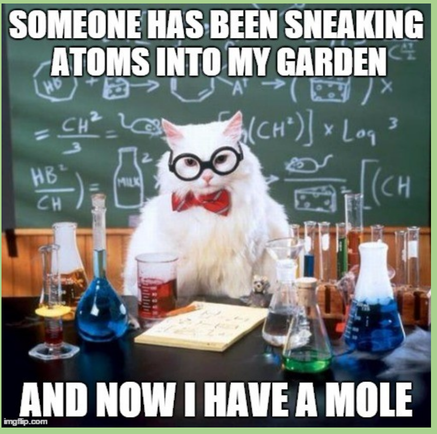
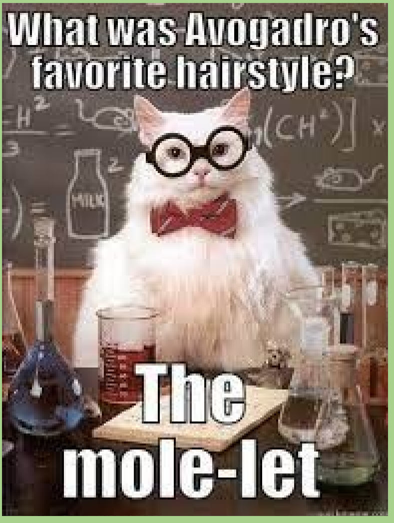
# Ch 6. Quantifying atoms and compounds (The mole)




**2023**




**AREA OF STUDY 2** HOW ARE MATERIALS QUANTIFIED AND CLASSIFIED?

Key knowledge:

- *the relative isotopic masses of isotopes of elements and their values on the scale in which the relative isotopic mass of the carbon-12 isotope is assigned a value of 12 exactly*
- *determination of the relative atomic mass of an element using mass spectrometry (details of instrument not required)*
- *Avogadro's constant as the number $6.02 \times 10^{23}$ indicating the number of atoms or molecules in a mole of any substance; determination of the amount, in moles, of atoms (or molecules) in a pure sample of known mass*
- *determination of the molar mass of compounds, the percentage composition by mass of covalent compounds, and the empirical and molecular formula of a compound from its percentage composition by mass*

Dr Matthews, Mr Tran, Ms Williams and Mr Zwack

## 6.1 Introduction

### Quantifying atoms and compounds

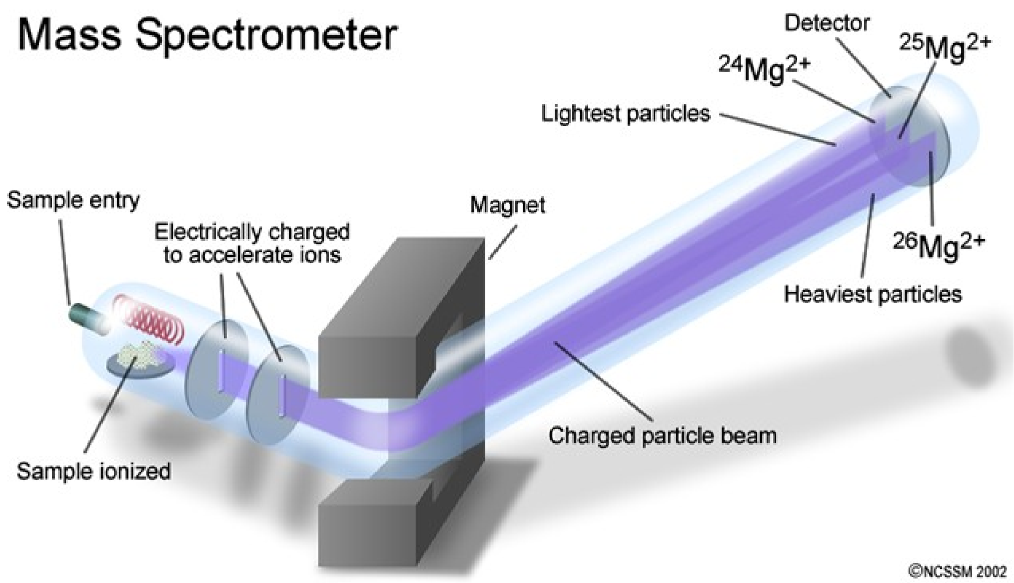
Atoms are tiny – so tiny that their size is difficult to comprehend. So how would we measure atoms?

Mass spectrometry is a device used to measure the masses of individual particles. When comparing the masses of the particles we can use formulas to calculate (roughly) how many particles would exist in a sample(s).

The mole concept, which is central to most chemical calculations, helps us to work with the vast numbers of atoms that are present in different types of substances. It allows a whole range of calculations to be performed (such as percentage composition and empirical formulas) which has commercial and industrial applications.

