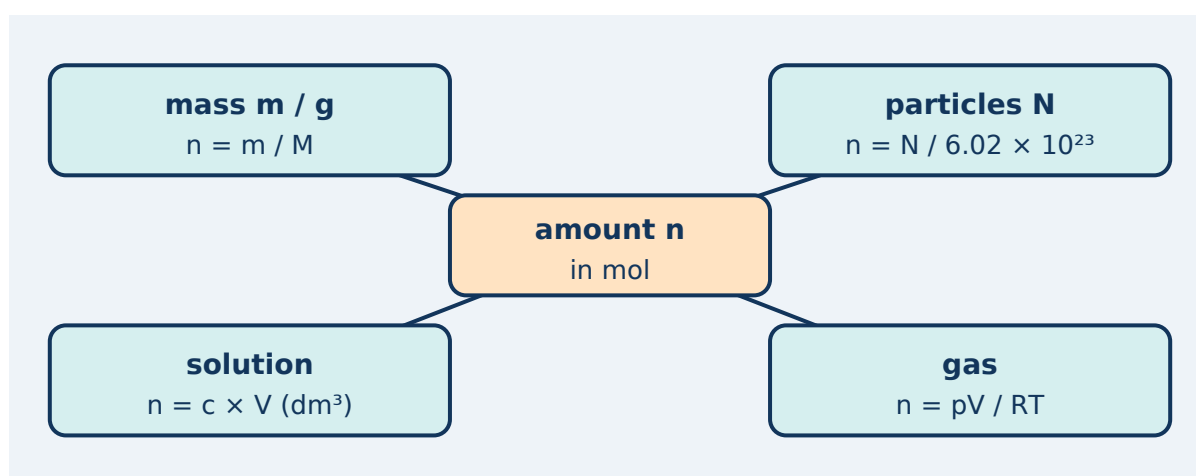
The mole links the masses we weigh to the particles that react. All amount calculations start from one quantity, n , measured in mol.

Definition

One **mole** is the amount of substance that contains 6.02×10^{23} particles (the Avogadro constant). The **molar mass** M is the mass of one mole in g mol^{-1} , equal numerically to the relative formula mass.

Formula

$n = m / M$ (m in g, M in g mol^{-1})
 $n = c \times V$ (c in mol dm^{-3} , V in dm^3)
 $n = N / 6.02 \times 10^{23}$ (N = number of particles)



Every route to the mole: mass, particles, solutions and gases.

Worked example 1

A farmer in Kenya dissolves 8.40 g of sodium hydrogencarbonate, NaHCO_3 , in 250 cm^3 of

water. Find its concentration.

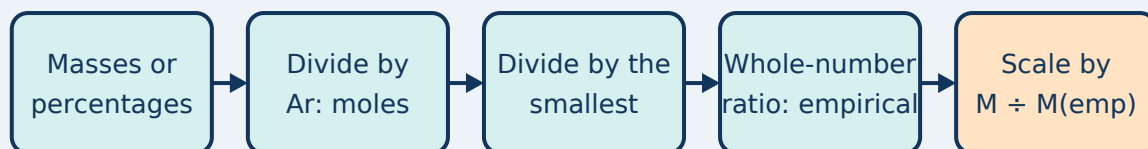
$$M = 23.0 + 1.0 + 12.0 + 48.0 = 84.0 \text{ g mol}^{-1}. n = 8.40 \div 84.0 = 0.100 \text{ mol}.$$

$$c = 0.100 \text{ mol} \div 0.250 \text{ dm}^3 = \mathbf{0.400 \text{ mol dm}^{-3}}.$$

How do you find an empirical and a molecular formula?

Definition

The **empirical formula** is the simplest whole-number ratio of atoms of each element in a compound. The **molecular formula** is the actual number of atoms in one molecule, a whole-number multiple of the empirical formula.



Example: 40.0 % C, 6.7 % H, 53.3 % O → CH₂O → C₆H₁₂O₆ (M = 180)

Five steps from composition data to the molecular formula.

Worked example 2

A sugar contains 40.0 % carbon, 6.7 % hydrogen and 53.3 % oxygen by mass, with M = 180 g mol⁻¹.

In 100 g: C = 40.0 ÷ 12.0 = 3.33 mol; H = 6.7 ÷ 1.0 = 6.7 mol; O = 53.3 ÷ 16.0 = 3.33 mol.

Divide by 3.33: C : H : O = 1 : 2 : 1, so the empirical formula is CH₂O (mass 30.0).

