INTRODUCTION TO GENERAL CHEMISTRY

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Introduction to general chemistry

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TABLE OF CONTENTS

1: Matter energy and their measurements

2: Elements

3: Compounds

4: Stoichiometry –the quantification of chemical reactions

Dedicated to Mr. Frank Reidy, a philanthropist who brought the author to the US

Mr. Frank Reidy

Dedicated to Mr. Frank Reidy, a philanthropist who brought the author to the US and who supported research on the medical application of pulsed electric fields at Frank Reidy Research Center For Bioelectrics, Old Dominion University, Norfolk, VA. The research resulted in developing techniques proven to cure some forms of cancer.

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CHAPTER OVERVIEW

1: Matter energy and their measurements

1.1: Matter and energy

Learning Objectives

- Define matter, element, molecule, compound, molecule, mixture, homogeneous and heterogeneous mixtures, the law of constant composition, states of matter, i.e., solid, liquid, gas, and plasma, energy and its types kinetic and potential energy, endothermic and exothermic and exothermic processes, and the law of conservation of energy.
- Be able to write and interpret symbols of elements, molecules, and compounds.

What is the matter?

Matter is anything that has mass and occupies space.

Matter is a natural material that makes up the universe. The matter comprises tiny particles called atoms held together by forces called bonds. The matter is classified as **pure** if it has a constant and a non-variable composition of the type of atoms. Pure matter is either an element or a compound.

Element

An element is pure matter that is composed of only one type of atom

For example, carbon, shown in Fig. 1.1.1, is an element. Elements can not convert to simpler matter by physical or chemical methods. There are around a hundred different elements known at this time. For example, hydrogen, oxygen, carbon, nitrogen, sodium, chlorine, iron, cobalt, gold, and silver are a few elements.

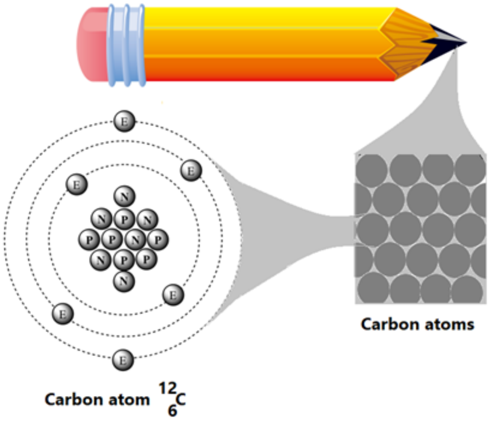


Figure 1.1.1: The pencil tip is carbon -an element composed of one type of atom, as shown in the model.

Symbol of an element

Symbols represent elements, the first alphabet of their English or non-English name, written in capital letters. For example, C for carbon, O for oxygen, and H for hydrogen. Usually, another alphabet is also chosen from the element's name and written as a small letter, e.g., He for helium, Co for cobalt. Some element symbols are derived from non-English names, e.g., Fe for iron is from its Latin name Ferrum, and Au for gold is from its Latin name Aurum.

Two consecutive capital letters do not represent an element; they may combine two elements.

CO is not a symbol of an element; it is a pure matter, a combination of carbon and oxygen bonded together in a 1:1 atom ratio.

Molecule

A molecule is a group of two or more atoms held together by forces called chemical bonds. The molecule is the smallest particle of matter that can exist freely. A single atom of some elements can exist freely and is also considered a molecule. For example, He, O_2, P_4, and S_8 are examples of elements having molecules composed of one, two, four, and eight atoms of the same element, respectively, as illustrated in Fig. 1.1.2. Although metal elements exist as a vast number of atoms bonded together by a special type of bond called metallic bonds, their symbol is that of a single atom, e.g., Fe for iron and Au for gold.

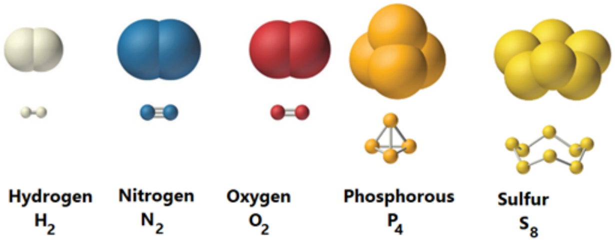


Figure 1.1.2: Models of molecules of some elements.

Compound

> A compound is a pure matter composed of atoms of two or more different elements in a constant whole-number ratio held together by chemical bonds.

The symbol of a compound is a combination of its constituent elements with a subscript to the right of the element symbol representing the whole number ratio of the atoms of the element in the compound. For example, H_2O symbolizes a compound called water composed of hydrogen (H) and oxygen (O) atoms in a 2:1 ratio. Similarly, NaCl symbolizes a table salt compound composed of sodium (Na) and chlorine (Cl) atoms in a 1:1 ratio. If the symbol of a compound also represents a molecule of the compound, it is called a **molecular formula**. For example, H_2O is a molecule formula of water. On the other hand, table salt is another class of compound composed of a vast number of atoms of its constituent elements arranged in a specific arrangement in 3D space called a **crystal lattice**, as illustrated in Fig. 1.1.3. When the compound symbol does not represent a molecule, it only means the simple whole-number ratio of the constituent elements; it is called the **formula unit**. For example, NaCl is a chemical formula of a compound called table salt.

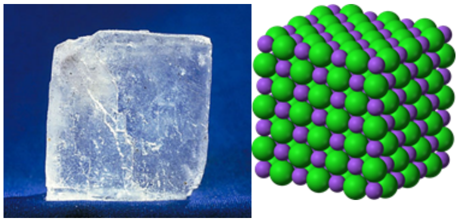


Figure 1.1.3: Sodium chloride (NaCl) –a compound, the crystal (left) and the model showing crystal lattice (right). Source: Halite(Salt)USGOV.jpg and Benjah-bmm27 (talk · contribs) / Public domain.

Law of definite proportion or law of constant composition

> A chemical compound always contains the number of atoms of its component elements in a constant ratio, or the ratio of masses of the constituent elements is a constant in a given compound.

Pure matter, i.e., elements or compounds, has a fixed proportion of atoms of element/s independent of the source or method of their preparation. It is also called a **chemical** or a **substance**. The atoms in a compound are held together by attractive forces called chemical bonds. Constituent elements in a compound can be separated only by breaking chemical bonds and making new chemical bonds which is a **chemical reaction**.

Mixture

> Two or more pure substances mixed such that ratio of the constituents is variable is called a mixture.

For example, table salt can be mixed with water, but the salt (NaCl) to water (H_2O) can be varied to give less salty or more salty water in a mixture. A mixture in which the components are thoroughly mixed, and the composition is constant throughout a given sample, is a **homogeneous mixture** or a **solution**. For example, table salt dissolved in water is an example of a homogeneous mixture or a solution. Other homogeneous mixtures include sugar dissolved in water; the air, a mixture of nitrogen, oxygen, carbon dioxide, and other gases; and metal alloys like brass, a mix of copper and zinc metals, etc.

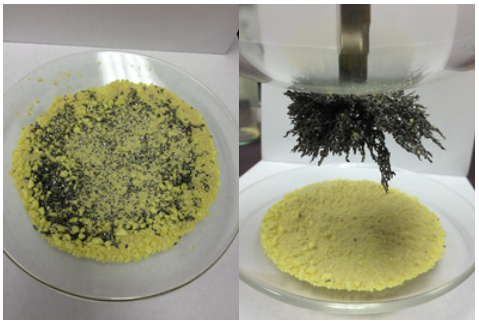


Figure 1.1.4: A heterogeneous mixture of iron and sulfur (left), separated by a magnet (right). Source: Asoult / CC BY (https://creativecommons.org/licenses/by/4.0)

It is a **heterogeneous** mixture if the miitsnents are not thoroughly mixed and the composition varies within different regions of a given sample. For example, sulfur (S) powder mixed with iron (Fe) filling is a heterogeneous mixture shown in Fig. 1.1.4. Other examples of heterogeneous mixtures include smoke which is a mixture of air and carbon particles; smog which is a mixture of liquid water droplets suspended in air; and orange juice which is a mixture of sugar, water, fiber particles, etc. Fig. 1.1.5 illustrates the classification of the matter described above.

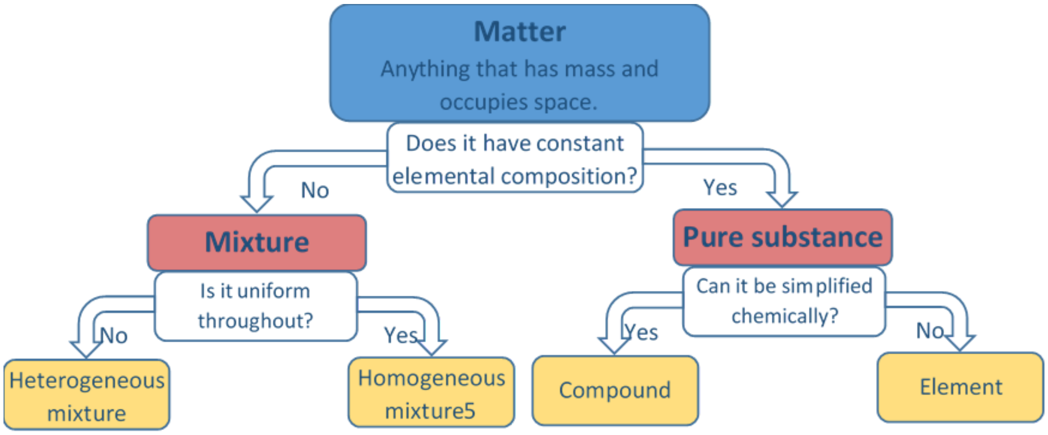


Figure 1.1.5: Classification of matter.

States of matter

Matter exists in one of the four physical states or phases, i.e., solid (s), liquid (l), gas (g), or plasma. Fig. 1.1.6 illustrates the four states of matter at the molecular level, and Fig. 1.1.7 shows examples of the four states of matter.

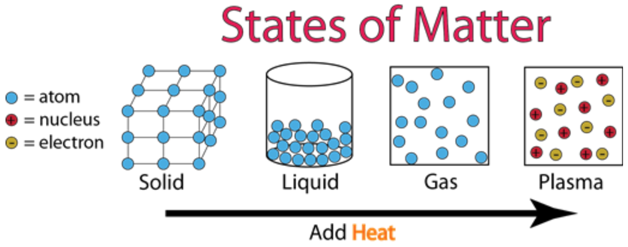


Figure 1.1.6: Four states of matter at the molecular level. Source: https://www.hiclipart.com/free-trans...mwpjm/download

Figure 1.1.7: Examples of the four states of matter. Clockwise from the top left are solid, liquid, plasma, and gas, represented by an ice sculpture, a drop of water, electrical arcing from a Tesla coil, and the air around clouds, respectively. Source: Spirit469 / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Solid-state

In the solid state**,** the particles, i.e., atoms or molecules, are very close to each other and held strongly by intermolecular forces. The particles can vibrate around their mean positions, but they cannot slide past each other. Expansion and contraction in a solid state are negligible. The solid has a fixed shape and a fixed volume.

Liquid state

In the liquid state, the particles are close enough to experience strong intermolecular interactions that usually do not let the particles cross the liquid boundary. Still, the particles can move around within the liquid. Consequently, the particles in a liquid can flow and acquire the shape of the container but have a fixed volume. Expansion and contraction are negligible in the liquid state.

Gas state

In the gas state, the particles are far apart. The intermolecular interactions are negligible in the gas phase due to the large distances between the particles. The gas molecules move in straight lines in random directions until they collide with other molecules or the walls of the container. The collisions are elastic; that is, the molecules bounce off like elastic balls, and the total kinetic energy of the system is conserved. If exposed to space, the particles keep moving into space. In other words, the particles in a gas can flow, acquire the shape of the container, and expand or contract to fill up the available space. The gases do not have a fixed shape and do not have a fixed volume.

Plasma state

In the plasma state, the particles are far apart like gases, and a portion of the negative charge of the particles, i.e., electrons, are separated from the positive charge potion, i.e., the nucleus. In other words, the atoms in the plasma state are ionized. The plasma state is not common on Earth but is the universe's most common state of matter. For example, the matter in the sun and stars is in the plasma state. Examples of the plasma state on Earth include the matter in the lightning bolts and electrical sparks.

What is energy

> Energy is a quantitative property transferred to an object and recognizable as performing work or as heat or light. In simple words: energy is the ability to do work.

What we commonly encounter other than matter is **energy**. There are two basic types of energies, i.e., the kinetic energy of moving objects and potential energy stored by the position of an object in a force field, e.g., gravitation potential energy under the gravity force and chemical potential energy under the electrical fields in the bonds, as illustrated in Figure 1.1.8.

Figure 1.1.8: Potential energy stored in the fuel is transformed into kinetic energy of the Harpoon missile launched on USS Thorn. (Copyright; Darantares, Public domain, via Wikimedia Commons)

Kinetic energy

The energy of moving objects is kinetic energy. The mathematical form of kinetic energy (KE) is $KE = \frac{1}{2}mv^2$, where m is the mass and v is the velocity of the moving object. Examples of kinetic energy include the energy of all moving things that we see around, like moving vehicles or a moving turbine that generates electricity. Thermal energy is also the kinetic energy of the atoms and molecules in matter.

Potential energy

Potential energy is due to the position of an object in a force field. Examples of force fields responsible for the potential energy include electric, magnetic, gravitational, and elastic forces. Examples of potential energies are electrical energy and gravitational energy. Light is potential energy due to moving electric and magnetic fields. Chemical energy is potential energy stored in chemical bonds in electrostatic potential energy.

Gravitation potential energy is due to position or height relative to the earth. The earth attracts other objects with force $F = mg$, where F is the force, m is the object's mass, and g is the acceleration due to gravity. When an object falls, the potential energy changes to several forms of energy, including kinetic energy, work against friction from air, sound, and work done in deformations when it hits the ground.

Chemical potential energy is due to chemical bonds that hold the atoms together in a molecule or compound through electrical forces between negative charge electrons and positive charge nuclei. Bond-forming always releases energy, and bond-breaking absorbs the same energy. Each bond has different bond energy. In chemical reactions, some bonds break, and some bonds form.

A combination of kinetic and potential energy is also possible, e.g., in mechanical waves. A sound wave is a mechanical wave that combines kinetic and potential energy –kinetic because particles move and potential due to the elasticity of the material in which the deformation (sound) is propagating.

