

OXFORD IB COURSE PREPARATION

CHEMISTRY

FOR IB DIPLOMA
COURSE PREPARATION

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OXFORD

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“ Francie came away from her first chemistry lecture in a glow. In one hour she had found out that everything was made up of atoms which were in continual motion. She grasped the idea that nothing was ever lost or destroyed. Even if something was burned up or left to rot away, it did not disappear from the face of the earth; it changed into something else – gases, liquids, and powders. ”

Betty Smith, *A Tree Grows in Brooklyn* (1943)

Chapter context

The excerpt above, from *A Tree Grows in Brooklyn*, outlines the two most fundamental concepts of chemistry: **atomic theory** and **conservation laws**. The immense diversity of matter in our Universe originates from just over a hundred basic building blocks, the **elements**, which combine with one another in various proportions.

Learning objectives

In this chapter you will learn about:

- **physical** and **chemical changes**
- the **atomic theory**
- the nature of **chemical elements**
- chemical **symbols**, **compounds** and **equations**
- **the mole** and **stoichiometric relationships**.



Key terms introduced

- Atoms, isotopes and chemical elements
- The elementary charge
- Ions, cations and anions
- Atomic number and mass number
- Ionic and covalent bonding
- Chemical equations, reactants and products
- Stoichiometry
- Valence
- Structural, molecular and empirical formulae
- The mole, molar mass and mole ratio
- Avogadro's Law
- Standard temperature and pressure (STP)
- The limiting reactant
- Reaction yield
- Green chemistry

1.1 The particulate nature of matter

Chemistry is the study of matter and its composition. *Matter* could be defined as anything that has mass and occupies space, while *energy* is anything that exists but does not have those properties. Matter and energy are closely associated with each other, and energy is often considered as a property of matter, such as the ability to perform work or produce heat. Although mass and energy can be converted into one another (for example, in nuclear reactors or inside the stars), chemistry studies only those transformations of matter where both mass and energy are *conserved*, that is, stay unchanged.

Matter exists in various forms. Every individual kind of matter having definite physical properties under given conditions (for example, iron, water or glucose) is called a *substance*. Substances can be isolated in pure forms, mixed together, or transformed into one another. Such transformations are called *chemical changes*, or *chemical reactions* (in contrast to *physical changes* that do not affect the identity of substances). For example, if we ignite a mixture of the two substances hydrogen and oxygen, an explosion occurs, and a new substance, water vapour, is produced. Therefore, the reaction between hydrogen and oxygen is a chemical process. In contrast, the condensation of water vapour into liquid water is a physical process, because both the vapour and the liquid are different states of the same substance, water.



Figure 1. Steam, liquid water and ice are the three states of water



Figure 2. Burning of charcoal (top) and sublimation of dry ice (bottom)



Key term

Atoms are the building blocks of all matter on Earth. There are many kinds of atom that differ in mass, size and internal structure, and they can combine in different ways.

A chemical **element** is a substance made of atoms of the same kind.

Question

1 Charcoal, the most common form of carbon, has been used for millennia as a source of heat. When burned in air, charcoal produces carbon dioxide, which is a colourless gas under normal conditions but can also exist as a white solid (known as “dry ice”) at very low temperatures. Above -78°C , dry ice sublimates without melting into gaseous carbon dioxide. Green plants use carbon dioxide and water to produce glucose and oxygen gas. State the nature of the change (physical or chemical) for each process described in the paragraph above.

Practical skills: Observable chemical changes

It is not always possible to distinguish between physical and chemical changes by observation. However, any spontaneous change in temperature, colour or state of matter requires a source of energy, and this energy is often chemical in nature. Observable chemical changes include spontaneous release or absorption of heat, change in colour or odour, formation of a precipitate, or release of gas (often appearing as bubbles in a liquid). Many violent processes, such as fires and explosions, are also caused by chemical changes. Finally, some chemical changes are difficult to reverse (for example, it is impossible to transform burned wood into its original state) while most physical changes are reversible.

Atoms

The building blocks of hydrogen, oxygen, water and all other chemical substances are called *atoms*. There are many kinds of atom that differ in mass, size and internal structure. A substance made of atoms of the same kind is called a *chemical element*. Currently 118 different elements are known, and this number is likely to grow in the future.

DP ready Theory of knowledge

Scientific vocabulary

The word “atom” is derived from the Greek *atomos*, which means “indivisible” and refers to a hypothesis that chemical elements cannot be split into simpler, more fundamental species. Democritus, an ancient Greek philosopher, thought that all matter consisted of invisible, indestructible and constantly moving particles of various shapes. Although now we know that subatomic particles do exist, the term “atom” is still used by scientists when they refer to the smallest unit of a chemical element. Scientific vocabulary develops along with our understanding of the natural world, and some terms change their meaning over time.



Figure 3. Democritus (circa 460–370 BC) on a Greek bank note

The existence of atoms was not universally accepted until the early 1800s, when the English scientist John Dalton used his atomic theory for explaining various chemical phenomena. In particular, he suggested that the observed fact that elements combine together only in certain proportions was the result of their atomic composition. Indeed, one, two or more atoms of one element can combine with one, two or more atoms of another element, but no combination can involve a fractional number of atoms.

Based on these and other observations, Dalton's theory can be summarized as follows:

- chemical elements consist of very small particles called atoms
- all atoms of a specific element are identical but differ from atoms of other elements
- chemical compounds are formed by atoms of two or more elements in whole-number ratios
- chemical reactions involve combination, separation or rearrangement of atoms
- atoms cannot be created, subdivided or destroyed.



Figure 4. John Dalton (1766–1844)

DP ready Nature of science

Scientific theories

Although the ideas of Democritus and other ancient philosophers look very similar to the modern concept of atoms, their theories were not scientific, as they were derived purely by reasoning and lacked any experimental evidence. In contrast, Dalton's theory was scientific, as it provided a simple and elegant explanation for existing observations (such as the law of conservation of mass and the law of definite proportions) and had predictive power. Nevertheless, some postulates of Dalton's theory were disproved by later discoveries. This is the eventual fate of all scientific theories, which are constantly tested against experiments, and modified or replaced by new, more accurate concepts and models.

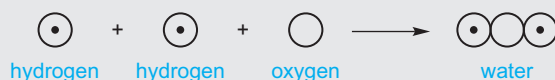
Using his theory, Dalton identified six elementary substances (hydrogen, carbon, nitrogen, oxygen, sulfur and phosphorus) and determined their *relative atomic masses* (this term is defined more precisely later in this section). To do so, he assigned the lightest atom, hydrogen, a mass of one unit and then deduced the masses of other atoms from the percentage composition of their compounds with hydrogen. Although these atomic masses were often inaccurate, Dalton was the first scientist who quantitatively described atoms in terms of their mass. To recognize the importance of this achievement, the International Union of Pure and Applied Chemistry (IUPAC) has adopted the name "dalton" for the unified atomic mass unit, which will be discussed later in this topic.

Worked example: Deducing relative atomic masses using mass percentages

1. Atoms of hydrogen and oxygen combine together in a 2:1 ratio to form water. The mass percentage of hydrogen in water is 11%. Assuming that the relative atomic mass of hydrogen is 1, deduce the relative atomic mass of oxygen.

Solution

Let's represent the formation of water in the same way as John Dalton did over two centuries ago:



If the smallest unit (molecule) of water contains two hydrogen atoms, their combined relative mass will be $2 \times 1 = 2$. This mass makes up 11% of the total mass of water.

Therefore, the relative mass of one water molecule will be $(2/11\%) \times 100\% \approx 18$.

The relative atomic mass of oxygen is therefore $18 - 2 = 16$.

Note that the ratio alone does not tell us anything about the actual number of atoms in a molecule. For example, the water molecule could contain four hydrogen and two oxygen atoms, or six hydrogen and three oxygen atoms, and so on. However, in all cases the relative atomic mass of oxygen would be the same. You can confirm this by repeating the above calculations for any larger molecule containing hydrogen and oxygen in a 2:1 ratio.

Question

- 2 Ammonia contains atoms of nitrogen and hydrogen in a 1:3 ratio. The mass percentage of nitrogen in ammonia is 82%. Deduce the relative atomic mass of nitrogen. (If you want to use John Dalton's notation, draw the nitrogen atom as a circle with a vertical line inside.)

Soon after Dalton formulated his theory, the relative atomic masses of many elements were determined. However, the nature of the atom remained a mystery for another century, until the scientific community accumulated enough evidence to suggest that atoms consisted of even smaller structural units.

DP ready Nature of science

The scientific method

Since the 17th century, the development of natural sciences has been based on systematic observation, measurement and experimentation. The experimental evidence was used to formulate, test and modify hypotheses, which were aimed to explain natural phenomena and predict the outcome of future experiments.

The most successful hypotheses were eventually developed into scientific theories. This approach is known as the *scientific method*.

Although scientists use various approaches to obtaining, analysing and interpreting experimental evidence, they have adopted common terminology and follow a certain way of reasoning that involves deductive and inductive logic through analogies and generalizations. Mathematics, the main language of science, requires no translation and can be understood by any scientist around the world.

Inside the atom

In 1897, the British physicist J. J. Thomson demonstrated that high-energy electric beams (so called *cathode rays*) contained negatively charged particles approximately 1,800 times lighter than a hydrogen atom. These particles, now known as *electrons* (symbol e^-), could be emitted by any element but always had exactly the same mass and charge. Therefore, Thomson suggested that electrons were constituent parts of every atom.

Twelve years later, the New Zealand-born British physicist Ernest Rutherford and his team bombarded a piece of gold foil with positively charged α -particles, the exact nature of which was unknown at that time. While most of the particles passed through the foil without changing course, some of them were repelled or deflected by large angles. These results suggested that almost all the mass of atoms was concentrated in a small, positively charged *nucleus* surrounded by electrons. When an α -particle passed close to a nucleus, it was repelled or deflected. However, the small atomic nuclei were easy to miss, so the majority of α -particles passed through the foil without any resistance.

