# Quantitative skills

**Problem Solving** is a skill that you will need to develop for all aspects of your degree in Chemistry. It applies equally to solving problems with a **numerical** answer (**quantitative** result) or with a **conceptual** answer (**qualitative** result).

## What are the key steps to solving a problem?

* **Understand the question:** What am I being asked to work out?
* **Consider the context**: What information and/or restrictions have I been given?
* **Choose a method**: What formula or approach can I use to answer the question? Is this method appropriate to the context of the question?
* **Interpret the result:** Does my answer make sense? Does it answer the question? Does it meet the criteria set out in the question?

This is a **cycle** where steps can/should be repeated until a final result is achieved.

## How do you write a quantitative result?

## Scientific notation

p = 1.00 x 105 Pa

## Vector or Scalar?

* A **scalar** quantity only has a magnitude (size)
  + *Examples*: Energy, wavelength, work
  + Variables in *italics* are scalars: *E*, *λ, W*
* A **vector** is a quantity that has both magnitude (size) and direction.
  + *Examples*: Force, momentum, electric field
  + Variables in **bold** are vectors: **F**, **p**, **E**
  + We often define vectors in term of components within a given coordinate system.

*Example*: the position vector which describes a location in 3D space can be expressed in Cartesian coordinates:

## How do you know if the result makes sense?

## Units

* **All** quantitative answers have **two** parts: the **numerical** part and the **units**.
* **All** quantitative answers **must** be reported with the appropriate **units**.
* The **absence of units** means that the quantity is **dimensionless.** That means that the physical quantity being reported has no units.
  + *Examples:* quantum number, order of a reaction, absorbance
* Sometimes experimentally measured quantities have **arbitrary units**. In this case, quantitative results are obtained through calibration or an internal reference.
  + *Example*: intensity in an NMR spectrum

## Order of magnitude

* How big do you expect the answer to be?
* Do not forget to consider the unit prefix!

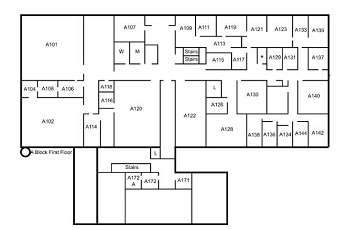
## Sign/Direction

* Should my answer be positive or negative?
* For vector quantities, does the direction make sense?

## Significant figures

* How precise is my answer? How many decimal places should I use?

# Example 1: Estimate the volume of room C/A 101



## Step 1. Understand the question

**Volume**

## Step 2. Consider the context

Estimate (no dimensions given)

## Step 3. Choose a method

**Assume a simple rectangular box**

**V = length x width x height**

## Step 4. Interpret the result

Consider the potential solutions to this problem listed below. Which answers can immediately be eliminated? Why?

1. *V* = 1.5 km wrong unit (distance!)
2. *V* = 120 L too small!
3. *V* = 250 cm3 too small!
4. *V* = 500 no units
5. *V* = 100 m2 wrong units (area)
6. *V* = 20 km3 too large!
7. *V* = - 250 m3 cannot be negative
8. *V* = 2 x 105 nm3 too small!
9. *V* = 1000 dm3  too small!
10. *V =* 8.5 x 105 L reasonable (850 m3)
11. *V* = 1000 m3 reasonable
12. V = 1.2 x 104 m3 too large

# Unit Conversion

## Table 1. SI base units

| **quantity** | **unit** | **symbol** |
| --- | --- | --- |
| mass | kilogram | kg |
| time | second | s |
| distance | meter | m |
| temperature | kelvin | K |
| electric current | ampere | A |
| amount of a substance | mole | mol |
| luminous intensity | candela | cd |

## Table 2. Common units

| **quantity** | **unit** | **Symbol for SI unit** | **SI base units** |
| --- | --- | --- | --- |
| frequency | hertz | Hz | s-1 |
| force | newton | N | kg m s-2 |
| pressure | pascal | Pa | kg m-1 s-2 (= N m-2) |
| energy | joule | J | kg m2 s-2 (= N m) |
| temperature | kelvin | K | K |
| electric charge | coulomb | C | A s |
| electric potential | volt | V | kg m2 s-3 A-1 (= J C-1) |
| capacitance | farad | F | kg-1 m-2 s4 A2 (= C V-1) |
| resistance | ohm | Ω | kg m2 s-3 A-2 (= V A-1) |
| power | watt | W | kg m2 s-3 (= J s-1) |