Exothermic and endothermic reactions

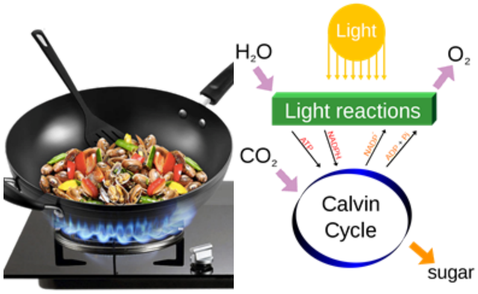


Figure 1.1.9: Combustion of methane –an example of an exothermic reaction that releases energy as the heat used for cooking (left), and photosynthesis - an example of an endothermic reaction that absorbs energy (right). Source: https://www.hiclipart.com/free-trans...imhhh/download and https://www.hiclipart.com/free-trans...-clipart-mslhq

The balance between the energy needed to break the bonds and the energy released from forming new bonds determines whether the chemical reaction releases or absorbs energy. Chemical reactions that release energy are called **exothermic** reactions. For example, the combustion of methane gas in kitchen burners releases energy. A reaction that absorbs energy is called an **endothermic** reaction. For example, photosynthesis converts carbon dioxide and water to glucose by absorbing sunlight, as illustrated in Fig. 1.1.9.

Law of conservation of energy

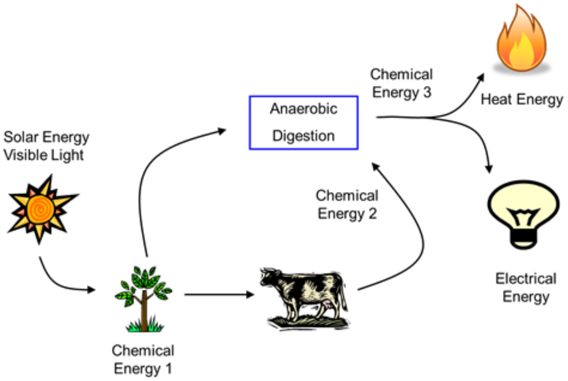


Figure 1.1.10: Energy can transform from one form to another, but energy can neither be created nor destroyed. Source: https://www.hiclipart.com/free-trans...muhlp/download

> The energy conservation law states that energy can transform from one form to another, but the total energy of an isolated system remains the same.

Energy can transform from one form to another through work or heat. An oscillating pendulum is an example of kinetic and gravitational potential energy periodically transforming into each other through work. Radiation energy in sunlight transfers to chemical energy during photosynthesis, heat, and work during glucose metabolism, but the total energy remains the same, as illustrated in Figure 1.1.10.

1.2: What is chemistry?

Learning Objectives

- Define chemistry, physical properties, physical process, intensive and extensive properties, chemical properties, chemical process, and the law of multiple proportions.
- Be able to write and interpret chemical equations.
- Understand the scientific method and its steps, including observation, hypothesis, experiment, conclusion, law, theory, and how theory evolves knowledge.

> Chemistry is the study of matter. More specifically, chemistry studies matter's composition, properties, and transformations.

The properties of matter are of two types, physical properties, and chemical properties, as illustrated in Fig. 1.3.1.

Figure 1.2.1: Chemical property relates to elemental composition and its changes. Physical property relates to appearance and its change. Source: https://www.hiclipart.com/free-trans...mnxsm/download

Physical property and physical process

Physical property

> Physical property is the property that, when observed, does not change the elemental composition of the matter.

Examples include color, mass, volume, electrical conductivity, and heat conductivities.

Intensive properties

Physical properties that do not depend on the amount of matter are called intensive properties, e.g., color, density, and heat conductivity.

Extensive properties

Physical properties that depend on the amount of the substance, like, mass and volume, are called extensive properties.

Physical process

> Any process that changes the matter somehow but does not change the elemental composition is called a physical process.

For example, melting solid to liquid or boiling liquid to a gas state are physical processes.

Mixtures can be separated using physical processes based on the differences in the physical properties of the constituents. Fig. 1.3.2 demonstrates that a magnetic material like iron can be separated from a nonmagnetic material like sulfur using a magnet.

The filtration process can separate a heterogeneous mixture of liquid and solid, like sand in water. Water passes through the filter paper leaving behind the sand particles on the filter.

The distillation process can separate homogeneous mixtures of solids in liquids or liquids in liquids based on the difference in the boiling points of the components. For example, salt dissolved in water separates by distilling off the water, leaving behind the solid salt. Distillation can also separate a mixture of two or more liquids if their boiling points differ; e.g., a distillation of crude oil separates the components based on their boiling points.

Chromatography is another technique often used to separate mixtures. For example, a mixture of inks is adsorbed on a porous paper and separated by ascending through the capillaries in the paper. The component of the ink mixture separate because some components have more ability to stay adsorbed in the solid phase and less ability to solubilize in the liquid phase than the other components. Fig. 1.3.2 Illustrates the physical separation processes described.

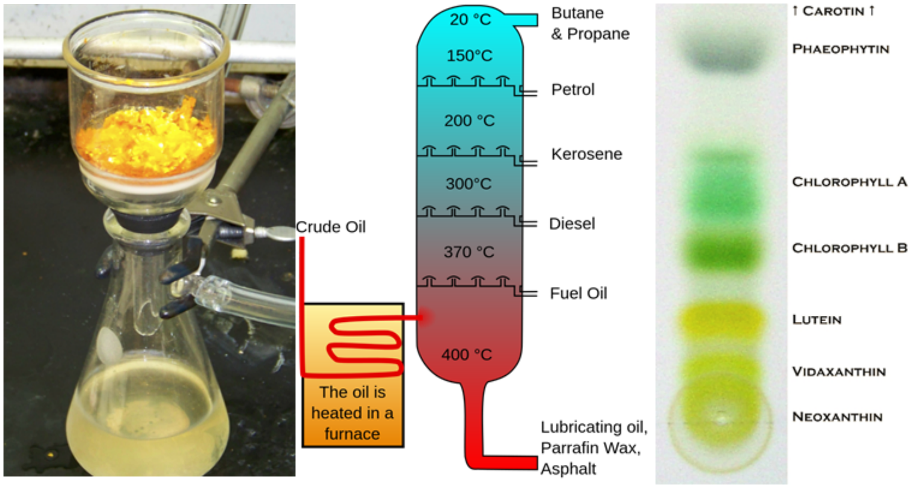


Figure 1.2.1: Filtration (left), a distillation of crude oil (middle), and chromatography of chlorophyll and other pigments of a leaf extract (right). Source: a) Smokefoot / Public domain, b) Crude_Oil_Distillation-fr.svg: Image originale:Psarianos, Theresa knott ; image vectorielle:Rogilbertderivative work: Utain () / CC BY-SA (http://creativecommons.org/licenses/by-sa/3.0/), c) No machine-readable author provided. Flo~commonswiki assumed (based on copyright claims). / CC BY-SA (https://creativecommons.org/licenses/by-sa/2.5)

Chemical property and chemical process

Chemical property

> Chemical properties relate to the change in the elemental composition of the matter.

For example, methane (CH_4) in natural gas is combustible -this is a chemical property. It means methane (\ce{CH4}\)) and oxygen (\ce{O2}\)) change their elemental composition to become carbon dioxide (\ce{CO2}\))and water (\ce{H2O}\)) and release heat after ignition.

Chemical process

> A process that changes the elemental composition is called a chemical process or chemical reaction.

For example, photosynthesis is a chemical process that converts carbon dioxide and water to glucose using energy from sunlight.

Chemical equation

> A chemical equation represents a chemical reaction in the form of symbols of elements and compounds involved.

Substances consumed in a chemical reaction are **reactants;** the substances formed are **products**. The reactants are written on the left side, separated by a plus sign, followed by an arrow, and products are on the right side of the arrow, as illustrated in Fig. 1.3.3. For example, the following chemical equation represents the combustion of methane.

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

Note that the chemical formula without any preceding number, e.g., O_2 and CO_2, represents one molecule or a unit amount of the chemical. The number preceding the formula is called the **coefficient**, and it represents the number of particles or the number of units involved. For example, the coefficient of 2 in $2H_2O$ in the above chemical equation represents two molecules of water formed or two moles of water formed, where the mole is the unit amount. Note that the chemical composition has changed in the chemical reaction. Before, one substance was carbon and hydrogen atoms in a 1:4 ratio, and the other substance was oxygen atoms. After the reaction, one substance is carbon and oxygen atoms in a 1:2 ratio, and the other is hydrogen and oxygen in a 2:1 proportion.

The physical state of matter is sometimes shown in a chemical equation by the following symbols: (s) for solid, (l) for liquid, (g) for gas, and (aq) for a substance dissolved in water, as illustrated in Fig. 1.3.3.

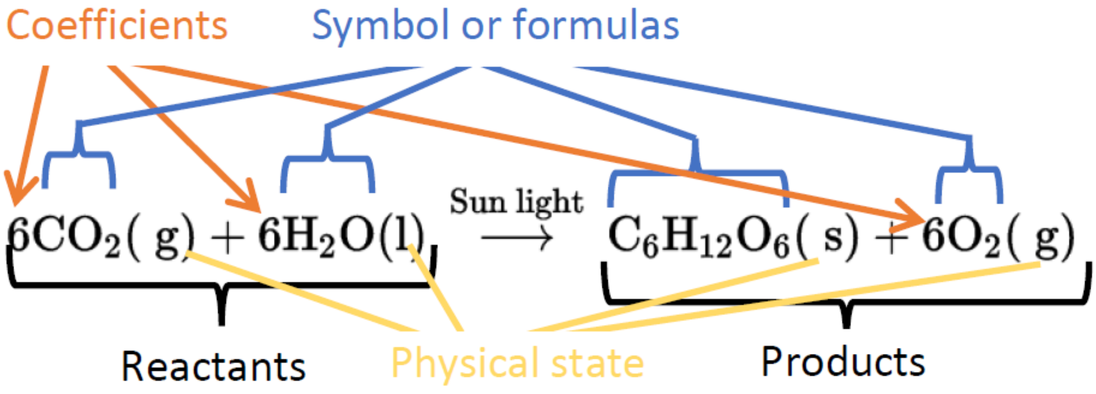


Figure 1.2.3: Components of a chemical equation (Copyright: Public domain).

Scientific method -how does science make progress?

Chemistry is one branch of science. Science knowledge is gathered systematically from generation to generation through the scientific method.

> The scientific method starts with making observations, giving a tentative explanation, i.e., hypotheses, testing the hypothesis, i.e., experiment, and deducing a conclusion from the investigation. A truth found through repeated experiments becomes a law, and a comprehensive explanation of related findings gathered over time becomes a theory.

Figure 1.2.4 illustrates these scientific method steps and is described below.

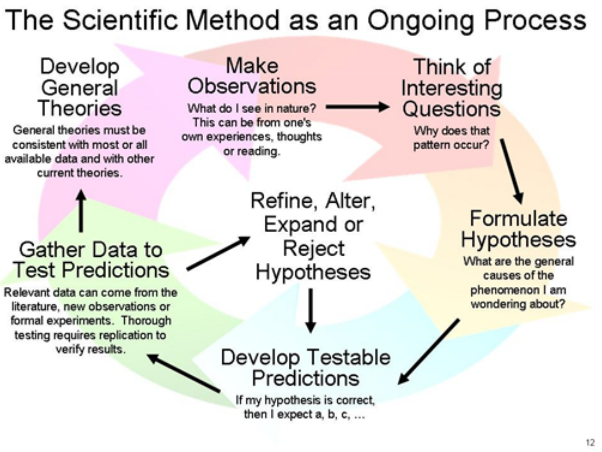


Figure 1.2.4: Illustration of the scientific method. Source: Whatiguana / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

Observation

Observation is the active acquisition of information from a primary source. For example, you fill the air in a car tire and notice that the pressure reading on the gauge increases. This is an observation.

Hypothesis

A hypothesis is a tentative explanation of the observation or a law based on available scientific knowledge. For example, John visits a friend and starts sneezing. The friend says I have a cat, and you might be allergic to cats. This tentative explanation of

John's sneezing is a hypothesis.

Experiment

Experiments test the hypothesis. For example, John visits another friend with a cat to determine whether he is allergic to cats. If he sneezes in this experiment, it supports the hypothesis. If he does not sneeze, the experiment disproves the hypothesis.

Conclusion

A hypothesis proven true becomes a conclusion. The hypothesis is rejected or revised if the experiment results do not support it. For example, scientists worldwide and in different periods attempted to convert other metals to gold and failed every time. It concluded that elements do not transform into the more simple matter by any physical or chemical reaction.

Law

It becomes law if an observation is universally true in repeated experiments. Examples of law are the following.

1. The pressure of any gas is directly proportional to the amount of gas if temperature and volume are kept constant, is Avogadro's law.
2. The proportion of atoms of different elements in a compound is always the same, a **law of constant proportion**.
3. Mass before any chemical reaction is the same as after the chemical reaction, i.e., mass is conserved in any chemical reaction or process, a **law of conservation of mass.**

Theory

A theory is a comprehensive explanation based on scientific principles to explain several laws and conclusions on a related topic. For example, the knowledge gathered over time on the properties of matter led Dalton to put forward Dalton's atomic theory.

Dalton's atomic theory

Postulates of Dalton's atomic theory are:

1. elements are composed of tiny indivisible particles called atoms;
2. atoms of any one element are identical to each other but different from atoms of any other element;
3. Atoms of different elements react with each other in a constant whole-number ratio to produce a compound;
4. atoms in a compound separate and recombine to give new material. Still, the atoms are neither created nor destroyed in the reaction.

These postulates explain the properties of the matter described in the previous sections. For example, elements can not convert to simpler substances by any physical or chemical process because they are composed of one type of atom, and atoms are indivisible according to the first postulate. Compounds can convert to elements by the chemical reaction because the atoms in the compounds can separate and recombine according to the fourth postulate.

What happens after a theory is accepted?

The theory goes through the test of time. If it keeps explaining the results of future experiments, it remains valid. It is either rejected or revised if it is disproved or cannot explain some observations of future investigations. For example, "atoms are not divisible" is no more considered valid. According to current knowledge, atoms can divide into **subatomic particles** like electrons, protons, and neutrons. However, the subatomic particles do not represent the element anymore.

"Atoms of the same element are the same" has been revised because isotopes are atoms of the same element that are different in some respects. The statement "atoms are neither created nor destroyed" is still valid for chemical reactions but does not hold in nuclear reactions where atoms of one element can convert to atoms of other elements. Similarly, matter can be converted into energy and vice versa in nuclear reactions, following Einstein's famous equation: $E = mc^2$, where E is energy, m is mass, and c is the speed of light. It means the law of conservation of mass and the law of conservation of energy are not valid individually in a nuclear reaction. Still, the mass and energy together are conserved in nuclear reactions. These are examples of revisions made in theory over time.

The theory is a basic knowledge that allows the prediction of new laws and leads to new ideas on related concepts. For example, Dalton predicted the law of multiple proportions, also known as Dalton's law, i.e., if atoms of two elements can combine in one whole number ratio to give a specific compound, they may also mix in another whole number ratio to give another compound.

Law of multiple proportions

When two elements form more than one compound, the proportions of the atoms of elements in those chemical compounds can be expressed in small whole-number ratios, or the ratio of the masses of the second element in the two compounds that combines with a fixed mass of the first, is a small whole number ratio.