In 1911, Rutherford summarized the results of his experiments by proposing the *planetary model of the atom*, also known as the *Rutherford model* (figure 7). In this model, negatively charged electrons orbit the positively charged atomic nucleus in the same way as planets orbit the Sun. Just as the Sun contains 99.8% of the solar system's mass, the atomic nucleus contains over 99.9% of the mass of the entire atom. However, instead of gravity, electrostatic attraction holds the electrons around the nucleus.

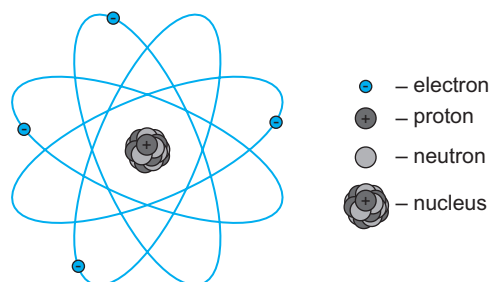


Figure 7. The Rutherford model of the atom

Rutherford was able to estimate the diameter of the atomic nucleus. He found that it was about 10^{-14} m, or 10,000 times smaller than the atomic diameter (about 10^{-10} m). If we could enlarge the atom to the size of a football stadium, the nucleus would look like a golf ball in the middle of the field.

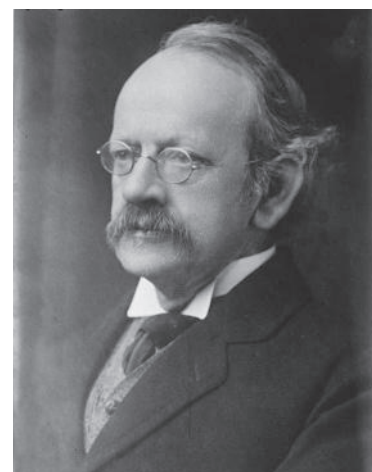


Figure 5. J. J. Thomson (1856–1940)

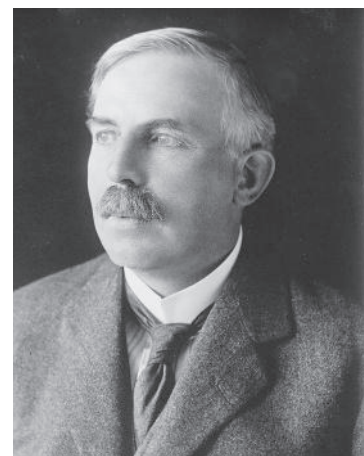


Figure 6. Ernest (Lord) Rutherford (1871–1937)

DP ready Nature of science

Wave–particle duality

According to modern theories, the electrons in an atom do not orbit the nucleus but rather fill the whole volume of the atom as diffuse clouds. By doing so, electrons demonstrate the properties of particles and waves at the same time. This peculiar behaviour could not be explained by the planetary theory, which was eventually replaced by the quantum model of the atom. Nevertheless, the main concept of the Rutherford model – a small, dense, positively charged nucleus surrounded by negatively charged electrons of negligible mass – has been confirmed by various experiments and still remains in use as an excellent visualization of the atomic structure.



Internal link

You can read about the quantum model of the atom in **2 Electron structure and chemical bonding**.

Later studies showed that atomic nuclei contain two types of subatomic particle: positively charged *protons* (symbol p) and uncharged *neutrons* (symbol n). Both particles have approximately the same mass (about 1.67×10^{-27} kg) while the mass of the electron is over 1800 times lower, about 9.11×10^{-31} kg. These masses are extremely small: a proton is as many times lighter than a golf ball as the golf ball is lighter than the Earth.

Since the masses of atoms and subatomic particles are so small, they are awkward to work with and take a lot of space when written. Therefore, they are often expressed in *unified atomic mass units* (symbol u), or *daltons* (symbol Da):

$$1 \text{ u} = 1 \text{ Da} \approx 1.66 \times 10^{-27} \text{ kg}$$

$$m(\text{p}) \approx m(\text{n}) \approx 1.01 \text{ u}$$

$$m(\text{e}^-) \approx 0.000549 \text{ u}$$

The unified atomic mass unit is traditionally used in chemistry, while the dalton is more common in biochemistry and molecular biology, especially for expressing the masses of large organic molecules. In this book, we will be using the unified atomic mass unit.

In simple calculations, the masses of protons and neutrons are often rounded to 1 u each, and the masses of electrons in atoms are considered negligible. For example, an atom of sodium contains 11 protons, 12 neutrons and 11 electrons, so its mass can be found as $11 \times 1 + 12 \times 1 + 11 \times 0 = 23 \text{ u}$. The exact mass of this atom determined experimentally is 22.99 u, which is very close to our approximate value.



DP link

You will learn why the mass of a proton is not exactly 1 u if you study **C.7 Nuclear fusion and nuclear fission** in the IB Chemistry Diploma Programme.



Key term

The electric charge carried by a single electron is known as the **elementary charge (e)** and has a value of approximately 1.602×10^{-19} C. The charges of subatomic particles are commonly expressed in elementary charge units. For example, the charge of an electron can be represented as $-e$, and the charge of a proton as $+e$. The symbol e is often omitted, so it is customary to say that an electron and proton have charges of -1 and $+1$, respectively.

Question

- 3 An atom of aluminium contains 13 p, 14 n and 13 e^- . Calculate the mass of this atom in u and kg.

Relative atomic masses (A_r) are numerically equal to the masses of atoms in u but have no units. For example, the A_r of the sodium atom is 22.99. Note that John Dalton assumed that hydrogen had $A_r = 1$ while in modern chemistry it has an A_r of 1.01. The reason for this will become clear in *1.3 Stoichiometric relationships*, when we will introduce the concept of the mole.

The electric charges of the proton and the electron have opposite signs but identical magnitude, the *elementary charge*. Since the atom as a whole is electrically neutral, it must contain the same number of protons and electrons. If an atom loses one or more electrons, it develops a net positive charge and becomes a *cation*. Similarly, if an atom gains one or more electrons, it develops a net negative charge and becomes an *anion*. Cations and anions, collectively known as *ions*, are often formed in chemical reactions, so the number of electrons in a given atomic species can vary.

However, chemical changes do not affect atomic nuclei, so the numbers of protons and neutrons in a given atomic species remain constant. The number of protons in the nucleus, also known as the *atomic number* (Z), is numerically equal to the nuclear charge, as

each proton has a charge of +1. In turn, the nuclear charge defines the chemical properties of the atom, such as its ability to lose, gain or share electrons and interact with other species.

The atomic number is the most fundamental characteristic that distinguishes one chemical element from another. All atoms of a given element have the same number of protons in their nuclei and thus the same atomic number. In contrast, the number of neutrons (N) can vary among the nuclei of the same element, as neutrons do not affect the nuclear charge and thus have very little effect on the chemical properties of the atom.

The elements

In chemistry, the elements are represented by their *symbols*, which consist of one or two letters and are derived from the element names. For example, the chemical symbol for hydrogen is H (the first letter of *hydrogen*), and the chemical symbol for iron is Fe (the first two letters of the Latin *ferrum*, iron). Chemical elements and their symbols are listed in table 1 and in the periodic table at the back of this book.

If you look closely at the fourth column of table 1, you will notice that most A_r values are very close to whole numbers. For example, $A_r(\text{H}) = 1.01 \approx 1$ and $A_r(\text{Na}) = 22.99 \approx 23$. Some elements (Mg, Cl, Fe and Cu), however, do not obey this rule: their A_r values differ significantly from whole numbers. Such elements consist of several *isotopes*. For example, chlorine has two common isotopes with relative atomic masses of 35 and 37. In naturally occurring chlorine, these two isotopes are mixed in a ratio that produces the *average* relative atomic mass of 35.45.

Table 1. Common chemical elements

Symbol	Name	Atomic number (Z)	Relative atomic mass (A_r)	Notes
H	hydrogen	1	1.01	
He	helium	2	4.00	
C	carbon	6	12.01	
N	nitrogen	7	14.01	
O	oxygen	8	16.00	
F	fluorine	9	19.00	
Na	sodium	11	22.99	Latin <i>natrium</i>
Mg	magnesium	12	24.31	
Al	aluminium	13	26.98	
P	phosphorus	15	30.97	
S	sulfur	16	32.07	
Cl	chlorine	17	35.45	
K	potassium	19	39.10	Latin <i>kalium</i>
Ca	calcium	20	40.08	
Fe	iron	26	55.85	Latin <i>ferrum</i>
Cu	copper	29	63.55	Latin <i>cuprum</i>

Key term

Ions are atoms that have lost or gained one or more electrons and thus have a net charge. **Cations** have a positive charge (have lost electrons), and **anions** have a negative charge (have gained electrons).

The number of protons in the nucleus is the **atomic number (Z)**.

Key term

Isotopes are atoms with the same number of protons but different numbers of neutrons in their nuclei.

The **mass number (A)** is the total number of protons and neutrons in the nucleus.

The total number of protons and neutrons in the nucleus is known as the *mass number* (A). To distinguish between isotopes, their mass numbers are often written as superscript indices to the left of the element symbol. For example, chlorine-35 can be represented as ^{35}Cl , and chlorine-37 as ^{37}Cl . It is also common to show the atomic number (Z) as a subscript index directly beneath the mass number. Since each atom of chlorine has 17 protons in its nucleus, chlorine-35 and chlorine-37 can be represented as $^{35}_{17}\text{Cl}$ and $^{37}_{17}\text{Cl}$, respectively. We can always find the number of neutrons (N) in the nucleus as the difference between its mass number and atomic number:

$$N = A - Z$$

For example, $^{35}_{17}\text{Cl}$ has $35 - 17 = 18$ neutrons, and $^{37}_{17}\text{Cl}$ has $37 - 17 = 20$ neutrons.