## Table 3. Metric System Prefix Table

| Prefix | Symbol | Multiplier | Exponential |
| --- | --- | --- | --- |
| tera | T | 1,000,000,000,000 | 1012 |
| giga | G | 1,000,000,000 | 109 |
| mega | M | 1,000,000 | 106 |
| kilo | k | 1,000 | 103 |
| hecto | h | 100 | 102 |
| deca | da | 10 | 101 |
| - | - | 1 | 100 |
| deci | d | 0.1 | 10-1 |
| centi | c | 0.01 | 10-2 |
| milli | m | 0.001 | 10-3 |
| micro | µ | 0.000001 | 10-6 |
| nano | n | 0.000000001 | 10-9 |
| pico | p | 0.000000000001 | 10-12 |
| femto | f | 0.000000000000001 | 10-15 |

## Table 4. Some common non-SI units

| Name | Symbol | Quantity | Definition |
| --- | --- | --- | --- |
| calorie | cal | energy | 4.184 J |
| angstrom |  | distance | 10-10 m |
| mile | mi | Distance | 1609 m |
| Celsius | °C | temperature |  |
| minute | min | time | 60 s |
| hour | h or hr | time | 3600 s |
| day | d | time | 86 400 s |
| litre | L | volume | 1 dm3 = 10-3 m3 |
| tonne | t | mass | 1 t = 103 kg |
| atmosphere | atm | pressure | 1.013 x 105 Pa |

# Unit conversion guide

**Step 1:** Determine the relationship between the current unit and the desired unit. Refer to Tables 1 - 4 for useful unit relationships.

e.g. 1000 mL = 1 L; 103 mg = 1 g = 10-3 kg; 1 hr = 60 min; 1 mL = 1 cm3

**Step 2:** Convert the relationship from (step 1) to a fraction with the desired unit on top and the current unit on the bottom.

Conversion from L to mL:

Conversion from kg to mg:

Conversion from minutes to hours:

Conversion from cm3 to mL

**Step 3:** To change multiple units at once, or to change a single unit in multiple steps, generate a conversion fraction for each desired change in unit and multiply together. If the unit is expressed with a power > 1, apply the same power to the entire fraction.

Conversion from cm3 to L in two steps

Conversion from m2 to mm2

**Step 4:** Multiply the quantity by the conversion fraction(s). The old unit will cancel leaving the new desired unit. This is equivalent to multiplying by 1 because the top and bottom of the conversion factions are (by design) equal.

Conversion from 0.25 L to mL:

Conversion from 3.45 x 10-4 kg to mg:

Conversion from 275 minutes to hours:

Conversion from 256 cm3 to L in two steps

Conversion from 6.43 x 10-7 m2 to mm2

**Step 5:** Check the result. Has the value of the quantity increased or decreased? Does this make sense relative to the change in unit? If the new unit is smaller the value should increase. If the new unit is bigger the value should decrease.

**Example 1:** convert *V* = 2 x 105 nm3 to m3

**Example 2:** convert *V* = 8.5 x 105 L to m3

## Using units to verify an equation

For any equation the units on both sides of the equation must be equivalent. Units of terms added/subtracted in an equation also have to be the same within an equation. Therefore, unit analysis can be used to verify an equation.

**Example:** Kinetic energy is given by the following relationship. Show that the units of the quantities on the right-hand-side (RHS) of the equation are equal to the unit on the left-hand-side (LHS).

RHS:

Units of *m* mass 🡪 kg

Units of *v* velocity 🡪 m s-1

Total units = kg (m s-1)2 = kg m2 s-2

LHS:

Units of *KE* energy 🡪 J

From Table 2: 1 J = 1 kg m2 s-2. Therefore, the units on the RHS and the LHS match.

# Quantitative Skills: Take Home Messages

## Problem solving

It is important to think about what the question is asking, consider what information you have available and to ask the question: does my answer make sense? This will help you in exams but more crucial in ‘real life’ (i.e. research, the lab) where the answer is not necessarily known.

## Units

* Memorising equations will only get you so far. It is impossible to remember everything and many quantities have similar or the same variables (e.g. p can be pressure or momentum). Need to understand the context.
* Units can help to provide a solution for how to solve a problem. This is especially true in situations like making up solutions in the lab. Make sure your units cancel out when you calculate volumes, masses, concentrations etc.
* In any equation, the units on each side need to be the same.
* Units of quantities added/subtracted need to be the same. (No adding apples to oranges unless you are counting ‘fruit’!)
* If you have the same unit on the top and bottom of a fraction, they cancel out.
* The ability to work comfortably with units and to convert between different units is a skill that will benefit you throughout your degree and future career.
* Including units in all steps of your calculations will help avoid errors.
* When doing unit conversions, the best way to avoid errors is to write down each step of the conversion. It is very easy to make mistakes when you do these conversions in your head – particularly in a high pressure environment like an exam.