For example, hydrogen and oxygen atoms can mix in a 2:1 ratio to provide water (H_2O). Still, they can also combine in a 2:2 ratio to give hydrogen peroxide (H_2O_2), a different compound. Similarly, carbon and hydrogen combine in a 1:4 ratio to make methane (CH_4); they can combine in a 2:6 ratio to make another ethane compound (C_2H_6).

1.3: Measurements

Measurements are an essential part of making observations needed to develop science. Several measurements are commonly done in everyday life, as illustrated in Fig. 1.3.1. The measured values have two components: a number and a unit.

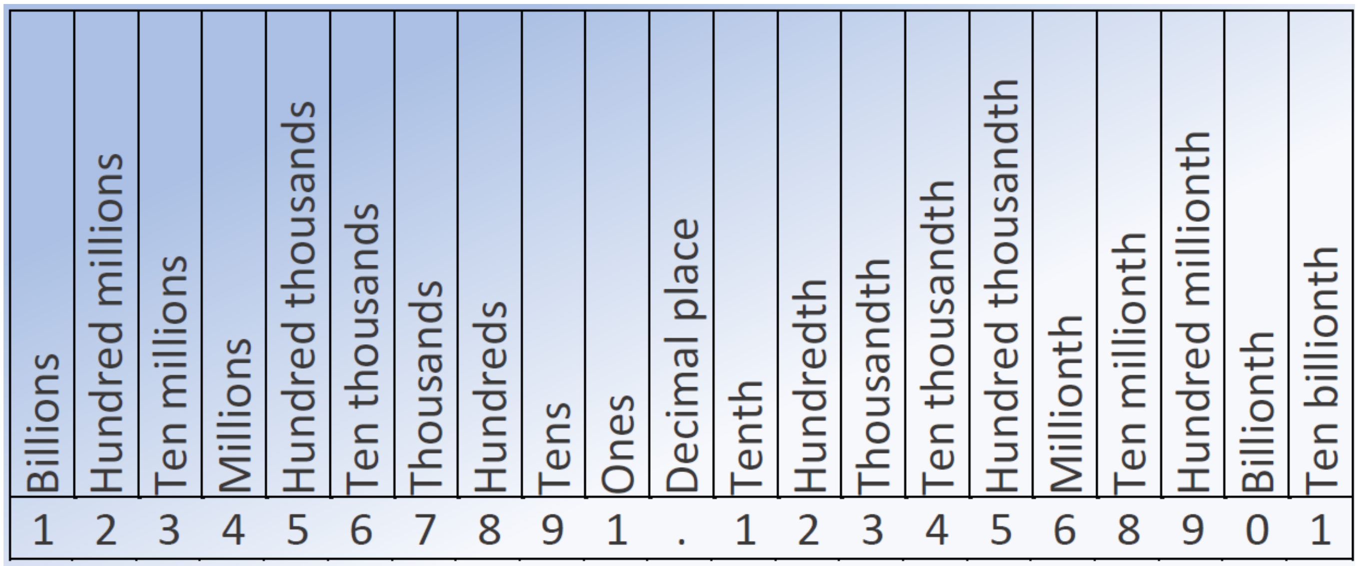
Figure 1.3.1: Measurements of mass, length, time, and temperature are part of daily life. Source: https://www.hiclipart.com/free-trans...xnlrr/download

Numbers

The numbers are composed of digits. The digits are 0, 1, 2, 3, 4, 5, 6, 7, 8, and 9. The digits are written in a row in the number, e.g., 123, which means one hundred and twenty-three. The numbers include a decimal point. If the decimal point is not marked, it is assumed to be present at the right of the number. For example, 123 is 123. by conversion, with the decimal point shown in red font.

Place value of a number

The digits have place values. The place values are relative to the decimal point, i.e., the 1st digit to the left of the decimal point is ones, the 2nd is tens, 3rd is hundreds, and so on. The digit 1st to the right of the decimal point is tenth, 2nd is a hundredth, 3rd is thousandth, and so, as shown in Fig. 1.3.2. For example, in 231.45, the digit 2 is hundreds, i.e., 200, 3 is tens, i.e., thirty, 1 is ones, that is one, 4 is tenth, i.e., four divided by ten, and 5 is hundredth, that is five divided by hundred.



Billions	Hundred millions	Ten millions	Millions	Hundred thousands	Ten thousands	Thousands	Hundreds	Tens	Ones	Decimal place	Tenth	Hundredth	Thousandth	Ten thousandth	Hundred thousandth	Millionth	Ten millionth	Hundred millionth	Billionth	Ten billionth
1	2	3	4	5	6	7	8	9	1	.	1	2	3	4	5	6	8	9	0	1

Figure 1.3.2: Place values of numbers.

Sign of a number

Numbers have signs, either +ve or -ve, to the left of a number, e.g., -23.4 and +430. By conversion, no sign means +ve. The signs are relative to zero; the -ve sign means the number is less than zero, and the +ve sign means the number is more than zero.

The number and the sign in calculations

The rules for the sign in a calculated answer are the following.

1. When two positive numbers add, the answer has a +ve sign, e.g., 3+2 = 5.
2. When two negative numbers add, the answer has –ve sign, e.g., -4 + (-2) = -6.
3. When two numbers having opposite signs add, subtract the smaller number from the larger number, and the answer has the sign of the larger number. For example, -5 +3 = -2.
4. In subtraction, change the sign of the subtracted number and then follow the addition rules. For example, subtract 3 from 5: 5-(+3) = 5-3 = 2. Note that 3 is subtracted, and its sign changed before operating addition. Another example: subtract -6 from 2: 2-(-6) = 2+6 = 8
5. When two positive numbers multiply, the answer has a +ve sign, e.g., 2x3 = 6.
6. When two negative numbers multiply, the answer has a +ve sign, e.g., (-4) x (-3) = 12.
7. When the two numbers multiplied have opposite signs, the answer has a –ve sign, e.g., (-3) x 2 = -6 and 4 x (-4) = -16.
8. When a number is divided by another number, it follows multiplication rules for the sign. For example, $\frac{-4}{-2}=2,\quad \frac{4}{2}=2,\quad \frac{-4}{2}=-2,$ and $\frac{9}{-3}=-3$.

Figure 1.3.3: Battery % remaining.

Percentage calculations

The percentage (%) is the part out of a hundred, as illustrated in Fig. 1.3.3. The percentage is calculated as part divided by the total and then multiplied by a hundred, i.e.:

$$\text{percentage }\% = \frac{\text{Part amount}}{\text{Total amount}} \times 100$$

✓ Example 1.3.1

Calculate the percentage of aspirin if there is 81 mg aspirin in a 325 mg tablet?

Solution

part = 81 mg aspirin, Total = 325 mg tablet

Formula:

$$\text{percentage } = \frac{\text{Part amount}}{\text{Total amount}} \times 100$$

Plug in values in the formula and calculate:

$$\text{Percentage } = \frac{81\text{mg aspirin}}{325\text{mg tablet}} \times 100 = 25\%\text{ aspirin}$$

✓ Example 1.3.2

A piece of 18K green color gold jewelry has 7.5 g gold, 2.0 g silver, and 0.5 g copper. Calculate the percentage of gold in the jewelry?

Solution

Part = 7.5 g gold, Total = 7.5 g gold + 2.0 g silver + 0.5 g copper = 10 g jewelry.

Plug in values in the formula and calculate:

$$\text{percentage } = \frac{\text{Part amount}}{\text{Total amount}} \times 100 = \frac{7.5\text{ggold}}{10\text{ g}} \times 100 = 75\%\text{gold}$$

Writing numbers in scientific notation

Sometimes the given number is too large or too small to be easily written, read, and grasped. Scientific notation is one approach to changing a too large or a too-small number into an easily readable and writable number. The following steps convert a given number to scientific notation.

> 1. Move the decimal point to the right or the left side, one digit at a time, till the largest non-zero digit becomes one's place.
>
>   For example, move the decimal in 12,700,000 seven times to the right  to obtain 1.27, and move the decimal in 0.000,006 six-time to the left  to get 6. The numbers 1.27 and 6 obtained are the coefficients of the scientific notation.
> 2. The coefficient is multiplied by 10^x, where x is a power of ten. The power of ten equals the number of times the decimal moved. The sign of the power is +ve if the decimal moved to the left and -ve if the decimal moved to the right. For example, 12,700,000 in scientific notation is 1.27×10^7, and 0.000,006 is 6×10^{-6}.

Units

Physical properties like mass, length, and temperature are measured. The measured value is a combination of a number and a unit, as illustrated in Fig. 1.3.4. For example, a person's height is 1.83 meters, where 1.83 is a number and a meter is a unit.

> Units are quantities defined by the standard that peoples agree to use as a reference.

For example, the meter is defined as the distance light travels in a vacuum in $\frac{1}{299,792,458}$ of a second.

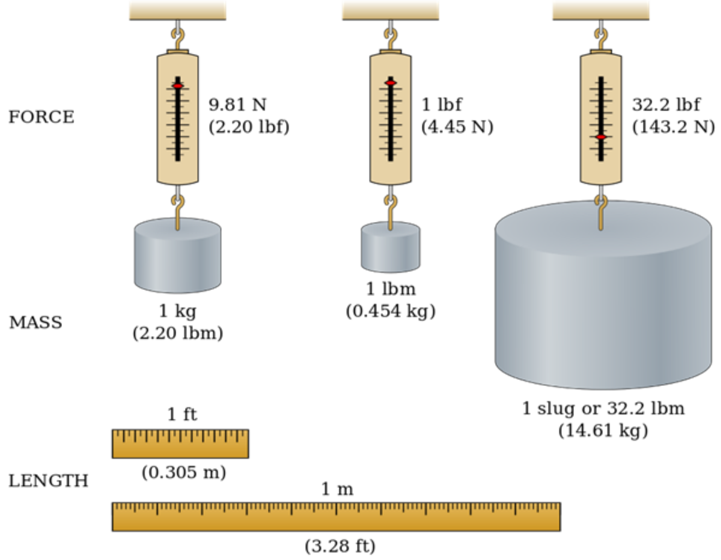


Figure 1.3.4: Measurement is a combination of a number and a unit. Source: https://www.hiclipart.com/free-trans...lzufr/download

Systems of units

There are different sets of units used in different systems of units. For example, 1.83 meters and 6.00 feet show the same length value but using a unit of ‘meter’ from the international system of units (SI) and ‘foot’ from the English system of units. The international system of units (SI) is universally used in scientific work. There are seven base units in SI, as listed in Table 1.

Table 1: Base units in the International System of Units (SI).

Measurement	**Unit**	**Abbreviation**
Time	second	s
Length	meter	m
Mass	kilogram	kg

Measurement	Unit	Abbreviation
Temperature	kelvin	K
Amount of substance	mole	mol
Electric current	ampere	A

Note

The following section is based on the 2019 redefinition of the SI base units: https://en.Wikipedia.org/wiki/2019_redefinition_of_the_SI_base_units#Kilogram, accessed on May 2nd, 2020

Time

Time is the progress of existence and events that occur in succession from the past through the present to the future.

In old times, the time measuring device was the hour sandglass shown in Fig. 1.3.5. The basic unit of time is second (s), a standard unit of time in all the measurements systems. Other units of time are minute (min) which is equal to 60 s, and hour which is equal to 60 min or 3600 s.

Definition: Second

The duration of 9,192,631,770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the cesium 133 atoms at a temperature of 0 K.

Figure 1.3.5: German; Half-hour sandglass; Horology. Source: Metropolitan Museum of Art / CC0

Length

Length is a measure of distance, i.e., a numerical measurement of how far apart the objects or points are.

Fig. 1.3.6. illustrated the concept of length. The SI unit of length is a meter (m).

Meter

The meter is defined as the distance that light travels in a vacuum in $\frac{1}{299,792,458}$ of a second.

Figure 1.3.6: Measure of length. Source: https://www.hiclipart.com/free-trans...nhlxx/download

Mass

> The mass of an object is a measure of its inertia.

Inertia is the resistance of any physical object to any change in its velocity. Mass determines the strength of the gravitational attraction of an object to another object -a property commonly used in modern balances for mass measurements, as shown in Fig. 1.3.7. SI unit of mass is the kilogram (kg).

> **Kilogram**
>
> Earlier definition: The mass of one cubic decimeter of water at the melting point of ice.
>
> Current definition: Kilogram (kg) is defined by taking the fixed numerical value of the Planck constant h to be $6.62607015 \times 10^{-34}$ when expressed in the unit $kg{\cdot}m^2{\cdot}s^{-1}$.

Figure 1.3.7: Laboratory Analytical balance. Source: https://www.hiclipart.com/free-trans...bbigu/download

Temperature

Temperature is a physical property of matter that expresses hotness or coldness, as illustrated in Fig. 1.3.8.

> Temperature is a manifestation of the thermal energy of the matter, which is a source of the flow of energy in the form of heat from a hot object to a cold object when they are in contact with each other.

The SI unit of temperature is Kelvin (K).

Kelvin

Kelvin (K) is defined by taking the fixed numerical value of the Boltzmann constant k to be 1.380649×10^{-23} when expressed in the unit $kg{\cdot}m^2{\cdot}s^{-2}{\cdot}K^{-1}$.

A 0 K, also called absolute zero, is the temperature of a matter at which no energy can be removed as heat from the matter. The freezing point of water is 273.15 K, and the boiling point of water is 373.15 K.

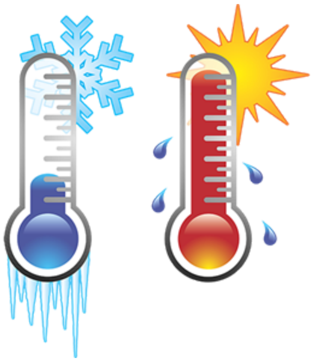


Figure 1.3.8: An illustration of temperature. Source: https://www.hiclipart.com/free-trans...txxww/download

Amount of substance

In chemistry, the amount of substance (n) measures the number of specified elementary entities. The elementary particles in chemistry are usually atoms in the case of elements and molecules or formula units in the case of compounds. SI unit of the amount of a substance is a mole (mol).

Mole (mol)

Mole is exactly 6.02214076×10^{23} elementary entities.

Fig. 1.3.9 illustrates one mole of aluminum, copper, and carbon. The molar mass is the mass in grams of one mole of that substance, i.e., the mass of 6.02214076×10^{23} atoms or molecules. Usually, the number of particles is shown with four significant figures, i.e., 6.022×10^{23} atoms or molecules in one mole of the substance.