Figure 8. Smoke detectors contain radioactive isotopes



DP link

Radioactive materials are used in industry, medicine and even household devices, such as smoke detectors. These and many other applications are discussed in **C.3 Nuclear fusion and fission** and **D.8 Nuclear medicine** in the IB Chemistry Diploma Programme.

DP ready Nature of science

Radioactivity

Isotopes are known for all chemical elements. Stable isotopes can exist indefinitely, while *radioisotopes* decompose with time. This decomposition, known as *radioactivity* or *radioactive decay*, can produce a variety of high-energy particles, including electrons, neutrons, photons and nuclei of other elements. For example, the α -particles used in Rutherford's experiments were later identified as nuclei of helium-4, each consisting of two protons and two neutrons (^4_2He). They are produced by the radioactive decay of radium-226 as follows:



The second product in the above *nuclear equation*, the gas radon-222, is also radioactive. Since radium-226 is naturally present in many minerals, radon-222 is constantly released from soil and may accumulate in poorly ventilated buildings. The levels of radon in particularly affected areas are monitored by authorities and ordinary people, who often keep portable radiation detectors in their homes.

Electrons and ions

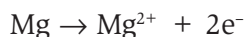
So far, our study of the atom has been focused on the nucleus. It is now time to have a closer look at the electrons, which occupy 99.999999999% of the atom's volume and are largely responsible for any chemical changes.

As you know already, the number of electrons in an atom is equal to the number of protons in its nucleus. For example, the nucleus of a sodium atom contains 11 protons, so this atom must have 11 electrons. In chemistry, atoms are represented by the same symbols as elements, so Na may refer to either a single sodium atom or, more generally, sodium as a type of atom.

When an atom loses electrons, it becomes an ion with a net positive charge (cation). This charge must be shown as a superscript index to the right of the element symbol. For example, sodium atoms readily lose one electron to produce sodium cations, Na^+ :



Similarly, magnesium atoms lose two electrons each, producing doubly charged magnesium cations:

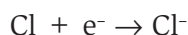


The reason why some elements produce singly charged ions while others tend to form multiply charged ions will be discussed in the next chapter. For now, it is sufficient to understand that each element tends to lose, gain or share only a certain number of electrons. As you will see, this ability explains the fact that elements combine with one another in definite proportions.

Monoatomic cations have the same names as the elements from which they are formed. When it is clear that we are talking about a cation, the words “cation” or “ion” can be omitted, so “magnesium” can refer to an atom, a chemical element, or a magnesium cation.

Cations may also consist of more than one atom. Such *polyatomic*, or *molecular*, cations often have common names ending with the suffix “-onium” (for example, the ammonium ion, NH_4^+).

Some elements, such as chlorine and sulfur, tend to gain electrons from other atoms and produce negatively charged ions (anions):



Monoatomic anions are named by combining a part of the element name with the suffix “-ide”, as shown in table 2.

Table 2. Common monoatomic anions and their names

Element		Anion	
Symbol	Name	Symbol	Name
H	hydrogen	H^{-}	hydride
N	nitrogen	N^{3-}	nitride
O	oxygen	O^{2-}	oxide
F	fluorine	F^{-}	fluoride
P	phosphorus	P^{3-}	phosphide
S	sulfur	S^{2-}	sulfide
Cl	chlorine	Cl^{-}	chloride
Br	bromine	Br^{-}	bromide
I	iodine	I^{-}	iodide

The names of polyatomic anions usually end with “-ate” (for example, the sulfate ion, SO_4^{2-}) or “-ite” (for example, the sulfite ion, SO_3^{2-}).

If we need to show the ionic charge of a specific isotope, all indices can be added to a single chemical symbol. For example, the anion of sulfur-32 can be represented as ${}_{16}^{32}\text{S}^{2-}$ or ${}^{32}\text{S}^{2-}$.



Internal link

The charges on ions are examined in **2 Electron structure and chemical bonding**.



Internal link

Polyatomic anions are discussed in more detail in **3 Inorganic chemistry**.

Question

- 4 Complete the table below by deducing the composition, names and/or symbols of atoms and ions.

Symbol	Name	Mass number (A)	Number of		
			neutrons	protons	electrons
	hydrogen cation		0		
		1			1
	hydride		0		
${}^{27}_{13}\text{Al}^{3+}$					
	chloride	35			
${}^{14}_7\text{N}^{3-}$					

Before moving on to the next topic, check that you have solved all the problems in the text and developed a working knowledge of atomic structure. You are also advised to review the information given in tables 1 and 2. Although you do not have to memorize the symbols and names of all elements, by now you should be able to recognize at least some of them, such as hydrogen (H), oxygen (O), sodium (Na) and chlorine (Cl), without checking the book.

1.2 Chemical substances, formulae and equations

Atoms and ions are the smallest units of matter that still possess certain chemical properties. While these species can exist individually, they tend to combine together and form chemical substances.

Elementary substances contain atoms of a single element while *chemical compounds* contain atoms of two or more elements bound together by chemical forces. For example, magnesium metal is an elementary substance, as it contains only one type of atom, Mg. Similarly, sulfur (S) is another elementary substance composed of sulfur atoms only. In contrast, magnesium sulfide is a chemical compound, as it consists of two different, chemically bound atomic species, Mg and S (figure 9).



Figure 9. Magnesium (left), sulfur (middle) and magnesium sulfide (right)

Practical skills: Mixtures and pure substances

If we grind magnesium metal and sulfur into fine powders and mix them together at room temperature, both elements will retain their chemical identities. For example, we will still see shiny particles of magnesium and yellow crystals of sulfur in this mixture under a microscope. Moreover, we will be able to separate this mixture into individual substances by shaking it with water: sulfur will float on the surface of water while magnesium will sink to the bottom. Finally, the mixture of magnesium and sulfur has variable composition, as we can mix these substances together in any proportion.

However, if we heat up the mixture of magnesium and sulfur, a vigorous reaction occurs, and the mixture turns into a white powder of magnesium sulfide. It will look like white crystalline material under a microscope, and we will not be able to isolate magnesium and sulfur from this compound by any physical methods. Therefore, magnesium sulfide is a pure substance. It has a definite composition (equal number of magnesium and sulfur atoms), and its properties differ from those of both the original substances (magnesium and sulfur) and their mixture.

Mixtures in which the components are clearly visible are called *heterogeneous* (from the Greek *heteros* “other”). The mixture of magnesium and sulfur is an example of a heterogeneous mixture. Other mixtures can be blended so well that they have uniform composition, and every part of the mixture has exactly the same properties. Such mixtures are called *homogeneous* (from the Greek *homos* “same”). Air, sea water and most metal alloys are examples of homogeneous mixtures.

**Internal link**

The most common homogeneous mixtures, aqueous solutions, will be discussed in **4 Solutions and concentration**.

Types of bonding: Ionic bonding

There are several ways in which atomic species can combine together. The first and probably the most obvious way is the electrostatic attraction between oppositely charged ions, which is known as *ionic bonding*. For example, magnesium sulfide consists of magnesium cations, Mg^{2+} , and sulfide anions, S^{2-} . In solid magnesium sulfide, these ions form a regular, highly symmetrical arrangement, known as the *crystal lattice*, in which each ion is surrounded by ions of the opposite charge (figure 10). Other ionic compounds, such as sodium chloride (table salt), have similar structures.

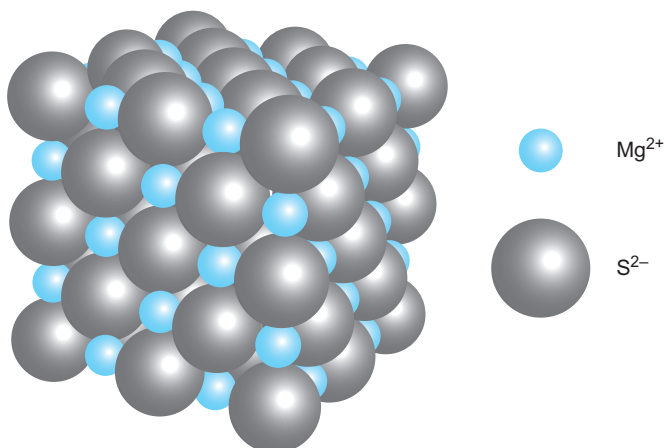
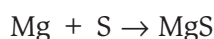


Figure 10. Crystal structure of magnesium sulfide

The formation of magnesium sulfide can be represented by the following *chemical equation*:

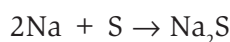


Key term

Ionic bonding is the electrostatic attraction between oppositely charged ions that holds them together in a compound.

In a **chemical equation**, substances are represented by symbols for the elements in their **chemical formulae**. The **reactants** are shown on the left, followed by a **reaction arrow** that shows that a change has occurred and then the **products** of the reaction are shown on the right.