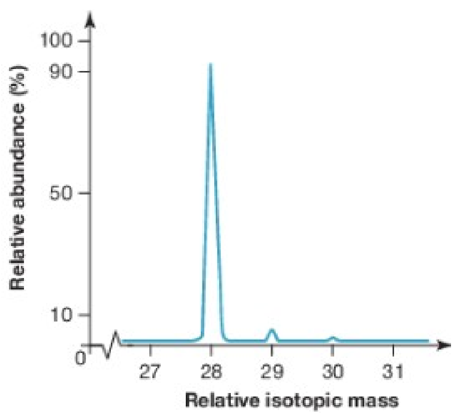
## 6.2 Relative isotopic mass and the carbon-12 scale

### The mass spectrum




The **mass spectrometer** is an analytical tool used to separate particles by mass and charge. For Unit 1 chemistry it can be used to calculate the relative isotopic mass of different elements. The reading produced from a mass spectrometer is called a mass spectrum. To read a mass spectrum:

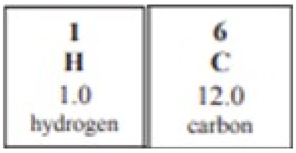
- The number of peaks indicates the **number of isotopes.**
- Read the x-axis to determine the **relative isotopic mass** (mass: charge ratio).
- The relative heights of the peaks correspond to the **relative abundance** of each isotope.




Recall:

- **Isotopes** are members of a family of an element that all have the **same number of protons** but **different number of neutrons.**
- **Relative isotopic mass** refers to the mass of an individual isotope of an element on the relative atomic mass scale, in comparison to the mass of the carbon-12 isotope.
- **Relative abundance** is the percentage of atoms with a specific atomic mass found in a naturally occurring sample of an element.

## Relative isotopic mass




The relative isotopic mass ($I_r$) is the mass of each isotope compared to carbon-12.

Hydrogen has a relative mass of 1 because the mass of H (1.66 x $10^{-24}$ g) is 12 times less than the mass of carbon (1.99 x $10^{-23}$ g).

**TABLE 6.1** Masses of atoms of three elements

| Element | Protons | Neutrons | Protons + neutrons | Mass relative to carbon-12 |
|---|---|---|---|---|
| $^{1}_{1}H$ | 1 | 0 | 1 | $\frac{1}{12} \times 12 = 1$ |
| $^{12}_{6}C$ | 6 | 6 | 12 | $\frac{12}{12} \times 12 = 12$ |
| $^{59}_{27}Co$* | 27 | 32 | 59 | $\frac{59}{12} \times 12 = 59$ |

*While cobalt, Co, has 22 isotopes, only one isotype is naturally occurring, $^{59}Co$.

Therefore, using the provided definition:

$$\text{Relative isotopic mass} = \frac{\text{mass of an atom of the isotope}}{\text{mass of an atom carbon} - 12} \times 12$$

### Extension- How mass spectrometers work

- Read at home
- Pg 230 (read additional document for more information)

## Significant figures

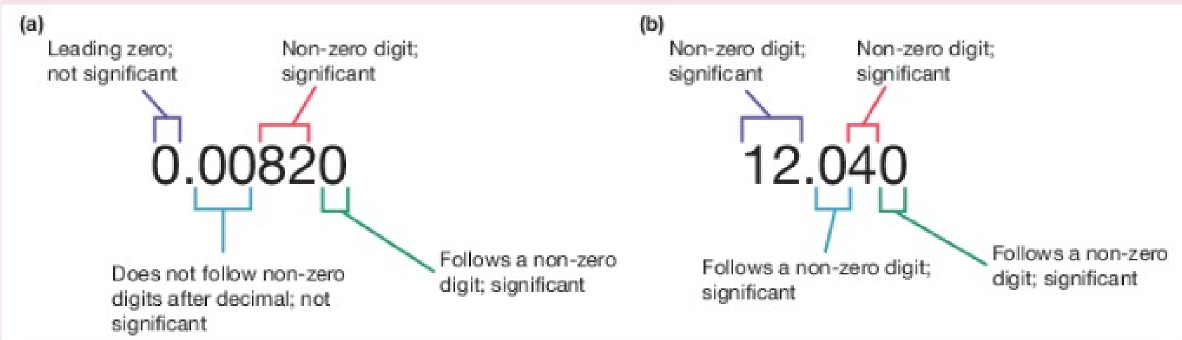
The number of significant figures we give in our answer depends on the number of significant figures we are given in the question. We take the number of significant figures from the number which has the **least** number of significant figures.

The best way of showing the number of significant figures is to put all data into **standard form** or **scientific notation**.

Notes:

- non-zero integers **always** count as significant figures
- leading zeros do **NOT** count as significant e.g. 0.05 has 1 significant figure
- captive zeros **always** count as significant e.g. 505 has 3 significant figures
- trailing zeros are **traditionally** significant only if the number contains a decimal point e.g. 0.500 has 3 significant figures (VCAA stipulates that trailing zeros are **ALWAYS** significant)

**FIGURE 6.7** Examples of significant figures: (a) three significant figures and (b) five significant figures




**Polar dissolves polar**

Remember that for a substance to be polar:

- its molecules must contain polar bonds
- its shape must be asymmetrical.

If the above are not satisfied, the substance is not polar.