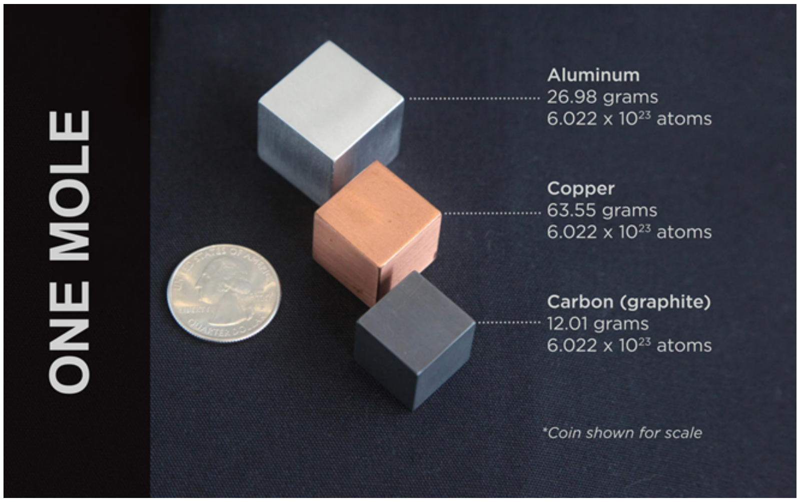


Figure 1.3.9: Amount in one mole of aluminum, copper, and carbon shown relative to US Quarter coin.

Source: Public information, photo: R. Press/NIST; graphic design: N. Hanacek/NIST

Electric current

> Electric current is the flow rate of electric charge past a point or a region.

It could be the flow of electrons in electric wires or the flow of cations and anions in opposite directions as in electrolytes, as illustrated in Fig. 1.3.10. The SI unit of current is ampere (A).

Definition: Ampere (A)

Ampere (A) is defined by taking charge of an electron (e) to be $1.602176634\times10^{-19}$ coulomb (C), where C is equivalent to ampere-second (A.s).

Figure 1.3.10: Illustration of the definition and direction of electric current, i.e, the current (I) is the rate of flow charges (Q) per unit time (t). Source: And1mu/ CC-BY-SA-4.0, https://commons.wikimedia.org/wiki/F...ricCurrent.gif

Luminous intensity

> Luminous intensity measures the wavelength-weighted power emitted by a light source in a particular direction per unit solid angle.

The solid angle is measured in steradian (sr), analogous to the radian. The radian is a planar angel that gives the length of the circumference of a circle, and the steradian is a 3D angle, like a cone, that gives an area on the surface of a sphere, as shown in Fig. 1.3.11.

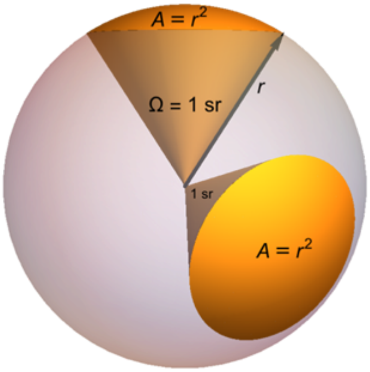


Figure 1.3.11: A solid angle is a three-dimensional analog of a circular angle that relates a portion of the volume of a sphere to the surface area it subtends. If that area equals the sphere’s radius squared, the solid angle is one steradian. This diagram displays two solid angles of one steradian, viewed from different directions. Source: Andy Anderson / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

SI unit of luminous intensity in a given direction is Candela (cd).

Candela (cd)

Candela (cd) is defined by taking the fixed numerical value of the luminous efficacy of monochromatic radiation of frequency 540×10^{12} Hz, K_{cd}, to be 683 $cd\cdot sr\cdot W^{-1}$, or $cd\cdot sr\cdot kg^{-1}\cdot m^{-2}\cdot s^{3}$, where **W is watt** –a SI unit of power described by $kg.m^{2}.s^{-3}$.

Prefixes in SI

In several situations, the measured number with the base unit is either too large or too small. For example, a person's height is comfortable to represent in the meter as the height is usually in a 1 m to 2 m range. However, the diameter of the earth, i.e., 12,700,000 m, and the diameter of red blood cells, i.e., 0.000,006 m, are too large and too small, respectively. The unit needs to be revised so that the number with it is easy to read and write.

> Prefixes are used in SI to increase or decrease the base unit by order of tens.

For example, kilo (k) means a thousand times, i.e., 1 km means 1000 m and 1 kg means 1000 g. Similarly, micro (µ) means one-millionth time, i.e., 1 µm is 10^{-6} m, and 1 µg is 10^{-6} g. Table 2 lists commonly used prefixes in SI.

Table 2: Commonly used prefixes in SI (note: m means "meter" in SI units, but as a prefix, it means "mili")

Prefix	**Means**	**Abbreviation**
Gega	10^9	G
Mega	10^6	M
Kilo	10^3	k
Deci	10^{-1}	d
Centi	10^{-2}	c
Mili	10^{-3}	m
Micro	10^{-6}	µ
Nano	10^{-9}	n
Pico	10^{-12}	p

A new unit may be defined and used if there is no appropriate prefix available in SI for some specific type of measurement. For example, the diameter of atoms varies in the range of 1 x 10^{-10} m to 5 x 10^{-10} m, where the prefix pico (p, 10^{-12}) is too small, and the prefix nano (n, 10^{-9}) is large. A new unit called **angstrom** (Å) is defined as 1Å = 10^{-10} m for reporting atomic diameter and inter-atomic distances.

Derived units

> The units in SI other than the seven base units are Derived units obtained by combining the base units.

For example, The SI unit of volume is meter-cube (m^3), equal to the space occupied by a cube of 1m on each edge, as illustrated in Fig. 1.3.12.

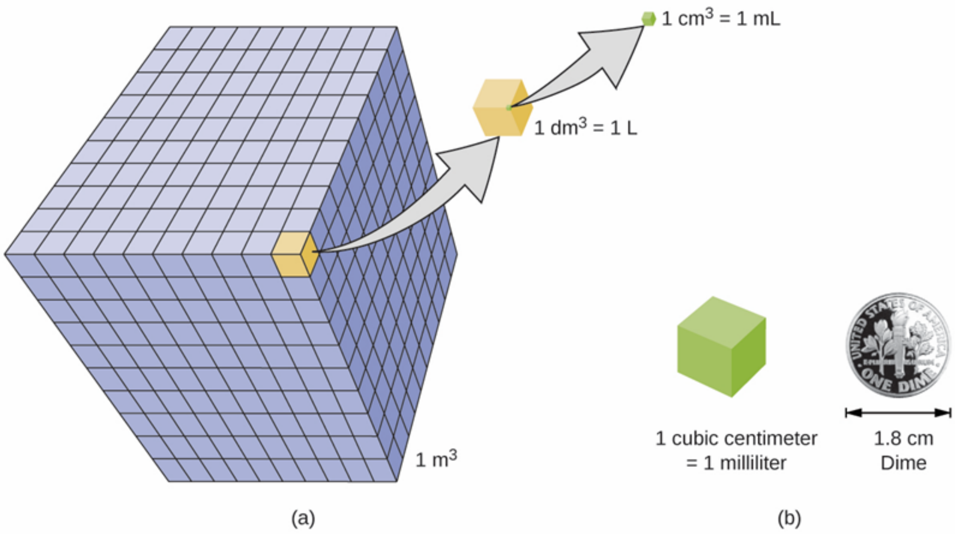


Figure 1.3.12: Relative volume in m^3, dm^3 and cm^3. Diagram of a 10x10x10 cubes. The small cubes represent one decimeter-cube (dm^3); the big cube represents one meter-cube (1 m^3). The purpose is to show that even though there is 10 dm in 1 m, there are 1000 dm^3 in 1 m^3. More generally, it shows that the conversion factor between units of volume is the cube of the conversion factor between corresponding length units. Source: Download for free at https://openstax.org/details/books/chemistry

Usually, the volume is reported in decimeter-cube (dm^3), commonly known as liter (L). One liter is a volume occupied by a cube that is one dm on each edge. Another commonly used unit of volume is the centimeter-cube (cm^3), which is also called cc or mL.

One mL is the volume occupied by a cube that is one cm on each edge. The dm^3 is a thousandth of m^3, and cm^3 is the thousandth of $dm^{3,}$ i.e., 1000 dm^3 = 1 m^3, and 1000 cm^3 = 1 dm^3, as illustrated in Fig. 1.3.11.

Relationship of SI units with metric and English system of units

SI was developed from the metric system. Some basic units are different, but both systems have much in common, using the same prefixes. The English system of units uses a different set of units except for the common unit of time. Table 3 compares the standard measuring units in the three systems of measurement.

Table 3: Common measurement units in three conventional systems of measurements

Quantity	English unit	Metric unit	SI unit	Relationships
Mass	Pound (lb)	Gram (g)	Kilogram (kg)	1 kg = 2.205 lb 1 kg = 1000 g
Length	Foot (ft)	Meter (m)	Meter (m)	1 m = 3.281 ft
Volume	Quart (qt)	Liter (L)	Cubic meter (m^3)	0.946 L = 1 qt 1 m^3 = 1000 L
Energy	calorie (cal)	calorie (cal)	Joule (J)	4.184 J = 1 cal
Temperature	Degree Fahrenheit (°F)	Degree Celsius (°C)	Kelvin (K)	°F = (1.8 × °C) + 32 K = °C + 273.15

1.4: Significant Figures

Significant figures are related to errors associated with the measured numbers. It is important to understand the significant figures because when calculations are made using numbers with errors, the answer cannot have less error than the error in any original number. The answer needs correction for the significant figures.

Precision and accuracy

The measured numbers have two types of errors, systematic and random errors, that determine the accuracy and precision of the measured number, as illustrated in Fig. 1.4.1.

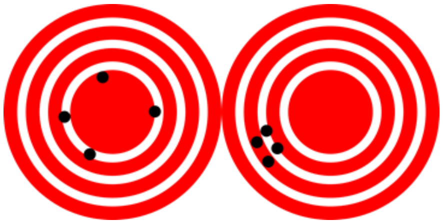


Figure 1.4.1: Representation of high accuracy with less precision (left) and low accuracy with high precision (right). Source: DarkEvil / Public domain

Systematic errors

Systematic errors are constant, i.e., they have the same value in every measurement. For example, meter rod is a little short or a little long than a meter, it will introduce a systematic error. Systematic errors usually happen due to inaccurate calibration of the measuring instrument. The systematic errors determine how much the measured value differs from the actual value.

Random errors

Random errors are the statistical variability of the measured number. Random errors vary from one observation to another. Random errors cancel out if many measurements are taken and averaged. Scientific measurements are usually taken at least in triplicate and averaged to minimize random errors. The random errors determine how close the repeat measured numbers are to each other.

Accuracy

> Accuracy or trueness of the measurement is defined as how close the average value is to the actual value.

The closer the average is to the actual value, the more accurate or true it is, as illustrated in Fig. 1.4.1. The trueness depends on systematic errors, i.e., less systematic error, more accurate the average.

Precision

> Precision is defined as how close the individual measurements are to each other.

The closer the individual values are to each other, the more precise the measurement is, irrespective of whether it is accurate or not, as illustrated in Fig. 1.4.1. Precision depends on random errors, i.e., more substantial random errors mean less precision.

Exact and inexact number

There are two types of numbers, count numbers that are exact and measured numbers that are inexact.

> If the value is a counted number, it is an **exact number**.

That is, there is no error in it. For example, a purchase of one dozen oranges contains exactly 12 nos of oranges; it can not be 11.5 or 12.5.

Inexact numbers and error range

When a value is measured, it comes with an error of measurement.

> A measured number with an error is called an **inexact number**.

For example, when the same one dozen oranges are purchased by mass, the balance may read it 1572.6 g, or 1573 g, or 1570 g, depending on whether the smallest digit that the balance displays is 0.1g, 1 g, or 10 g. Suppose the balance is accurate to 1 g and reports the mass 1573 g; the actual mass may be anywhere in the range of 1572.5g-to-1573.4g. The smallest measured digit, i.e., the number in one's place, in this case, is an **estimated number** associated with an error. By convention, the estimated digit has ±1 errors associated with it. For example, the above-mentioned measured numbers are reported in science as 1572.**6** g ± 0.1 g, 157**3** g ± 1 g, or 15**7**0 g ± 10 g, respectively. The estimated digits are shown in bold fonts in the examples.

The smallest digit in the display of digital instruments is an estimated number. In measurement using instruments that do not have a digital display, the smallest digit marked on the instrument plus one digit less than the minimum marked digit is added to the reported value. The smallest reported digit is an estimated digit. For example, the length of the pencil in Fig 1.4.2 is reported as 17.**7** cm using the ruler on the bottom, where 17 includes the smallest digit marked on the ruler, and the last digit, i.e., 0.7 is an estimated digit. By convention, the error range in this value is shown as 17.**7** ± 0.1. The same length is 17.7**0** cm using the ruler on the top in Fig. 1.4.2l, where 17.7 includes the smallest digit marked on the ruler, and the last reported digit, i.e., 0, is an estimated digit. By convention, the error range in this value is shown as 17.7**0** ± 0.01. The estimated digits are marked in bold fonts.

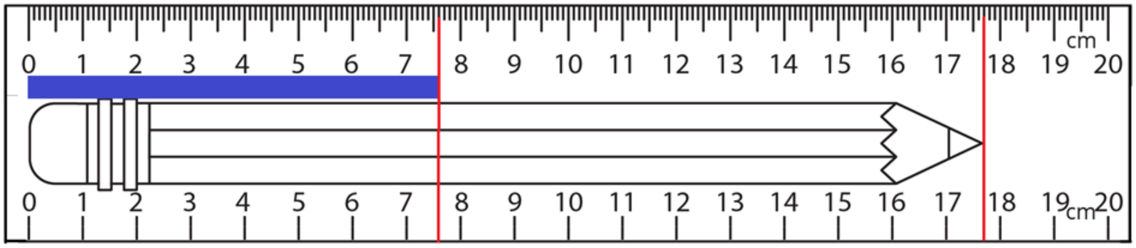


Figure 1.4.1: Illustration of measurements that yield inexact numbers. The length of a blue rectangle is 7.6**0** ± 0.01 cm by using a more accurate ruler on the top and 7.**6** ±0.1 cm by using a less accurate ruler on the bottom. The estimated digit is marked in bold fonts.

Rules to determine the significant figures in measured numbers

Significant figures

All the digits reported in the measured value, including the estimated digit, are significant figures (SF).

For example, 1572.6 g, 1573 g, and 1570 g have significant figures of 5, 4, and 3, respectively.

Caution

Note that zero in the last reading 1570g is not significant; it is a placeholder zero that is needed to place the estimated digit 7 at tens place.

It is crucial to find significant figures in measured numbers because, when they are used in calculations, the answer cannot have less error than the maximum error in any measured number used in the calculation. The rules to determine the significant numbers in a measured number are the following.

1. All non-zero digits are significant, e.g., 1572 has 4 SFs. The zeros may or may not be significant. In the following examples, the zeros in bold fonts are nonsignificant.
2. Zeros between non-zero digits are significant, e.g., 1305.6 has 5 SFs.
3. Leading zeros are not significant, e.g., **0.0**134 has 3 SFs.
4. Trailing zeros are not significant if there is no decimal point present, e.g., 157**0** has 3 SFs. Trailing zeros are significant if the decimal point is present, e.g., 1570. has 4 SFs because the decimal point is present. Similarly, **0.0**124 has 3 SFs, but **0.0**1240 has 4 SFs because the decimal point is present.
5. Confusion arises when more than one trailing zeros and the decimal point is absent. For example, 1500 g has 2 SFs by convention, but if the balance was accurate to 10 g, one of the zero was an estimated digit and was significant. Converting the number to a scientific notation resolves this issue. The coefficient part of the scientific notation shows all the significant figures in the measurement. For example, the number 1500 g, if shown in scientific notation as 1.5 x 10^3 has 2 SFs, but the same number shown as 1.50 x 10^3 has 3 SFs.