In this equation, the elementary substances (magnesium metal and sulfur) are represented by the same symbols as their chemical elements (magnesium and sulfur, respectively). Since these substances undergo chemical changes by reacting with each other, they are called *reactants*. In chemical equations, reactants are traditionally placed on the left and followed by a *reaction arrow* that shows the direction of the reaction. The arrow points at the *reaction product(s)* formed as a result of the chemical changes. In our case, the reaction product is magnesium sulfide, MgS. The *chemical formula* MgS represents a chemical compound of a definite composition (magnesium and sulfide ions combined in 1:1 ratio). This formula also shows that magnesium sulfide is electrically neutral, as positive charges of Mg²⁺ ions in this compound are compensated by exactly the same number of negative charges of S²⁻ ions. If needed, the ionic nature of magnesium sulfide can be shown explicitly as Mg²⁺S²⁻. However, in chemical formulae of neutral species, the ionic charges of individual elements are usually omitted. It is important to understand that any chemical compound or elementary substance must be electrically neutral as a whole. The ions of the same sign repel one another, so they cannot stay together in any significant quantity unless their charges are cancelled by the ions of the opposite sign. If we could somehow place 1 g of only Mg²⁺ ions together, their electrostatic repulsion would produce an explosion more powerful than the simultaneous detonation of all nuclear weapons in the world! The need to balance ionic charges is one of the reasons why chemical elements combine with one another in definite proportions. Ions of different charge magnitudes can form compounds together. For example, sodium atoms produce singly charged ions, Na⁺, while sulfur atoms form doubly charged ions, S²⁻. To balance these charges, we need twice as many Na⁺ ions as S²⁻ ions. Therefore, sodium and sulfur combine together in a 2:1 ratio in sodium sulfide:



In this equation, the *stoichiometric coefficient* 2 placed before the symbol of the sodium atom shows that two atoms of sodium react with each sulfur atom. (The stoichiometric coefficient 1 before S and Na₂S is omitted, as it would normally be omitted in any other expression, such as “2x + y = z”.) Note that the expression “2Na + S” shows only the ratio of the atoms, not their exact quantities: it might be ten billion sodium atoms and five billion sulfur atoms.

The *subscript index* 2 placed after the symbol of sodium in the formula of sodium sulfide, Na₂S, has a slightly different meaning. This index shows the exact number of Na⁺ ions in the smallest structural unit of sodium sulfide. While the stoichiometric coefficients (numbers before chemical symbols and formulae) can vary among equations, the subscript indices for each particular compound must always stay the same. This distinction will become clear as you study more examples.



Key term

The term **stoichiometry** is derived from two Greek words, *stoicheion* “element” and *metron* “measure”, and refers to the relationship between the amounts of substances participating in a chemical reaction. In a broader sense, this term is used to describe any quantitative relationships in chemistry, such as percent composition of compounds, reaction yields, volume ratios and so on; see [1.3 Stoichiometric relationships](#).

To deduce a formula of an ionic compound, all we need to know is the charges of the ions involved. Most of these charges can be deduced from the periodic table, which we will discuss in the next chapter. For now, it is sufficient to know that the cations of sodium (Na^+) and potassium (K^+) are singly charged, magnesium (Mg^{2+}) and calcium (Ca^{2+}) form doubly charged cations, and aluminium forms a triply charged cation (Al^{3+}). The charges and names of all common anions are listed in table 2.

Worked example: Deducing formulae of ionic compounds

WE

2. Write the formula of calcium phosphide. (This compound will contain ions of Ca^{2+} and P^{3-} .)

Solution

To produce a neutral compound, the total charge of Ca^{2+} ions must be exactly countered by the total charge of P^{3-} ions.

The lowest common multiple of 2 and 3 is 6, so we need three Ca^{2+} ions ($2 \times 3 = 6$ positive charges) and two P^{3-} ions ($3 \times 2 = 6$ negative charges).

Therefore, the formula of calcium phosphide is Ca_3P_2 .

Question

Q

5 Complete the table below by deducing the formulae and names of ionic compounds. One cell is already filled as an example.

	Cl^-	O^{2-}	N^{3-}
Na^+			
Ca^{2+}		CaO calcium oxide	
Al^{3+}			

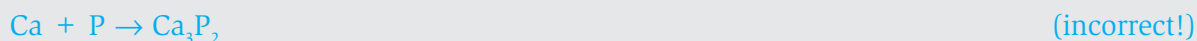
Worked example: Balancing equations

WE

3. Balance the equation for the production of calcium phosphide above.

Solution

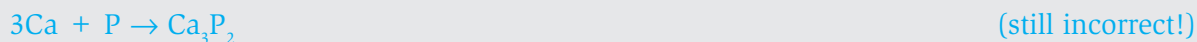
If we want to represent the formation of calcium phosphide by a chemical equation, we must not forget about the stoichiometric balance: the number of atoms of each kind on both sides of the equation must be the same. For example, the following equation is not balanced:



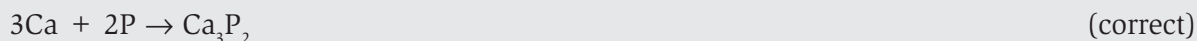
It contains one Ca atom on the left but three Ca atoms on the right. Similarly, there is one P atom on the left but two P atoms on the right.

To balance an equation, we can change the stoichiometric coefficients before any substances (reactants and/or products) but not the subscript indices that show the ratio of the atoms in chemical formulae of compounds.

Start by balancing calcium by placing the coefficient 3 before Ca on the left:



Now calcium is balanced, but phosphorus is not. We can correct it by placing 2 before P on the left:



Both elements are now balanced, so the equation is complete.

It is good practice to balance all chemical equations you write, as it will help you to avoid errors in stoichiometric calculations (see 1.3 *Stoichiometric relationships*).

Question

- 6 Write and balance chemical equations for the formation of each ionic compound from question 5.

Key term

Covalent bonding occurs when a pair of electrons is shared between two atoms. The electrostatic attraction between the nuclei of each atom and these electrons holds the atoms together.

The term **covalent** is related to the word **valence**, which in turn is derived from Latin *valentia* (“power”). In chemistry, *valence* is the ability of atoms to form **covalent bonds** with one another. An atom is said to be **monovalent** if it can form only one covalent bond; **divalent** atoms form two covalent bonds, and so on.

Key term

In **structural formulae**, each covalent bond is shown as a line between atom symbols.

Molecular formulae show the number of atoms in a molecule, but not necessarily how they are joined.

Types of bonding: Covalent bonding

Although ionic compounds are very common in chemistry, there are other types of chemical bonding. *Covalent compounds* are formed when atoms share their electrons rather than transferring them completely from one element to another. For example, the lightest element, hydrogen, exists in the form of a diatomic *molecule*, H_2 , where the two hydrogen atoms have a common pair of electrons. If we draw electrons as dots near the element symbols, the formation of H_2 from two hydrogen atoms can be represented by the following scheme:



Electrons are charged negatively while the atomic nuclei have positive charges. When a pair of electrons is shared between two atoms, both nuclei are electrostatically attracted to these electrons. In other words, shared electrons act as a “glue” that holds the atoms together. This type of chemical bonding is called *covalent bonding*, and each pair of shared electrons is treated as a separate *covalent bond*.

A hydrogen atom has a single electron, so it is *monovalent* in all its compounds. Another element that is usually monovalent is chlorine. Oxygen is *divalent*, and nitrogen is usually *trivalent*. All these elements form stable diatomic molecules with one or more shared electron pairs. Covalent molecules are often represented by *structural formulae*, where each covalent bond is shown as a line (figure 11).

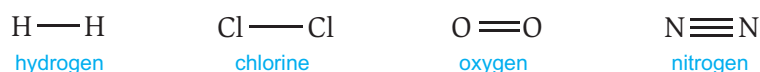
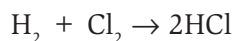


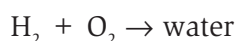
Figure 11. Structural formulae of some diatomic molecules

Since these diatomic molecules are the smallest structural units of elementary hydrogen, chlorine, oxygen and nitrogen, their formulae in chemical equations must be written as H_2 , Cl_2 , O_2 and N_2 , respectively, rather than H, Cl, O and N. Such formulae are known as *molecular formulae*, as they show the exact number of atoms in each molecule. For example, the reaction between hydrogen and chlorine is represented by the following equation:

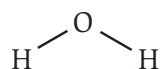


The product of this reaction, hydrogen chloride, HCl, is another covalent molecule that contains a single covalent bond between hydrogen and chlorine. Generally, the formulae of covalent compounds are constructed in the same way as the formulae of ionic compounds, except that the valences of atoms are used instead of ionic charges.

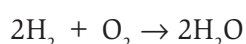
For example, water can be produced by the reaction of hydrogen with oxygen:



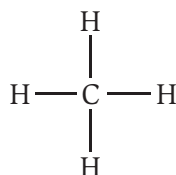
Therefore, we can expect that a molecule of water consists of H and O atoms. Since oxygen is divalent, it will form bonds with two monovalent hydrogen atoms:



Thus, the formula of water is H_2O . Now we can complete and balance the equation:



If the valence of an element is unknown, we can often deduce it from the formula of a covalent compound. For example, the major component of natural gas, methane, has the formula CH_4 . Since hydrogen is monovalent, carbon will need to form four covalent bonds to hold four hydrogen atoms. Therefore, carbon is tetravalent, and the formula of methane can be drawn as follows:



Methane is the simplest *organic compound*, as it contains both carbon and hydrogen atoms. We will discuss its structure and properties in the last chapter of this book.

Question

- Draw the structures of the following covalent molecules, representing each covalent bond as a line: HF, H_2S , NH_3 , CF_4 , CO_2 .
- For each compound in Question 7, write and balance a chemical equation where this compound is formed from elementary substances.

DP ready Nature of science

Trivial and systematic names

Many covalent compounds have trivial names, such as water (H_2O), ammonia (NH_3) and silica (SiO_2). These names are so common that they are likely to stay in use for a very long time, both in chemical literature and everyday life. Some of these trivial names are introduced throughout this book. However, scientists also have *systematic names* for these substances, which are constructed in the same way as those for ionic compounds:

H_2O – hydrogen oxide

NH_3 – hydrogen nitride

SiO_2 – silicon oxide



Internal link

You will learn more about systematic nomenclature of inorganic compounds in **3 Inorganic chemistry**.