**Q.** Determine the number of significant figures in the following examples

| | | |
|---|---|---|
| 70 | 0.00005 | 0.01 |
| 9500 | 85 | $4.2 \times 10^3$ |
| $4.15 \times 10^2$ | 872,000 | 0.000450 |

**Q.**

a. Convert each example to 3 significant figures in scientific notation format

b. Round the numbers to their indicated s.f. (inc. scientific notation)

| | |
|---|---|
| 0.000030<br><br>Round 7.994 to 2 significant figures. | 8.0<br><br>Round 10.356 to 3 significant figures. |
| 10.4<br><br>Round 0.08907654 to 1 significant figure. | 0.09<br><br>Round 89.98 to 3 significant figures. |
| 90.0<br><br>Round 45678 to 1 significant figure. | 50000<br><br>Round 136000 to 2 significant figures. |

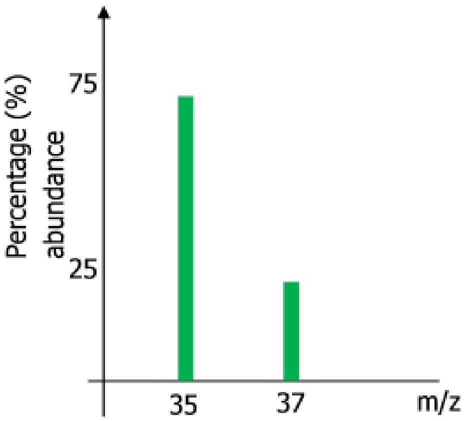
Relative atomic mass ($A_r$)

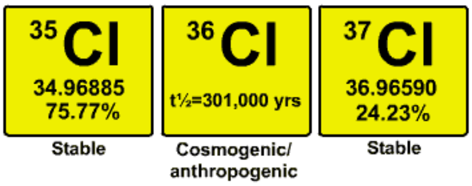
The **mass spectrum** of an element is used to calculate the **relative atomic mass ($A_r$).**

## Relative atomic mass

The relative atomic mass of an element can be calculated from the following formula:

$$A_r = \frac{(\text{RIM of first isotope} \times \%\,\text{abundance}) + (\text{RIM of second isotope} \times \%\,\text{abundance}) + \ldots}{100}$$




**Q1.** Calculate the relative atomic mass for chlorine.

$$\boldsymbol{A_r(Cl)} = \frac{\sum(I_r \text{ x } \%\, abundance)}{100}$$
$$= \frac{(34.96885 \text{ x } 75.77 + 36.96590 \text{ x } 24.23)}{100}$$
$$= \mathbf{35.45}$$

**Q** Calculate the relative atomic mass for silicon to 3 significant figures given:
Isotope $^{28}Si$, relative isotopic mass = 27.977, abundance = 92.23%
Isotope $^{29}Si$, relative isotopic mass = 28.976, abundance = 4.67%
Isotope $^{30}Si$, relative isotopic mass = 29.973, abundance = 3.1%

**Q** Lithium consists of two isotopes. One isotope, $^{6}Li$, has a relative isotopic mass of 6.02 and an abundance of 7.42%. The other isotope, $^{7}Li$, has a relative isotopic mass of 7.02 and an abundance of 92.58%.

a. Is the relative atomic mass closer to six or seven? Explain your answer

b. Calculate the relative atomic mass of lithium

**Q** Copper has two isotopes: $^{63}Cu$, which has the relative isotopic mass of 62.93, and $^{65}Cu$, which has the relative isotopic mass of 64.92. The proportions of each isotope are 69.15% and 30.85% respectively. Calculate the relative atomic mass, $A_r$, of copper.

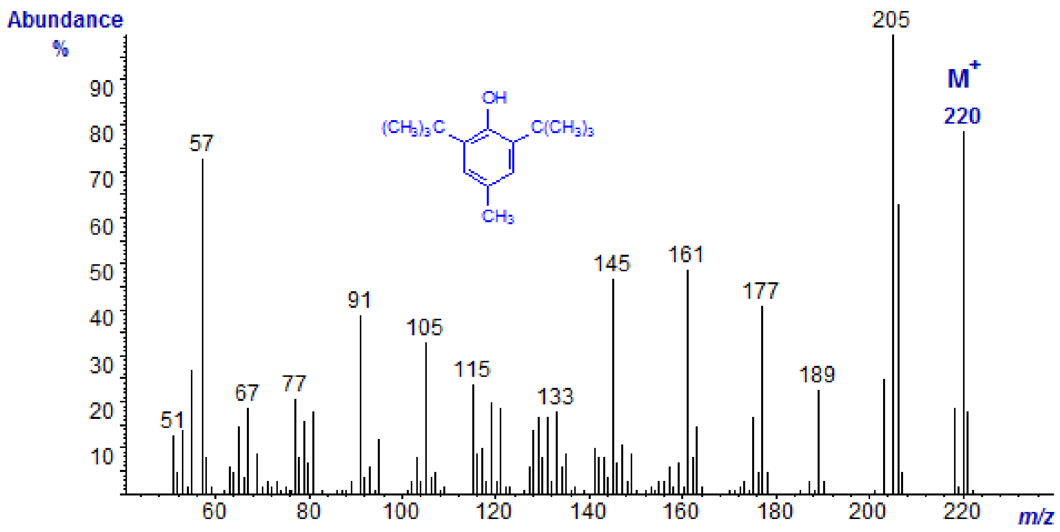
**Q** The relative atomic mass of rubidium is 85.47. The relative isotopic masses of its two isotopes are 84.95 and 86.94. Calculate the relative abundances of the isotopes in naturally occurring rubidium.
Hint: Abundance of lighter isotope = x
Hint 2: Abundance of heavier isotope must be 100 – x

**Q** The relative atomic mass of copper is 63.54. The relative isotopic masses of its two isotopes are 62.95 and 64.95. Calculate the relative abundances of the isotopes in naturally occurring copper.

**Relative molecular mass ($M_r$)**

The relative molecular mass ($M_r$) is the mass of one molecule of that substance relative to the mass of a $^{12}C$ atom taken as 12 units exactly.