Rounding the calculated answer involving inexact numbers

When inexact numbers are used in calculations, the answer needs to be rounded to an appropriate number of significant figures, determined by the following rules.

Rules of rounding

1. A number is rounded by keeping the larger digits equal to significant figures and dropping or replacing the remaining smaller digits with placeholder zeros. The placeholder zeros are in bold fonts in the following examples. For example, 13543 becomes 135**00** when rounded to three significant.
2. If the largest digit dropped is 4 or less than 4, it is simply dropped. For example, 23145 becomes 231**00**, when rounded to three significant figures.
3. If the largest digit dropped is 5 or more than 5, then the smallest digit retained is increased by one. For example, 13543 becomes 14**000** when rounded into two significant figures.

Rules for determining the significant figures in a calculated answer

In the following rules, the track of significant figures that dictate the significant figures in the answer is kept by using bold fonts.

1. In addition and subtraction, the answer has the same number of decimal places as the number with the smallest number of decimal places in the original numbers. For example, 13.**2** + 12.252 = 25.**4**52 is rounded to 25.**5** to keep one decimal place.
2. In multiplication and division, the answer has the same number of significant figures as the original number with the smallest number of significant figures. For example, 1.35 x **2.1** = **2.8**35 is rounded to 2.8.

Note

If mathematical operations are performed in a series of steps, keep track of the significant figures but do not round off intermediate answers. Carry as many digits as possible from the intermediate answers to the next calculation step. Round off the final answer following the above rules. For example, (13.**2** + 12.252) x (1.35 x **2.1**) = **25.4**52 x **2.8**35 = **72**.15642 is round to 72 in agreement with **2.8**35 that should have been rounded to 2.8 in a one-step calculation. Rounding the intermediate answers will lead to incorrect final answer of 71 instead of more correct 72, i.e. (13.2 + 12.252) x (1.35 x 2.1) = 25.5 x 2.8 = 71

Caution

Exact numbers have an unlimited number of significant figures, which means they do not restrict the significant figures in the calculated answer.

Example 1.4.1

If 12 oranges weigh 1572.6 g calculate the mass of 1 orange in grams?

Solution

$$1572.6 \text{ g}/12 = 131.05 \text{ g}$$

Explanation: The answer has 5 SFs because 12 is a counted number and exact. The only inexact number in the calculation that dictates the significant figures in the solution is 1572.6, which has 5 SFs.

Example 1.4.2

One dozen oranges were were sold 11 times. Calculate the total oranges sold?

Solution

$$12 \times 11 = 132 \text{ oranges}$$

> Explanation: The answer is not rounded because both the numbers in the calculation are exact, so the answer is also exact with unlimited significant figures.

1.5: Unit conversions

Conversion of values in one unit to the same value in another unit, as illustrated in Figure 1.5.1 is often needed in scientific calculations. The unit conversion includes the following.

- Conversion of the same type of measurement in the same system of measurement, e.g., conversion of a measured value of the length in meters to kilometers in SI;
- conversion of the same type of measurement in different systems of measurements, e.g., conversion of a measured value of the length in kilometers from SI to miles in the English system; and
- conversion of one type of measurement to another type of measurement, e.g., conversion of a measured value of the mass in g to volume in mL of a substance using the density of the substance.

Figure 1.5.1: Illustration of unit conversions. Source: https://www.hiclipart.com/free-trans...fksbi/download

Conversion factors

The conversion factors are derived from equality between the given unit and the desired unit. For example, 1 cm = 10^{-2} m is equality between centimeter and meter. The conversion factors are derived from the equality by the following steps.

Both sides of the equality are divided by one side to get one conversion factor. For example, $1=\frac{10^{-2}\ m}{1\ cm}$, which is a conversion factor for cm to m.

Then both sides are divided by the other side of the equality to get the second conversion factor. For example, $1=\frac{1\ cm}{10^{-2}\ m}$, which is a conversion factor for m to cm.

Since both the conversion factors are equal to one, multiplying a value with a conversion factor changes the number and the unit, such that the new number and the new unit together represent the same value. The unit of the given number should be opposite to the same unit in the conversion factor, i.e., numerator versus denominator or denominator versus numerator, to cancel them out and leave the desired unit in the answer. For example, 1.83m is converted to cm unit using the conversion factor $\frac{1\ cm}{10^{-2}\ m}$ as:

$$1.83\ \cancel{\text{m}}\times\frac{1\ \text{cm}}{10^{-2}\ \cancel{\text{m}}}=183\ \text{cm}$$

Keep track of the units that cancel out and the unit left in the answer. If all the units cancel out, leaving only the desired unit means the chosen conversion factor is correct. An incorrect conversion factor leads to an unwanted unit in the answer, e.g., in the above calculation if incorrect conversion factor is chose, it will lead to:

$$1.83\ m\times\frac{10^{-2}\ m}{1\ \text{cm}}=0.0183\frac{\text{m}^2}{\text{cm}}$$

, where no unit is canceled and the answer has units that are not the desired. It means an incorrect conversion factor was employed.

Converting the same type of measurement in the same system

The prefixes in the SI, listed in section 1.3 Table 2, establish equality between the base and the prefixed units. For example, centi (c) means 10^{-2}. Therefore

$$1\ \text{cm}=10^{-2}\ \text{m}$$

1cm = 10^{-2} m is an equality that gives two conversion factors:

$$\frac{1\ cm}{10^{-2}\ m} \text{ and } \frac{10^{-2}\ m}{1\ cm}$$

Some of the common qualities in SI are listed in Table 1 and the English system in Table 2.

Note

The prefixes are exact numbers. The equalities within the same system of measurement are exact numbers. Therefore the equalities and the conversion factors derived from them are exact numbers. Significant figures in the answers involving exact and inexact numbers are dictated by inexact numbers only.

Example 1.5.1

Convert 325 cm to m units?

Solution

$$325\ \cancel{cm} \times \frac{10^{-2}\ m}{1\ \cancel{cm}} = 3.25\ m$$

Note that in this example, the answer has the significant figures the same as in the given number because the conversion factor within the same system of measurement is numbers.

Table 1: Some of the common equalities in SI

Length	Mass	Volume
1 km = 1,000 m	1 kg = 1,000 g	1 L = 10 dL
1 m = 100 cm	1 g = 1,000 mg	1 L = 1,000 mL
1 m = 1,000 mm	1 mg = 1,000 µg	1 L = 1,000,000 µL
1 cm = 10 mm	10-1	1 dL = 100 mL
		1 mL = 1 cm^3 = 1 cc

Table 2: Some of the common equalities in the English System

Length	Mass	Volume
ft = 12 in.	1 lb = 16 oz	1 qt = 4 cups
1 yd = 3 ft	1 ton = 2,000 lb	1 qt = 2 pints
1 mi = 5,280 ft		1 qt = 32 fl oz
		1 gal = 4 qt

Conversion of the same type of measurement in different systems

Table 3 lists some common qualities between SI and the English systems.

> These equalities between different systems usually have one side in the equality, which is the number 1, as exact, while the other side is considered an inexact number.

For example, 1 kg = 2.205 pounds (lb) has an exact number (1 kg) on the left side but an inexact number (2.205 lb) with 4 SFs on the right. Remember that only the inexact numbers dictate the significant figures in the answer.

> There are some exceptions to the above general rule. Some equalities between units in different systems are defined and considered exact. They are stated to be exact in the reference tables.

For example, 1 inch = 2.54 cm is defined, which means both sides are the exact number.

Table 3: some of the common SI-to-English system equalities

Length	Mass	Volume
2.54 cm = 1 in. **defined and exact**	1 kg = 2.20 lb	946 mL = 1 qt
1 m = 39.4 in.	454 g = 1 lb	1 L = 1.06 qt
1 km = 0.621 mi	28.4 g = 1 oz	29.6 mL = 1 fl oz

Conversion of one type of measurement to another

Sometimes, equality between two different units is known under specific conditions. For example, **density (d)** which is mass (m) per unit volume (V), is a relationship between mass and volume of a given substance, i.e., $d = \frac{m}{v}$. The density is a conversion factor used to convert the volume to the mass of a substance. Reciprocal density, i.e., $\frac{1}{d} = \frac{v}{m}$, is the second conversion factor that converts the mass to the volume of the substance.

✓ Example 1.5.2

The density of ethanol at 20 ^{o}C is 0.7893 g/mL; what is the mass of 10.0 mL of ethanol?

Solution

Multiply the given volume with the conversion factor that has volume in the denumerator, i.e., \(frac{m}{v} to get the mass desired.

$$10.0\ \cancel{\text{mL}} \times \frac{0.7893\ \text{g}}{1\ \cancel{\text{mL}}} = 7.89\ \text{g}$$

Note that 1mL is exact, and 10.0 and 0.7893 are inexact numbers with 3SF and 4 SF, respectively. The answer has 3 SFs.

✓ Example 1.5.3

The density of gold is 19.30 g/mL; what is the volume of 10.123 g of gold?

Solution

Multiply the given mass with the conversion factor that has a mass in the denumerator, i.e., $fracvm$ to get the mass desired.

$$10.123\ \cancel{\text{g}} \times \frac{1\ \text{mL}}{19.30\ \cancel{\text{g}}} = 0.5245\ \text{mL} \tag{1.5.1}$$

Conversion factors derived from chemical equations

Chemical equations show relationships or equalities between reactants and products measured in **moles**. Mole is a SI unit for the amount of substance. Mole equals 6.02 x 10^{23} particles (atoms or molecules) of the substance. Like dozen means 12 of something, mole means 6.02 x 10^{23} atoms of element or molecules/formula units for compounds in a chemical equation.

> For calculations in chemistry, the number of moles of a substance is considered equal to its coefficient in a balanced chemical equation.

For example:

$$2\,H_2 + O_2 \longrightarrow 2\,H_2O$$

gives the following equalities and their corresponding conversion factors:

1. equality: 1 mole O_2 = 2 moles H_2, conversion factors: $\frac{1\ \text{mol}\ O_2}{2\ \text{mol}\ H_2}$ and $\frac{2\ \text{mol}\ H_2}{1\ \text{mol}\ O_2}$
2. equality: 1 mole O_2 = 2 mole H_2O, conversion factors: $\frac{1\ \text{mol}\ O_2}{2\ \text{mol}\ H_2O}$ and $\frac{2\ \text{mol}\ H_2O}{1\ \text{mol}\ O_2}$ and

3. equality: 2 moles H_2 = 2 moles H_2O, conversion factors: $\frac{2\ \text{mol}\ H_2}{2\ \text{mol}\ H_2O}$ and $\frac{2\ \text{mol}\ H_2O}{2\ \text{mol}\ H_2}$.

The use of these conversion factors in the calculation is explained in the following example.

✓ Example 1.5.4

If 5 moles of oxygen (O_2) is consumed, how many moles of water are produced by the chemical equation mentioned above?

Solution

Given: 5 mol O_2, Desired: ? mol H_2O

Multiply the given quantity with the conversion factor that has the given unit in denumerator and the desired unit in the numerator:

$$5.0\ \cancel{\text{mole}\ O_2} \times \frac{2\ \text{mole}\ H_2O}{1\ \cancel{\text{mole}\ O_2}} = 10\ \text{mole}\ H_2O$$

Unit conversion involving more than one conversion factor

Often, there is no direct conversion factor between the given unit and the desired unit. In this situation, convert the given unit to another unit that can, later on, be linked with the desired unit, as explained in the following examples.

✓ Example 1.5.5

How many μg are in 10.0 mg?

Solution

Problems like this can be solved in two steps: i) by converting the given unit to the base unit and then, ii) converting the base unit to the desired unit:

$$10.0\ \cancel{mg} \times \frac{10^{-3}\ g}{1\ \cancel{mg}} = 1.00 \times 10^{-2}\ g$$

$$1.00 \times 10^{-2}\ \cancel{g} \times \frac{1\ \mu g}{10^{-6}\ \cancel{g}} = 1.00 \times 10^{4}\ \mu g$$

Note that the first conversion factor converts mg to g, and then the second conversion factor converts g to the desired unit μg. The same calculation can be done using two conversion factors in a rwo:

$$10.0\ \cancel{\text{mg}} \times \frac{10^{-3}\ \cancel{\text{g}}}{10\ \cancel{\text{mg}}} \times \frac{1\ \mu g}{10^{-6}\ \cancel{\text{g}}} = 1.00 \times 10^{4}\ \mu g$$

✓ Example 1.5.6

What is 100. km/h speed in m/s, where h represents hours?

Solution

This problem asks to convert two units, i.e., km to m and h to s. First convert one unit and then follow on to convert the second unit as:

$$\frac{100.\ \cancel{\text{km}}}{\cancel{\text{h}}} \times \frac{10^{3}\ \text{m}}{1\ \cancel{\text{km}}} \times \frac{1\ \cancel{\text{h}}}{60\ \cancel{\text{min}}} \times \frac{1\ \cancel{\text{min}}}{60\ \text{s}} = 27.8\ \text{m/s}$$

Note that the first conversion factor converts km to m, and then two conversion factors are needed to convert h to s via min.

✓ Example 1.5.7

A prescription says a dosage of 0.225 mg of Synthroid to be taken once a day. If tablets in stock contain 75 µg of Synthroid, how many tablets are needed per day?

Solution

The given mass is in mg, while the equality "1 tablet = 75 µg" takes mass in µg. First convert mg to base unit, i.e., g, then from g to needed unit, i.e., µg, and finally take appropriate conversion factor from the two given by the equality to convert µg to tablet, i.e., three conversion factors in a row:

$$0.225\ \cancel{\text{mg}} \times \frac{10^{-3}\ \cancel{\text{g}}}{1\ \cancel{\text{mg}}} \times \frac{1\ \cancel{\mu\text{g}}}{10^{-6}\ \cancel{\text{g}}} \times \frac{1\ \text{tablet}}{75\ \cancel{\mu\text{g}}} = 3.0\ \text{tablet}$$

✓ Example 1.5.8

A healthy person has 16% body fat by mass. Calculate the mass of fat in kg of a person who weighs 180. lb?

Solution

Given: mass of a person = 180. lb, Desired: mass of body fat in kg.