Types of bonding: Metallic bonding

In addition to ionic and covalent compounds, atoms of certain elements combine together by *metallic bonding*. As suggested by the name, this type of bonding usually occurs in metals. Atoms of metals lose their electrons easily, producing cations. The free electrons are distributed throughout the whole volume of the metal, holding the cations together by electrostatic attraction. This type of bonding is similar to both ionic bonding (as it involves ions) and covalent bonding (as the electrons act as a “glue” between the atoms). However, in contrast to ionic bonding, metals contain only positively charged ions (cations), with the negative charges of the free-moving electrons balancing the charges on the cations. And in contrast to covalent bonds, which are *localized* between specific atoms, the metal bonding is *delocalized*, so all metal cations are bonded to one another by a single cloud of shared electrons.

In chemical equations, metallic substances are represented by their element symbols without any subscript indices (for example, Na or Fe), as the total number of metal atoms in a sample can vary. If several metals are present in the same sample, their atoms may share electrons with one another and form an *alloy*. Since alloys have variable composition, they are not considered chemical compounds but rather mixtures or solid solutions.

Further discussion of ionic, covalent and metallic bonding requires more detailed knowledge of the electron structure of chemical elements, which you will explore in the next chapter. Then, in the same chapter, you will see how the type of chemical bonding in various compounds can be predicted, and how it affects the properties of these compounds.

States of matter

So far, we have considered individual atoms and molecules without paying much attention to the physical properties of substances. It is now time to review the states of matter and the way they are represented in chemical formulae and equations.

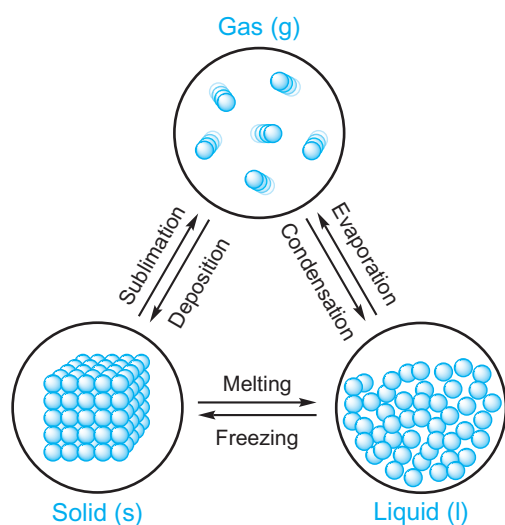
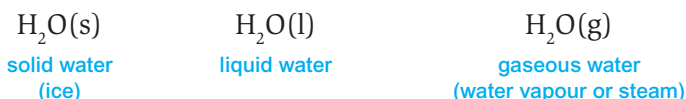


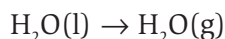
Figure 12. States of matter and physical changes

As you probably know, the three most common states of matter are solid, liquid and gaseous (figure 12). In solid substances, every atom, ion or molecule occupies a certain position owing to strong attractive forces between these particles. Solids are almost incompressible, and have definite volume and shape. In liquids, the forces between particles are weaker, so atoms, ions or molecules can move around but cannot get far away from each other. As a result, liquids are also almost incompressible and have definite volume but no definite shape. In gases, the attractive forces between particles are negligible, so atoms or molecules move freely and generally faster than in liquids. Gases can be compressed and have no definite volume or shape, so they fill the whole volume of the vessel.

To specify the state of a substance, we show the first letter of the state (“s” for solid, “l” for liquid and “g” for gaseous) in brackets after the formula, for example:

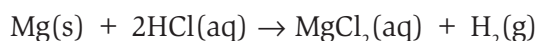


Using these state symbols, we can represent physical changes in the same way as chemical. For example, evaporation of liquid water can be shown as follows:



A special symbol, “(aq)”, is used for substances or ions in aqueous solutions. For example, the expression “NaCl(aq)” tells us that sodium chloride is dissolved in water while “NaCl(s)” refers to the individual compound (solid sodium chloride). Please note the difference between liquid and aqueous states: the expression “NaCl(l)” means that sodium chloride is molten and probably has a very high temperature, as this salt melts at 801°C (1074 K).

In chemical equations, states are particularly important when we discuss reactions in aqueous solutions, thermal effects, reaction rates and chemical equilibrium. Many substances behave differently depending on whether they are in their pure form or dissolved in water, so we need to know their states to write the correct chemical equation. In addition, the states of reactants and products can provide some information about the reaction conditions and observable chemical changes, such as the release of a gas or the formation of a precipitate, for example:



The above equation tells us that solid magnesium metal reacted with an aqueous solution of hydrogen chloride, producing bubbles of a gas (hydrogen) and an aqueous solution of magnesium chloride. We can also predict that the amount of magnesium decreased and, if the reaction went to completion, the metal eventually disappeared. Finally, the equation tells us that magnesium chloride is soluble in water, as otherwise it would produce a solid precipitate, $\text{MgCl}_2(\text{s})$.

Showing states of all reactants and products is good practice, and in this book we will use state symbols in most equations; any exceptions will be explained in the text.

Question

- 9 Using equations and state symbols, represent all physical and chemical changes described in question 1 on page 2. The formula of glucose is $\text{C}_6\text{H}_{12}\text{O}_6$.



Internal link

Reactions in aqueous solutions are discussed later, in **4 Solutions and concentration**. Thermal effects, reaction rates and chemical equilibrium are all covered in **5 Thermochemistry, kinetics and equilibrium**.

You have now learned how the composition and transformations of chemical substances can be represented by chemical formulae and equations. In the next topic, you will see how these formulae and equations can be used for quantitative description of matter and stoichiometric calculations.

1.3 Stoichiometric relationships

Atoms and molecules are so small that their masses cannot be measured directly. Even a million atoms of lead, Pb, the heaviest stable element, would have a mass of only 3.4×10^{-16} g, which is too small to be weighed even on the most sensitive laboratory balance. At the same time, the number of Pb atoms in 1 g of lead is a huge number, about 2.9×10^{21} , which is hard to imagine, let alone count. Therefore, chemists need a unit allowing them to work comfortably with both very small masses and very large numbers of atoms. This unit, the *mole*, was devised in the 19th century and quickly became one of the most useful concepts in chemistry.

The mole

In 1971, the 14th General Conference of Weights and Measures adopted the mole (symbol “mol”) as one of the base SI units.



Key term

The **mole** was defined as the *amount of substance* that contains as many elementary entities (atoms, molecules, ions, electrons or other particles) as there are atoms in 0.012 kg (or 12 g) of carbon-12.

DP ready Nature of science

The International System of Units

The International System of Units (SI, abbreviated from French *Système international d'unités*) is the system of measurement most widely used by scientists. Its building blocks are the seven base units: length (metre, m), mass (kilogram, kg), time (second, s), electric current (ampere, A), temperature (kelvin, K), amount of substance (mole, mol) and luminous intensity (candela, cd). All other units, such as those of volume (m^3), density (kg m^{-3}), energy (joule, J, where $1 \text{ J} = 1 \text{ kg m}^2 \text{ s}^{-2}$) and so on, are derived from the seven base units. The use of universal and precisely defined units is extremely important, as it allows scientists from different countries to understand one another and share the results of their discoveries. Base and derived SI units, physical constants and useful expressions are listed in the appendix.

The number of atoms in 12 g of $^{12}_6\text{C}$ is known with very high precision. Its current value is $6.022140857 \times 10^{23}$, but it might be revised slightly in the future. In all our calculations, we will use the rounded value 6.02×10^{23} .

The *Avogadro constant* (N_A) is the conversion factor linking number of particles and number of moles. It has the unit of mol^{-1} :

$$N_A = 6.02 \times 10^{23} \text{ mol}^{-1}$$

In chemical calculations, the Avogadro constant is used in the same way as any other conversion factor. For example, to convert kilograms into grams, we need to multiply the mass in kg by 1000. Similarly, to convert the amount of substance (n) into the number of atoms or any other structural units (N), we need to multiply that amount by N_A :

$$N = n \times N_A$$

Worked example: Using the Avogadro constant

4. Calculate the amount of lead in a sample containing 2.9×10^{21} atoms of this element.

Solution

$$N = n \times N_A \quad \text{rearrange to } n = \frac{N}{N_A}$$

$$n = 2.9 \times 10^{21} / 6.02 \times 10^{23} \text{ mol}^{-1} \approx 0.0048 \text{ mol} = 4.8 \text{ mmol.}$$

Question

10 Calculate:

- a) the number of atoms in 2.5 mol of sodium metal;
 b) the number of molecules in 0.25 mol of water;
 c) the number of atoms in 0.25 mol of water.

DP ready Theory of knowledge**Mole Day**

Every year, October 23 (written as 10/23 in the USA) is celebrated by many chemists as Mole Day. The event begins at 6.02am and ends at 6.02pm. Combined together, the time and date resemble the Avogadro constant, $6.02 \times 10^{23} \text{ mol}^{-1}$. This constant is named after the Italian scientist Amedeo Avogadro, who made a significant contribution to chemistry by showing that equal volumes of gases under the same conditions contain equal numbers of molecules. Schools and other organizations around the world celebrate Mole Day with various activities related to the mole with the aim to foster public interest in chemistry.



Figure 13. Amedeo Avogadro (1776–1856)

Calculations involving chemical formulae

By definition, the *molar mass* of carbon-12 is exactly 12 g mol^{-1} (as 12 g of this isotope contains exactly 1 mol of carbon atoms). Molar mass expressed in g mol^{-1} has the same numerical value as relative atomic mass (A_r), which is a unitless quantity:

$$M(^{12}\text{C}) = 12 \text{ g mol}^{-1}$$

$$A_r(^{12}\text{C}) = 12$$

For molecular species, we use the term *relative molecular mass* (M_r) instead of relative atomic mass (A_r). The M_r values are also unitless. To find the relative molecular mass of a compound, we need to add together the A_r values of all atoms in this compound.

Key term

The **molar mass** (M) of a chemical substance in g mol^{-1} is the mass of 1 mol of that substance.