The relative molecular mass can be determined by using the **periodic table** or a **mass spectrometer**. The relative molecular mass is equal to the sum of the relative masses of the atoms in the molecule.




**E.g.** The relative molecular mass of carbon dioxide ($CO_2$)

$A_r$ (C) = 12.0
Ar (O) = 16.0
$M_r$ ($CO_2$) = 1 * $A_r$ (C) + 2* $A_r$ (O)

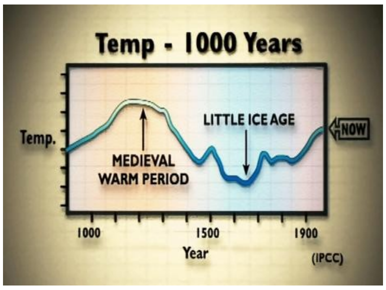
= 1 * 12.0 + 2 * 16.0
= 44.0

## 6.3 Avogadro's constant and the mole

### Avogadro's constant

It is difficult to count atoms individually. For many items we count by a larger unit.
Some everyday groups:

Pair =
Dozen =
Century =
Millennium =
Mole =




Avogadro's constant is equal to $6.02 \times 10^{23}$ which can be used as a reference to determine the amount of atoms or molecules in a **mole** of any substance.

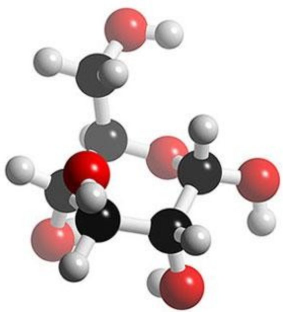
### The mole

For atoms we count by the **mole**. It is referred to as the 'amount of substance', with the symbol **n** and the unit **mol**.

When referring to a mole of a substance, it is important to indicate which particle is being specified. For example, one mole of oxygen molecules ($O_2$) would actually contain two mole of oxygen atoms (O).

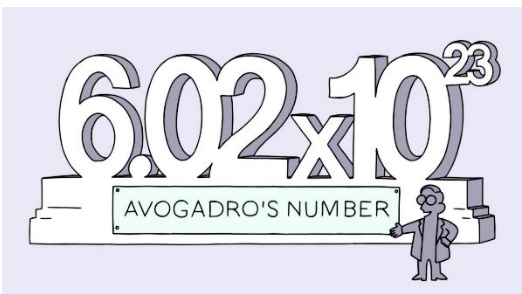
One mole of any substance contains exactly $6.022140 \times 10^{23}$ elementary entities.

There are $6.02 \times 10^{23}$ atoms in 12g of $^{12}C$. By using Carbon-12 as a common reference, we are able to find out the mass of one mole of any element. E.g. In 16g of O there are $6.02 \times 10^{23}$ particles of oxygen.



1 mol of glucose ($C_6H_{12}O_6$) contains 24 mol of atoms

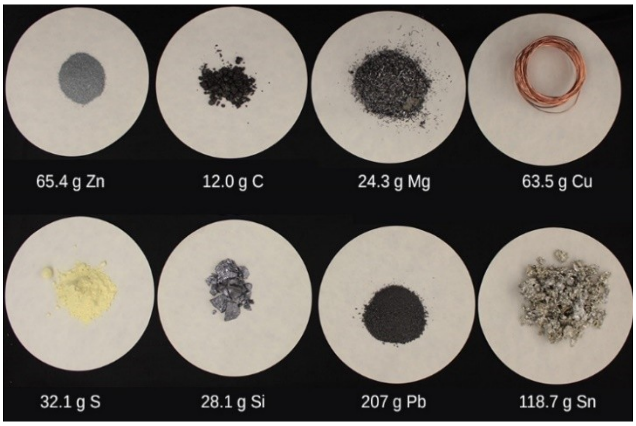
This is known as **Avogadro's Number ($N_A$).**
**$N_A = 6.02 \times 10^{23}$ mol$^{-1}$**



**Practical: Determine one mole**

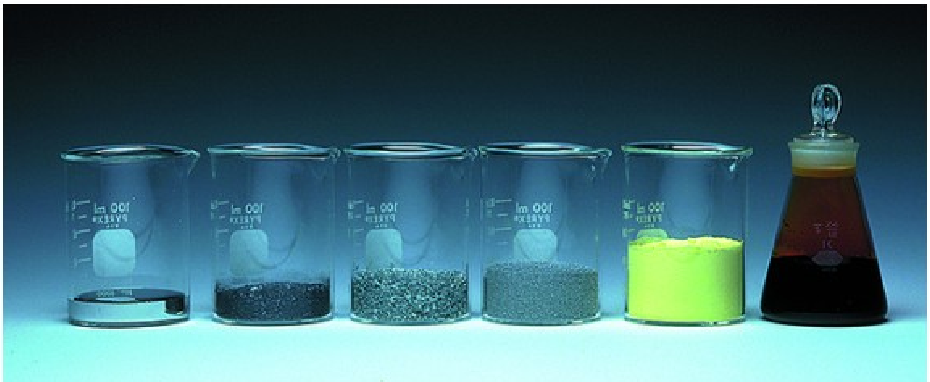
**Aim:** To determine the mass of exactly one mole of substances supplied to you by your teacher.