16% body fat by mass means: 16 lb body fat = 100 lb body mass, and the equality kg and lb is: 1 kg = 2.20 lb. Take one conversion factor from each equality such that the units cancel out leaving the desired unit in the answer:

$$180.\ \cancel{\text{lb body mass}} \times \frac{16\ \cancel{\text{lb body fat}}}{100\ \cancel{\text{lb body mass}}} \times \frac{1\ \text{kg body fat}}{2.20\ \cancel{\text{lb body fat}}} = 16\ \text{kg body fat}$$

Note that there are three inexact numbers in the calculation, i.e., 180, 16, and 2.20, and the answer as two significant figures in agreement with the smallest significant figure among the inexact numbers.

1.6: Equations and graphs

Equalities where both sides have a single term, i.e., monomial, lead to the conversion factors. If one or both sides of the equality have more than one term, i.e., polynomial, it leads to a formula that does the same job, i.e., to convert units. Temperature conversion equations and ideal gas equations and the manipulation procedure of these equations are described below as examples of how to manipulate the questions needed for making calculations.

Temperature conversion equations

There are three temperature scales in common use: Celsius (^oC), Kelvin (K), and Fahrenheit (^oF), illustrated in Fig. 1.6.1.

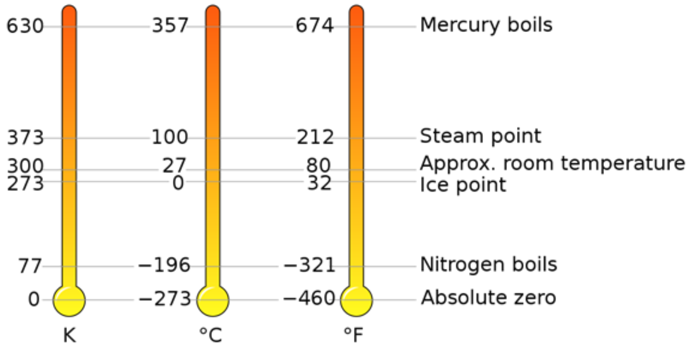


Figure 1.6.1: Relations among temperature scales in common use. Source: MikeRun / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

Celsius (^oC)

The Celsius scale has O ^oC at the freezing point of water and 100 ^oC at the boiling point of water. Celsius is the base unit of temperature in the metric system.

The Kelvin scale

Kelvin is the base unit of temperature in the SI. The freezing point of water is 273.15 K, and the boiling point of water is 373.15 K. For most practical purposes, the freezing point of water is reported as 273 K and the boiling point 373 K, i.e., accurate to three significant figures. Celsius scale units are the same size but shifted up by 273 compared to the Kelvin scale. So, the relationship between Kelvin and Celsius is:

$$T_K = T_C + 273,$$

where T_K is the temperature in Kelvin, and T_C is the temperature in degrees Celsius. This equation converts temperature in Kelvin to temperature in Celsius.

A 0 K, also called absolute zero, is the temperature of a matter at which no energy can be removed as heat from the matter. There is no negative temperature on the Kelvin scale.

Fahrenheit (^oF)

Fahrenheit is the base unit of the English system, with 32 ^oF at the freezing point of water and 212 ^oF at the boiling point of water. Fahrenheit is $\frac{5}{9}$ times shorter and shifted up by 32 than Celsius. So the relationship between the two is:

$$T_F = \frac{9}{5} \times T_C + 32,$$

where T_F is the temperature in Fahrenheit, and T_C is the temperature in degrees Celsius. This equation converts temperature in Celsius to temperature in Fahrenheit.

Manipulating temperature conversion equations

The equation for converting Celsius to Fahrenheit is:

$$T_F = \frac{9}{5} \times T_C + 32,$$

Addition or subtraction of the same number on the two sides of an equation does not change the equality. Subtracting 32 from both sides of the above equation leads to:

$$T_F - 32 = \frac{9}{5} \times T_C + \cancel{32} - \cancel{32},$$

$$T_F - 32 = \frac{9}{5} \times T_C.$$

Multiplication or division by the same number on both sides of an equation does not change equality. Remember that multiplication or division should apply to every term on either side of the equality. Enclose the side with more than one term in small brackets and then do the multiplication of division operation so that it applies to each term in the bracket. Multiplying both sides of the above equation with $\frac{5}{9}$ leads to:

$$\frac{5}{9} \times (T_F - 32) = \frac{5}{\cancel{9}} \times \frac{9}{\cancel{5}} \times T_C$$

$$\frac{5}{9} \times (T_F - 32) = T_C$$

Swapping the sides of an equation does not change equality. Swapping the sides in the above equation to bring T_C to the left:

$$T_C = \frac{5}{9} \times (T_F - 32)$$

This is the equation for Fahrenheit to Celsius conversion.

The procedure of rearranging an equation described above applies to all algebraic equations. For example, start with a relationship that converts Celsius to Kelvin:

$$T_K = T_C + 273,$$

subtract 273 from both sides:

$$T_K - 273 = T_C + \cancel{273} - \cancel{273},$$

$$T_K - 273 = T_C,$$

and finally swap the left and right side to bring T_C to the left:

$$T_C = T_K - 273.$$

This is the equation for Kelvin to Celsius conversion.

Ideal gas equation

The ideal gas equation relates more than two variables:

$$PV = nRT,$$

where P is pressure, V is volume, n is the amount of gas in moles, T is the temperature (in K), and R is the proportionality constant called an **ideal gas constant**. Dividing both sides of the equation with V leads to:

$$P \times \frac{V}{V} = \frac{nRT}{V},$$

$$P = \frac{nRT}{V}.$$

It allows calculating the pressure of a gas sample if the amount in moles, temperature in kelvin, and volume of the gas sample are known, along with the value of the constant R in the consistent units. Similarly, rearranging the equation leads to formulas for calculating, V, T or n of a gas sample:

$$V = \frac{nRT}{P}, \quad T = \frac{PV}{nR}, \quad \text{and} \quad n = \frac{PV}{RT}$$

Graphs

The graph is a visual presentation of a relationship between two variables. Fig. 1.6.2 shows a graph that presents a relationship between the volume and pressure of a given amount of gas at a constant temperature, known as Boyle's law.

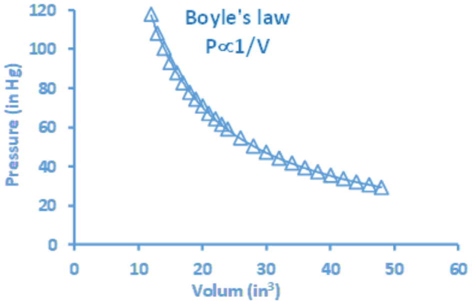


Figure 1.6.2: Boyle's law –the relationship between pressure and volume of a given amount of gas at a constant temperature.

The typical components of a graph are the following.

1. A title that tells what the graph is about, e.g., "Boyle's Law: " in the graph of Fig. 1.6.2.
2. Axes: the x-axis is a horizontal line, and the y-axis is a vertical line. Axes usually have an evenly distributed scale starting from zero. The x-axis represents the independent variable, and the y-axis represents the dependent variable. For example, volume is independent, and pressure is the dependent variable in Fig. 1.6.2.
3. Axes labels that tell the variable's name and the units of measurement. For example, volume (in^3) and pressure (in Hg), where in^3 and in Hg are the units of the variables.
4. Symbols representing experimental points. For example, Δ symbols in Fig 1.6.2, at the crossing of a vertical line starting from an experimental value independent variable on the x-axis and a horizontal line starting from the corresponding value of the dependent variable on the y-axis.
5. A curve connects the experimental points and shows the trend in the relationship. For example, the cure in Fig. 1.6.2 tells that the pressure decreases as the volume increases.

Interpretation of a graph

Interpretation is reading the trend or relationship between the variables plotted. For example, Fig. 1.6.2 shows that the pressure decreases as the volume of gas increases. The curve also allows reading the value of one variable from the value of the other. For example, if the volume is 30 in^3, the pressure would be ~50 in Hg. To read: draw a vertical line from the given value on the x-axis and a horizontal line from the point where the vertical line crosses the curve. Then, read the value where the horizontal line meets the y-axis. The process is reversed when the given value is of the dependent variable on the y-axis, and the desired is the corresponding value of the independent variable on the x-axis. For example, if the pressure is 40 in Hg, the volume is about 35 in^3. Fig. 1.6.3 is another example of a graph that shows a relationship between the molar mass and density of the gases at a constant temperature. The cure in this graph tells that the density of gases increases as the molar mass increases.

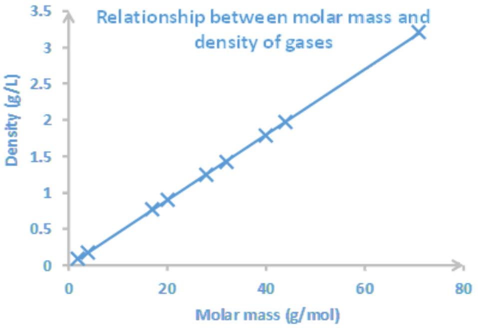


Figure 1.6.3: Curve showing gases having lower molar masses are less dense at the same temperature.

1.7: Density and specific gravity measurements

Density

Density is the mass-to-volume ratio of a substance.

Density is a physical characteristic of matter. Each substance has a characteristic density that can be used as one hint in identifying a substance.

Gases have very low density, usually expressed in g/L. For example, air density is around 1.224 g/L at sea level and 15 ^{o}C. The density of liquids and solids is usually expressed in g/mL. For example, the density of water at 4 ^{o}C is 1.00 g/mL.

Objects that are less dense than water float, and the denser objects than water sink in the water. For example, oil is less dense than water and floats on water. Metals are denser than water and sink in water. The density of some common substances is listed in Table 1

Table 1: Densities of some common substances

Substance	Density (g/mL)
hydrogen	0.000089
carbon dioxide	0.0019
ethyl alcohol	0.7893
water	1.00
magnesium	1.74
table salt	2.16
aluminum	2.70
iron	7.86
copper	8.92
silver	10.50
lead	11.34
mercury	13.59
gold	19.30

Density measurement

Density (d) is calculated from the mass (m) and volume (V) of a substance by the formula:

$$d=\frac{m}{V}$$

Mass is usually measured using an analytical balance. The volume of liquids can be measured using a graduated cylinder, pipet, or density bottle. The volume of regular solids can be calculated from the geometric parameters. For example, the volume of a rectangle is equal to length x width x height. The volume of a cube is equal to the edge length cubed.

The volume of an irregular shaped sold is usually measured because the substances that are denser than water sink and displace an equal amount of water. Fig. 1.7.1 illustrates the density measurement of an irregular-shaped solid object that sinks in water, as explained in the following example.

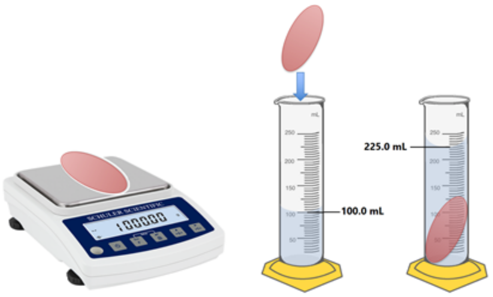


Figure 1.7.1: Measuring mass, volume, and density of an irregular solid object. Source: modified images from https://www.hiclipart.com

Example 1.7.1

Wwhat the density of the object in Fig. 1.7.1?

Soution

the mass (m) of the object on balance is 1000.00 g. The volume of the object is equal to the volume of the water displaced by the object, which is 225.0 mL – 100.0 mL = 125.0 mL.

$$d = \frac{m}{V} = \frac{1000.00\text{ g}}{125.0\text{ mL}} = 8.000\,\frac{\text{g}}{\text{ml}}$$

Caution

Most of the time, Calculators give more significant numbers and sometimes less than needed; both need correction. In example 1.7.1, the calculator displays 8, i.e., one significant figure, but three zeros are added to make four significant figures.

Bone density and osteoporosis

Osteoporosis is a bone disease associated with decreased bone density, particularly in older adults. Bones always lose and gain calcium, magnesium, and phosphate. In childhood, the bones build faster than decay, but in old age, the process reverses, and the bones start to thin, loos strength, and become more prone to fracture, as illustrated in Fig. 1.7.2. Hormonal changes, diseases, and some medications contribute to bone thinning. Severe loss of bone density is called osteoporosis.

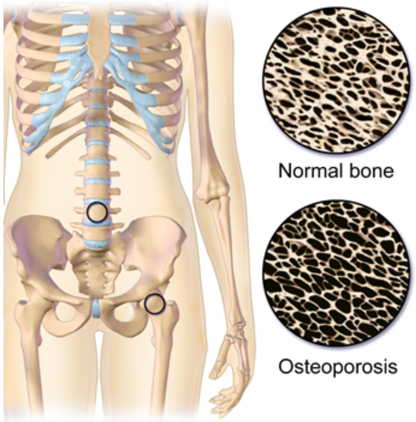


Figure 1.7.2: Illustration of Osteoporosis as a result of bone density decrease. Source: BruceBlaus / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

Specific gravity

Specific gravity is the ratio of the object's density to the density of water, i.e.:

$$\text{Specific gravity } = \frac{\text{Density of an object}}{\text{Density of water}}$$

Specific gravity is the ratio of the object's density to the density of water, i.e.:

$$\text{Specific gravity } = \frac{\text{Density of an object}}{\text{Density of water}}$$

The units cancel out in the ratio. Therefore, the specific gravity is a unitless number. The density of water is 1.0 g/mL at room temperature, so the specific gravity is equal to the density of the object expressed without a unit.

When substances dissolve in water, the density of the solution is usually different from pure water. For example, the density of whole blood for humans is ~1.060 g/mL. The density of urine varies in the range of 1.0050 g/mL to 1.030 g/mL. Both the blood and urine have dissolved substances in water that increase the density from that of pure water. Both high and low density or specific gravity than the normal range of urine indicates medical problems. An increase in the specific gravity of urine indicates that it is due to an increase in the solutes caused by dehydration, diarrhea, or infection. Similarly, a decrease in solute concentration decreases the specific gravity of urine, which indicates medical problems like renal failure.

Specific gravity measurement

The specific gravity is usually measured using an instrument called a hydrometer. The hydrometer partially submerges in the liquid sample, and the reading on the scale at the air-water junction point is recorded, as illustrated in Fig. 1.7.3.

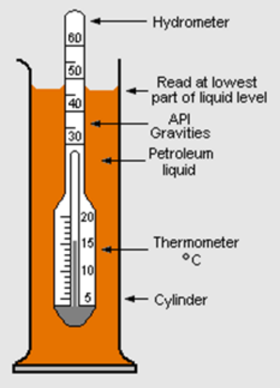


Figure 1.7.3: Schematic drawing of an API hydrometer combined with a thermometer. Source: Milton Beychok, CCO

1.8: Heat and its measurements

Heat

Heat is energy in transfer to and from a thermodynamic system by a mechanism other than the work or the transfer of matter.

Energy exists in different forms, but energy transforms from one form to another through work or heat. In chemical reactions, a significant portion of energy transfer happens through heat. Green leaves in plants trap the energy from light and store it as chemical energy in the form of glucose synthesized from water and carbon dioxide, as illustrated in Fig. 1.8.1.