Worked example: Calculating the relative molecular mass

5. The formula of water is H_2O . Calculate its relative molecular mass and molar mass.

Solution

The molecule contains two hydrogen atoms and one oxygen atom.

From table 1, $A_r(\text{H}) = 1.01$ and $A_r(\text{O}) = 16.00$, so:

$$M_r(\text{H}_2\text{O}) = 2 \times 1.01 + 16.00 = 18.02.$$

Since M_r and M have the same numerical value, $M(\text{H}_2\text{O}) = 18.02 \text{ g mol}^{-1}$.

Question

11 Calculate relative molecular masses and molar masses of the following substances:

- a) elementary chlorine, Cl_2 ; b) ammonia, NH_3 ; c) sulfuric acid, H_2SO_4 .
 The A_r values of elements are given in table 1 and the periodic table.

Maths skills: Significant figures



Any measurement involves uncertainty, so the result of the measurement always has a limited number of *significant figures*. The length of a small object measured with a ruler typically has no more than three significant figures (sf) as shown in figure 14.

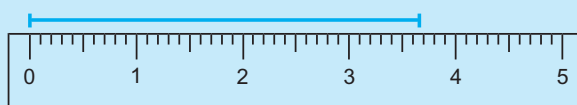


Figure 14. Measurement uncertainty when using a ruler

In this example, the measured length is 3.67 cm. The first two figures, 3 and 6, are certain, as the length is definitely greater than 3.6 but less than 3.7 cm. The last figure, 7, is uncertain, as the actual length could be 3.66 or 3.68 cm. There is absolutely no way of getting the fourth figure using this particular ruler, as we are not sure even about the third figure.

When the results of measurements are multiplied or divided, the value with the smallest number of sf determines the number of sf in the answer. For example, $3.67 \times 1.3 = 4.771 \approx 4.8$ (the answer must be rounded to two sf, as the second value has only two sf).

When the results of two or more measurements are added together or subtracted from one another, the value with the fewest decimal places determines the number of decimal places in the answer. For example, $3.67 + 1.3 = 4.97 \approx 5.0$ (the answer must be rounded to one decimal place, as the second value has only one decimal place).

In multi-step calculations, all intermediate results may be recorded with one or two extra significant figures, and only the final result should be rounded as explained above.

The amount, mass and molar mass of any substance are related as follows:

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

This is probably the most common expression in chemistry, as it is used in almost all stoichiometric calculations. Although the base SI unit of mass is kilogram, the masses of chemical substances are traditionally expressed in grams, and molar masses in g mol^{-1} .



Key term

The **mole ratio** of elements in a chemical compound is the ratio of the amounts of these elements in the compound. For example, one mole of water (H_2O) contains two moles of hydrogen atoms and one mole of oxygen atoms, so the mole ratio of hydrogen to oxygen in water is 2:1.

Question



- 12 The relative atomic mass of lead is 207.20. Calculate the amount of lead in 1.0 g of this metal.
- 13 Calculate the mass of 15 mol of sulfuric acid, H_2SO_4 .

The *mole ratio* can be used to calculate the percentage composition of a compound. (Unless stated otherwise, the term “percentage composition” refers to mass percentages.)

Worked example: Calculating percentage composition

WE

6. Calculate the percentage composition of water.

Solution

Let $n(\text{H}_2\text{O}) = 1 \text{ mol}$, then:

$$m(\text{H}) = 2 \text{ mol} \times 1.01 \text{ g mol}^{-1} = 2.02 \text{ g}$$

$$m(\text{O}) = 1 \text{ mol} \times 16.00 \text{ g mol}^{-1} = 16.00 \text{ g}$$

$$m(\text{H}_2\text{O}) = 1 \text{ mol} \times 18.02 \text{ g mol}^{-1} = 18.02 \text{ g}$$

$$\omega(\text{H}) = \frac{2.02 \text{ g}}{18.02 \text{ g}} \times 100\% \approx 11.2\%$$

$$\omega(\text{O}) = 100\% - 11.2\% = 88.8\%$$

Question

Q

14 Calculate the percent composition of sulfuric acid, H_2SO_4 .

In practice, chemists more often face the opposite problem of deducing the formula of an unknown compound from its percentage composition. The mass percentages of elements in a sample can be determined by various analytical techniques, such as fully automated combustion elemental analysis. In a typical experiment, the sample is burned in excess oxygen, and the volatile combustion products are trapped and weighed. These weights are then converted into mass percentages of chemical elements in the original sample.

Worked example: Deducing the empirical formula

WE

7. Deduce the formula of a compound that contains 3.05% hydrogen and 96.95% sulfur by mass.

Solution

First of all, we need to check whether the mass percentages add up to 100%:

$$3.05\% + 96.95\% = 100\%$$

Therefore the compound contains no other elements, and its formula can be represented as H_xS_y .

Let's assume that $m(\text{H}_x\text{S}_y) = 100 \text{ g}$, so the mass percentages of elements become numerically equal to their masses:

$$m(\text{H}) = \frac{100 \text{ g} \times 3.05\%}{100\%} = 3.05 \text{ g}$$

$$m(\text{S}) = 100 \text{ g} - 3.05 \text{ g} = 96.95 \text{ g}$$

$$n(\text{H}) = \frac{3.05 \text{ g}}{1.01 \text{ g mol}^{-1}} \approx 3.02 \text{ mol}$$

$$n(\text{S}) = \frac{96.95 \text{ g}}{32.07 \text{ g mol}^{-1}} \approx 3.02 \text{ mol}$$

$$n(\text{H}):n(\text{S}) = 3.02 \text{ mol}:3.02 \text{ mol} = 1:1.$$

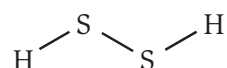
Therefore, the *empirical formula* of this compound is HS.

Key term

The **empirical formula** is the simplest integer ratio of elements present in the compound.

Empirical formulae, like the one found in worked example 7, are determined from experimental data. An empirical formula of a specific compound might or might not be the same as its molecular formula, which shows the exact number of atoms of each element in the molecule (see 1.2 *Chemical substances, formulae and equations*). In the worked example, the empirical formula HS seems unlikely, as we know that hydrogen is monovalent and sulfur is normally divalent, so the valences of these two elements do not match.

We can try to guess the correct molecular formula by multiplying the number of each atom in the empirical formula by the same factor (2, 3, and so on). For example, doubling the formula HS will produce H₂S₂, which corresponds to the following structure:



This compound, hydrogen disulfide, does exist, so the guess is probably correct. But we can never be sure about it without additional experimental evidence. Such evidence can be obtained by determining the molar mass of this compound.

Question

15 Deduce the empirical formula of a compound that contains 30.45% nitrogen and 69.55% oxygen by mass.

Key term

Avogadro's Law states that equal volumes of any two gases at the same temperature and pressure contain equal numbers of molecules.

Molar volume (V_m) of an ideal gas is equal to 22.7 dm³ mol⁻¹ at **standard temperature and pressure (STP)** ($T = 273 \text{ K (}0^\circ\text{C)}$ and $p = 100 \text{ kPa}$).

This in turn gives us the **ideal gas law**, $pV = \frac{m}{M} \times RT$.

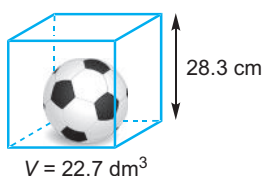


Figure 15. Molar volume of an ideal gas compared with a soccer ball

Calculations involving gases

In 1811, Amedeo Avogadro suggested that equal volumes of any two gases at the same temperature and pressure contain equal numbers of molecules. This hypothesis has been confirmed in many experiments and is now known as *Avogadro's Law*. An important consequence of Avogadro's Law is that under the same conditions, the mass of a certain volume of a gas or vapour is proportional to the molar mass of this gas:

$$m = \frac{V}{V_m} \times M$$

In this expression, V_m is the *molar volume* of an ideal gas, which is equal to 22.7 dm³ mol⁻¹ at $T = 273 \text{ K (}0^\circ\text{C)}$ and $p = 100 \text{ kPa}$ (figure 15). These conditions, known as *standard temperature and pressure (STP)*, are commonly used for comparing and determining the properties of gases. Although the molar volumes of real gases might differ slightly from 22.7 dm³ mol⁻¹, these differences are very small, so in this book we will assume that the standard V_m value can be applied to any gas.

If we know the mass and volume of a gas sample at STP, we can rearrange the above expression to find the molar mass of the gas:

$$M = \frac{m}{V} \times V_m$$

The ratio m/V is the gas *density* (ρ), so the molar mass of a gas and its density are related as follows:

$$M = \rho \times V_m$$

For example, if the unknown gas with the empirical formula HS has a density of 2.91 g dm^{-3} at STP, then:

$$M = 2.91 \text{ g dm}^{-3} \times 22.7 \text{ dm}^3 \text{ mol}^{-1} \approx 66.1 \text{ g mol}^{-1}$$

This value is very close to the molar mass of H_2S_2 (66.16 g mol^{-1}), which confirms our earlier suggestion.

Question

16 Calculate the molar mass of a gaseous oxide of sulfur and deduce its molecular formula if 0.250 dm^3 of this oxide at STP has a mass of 0.706 g .

If a substance is liquid or solid at STP, its molar mass can be determined under different conditions (typically at a higher temperature) using the *ideal gas law*:

$$pV = \frac{m}{M} \times RT$$

The *universal gas constant* (R) in this expression has a value of $8.31 \text{ J mol}^{-1} \text{ K}^{-1}$. To obtain the molar mass in g mol^{-1} , it is convenient to measure the pressure (p) in kPa, volume (V) in dm^3 , mass (m) in g and temperature (T) in K.

Temperatures in $^{\circ}\text{C}$ must be converted to kelvins: $T_{\text{K}} = T_{\text{C}} + 273.15$.