One Mole of Several Substances


**Q How do we find the mass of one mole of an element without experimentation? (Hint: periodic table)**

FIGURE 6.9 One mole each of mercury, zinc, silicon, aluminium, sulfur and bromine. The quantity of each of the substances shown contains $6.02 \times 10^{23}$ particles.

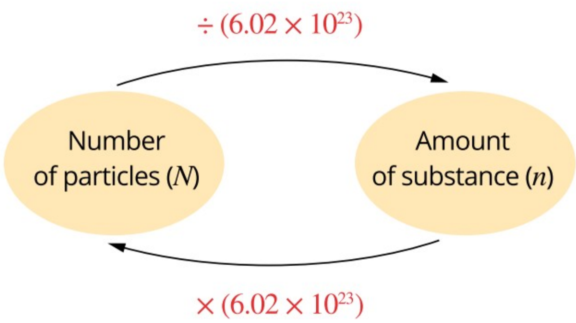


## Extension- Amedeo Avogadro

- Read at home
- Pg 238 (read additional document for more information)

**Using Avogadro's Number**

The connection between the mole and Avogadro's Number

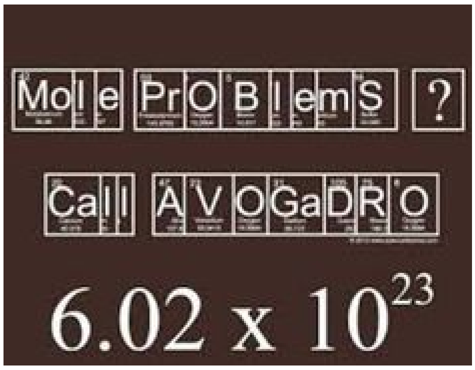



This can be written as:

$$n = \frac{N}{N_A}$$

n = the amount in mol
N = the number of specified particles

$N_A$ = Avogadro's Number ($6.02 \times 10^{23}$)




**Q** Calculate the number of molecules in 3.5 moles of water ($H_2O$)

**Q** Calculate the number of molecules in 1.6 moles of carbon dioxide ($CO_2$)

**Q** Calculate the number of oxygen atoms in 2.5 mol of oxygen gas ($O_2$)

**Q** Calculate the number of hydrogen atoms in 0.35 mol of methane ($CH_4$)

**Q** Calculate the amount, in mol, of ammonia molecules ($NH_3$) represented by $2.5 \times 10^{22}$ ammonia molecules

**Q** Calculate the amount, in mol, of magnesium atoms represented by $8.1 \times 10^{20}$ magnesium atoms

**Q** Calculate the amount, in mol, of hydrogen atoms in 0.75 mol of water ($H_2O$)

Molar Mass (M)

The molar mass (M) of an element is defined as the mass of **one mol** of the element; that is 6.02 x $10^{23}$ atoms of the element). The unit is grams per mol (g $mol^{-1}$). It is calculated by adding up the relative atomic masses of all elements within the chemical formula.

## Molar mass of carbon *atoms*

$$\text{Molar mass of carbon } atoms = \text{mass of 1 mol of C } atoms$$
$$A_r(C) = 12.0$$

$$\therefore \text{ mass of 1 mol of C } atoms = 12.0 \text{ g mol}^{-1}$$

That is,

$M(C) = 12.0 \text{ g mol}^{-1}$

$$\therefore \text{ 12.0 g of carbon contains } 6.02 \times 10^{23} \ atoms$$

## Molar mass of oxygen *atoms*

$$\text{Molar mass of oxygen } atoms = \text{mass of 1 mol of O } atoms$$
$$A_r(O) = 16.0$$

$$\therefore \text{ mass of 1 mol of O } atoms = 16.0 \text{ g mol}^{-1}$$

That is,

$M(O) = 16.0 \text{ g mol}^{-1}$

$$\therefore \text{ 16.0 g of oxygen contains } 6.02 \times 10^{23} \ atoms$$

## Ionic compounds

The $M_r$ of an ionic compound is found by adding the $A_r$ of each atom in the formula of the compound. For example:

$$\begin{aligned} M_r(CuSO_4) &= A_r(Cu) + A_r(Cu) + (4 \times A_r(O)) \\ &= 63.5 + 32.1 + (4 \times 16.0) \\ &= 159.6 \end{aligned}$$

The molar mass ($M$) of $CuSO_4$ is 159.6 g $mol^{-1}$.

That is,

$$M(CuSO_4) = 159.6 \text{g mol}^{-1}$$

**Q** Calculate the molar mass of oxygen gas ($O_2$)

**Q** Calculate the molar mass of sodium carbonate decahydrate ($Na_2CO_3.10H_2O$)

## Using Molar Mass

The connection between molar mass and the amount of substance is:

$$n = \frac{m}{M}$$

n = amount in mol
m = mass in grams
M = molar mass, in g $mol^{-1}$

$$\text{mass} \underset{\text{multiply by molar mass}}{\overset{\text{divide by molar mass}}{\rightleftarrows}} \text{moles}$$