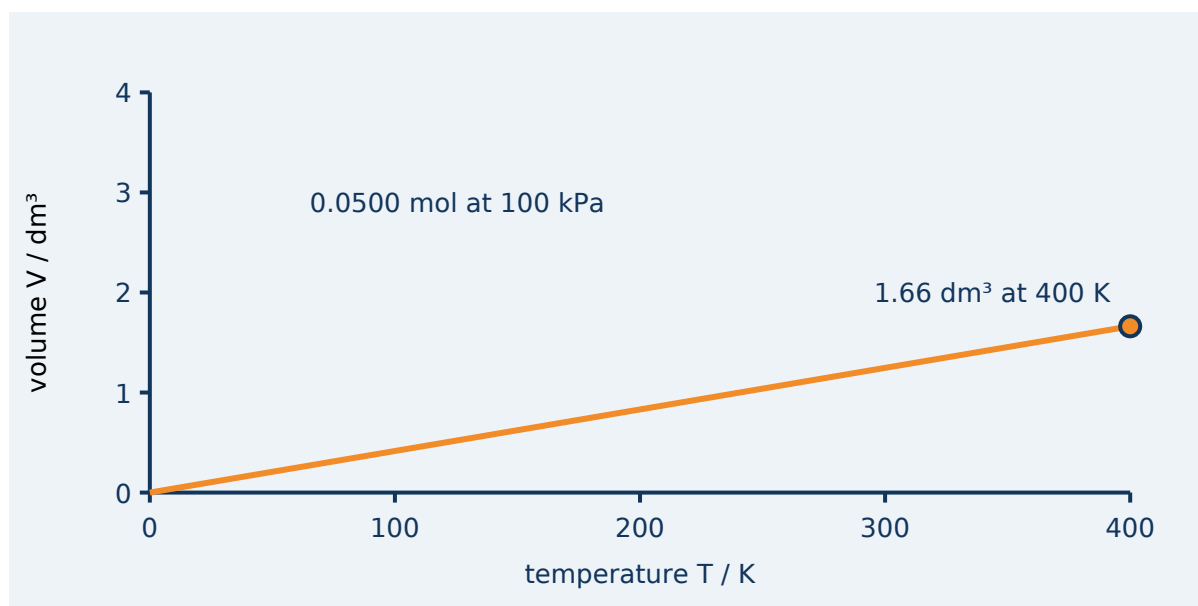
180 ÷ 30.0 = 6, so the molecular formula is **C₆H₁₂O₆**.

Common mistake

If a ratio comes out as 1 : 1.5, do not round to 1 : 2. Multiply every number by 2 to get 2 : 3. Only round when the value is within about 0.05 of a whole number.

How does the ideal gas equation work?

An ideal gas follows the equation $pV = nRT$. At a fixed pressure, doubling the kelvin temperature doubles the volume, as the graph shows.



At constant pressure and amount, V is proportional to T (kelvin).

Formula

$$pV = nRT$$

p = pressure in Pa, V = volume in m^3 , n = amount in mol, T = temperature in K, $R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$.

Convert	Rule
$^{\circ}\text{C}$ to K	add 273
cm^3 to m^3	multiply by 10^{-6}
dm^3 to m^3	multiply by 10^{-3}
kPa to Pa	multiply by 10^3

Worked example 3

Find the volume of 0.250 mol of gas at 27°C and 101 kPa.

$T = 300 \text{ K}$, $p = 101\,000 \text{ Pa}$.

$$V = nRT \div p = (0.250 \times 8.31 \times 300) \div 101\,000 = 6.17 \times 10^{-3} \text{ m}^3 = \mathbf{6.17 \text{ dm}^3}.$$

What is atom economy?

Definition

Atom economy = (relative formula mass of the desired product $\div$ sum of the relative formula masses of all products) $\times 100\%$. It measures how much of the reactant mass ends up in the useful product.

Fermentation, $\text{C}_6\text{H}_{12}\text{O}_6 \rightarrow 2\text{C}_2\text{H}_5\text{OH} + 2\text{CO}_2$, gives $(2 \times 46.0) \div 180.0 \times 100 = 51.1\%$, because carbon dioxide is also produced. Atom economy differs from percentage yield, which compares the actual mass obtained with the maximum possible mass.

Lina's tip

Write the unit of every number as you substitute. If the units of an ideal gas problem do not give m^3 at the end, you forgot to convert cm^3 , dm^3 or kPa .

Key points to remember

- $n = m / M$; $n = c \times V$; $n = N / 6.02 \times 10^{23}$
- $pV = nRT$ with p in Pa , V in m^3 , T in K , $R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$
- Empirical formula: divide masses by A_r , then by the smallest value
- Molecular formula = empirical formula $\times (M \div \text{empirical mass})$
- Atom economy = $\text{Mr desired product} \div \text{Mr all products} \times 100 \%$

Moles, formulae, gas volumes and atom economy: frequently asked questions

What is the difference between empirical and molecular formula?

The empirical formula is the simplest whole-number ratio of atoms, such as CH_2 . The molecular formula is the real number of atoms in a molecule, such as C_4H_8 . You need the molar mass to go from one to the other.

Why must temperature be in kelvin in $pV = nRT$?

The volume of a gas is proportional to the absolute temperature. A 0°C value would give zero volume, which is wrong. Always add 273 to the Celsius value.

Why must volume be in m^3 and pressure in Pa ?

The gas constant $R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$ uses SI units. One pascal times one cubic metre equals one joule, so the units cancel correctly only in Pa and m^3 .

Does a high atom economy mean a high yield?

No. Atom economy compares the masses in the balanced equation, whatever happens in the real experiment. A reaction can have a perfect atom economy yet a low percentage yield if it is incomplete or if product is lost.

How do you get the number of atoms in a sample?

Find the amount in mol , then multiply by 6.02×10^{23} . For atoms inside molecules, multiply by the number of atoms of that element in each formula unit.