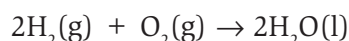
Question

17 A sealed container with a volume of 0.400 dm^3 was charged with 2.32 g of an unknown liquid and heated to 353 K until all liquid was vaporized. At that moment, the pressure in the container reached 124 kPa .

- Calculate the molar mass of the liquid.
- Deduce the molecular formula of the liquid if it contains 22.55% phosphorus and 77.45% chlorine by mass.

Calculations involving chemical equations

The stoichiometric coefficients in any chemical equation show the ratio between reactants and products. For example, the following equation represents the formation of water from molecular hydrogen and oxygen:



This equation tells us that each O_2 molecule reacts with two H_2 molecules, producing two molecules of water. In other words, the molecular ratio between H_2 , O_2 and H_2O is $2:1:2$.

Since the amount of each substance is proportional to the number of its molecules (or other structural units), the mole ratio between the reactants and products will be the same as their molecular ratio. In our example, each mole of oxygen will react with two moles of hydrogen, producing two moles of water.

In turn, mole ratios can be used to calculate mass and volume ratios. Therefore, if we know the amount, mass or volume of any substance participating in a chemical reaction, we can find the amounts, masses and volumes of all other reactants and products.

Worked example: Calculating amounts, masses and volumes

WE

8. Suppose that the above reaction produced 3.6 g of water. Calculate the amounts, masses and volumes of the reactants at STP.

Solution

$$M(\text{H}_2\text{O}) = 2 \times 1.01 + 16.00 = 18.02 \text{ g mol}^{-1}$$

$$n(\text{H}_2\text{O}) = 3.6 \text{ g} / 18.02 \text{ g mol}^{-1} \approx 0.20 \text{ mol}$$

$$n(\text{H}_2) = n(\text{H}_2\text{O}) = 0.20 \text{ mol}$$

$$n(\text{O}_2) = n(\text{H}_2\text{O}) / 2 = 0.20 \text{ mol} / 2 = 0.10 \text{ mol}$$

$$m(\text{H}_2) = 2 \times 1.01 \text{ g mol}^{-1} \times 0.20 \text{ mol} \approx 0.40 \text{ g}$$

$$m(\text{O}_2) = 2 \times 16.00 \text{ g mol}^{-1} \times 0.10 \text{ mol} \approx 3.2 \text{ g}$$

$$V(\text{H}_2) \text{ at STP} = 0.20 \text{ mol} \times 22.7 \text{ dm}^3 \text{ mol}^{-1} \approx 4.5 \text{ dm}^3$$

$$V(\text{O}_2) \text{ at STP} = 0.10 \text{ mol} \times 22.7 \text{ dm}^3 \text{ mol}^{-1} \approx 2.3 \text{ dm}^3.$$

Note that we cannot use V_m to calculate the volume of liquids, such as water in this example.

A single numerical value (in our case, the mass of the product) has allowed us to determine the quantities of all reacting species. This is the power of chemical equations: in just one line, they represent many qualitative and quantitative characteristics of the chemical change.

All calculations based on chemical equations begin from determining the amount of any species (reactant or product) present in the equation. Once that is done, other quantities can be calculated, as the amounts of all other reacting species are proportional to their stoichiometric coefficients. In turn, the mass of each substance and the volume of each gas can be found in one step by multiplying their amounts with M_r and V_m values, respectively.

Question

Q

18 The combustion of hydrogen sulfide proceeds as follows:



Calculate the volume of consumed oxygen and the masses of the reaction products if the volume of combusted hydrogen sulfide was 0.908 dm^3 . All volumes are measured at STP.

From Avogadro's law, it follows that the amount of a gaseous substance is proportional to its volume:

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

Therefore, the volumes of reacting species measured under the same conditions are proportional to the amounts of these species:

$$\frac{n_1}{n_2} = \frac{V_1}{V_2}$$

In turn, the amounts of reactants and products are proportional to their stoichiometric coefficients. As a result, if we know the volume of any gas consumed or produced in the reaction, the volumes of other gaseous substances can be found without calculating their amounts.

Worked example: Calculating volume using stoichiometric coefficients

WE

9. Deduce the volume of oxygen consumed in question 18.

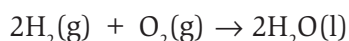
Solution

$$V(\text{O}_2) = \frac{3}{2} \times V(\text{H}_2\text{S}) = \frac{3}{2} \times 0.908 \text{ dm}^3 \approx 1.36 \text{ dm}^3$$

The limiting reactant

So far, we have assumed that all reactants are used up completely in the course of the reaction, and the final mixture contains only the reaction products. In real life, chemical reactions rarely go to completion, so some starting materials are often left over. In addition, one of the reactants may have been used in excess, so some of it will remain in the final mixture even if all other reactants are fully consumed.

For example, suppose that we mixed 1.0 mol of hydrogen with 3.0 mol of oxygen and ignited the mixture. As usual, hydrogen and oxygen will react in a 2:1 ratio, producing water:



The reaction will stop when all the hydrogen is consumed. If 1.0 mol of hydrogen has reacted with 0.5 mol of oxygen, another $3.0 - 0.5 = 2.5$ mol of oxygen remains unreacted. Therefore, the final mixture will contain 1.0 mol of water and 2.5 mol of oxygen.

It is helpful to record the amounts of all substances as follows:

	$2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{l})$		
$n_{\text{init}} / \text{mol}$	1.0	3.0	0
$\Delta n / \text{mol}$	-1.0	-0.5	+1.0
$n_{\text{fin}} / \text{mol}$	0	2.5	1.0

The first row under the equation represents the initial mixture, where the substances can be present in any proportions. Indeed, we can take any amounts of reactants and mix them together, regardless of stoichiometric coefficients.

The second row shows how the amount of each substance changes in the course of the reaction. The sign before each amount shows whether it decreases (for reactants) or increases (for products). These changes must be proportional to stoichiometric coefficients, as all substances are consumed or produced according to the equation.

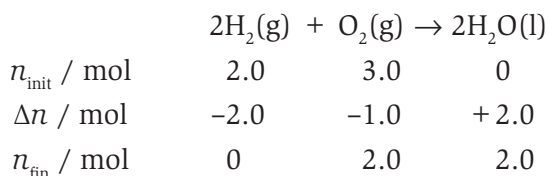
The last row represents the final mixture, where the amounts of all substances are calculated as $n_{\text{fin}} = n_{\text{init}} + \Delta n$. As with the initial mixture, the composition of the final mixture is not related to stoichiometric coefficients.

In this example, the amount of the reaction product (water) is limited by the amount of hydrogen, which is completely consumed in the reaction. In other words, hydrogen is the *limiting reactant*, while oxygen is present in excess.

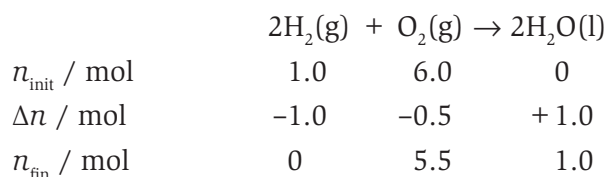
Key term

A **limiting reactant** is the reactant used up completely while other reactants are present in excess. It controls the amount of product formed in the reaction.

The concept of the limiting reactant is very important, as it allows us to determine the extent of reaction. For example, if we double the amount of hydrogen, the amount of water formed will also double:



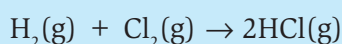
However, if we double the amount of oxygen (which was already in excess), the amount of water produced in the reaction will not change at all:



Therefore in this case, the larger the excess of oxygen we use, the greater amount of it will remain unreacted.

Question

19 Hydrogen and chlorine react with each other to produce hydrogen chloride:



A mixture of 4.54 dm³ of hydrogen and 2.27 dm³ of chlorine was heated until the reaction was complete. Calculate the volumes of each substance in the final mixture. All volumes are measured at STP.

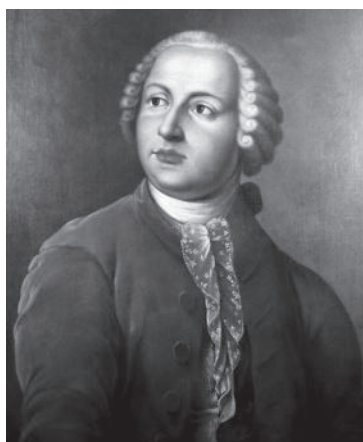


Figure 16. Top: Mikhail Lomonosov (1711–1765); bottom: Antoine Lavoisier (1743–1794)

The reaction yield

In any chemical reaction, the total mass of the reaction products is equal to the total mass of the consumed reactants. This principle, known as the *law of conservation of mass*, follows from the atomic theory. Since atoms cannot be created or destroyed, their total number and mass cannot be affected by chemical changes.

DP ready Nature of science

The law of conservation of mass

“Nothing comes from nothing” was one of the basic principles in ancient Greek philosophy. The first experimental evidence for the conservation of mass was obtained in 1748 by the Russian scientist Mikhail Lomonosov, who carried out chemical reactions in sealed vessels and found that chemical changes did not affect the total mass of the mixtures. However, the works of Lomonosov were almost unknown in most European countries, so it was over 25 years before the French chemist Antoine Lavoisier formulated this principle in 1774 and was commonly credited for its discovery. This example shows the importance of sharing knowledge and ideas: any discovery that is not reported properly remains hidden from the scientific community and has no effect on the progress of science.

Question

- 20 Calculate the masses of reactants and products in question 19 and verify that the law of conservation of mass is valid for the reaction between hydrogen and chlorine.
- 21 Magnesium metal (10.21 g) was burned in excess oxygen to produce magnesium oxide. Determine the initial volume of oxygen at STP if the volume of oxygen left after the reaction was 6.81 dm³ at STP.