**Q** Calculate the mass of 0.35 mol of magnesium nitrate ($Mg(NO_3)_2$)

**Q** Calculate the mass of 4.68 mol of sodium carbonate ($Na_2CO_3$)

**Q** Calculate the number of $CO_2$ molecules present in 22g of carbon dioxide

**Q** Calculate the number of pentyl ethanoate ($C_7H_{14}O_2$) molecules in each bee sting (1 x $10^{-6}$ g)

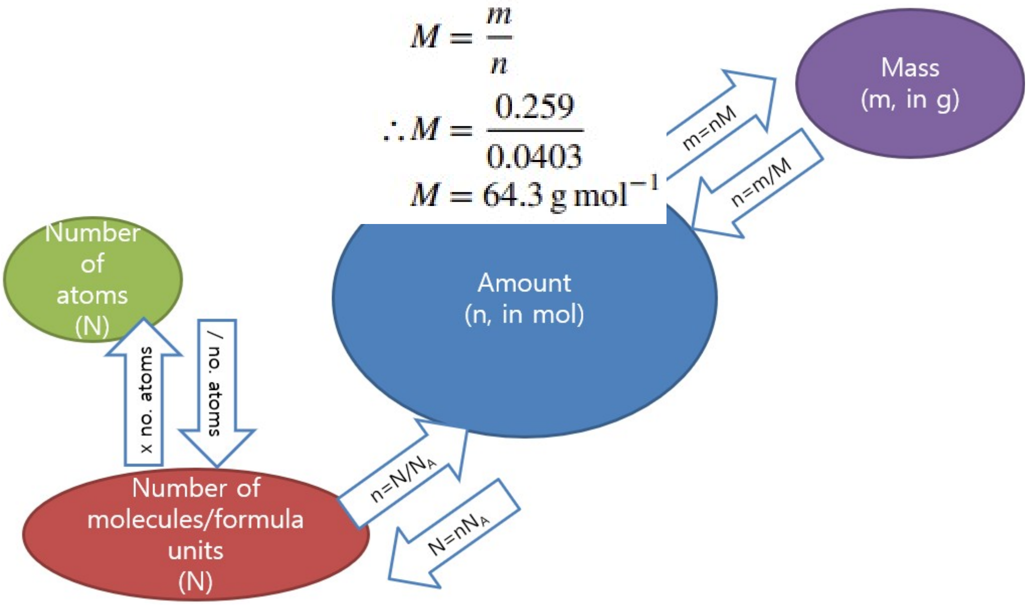
**Q** Calculate the number of atoms in a teaspoon (4.2g) of sucrose ($C_{12}H_{22}O_{11}$)

## 6.4 Using the mole concept

**Q** A sample of gas is collected from burning sulfur in air. The sample has a mass of 0.259 g. Through alternative methods, the number of moles in the sample was determined to be 4.03 x $10^{-3}$ mol.

From this information, calculate the molar mass of the compound to determine the composition of the gas sample

$$M = \frac{m}{n}$$
$$\therefore M = \frac{0.259}{0.0403}$$
$$M = 64.3 \text{ g mol}^{-1}$$




## Percentage composition

The percentage composition of a compound tells you the proportion **by mass** of the different elements in the compound Mining companies and many scientists are very interested in the **percentage composition** of compounds so that they can

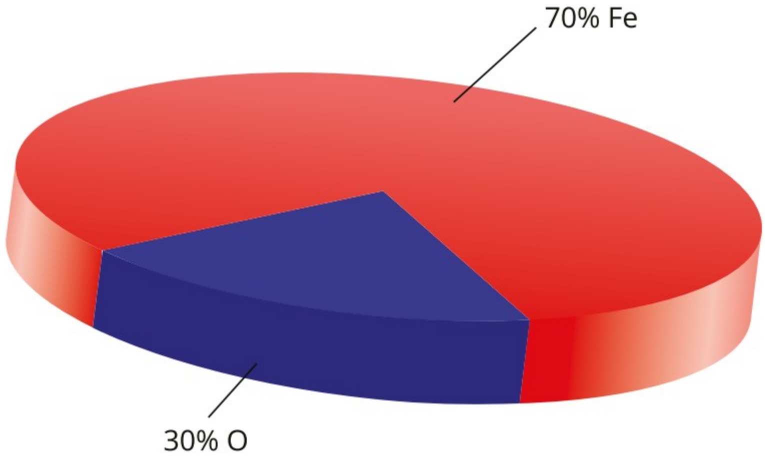



**FIGURE 5.4.2** The pie chart shows the percentage composition, by mass, of iron(III) oxide ($Fe_2O_3$).

determine the amount of product they can produce.

Q

$$\text{\% by mass of an element in a compound} = \frac{\text{mass of the element in 1 mol of the compound}}{\text{molar mass of the compound}} \times 100$$

$$\text{Percentage composition of copper} = \frac{\text{mass of copper}}{\text{molar mass of } Cu(OH)_2} = \frac{63.5}{97.5} \text{ X } \frac{100}{1} = 65.13\%$$

$$\text{Percentage composition of oxygen} = \frac{\text{mass of oxygen}}{\text{molar mass of } Cu(OH)_2} = \frac{32}{97.5} \text{ X } \frac{100}{1} = 32.82\%$$

$$\text{Percentage composition of hydrogen} = \frac{\text{mass of hydrogen}}{\text{molar mass of } Cu(OH)_2} = \frac{2}{97.5} \text{ X } \frac{100}{1} = 2.05\%$$

Calculate the percentage by mass of aluminium in alumina ($Al_2O_3$)

**Q** Calculate the percentage by mass of nitrogen in ammonium nitrate ($NH_4NO_3$)

**Empirical formula**

The empirical formula of a compound gives the simplest whole number ratio of the atoms or ions present in the compound. Note: formulas for ionic compounds are already in their simplest ratio.