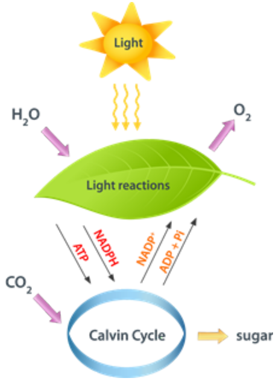


Figure 1.8.1: Photo-synthesis traps the light energy and stores it as chemical energy. Source: https://www.hiclipart.com/free-trans...gzitr/download

A reverse process happens when we eat food, i.e., the food substances are converted to carbon dioxide, water, and energy, as illustrated in Fig. 1.8.2. Some energy is used to maintain our body temperature at an average level. Another portion is used to drive chemical reactions that consume energy and synthesize substances we need.

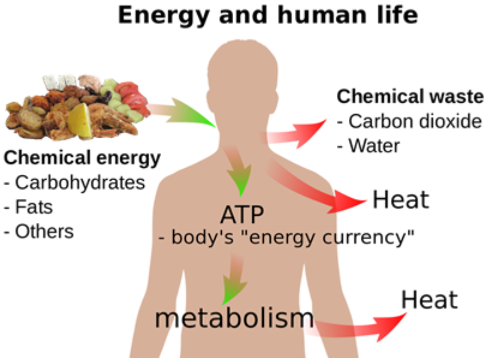


Figure 1.8.2: Basic overview of energy and human life. Source: Mikael Häggström / Public domain

Body Temperature

The human body continually loses energy as heat to the environment. The heat released by exothermic reactions in the food digestion process supplies the heat needed to maintain the body temperature at an average level. Human body temperature varies over a small range, as illustrated in Fig. 1.8.3. Hypothermia is <35.0 °C (95.0 °F), normal body temperate is 36.5–37.5 °C (97.7–99.5 °F), fever and hyperthermia is >37.5 or 38.3 °C (99.5 or 100.9 °F), Hyperpyrexia is >40.0 or 41.0 °C (104.0 or 105.8 °F).

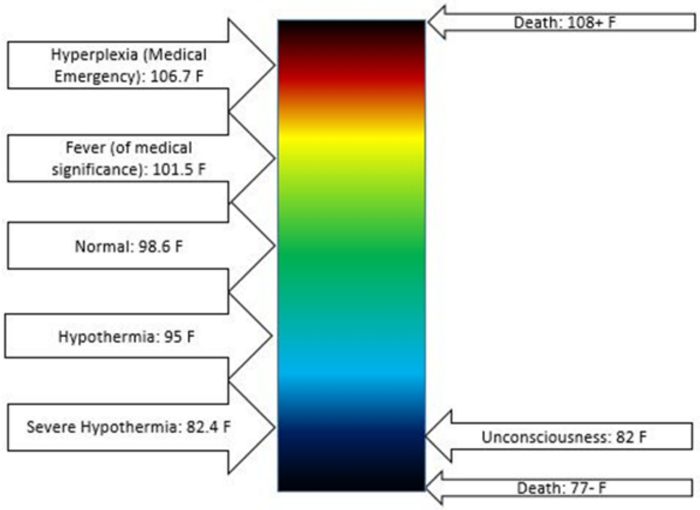


Figure 1.8.3: Variation in human body temperate. Source: Foxtrot620 / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

Measurement of heat

Temperature is a manifestation of the thermal energy of an object, but the temperature and the energy are not the same. Temperature is a measure of hotness or coldness, and it is intensive, and energy is an extensive physical property of matter. For example, 1 g of water has some energy, but 2 g of water at the same temperature has twice the energy.

Specific heat

The calory (c or cal) is a non-SI unit of heat, work, and energy.

The calory (c or cal)

The energy needed to raise the temperature of 1 g of water by 1 ^{o}C is 1 calory

The heat needed to raise the temperature of 2 g of water by 1 ^{o}C is 2 calory, and to raise the temperature of 2 g of water by 2 ^{o}C is 4 calory. That is, heat energy (q) is directly proportional to both the mass (m) and change in temperature (ΔT) of an object:

$$q \propto m\Delta T$$

Introducing a constant of proportionality, i.e., specific heat (C_s) changes the proportionality to equality, that is known as the **heat equation**:

$$q = C_s m\Delta T$$

, where C_s is Specific heat.

Specific heat of a substance

The heat energy needed to raise the temperature of 1g of a substance by 1 ^{o}C (or 1K) is specific heat if the substance.

The mathematical form of the definition of specific heat is:

$$C_S = \frac{q}{m\Delta T}$$

The units of specific heat are $\frac{cal}{g.^{\circ}\mathrm{C}}$, where cal is a non-SI unit of energy. The SI unit of energy is the joule (J). The following is an exact relationship between calory and joule:

$$1 \text{ cal} = 4.184 \text{ J (exact)}$$

So, the specific heat (C_s) in SI units is: $\frac{J}{g.^{o}C}$

The energy unit in nutrition and food is food calory or Calory (C) that is written with capital C, and it is equal to 1000 cal, i.e.,

$$\mathrm{C} = 1000\ \mathrm{cal} = 1\ \mathrm{kcal} = 4184\ \mathrm{J}$$

, where the capital letter C is food calory.

The specific heat is a characteristic physical property of a material. It varies because the energies of vibrational motions of bonds and other motions that contribute to the thermal energy content differ from material to material. Table 1 lists specific heats of some familiar materials.

Water has higher specific heat than other materials, i.e., it absorbs or releases more heat for the same change in temperature. The environmental temperature variation remains moderate in coastal areas because the temperature change of water is less for the same amount of energy absorbed or released. Note that the specific heat of liquid water is different from solid water (ice) and gaseous water (steam).

Table 1: Specific heat of some common substances

Substance	**Specific heat ($\frac{J}{g \cdot {}^{o}C}$)**
Al	0.902
C (graphite)	0.720
Fe	0.451
Cu	0.385
Au	0.128
NH_3 (ammonia)	4.70
H_2O (liquid)	4.184
H_2O (ice)	2.06
H_2O(steam)	2.00
C_2H_5OH (l) (ethanol)	2.46
$(CH_2OH)_2$ (l) (ethylene glycol, antifreeze)	2.42
CCl_4 (carbon tetrachloride)	0.861
Wood	1.76
Concrete	0.88
Glass	0.84

Calculations using specific heat

The specific heat values are used in the heat equation ($q = C_s m \Delta T$) to calculate the temperature change for a given amount of heat or the heat energy needed for a given temperature change of a material. A coffee cup calorimeter illustrated in Fig. 1.8.4 is commonly used. It consists of a coffee cup with a lid. It contains water in which the hot or cold object is immersed, or a chemical reaction is performed for heat exchange with the water. A wire loop is used to stir the water. A thermometer records the change in the temperature of the water. The heat absorbed or released by the water is calculated from the data of mass, specific heat, and temperature change of the water.

Figure 1.8.4: Photo of coffee cup calorimeter set. Source: Community College Consortium for Bioscience Credentials / CC BY (https://creativecommons.org/licenses/by/3.0)

✓ Example 1.8.1

Immersing a hot object in 50.0 grams of water in a coffee cup calorimeter increased the water temperature from 22.0 ^{o}C to 28.8 ^{o}C. How much heat is gained or lost by water?

Solution

Given: m = 50.0 g water, C_s = 4.184 (\frac{J}{g \cdot^{o} C}\), $\Delta T = T_f - T_i$ = 28.8 ^{o}C – 22.0 ^{o}C = 6.8 ^{o}C, Desired: heat gained or lost by water, i.e, q_{water} = ?

Calculations:

$$\mathrm{q_{water}} = \mathrm{C_s m \Delta T} = 4.184\frac{\mathrm{J}}{\mathrm{g}^{\circ}\mathrm{C}} \times 50.0\ \mathrm{g} \times 6.8^{\circ}\mathrm{C} = +1400\ \mathrm{J}$$

The +ve sign tells water gained 1400 J heat.

✓ Example 1.8.2

Ammonium nitrate (NH_4NO_3) is used as a cold pack in hospitals to decrease the temperature of a targeted skin area. When 3.21 g of NH_4NO_3 is dissolved in 50.0 g of water in a coffee cup calorimeter at 25.0 ^{o}C, the temperature decreases to 20.4 ^{o}C. What is the amount of heat absorbed or released by water?

Solution

Given: m of solution = 50.0g H_2O + 3.21 g NH_3NO_3 = 53.2 g, C_s = 4.184 (\frac{J}{g \cdot^{o} C}\), $\Delta T = T_f - T_i$ =20.4 ^{o}C - 25.0 ^{o}C = -4.6 ^{o}C, Desired: heat gained or lost by the solution, i.e, $q_{solution}$ = ?

Calculations:

$$\mathrm{q_{solution}} = \mathrm{C_s m \Delta T} = 4.184\frac{\mathrm{J}}{g^{\circ}\mathrm{C}} \times 53.2\ \mathrm{g} \times (-4.6^{\circ}\mathrm{C}) = -1.0 \times 10^{3}\ \mathrm{J}$$

The –ve sign tells water lost heat

Note

In the problems involving the heating of solution, the mass of solution includes the mass of water and the solute. It is assumed that the specific heat and density of the dilute solution are the same as that of pure water.

Example 1.8.3

Calcium chloride ($CaCl_2$) is used as a hot pack, i.e., to raise the temperature of a targeted portion of the skin. When $CaCl_2$ dissolves in water, heat is released by the process and absorbed by the surrounding water, increasing the temperature of the water.

When 5.00 g of $CaCl_2$ is dissolved in 50.0 g of water at 23^{o}C in a coffee cup calorimeter, the temperature rises to 39.2^{o}C. What is the amount of heat absorbed or released by water?

Solution

Given: m of solution = 50.0g H_2O + 5.00 g $CaCl_2$ = 55.0 g, C_s = 4.184 (\frac{J}{g \cdot^{o} C}\), $\Delta T = T_f - T_i$ =39.2 ^{o}C - 23.0 ^{o}C = 16.2 ^{o}C, Desired: heat gained or lost by the solution, i.e, $q_{solution}$ = ?

Calculations:

$$q_{\text{solution}} = C_s m \Delta T = 4.184 \frac{J}{g.^{\circ} C} \times 55.0 \text{ g} \times (16.2^{\circ} C) = 3.7 \times 10^{3} \text{ J}$$

The +ve sign tells water gained heat.

The energy released from foods

Foods and fossil fuels are carbon and hydrogen compounds and may also contain some other elements like oxygen, nitrogen, phosphorous, and sulfur. Fuels are used in combustion reactions to release heat for different purposes. The same combustion reactions happen in living systems in several steps to get energy from the foods. For example, the chemical equation for the combustion of glucose is:

$$C_6H_{12}O_6(s) + 6\,O_2(g) \longrightarrow 6\,CO_2(g) + 6\,H_2O(l) \quad \Delta H^{\circ} = -2803 \text{ kJ}$$

, where ΔH^{o} is the enthalpy of reaction, i.e., the heat evolved or absorbed at constant pressure conditions. This reaction releases 2803 kJ of energy as heat per mole of glucose. The –ve sign of ΔH^{o} tells that the reaction releases the energy, i.e., the reaction is exothermic. The same amount of energy is released when glucose is digested and converted to the same products in the living system under the same conditions.

Measurement of energy released from food

The heat released from the combustion of a substance is measured using a bomb calorimeter illustrated in Fig. 1.8.5. The substance is placed in a particular cell surrounded by an excess of oxygen. An electric spark ignites the substance, and the heat released causes a temperature increase in the water and the other materials in the meter. The heat capacity (C_{cp}), i.e., the product of the meter's average specific heat and mass and the water components, is calibrated before the experiment. The heat released from the given amount of the substance is calculated from the heat capacity and the measured temperate increase.

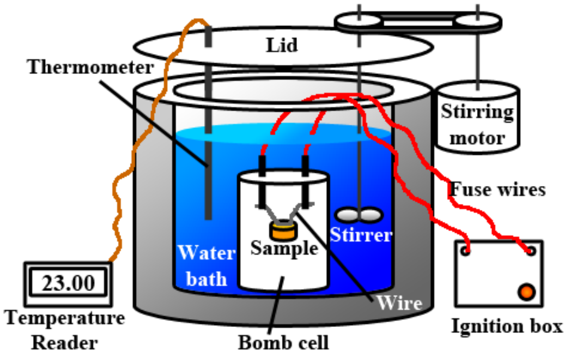


Figure 1.8.1: Bomb calorimeter. Source: Lisdavid89, CC BY-SA 3.0 <https://creativecommons.org/licenses/by-sa/3.0>, via Wikimedia Commons

Fuel value

The heat of combustion per g of a food is called the fuel value of the food

Glucose is one of the **carbohydrates**. Carbohydrates are food components that are compounds of carbon, hydrogen, and oxygen in which the ratio of hydrogen-to-oxygen is 2-to-1. The average fuel value of carbohydrates is 17 kJ/g.

The second major class of food is **fat**. For example, the chemical equation of tristearin $C_{57}H_{110}O_6$, which is a fat, is:

$$2\,C_{57}H_{110}O_6(s) + 16\,O_2(g) \longrightarrow 114\,CO_2(g) + 110\,H_2O(l) \quad \Delta H^\circ = -71609\text{ kJ}$$

The –ve sign with energy value tells the energy is released, or the reaction is exothermic. The average fuel value of fats is 38 kJ/g.

The third primary type of food is **protein**. Protein is mainly used as a building material in living systems, but it is also used as a source of energy. The average fuel value of protein is 17 kJ/g.

The average fuel values of the three major food components are listed in Table 2. These values are used to calculate the fule value of food servings, as explained in the following examples.

Table 2: Average fuel value of food components

Food	Fuel value kJ/g
Carbohydrates	17
Proteins	17
Fats	38

Example 1.8.1

Calculate the energy released from one cup of orange juice that contains 26 g of carbohydrates, no fat, and 2 g of protein.

Solution

Carbohydrate: $26\text{ g} \times 17\text{ kJ/g} = 442\text{ kJ}$
Protein: $2\text{ g} \times 17\text{ kJ/g} = 34\text{ kJ}$
Total energy released $= 476\text{ kJ}$

The energy value in kJ can be converted to food calories (C) by using the conversion factor based on the following relations.

$$\text{Food calory C } = 1000\text{ cal} = 1\text{ kcal} = 4184\text{ J}$$

1.9: Heat and changes in physical states of matter

Among the four physical states of matter, solid has the lowest thermal energy. Intermolecular forces in solids are strong and do not let the molecules slide past each other. The molecules and the bonds in them can still have vibrational motions that account for the thermal energy contents of the material.

The temperature reflects the thermal energy content of the material—the addition of heat increase the vibrational motions, and temperature increases. Ultimately, the solid changes to a liquid and the liquid changes to a gas phase as more heat is added, as illustrated in Figure 1.9.1.