When chemical reactions are carried out in a laboratory, the actual amounts of the reaction products are usually lower than the amounts predicted by the equation. This can happen for many reasons, including incomplete conversion of the reactants or simply because some product was lost during its isolation and purification. In such cases, we can calculate the *reaction yield*, which is the ratio of the practical and theoretical amounts of the product. Since the amount of an individual substance is proportional to its mass ($n = m/M$), the yield can also be found as the ratio of the practical and theoretical masses of the product:

$$\text{Yield} = \frac{n_{\text{pract}}}{n_{\text{theor}}} \times 100\% = \frac{m_{\text{pract}}}{m_{\text{theor}}} \times 100\%$$

Key term

Reaction yield is the ratio of the practical and theoretical amounts of the product.

Worked example: Calculating the percentage yield

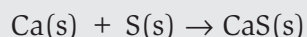
10. Suppose that we mixed 10.0 g of calcium metal and 9.62 g of sulfur, heated the mixture for some time, and collected 17.0 g of calcium sulfide, CaS. Calculate the yield of calcium sulfide.

Solution

First we need to find the amounts of all substances:

$$\begin{aligned} n(\text{Ca}) &= 10.0 \text{ g}/40.08 \text{ g mol}^{-1} \approx 0.250 \text{ mol} \\ n(\text{S}) &= 9.62 \text{ g}/32.07 \text{ g mol}^{-1} \approx 0.300 \text{ mol} \\ n(\text{CaS}) &= 17.0 \text{ g}/72.15 \text{ g mol}^{-1} \approx 0.236 \text{ mol.} \end{aligned}$$

According to the equation, the limiting reactant is calcium, as the two elements are consumed in a 1:1 ratio:



The theoretical amount of calcium sulfide is 0.250 mol (the same as the initial amount of the limiting reactant, calcium). However, the reaction produced only 0.236 mol of this compound, so the yield of calcium sulfide is:

$$(0.236 \text{ mol}/0.250 \text{ mol}) \times 100\% = 94.4\%.$$

The same result could be obtained through practical and theoretical masses of calcium sulfide:

$$\begin{aligned} m(\text{CaS})_{\text{theor}} &= 0.250 \text{ mol} \times 72.15 \text{ g mol}^{-1} \approx 18.0 \text{ g} \\ \text{Yield} &= (17.0 \text{ g}/18.0 \text{ g}) \times 100\% \approx 94.4\%. \end{aligned}$$

Question

- 22 Calculate the percentage yield of the reaction between 9.443 g of aluminium and 7.945 dm³ (STP) of oxygen that produced 17.13 g of aluminium oxide.

The yields of chemical reactions are particularly important in the chemical industry, where the loss of a tiny percentage of the final product could mean a significant drop in profit. At the same time, low reaction yields increase the amount of waste, which needs to be disposed of safely or reused. The development of highly efficient synthetic procedures with low environmental impact is reflected in the concept of *green chemistry*, which is now adopted by the majority of commercial and research organizations around the world.

DP ready Nature of science

Green chemistry

The term “green chemistry” was coined in 1991 by American chemists Paul Anastas and John Warner, who formulated 12 principles for their approach to chemical technology. These principles include the use of nonhazardous chemicals and solvents, reduction of energy consumption and waste production (“the best form of waste disposal is not to create it in the first place”), choice of renewable materials, and prevention of accidents. The philosophy of green chemistry has passed into national and international laws, which restrict the use of certain chemical substances and promote environmentally friendly technologies.



Internal link

Later you will see how the laws of stoichiometry can be applied to redox processes [3.3 Redox processes], electrolytes [4.2 Concentration expressions and stoichiometry], chemical energetics [5.1 Thermochemistry], kinetics [5.2 Chemical kinetics], equilibria [5.3 Chemical equilibrium] and acid–base reactions [6.3 The concept of pH].

Stoichiometry—a general approach

Solving a stoichiometry problem is often a challenge that requires handling a variety of data and performing multi-stage mathematical calculations. Although there is no single strategy, most problems can be approached as follows.

1. Write and balance the chemical equation(s) for any chemical changes mentioned in the problem.
2. Calculate the amounts of as many substances as you can using the formulae $n = m/M$ and $n = V/V_m$. If you know a mass percentage, convert it first to mass (if possible) and then to amount.
3. Write all known amounts of substances below their formulae in the chemical equation. Any missing values may suggest the next step of the solution.
4. Determine the limiting reactant and use stoichiometric coefficients to calculate the amount changes for all substances. Remember that these coefficients do not reflect the initial or final amounts of reactants and products.
5. Check the mass balance. The total mass of products must be equal to the total mass of reactants. If it is not the case, revise your solution.
6. Check that the answer makes sense. All percentages should add up to 100%, and no individual percentage can be greater than 100%. The yield of the final product must not exceed 100%. Finally, treat very low or very high percentages with caution.

These simple rules will help you to avoid many common errors and solve the problem in the fewest steps. We will continue the discussion of stoichiometric relationships in the next chapters of this book.

Chapter summary

In this chapter, you have learned about the atomic theory, chemical and physical changes, chemical formulae, equations and stoichiometry.

Before moving further, check that you have a working knowledge of the following concepts and definitions.

- All matter consists of atoms, which cannot be created or destroyed by chemical changes.
- The atom is the smallest unit of a chemical element.
- An atom consists of a small, dense, positively charged nucleus surrounded by negatively charged electrons.
- Atoms can form ions by losing or gaining electrons, or combine together into molecules by sharing electrons.
- Elementary substances contain atoms of one element while compounds contain atoms of two or more elements.
- Pure substances have definite compositions that can be represented by chemical formulae.
- An empirical formula shows the simplest integer ratio of atoms in a compound.
- A molecular formula shows the actual number of atoms in the molecule.
- One mole of any substance contains 6.02×10^{23} structural units.
- The amount, mass and molar mass of a substance are related by the expression $n = \frac{m}{M}$.
- One mole of any gas has a volume of 22.7 dm^3 at STP (273 K and 100 kPa).
- The amount and volume of a gas are related by the expression $n = \frac{V}{V_m}$.
- Chemical equations represent chemical changes where the reactants are transformed into the products.
- Stoichiometric coefficients show the mole ratio of the substances consumed or produced in the course of the reaction.
- The total mass of the reaction products is equal to the total mass of the reactants.
- The reaction yield is the ratio between the practical and theoretical amounts of the product.

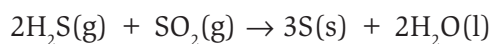
Additional problems

1. Ammonia (NH_3) is a colourless, strong-smelling, toxic gas that can be produced from hydrogen and nitrogen. Under a pressure of 1 MPa, ammonia condenses into a liquid at room temperature. Evaporation of liquid ammonia absorbs a significant amount of heat, which makes this compound a common refrigerant. Ammonia is flammable and typically produces nitrogen gas and water when burned in air. Identify all physical and chemical changes described in this paragraph and represent these changes using equations and state symbols.
2. Dalton's atomic theory consisted of five postulates, as explained in the text. Examine each of these postulates and suggest whether it agrees with the modern views on the atomic structure or not. Support your answer by specific examples.
3. Tritium is a radioactive isotope of hydrogen with a mass number of 3. State the number of protons, neutrons and electrons in an atom of tritium.
4. Naturally occurring sulfur has four isotopes with the following atomic percentages: ^{32}S (95.02%), ^{33}S (0.75%), ^{34}S (4.21%) and ^{36}S (0.02%). Calculate the average A_r value for sulfur. Suggest why your result differs slightly from the A_r value given in table 1.

5. Hydrogen peroxide (H_2O_2) and hydrazine (N_2H_4) are covalent molecules that contain single O–O and N–N bonds, respectively. Many molecules with such bonds decompose easily, producing large amounts of heat. Because of that, both hydrogen peroxide and hydrazine are used as fuel in rocket engines.
- Draw the structural formulae of hydrogen peroxide and hydrazine, representing covalent bonds with lines.
 - Decomposition of hydrogen peroxide produces water and an elementary substance while decomposition of hydrazine produces ammonia (NH_3) and another elementary substance. Deduce and balance chemical equations for these processes.
 - Suggest the most likely state symbols for all reaction products when liquid hydrogen peroxide and liquid hydrazine are used as rocket fuels.
6. To visualize the mole, a chemistry student decided to pile up 6.02×10^{23} grains of sand. Estimate the time needed to complete this project if an average grain of sand weighs 5 mg, and the student can shovel 50 kg of sand per minute.
7. Calculate the percentage composition of magnesium hydroxide, $\text{Mg}(\text{OH})_2$.
8. Calculate the density, in g dm^{-3} , of chlorine gas at: a) STP; b) 100°C and 30.0 kPa.
9. Carbon forms several gaseous compounds with fluorine. Deduce empirical, molecular and structural formulae for three of these compounds using the mass percentages and densities from the table below.

Compound	$\omega(\text{C}) / \text{mass \%}$	ρ at STP / g dm^{-3}
X	13.65	3.88
Y	24.02	4.41
Z	17.40	6.08

10. A reaction between hydrogen sulfide and sulfur dioxide proceeds as follows:



Deduce the limiting reactant and determine the molar composition of the final mixture if the initial mixture contained 11.35 dm^3 of hydrogen sulfide and 18.16 dm^3 of sulfur dioxide at STP.

11. Magnesium metal (100.0 g) was heated with an equal mass of elemental phosphorus until the reaction was complete. Determine the mass percentages of all substances in the final mixture.
12. Calcium carbonate (CaCO_3 , limestone) and calcium oxide (CaO , quicklime) are widely used in construction and steelmaking. Above 825°C , calcium carbonate decomposes into calcium oxide and carbon dioxide, CO_2 . Calculate the percentage yield of this reaction if the decomposition of 20.0 kg of calcium carbonate in an industrial furnace released 3.86 m^3 (STP) of carbon dioxide.