The empirical formula is calculated by converting the mass of each element into the number of moles of each element, and then changing that to a whole-number ratio.

Obtain the mass ($m$) of each element in a compound. → Calculate the amount, in mol, of each element present using the formula $n = \frac{m}{M}$. → Convert the mole of each element calculated in the previous step to a whole number ratio. → Write the empirical formula.

**Q** A compound of carbon and oxygen contains 27.3% carbon and 72.7% oxygen by mass. Calculate the empirical formula of the compound

| Step | Thinking | C | O |
|---|---|---|---|
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |

**Q** 0.50g of magnesium is heated and allowed to completely react with chlorine. 1.96g of white powder is formed. Determine the empirical formula of the compound

**Q** A compound of sulfur contains 2.4% hydrogen, 39.0% sulfur and 58.6% oxygen. Find the empirical formula of the compound.

**Q** A sample of potassium carbonate yielded 6.85g of potassium, 1.06g of carbon and 4.20g of oxygen upon analysis. Calculate its empirical formula

## Molecular formula

Molecules have both an empirical formula and a molecular formula. The molecular formula is the actual number of atoms of each element present in the molecule.

| Molecule | Molecular formula | Empirical formula |
|---|---|---|
| Water | $H_2O$ | $H_2O$ |
| Ethane | $C_2H_6$ | $CH_3$ |
| Carbon dioxide | $CO_2$ | $CO_2$ |
| Glucose | $C_6H_{12}O_2$ | $CH_2O$ |

Ionic compounds do not form molecules and hence do not have molecular formulas. Their formulas are technically already in empirical form.

The **molecular formula** is determined by **comparing the empirical formula** of a molecule to its **molar mass**.

Sample
Q A

$$\text{Number of empirical formula units in a molecule} = \frac{\text{molar mass of the compound}}{\text{molar mass of one empirical formula unit}}$$

The general steps in the determination of a molecular formula are shown in Figure 5.4.5.

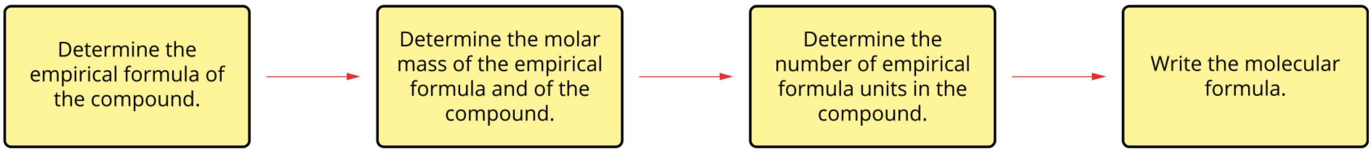
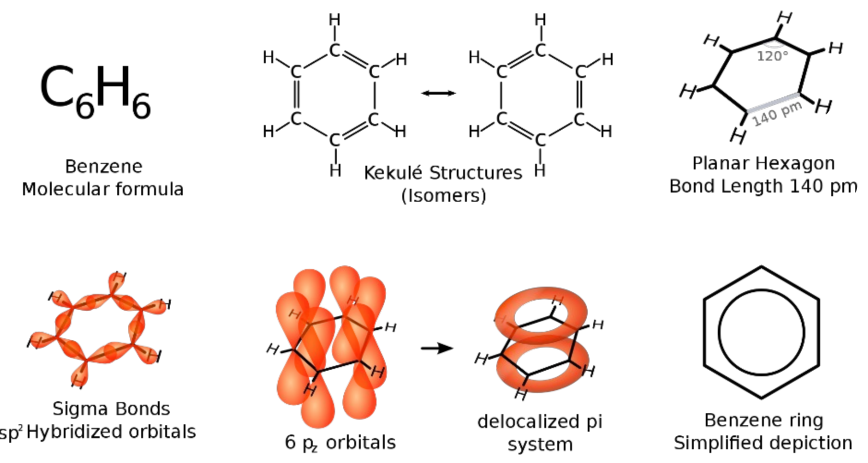



**FIGURE 5.4.5** Steps for calculating a molecular formula.

compound has the empirical formula CH. The molar mass of this compound is 78 g $mol^{-1}$. What is the molecular formula of the compound?




No. empirical formula units in a molecule =

$$\frac{\textit{molar mass of compound}}{\textit{molar mass of one empirical formula unit}}$$

$$= \frac{78}{13}$$

$$= 6$$

Therefore, the molecular formula = 6 x CH
= $C_6H_6$

**Q** A compound has the empirical formula $C_2H_5$. The molar mass of this compound was determined to be 58 g mol$^{-1}$. What is the molecular formula of the compound?

**Q** The production of ethanol as a sustainable fuel is growing rapidly across the world. Ethanol produced in this fashion is termed *bioethanol*. Analysis of a bioethanol sample revealed that it consisted of 52.2% carbon, 13% hydrogen and 34.8% oxygen by mass

a. Calculate the empirical formula of bioethanol
b. In a separation determination, the molar mass of bioethanol was found to be 46 g mol$^{-1}$. Calculate the molecular formula of bioethanol

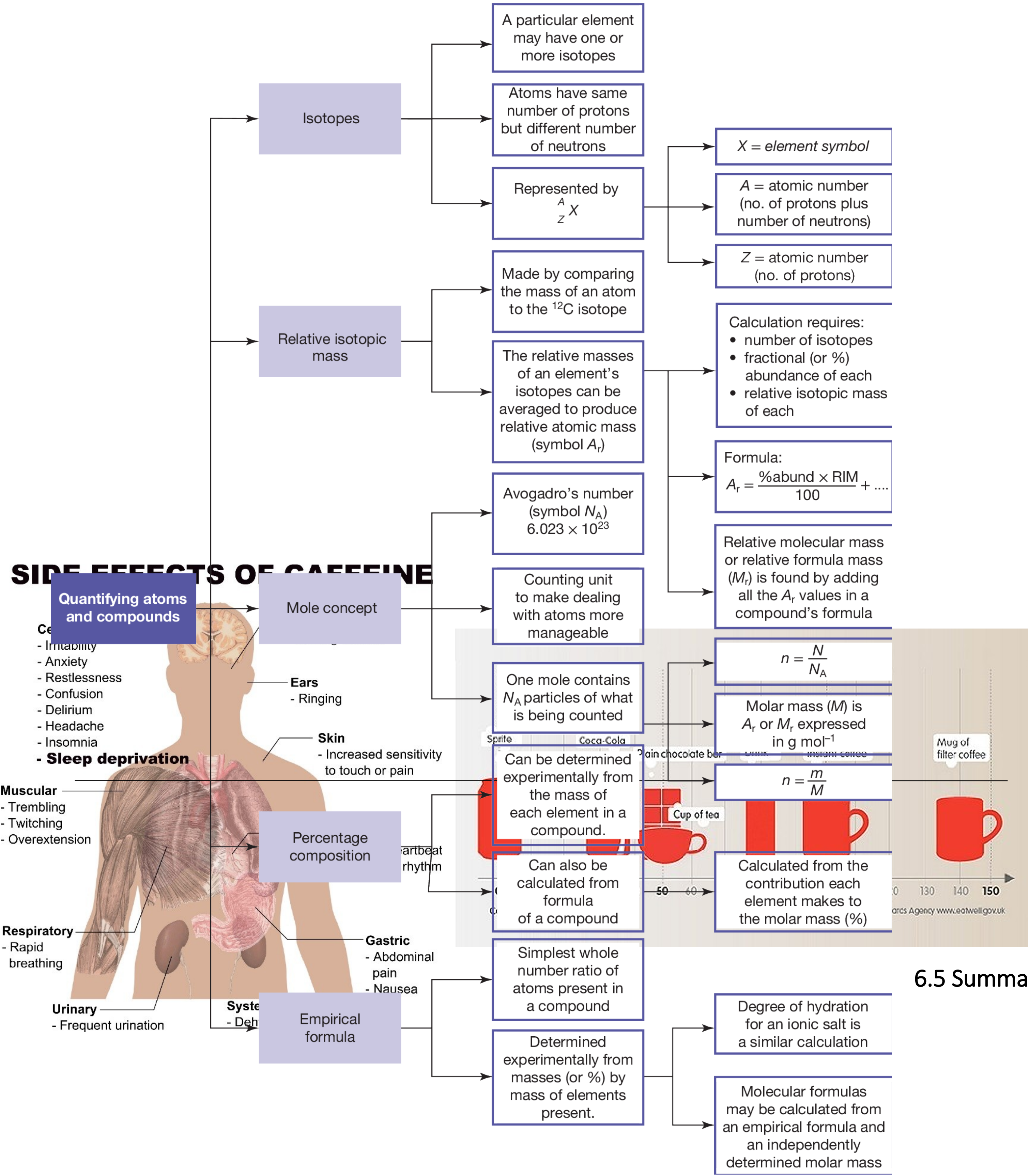
**Q** Another sustainable fuel is biodiesel. One of the compounds that it can be made from is stearic acid. Analysis of stearic acid determined that it consisted of 76.0% carbon, 12.7% hydrogen and 11.3% oxygen. Its molar mass was found to be 284 g mol$^{-1}$.

a. Calculate the empirical formula of stearic acid
b. Calculate the molecular formula of stearic acid

**Q** Caffeine contains 49.48% carbon, 5.15% hydrogen, 28.87% nitrogen and the rest oxygen.

a. Determine the empirical formula of caffeine
b. If 0.20 mol of caffeine has a mass of 38.8g, determine the molar mass of caffeine

c. Determine the molecular formula of caffeine
d. Determine the amount (mol) of caffeine molecules in 1.00g of caffeine
e. Determine the number of molecules in 1.00g of caffeine
f. Determine the number of atoms in 1.00g of caffeine




6.5 Summary

**Homework suggested questions:**

| Ex 6.2 | Ex 6.3 | Ex 6.4 | Ex 6.5 |
|---|---|---|---|
| **Exercises:** 1, 2, 3, 5a, 5c, 5e, 6, 9<br><br>**Exam:** 2, 3, 5 (the rest optional) | **Exercises:** 1a, 1c, 2, 3a, 3c, 4a, 4c, 5, 6, 7a, 7e, 8, 9, 10<br><br>**Exam:** 1, 2, 3, 5 (the rest optional) | **Exercises:** 1a, 1d, 2, 4, 5, 7, 8a, 8c, 9, 10<br><br>**Exam:** 1, 3, 5 (the rest optional) | Optional (all recommended) |