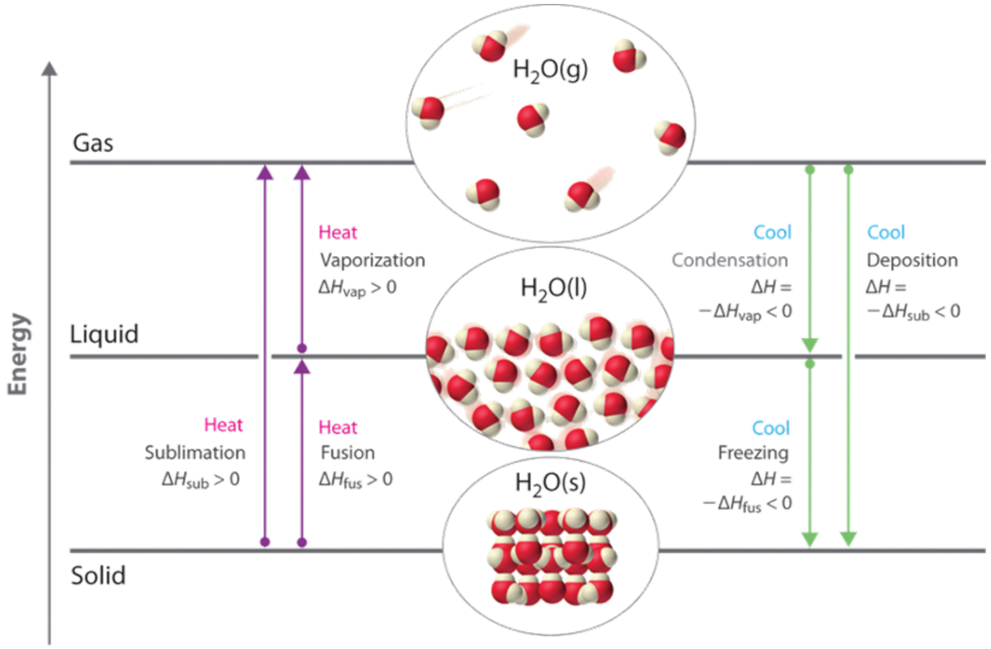


Figure 1.9.1: Illustration of the relationship between energy and phase changes of matter. Source: https://www.hiclipart.com/free-trans...poitg/download

Melting and freezing

When the temperature reaches the melting point of the solid upon heating, the temperature does not increase further, but the sold changes gradually to the liquid phase. The heat added at the melting point is used to change the particles from a well-arranged form in the solid to an irregular arrangement in the liquid phase. This process is called the melting of solid.

Heat of fusion (ΔH_{fus})

The energy needed to melt a unit amount of the substance is the heat of fusion (ΔH_{fus}).

The heat of fusion is usually expressed in the units of joules per gram ($\frac{J}{g}$) for the unit amount in grams or in joules per mole ($\frac{J}{mol}$) for the unit amount in moles.

If heat is removed from a substance at its melting point, the reverse of melting, i.e., freezing, happens, i.e., the liquid gradually changes from liquid to solid phase. The energy equal to the heat of fusion is released during the freezing process. Fig. 1.9.2 shows ice and water at 0 ^{o}C –an example of melting and freezing.

Figure 1.9.2: Ice and water at 0 ^{o}C –an example of melting and freezing. Source: Ulflund / CC0

Vaporization and condensation

After melting, the heat addition causes an increase in the temperature of the liquid until the boiling point is reached. Some of the molecules in a liquid have high enough kinetic energy to cross the liquid-gas boundary and become gas phase. This process is called vaporization.

Heat of vaporization (ΔHvap)

The energy needed to evaporate a unit amount of a liquid is called the heat of vaporization (ΔH_{vap}).

The heat of vaporization is usually expressed in the units of joules per gram ($\frac{J}{g}$) for the unit amount in grams or joules per mole ($\frac{J}{mol}$) for the unit amount in moles.

The reverse of evaporation is called condensation, which releases heat equal to the heat of vaporization. Fig. 1.9.3 demonstrates the co-existence of liquid and gas-phase bromine at room temperate through the simultaneous evaporation and condensation processes.

When the temperature reaches the boiling point of the liquid, the temperature does not increase further, but the added heat is used to evaporate the liquid. Heating increases the temperature of the gas phase after all of the liquid has changed to the gas phase.

Figure 1.9.3: Bromine at room temperature –an example of evaporation and condensation. Source: Alchemist-hp (pse-mendelejew.de) / CC BY-SA 3.0 DE (https://creativecommons.org/licenses...3.0/de/deed.en)

Sublimation and deposition

The solid can change directly to the gas phase without going through the liquid phase. This process is called sublimation.

The energy required in sublimation (ΔH_{sub}) is the addition of the heat of fusion and the heat of vaporization, i.e.,:

$$\Delta H_{\text{sub}} = \Delta H_{\text{fus}} + \Delta H_{\text{vap}}$$

The reverse of the sublimation is called deposition, i.e., the gas phase changes directly to the solid phase. Fig. 1.8.4 shows the sublimation of iodine crystals on a hot plate and deposition of iodine gas on an ice-cold watch glass.

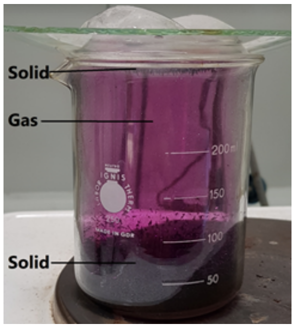


Figure 1.9.4: Iodine crystals on hot plate sublime by the heat and the gaseous iodine deposits on ice-cold watch galss. Source: Alvy16 / CC BY (https://creativecommons.org/licenses/by/4.0)

The sublimation is responsible for drying clothes below 0 ^{o}C conditions in cold areas. Sublimation is also used in freeze-drying vegetables and other foods. Bacteria can not grow on dried foods because they need some moisture to grow. Fig. 1.9.5 shows the terminologies related to the phase changes described in the previous paragraphs.

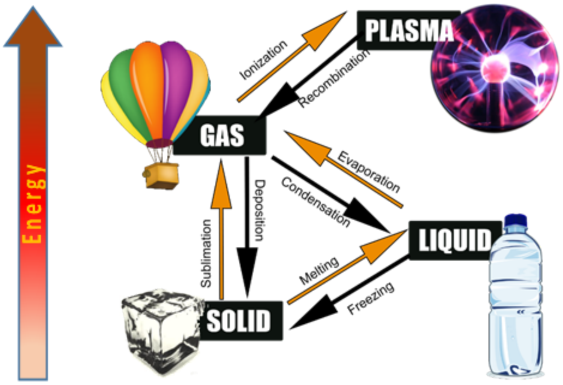


Figure 1.9.5: Nomenclature of the phase changes of matter. Source: https://www.hiclipart.com/free-trans...tfefi/download.

Heating curve

> A graphical presentation of the relationship of heat added versus the temperature change and phase changes of a matter is called a **heating curve**.

Fig. 1.9.6 shows the heating curve of water. The curve shows the heating of ice initially, followed by co-existing of solid and liquid at the freeing point, then hating of liquid water, then co-existing of liquid and gas phases at the boiling point, and finally the heating of steam –the gas phase of water. The reverse of the heating curve is called the **cooling curve**.

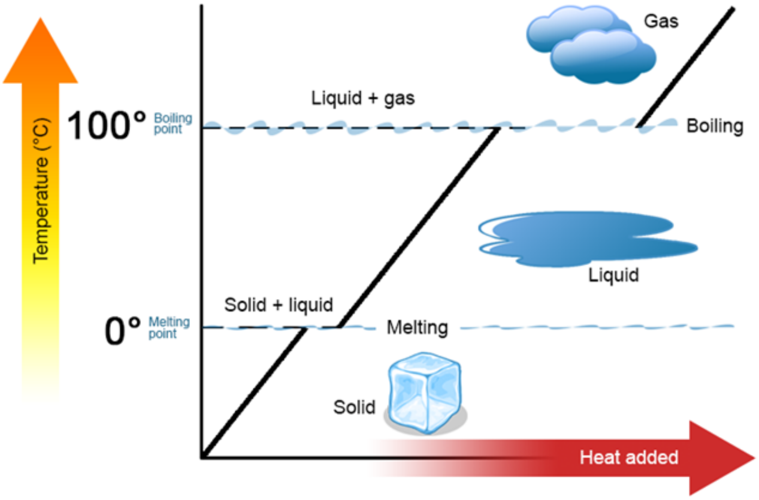


Figure 1.9.6: Heating curve of water. Source: Community College Consortium for Bioscience Credentials / CC BY (https://creativecommons.org/licenses/by/3.0)

Heat calculations on heating or cooling curves

The heat required or released can be calculated by using the specific heat of the substance's solid, liquid, and gas phases. The heat of fusion is needed at the freezing point, and the heat of evaporation is needed at the substance's boiling point. The heat calculation is explained in the following example.

✓ Example 1.9.1

Calculate the energy required to heat 10.0 g of ice from -20.0 °C to steam (water vapor) at 110 °C?

Solution

1st step –heating the ice from -20.0 °C to the melting point of the ice, i.e., 0.00 °C:

m = 10.0 g, C_s of ice = 2.06 $\frac{J}{g{\cdot}^{\circ}C}$, ΔT = 0.00 °C – (-20.0 °C) = 20.0 °C

$$\mathrm{q_1 = C_s m \Delta T = 2.06}\frac{J}{g\cdot{}^{\circ}\mathrm{C}}\times 10.0\ \mathrm{g}\times 20.0^{\circ}\mathrm{C} = 412\ \mathrm{J}$$

2nd step – melting of ice, multiply the heat of fusion with the amout of substance:

m = 10.0 g, ΔH_{fus} = 334 $\frac{J}{g}$.

$$\mathrm{q_2 = \Delta H_{fus}\ \times m = 334}\frac{J}{g}\ \times 10.0\ \mathrm{g} = 3340\ \mathrm{J}$$

3rd step –hating of the water from 0.00 °C to the boiling point of water, i.e., 100 °C:

m = 10.0 g, C_s of liquid water = 4.184 $\frac{J}{g{\cdot}^{\circ}C}$, ΔT = 100 °C – 0.00 °C = 100 °C

$$\mathrm{q_3 = C_s m \Delta T = 4.184}\frac{J}{g\cdot{}^{\circ}\mathrm{C}}\times 10.0\ \mathrm{g}\times 100^{\circ}\mathrm{C} = 4180\ \mathrm{J}$$

4th step – boiling of liquid water, multiply the heat of vaporization with the amount of the substance:

m = 10.0 g, ΔH_{vap} = 2260 $\frac{J}{g}$

$$\mathrm{q_4 = \Delta H_{vap}\ \times m = 2260}\frac{J}{g}\ \times 10.0\ \mathrm{g} = 22600\ \mathrm{J}$$

5th step –hating of the stem from 100 °C to 110 °C:

m = 10.0 g, C_s of steam = 2.00 $\frac{J}{g{\cdot}^{\circ}C}$, ΔT = 110 °C – 100 °C = 10.0 °C

$$q_5 = C_s m \Delta T = 2.00 \frac{J}{g \cdot {}^\circ C} \times 10.0\ g \times 10.0^\circ C = 200\ J$$

Total heat needed = $q_1 + q_2 + q_3 + q_4 + q_5 = 412\ J + 3340\ J + 4180\ J + 22600\ J + 200\ J = 30700\ J$

$$30700\ J \times \frac{1\ kJ}{1000\ J} = 30.7\ kJ$$

Note

The most significant portion of the heat is consumed in boiling the water to steam, i.e., 22.6 kJ out of 30.7 kJ total. The same amount of heat is released when the steam condenses. That is why the steam burn is much more severe than the burn by hot water.

CHAPTER OVERVIEW

2: Elements

2.1: Dalton’s atomic theory

Atom

Atom is the smallest particle of an element that retains the element's characteristics.

For example, gold is an element. Magnifying a section of the gold surface large enough would look like a packing of atoms, as illustrated in Fig. 2.1.1.

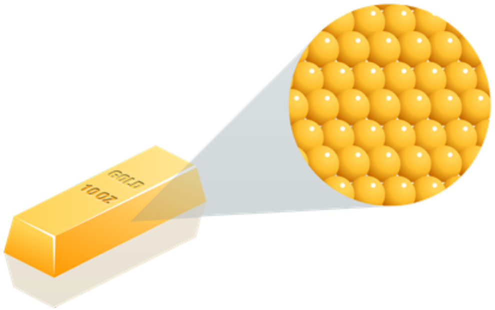


Figure 2.1.1: A piece of gold (right) is an element that is composed of particles called atoms, as shown in the model (left). Source: https://www.hiclipart.com/free-trans...ghixq/download.

Dalton's atomic theory was the first significant attempt to explain the basic knowledge of atoms gained over time. Postulates of Dalton's atomic theory are the following.

Postulates of Dalton's atomic theory

1. Elements are composed of tiny indivisible particles called atoms.
2. Atoms of an element are identical but different from atoms of any other element.
3. Atoms of different elements react with each other in a fixed whole numbers proportion to produce a compound.
4. Atoms in a compound can separate and recombine to give new substances. Still, the atoms are neither created nor destroyed in the reaction.

Dalton's atomic theory is the basis of the current atomic theory, though the atoms are no more considered ‘indivisible.’ According to the current knowledge, **subatomic particles** like electrons, protons, and neutrons compose the atoms. However, the subatomic particles do not represent the element.

2.2: Subatomic particles and a modern view of an atom

> Atoms are composed of fundamental subatomic particles: electrons, protons, and neutrons.

Electron was the first subatomic particle discovered. The discovery of electrons is related to the study of cathode rays and the basic knowledge of charges, i.e., there are two types of charges +ve and –ve; like charges repel each other; opposite charges attract each other as illustrated in Fig. 2.2.1; electric and magnetic field deflects the moving charges.

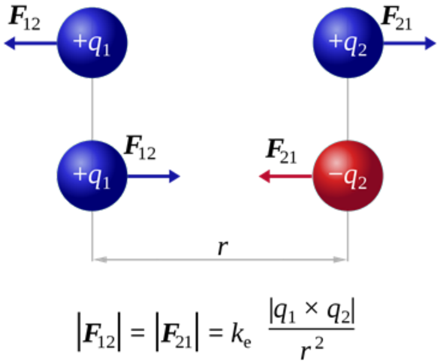


Figure 2.2.1: This diagram describes two equal (like) point charges repelling each other and two opposite charges attracting each other, with an electrostatic force F which is directly proportional to the product of the magnitudes of each charge and inversely proportional to the square of the distance between the charges. K_e is Coulomb's constant. Source: File:CoulombsLaw.svg: User:Dna-Dennis / *derivative work RJB1 / CC BY (https://creativecommons.org/licenses/by/3.0)

The discovery of the electron

Cathode rays

Cathode rays are a type of radiation emitted from a cathode (negatively charged electrode) when a high electric field is applied across a pair of electrodes under reduced pressure conditions, as illustrated in Fig. 2.2.2. The cathode rays travel in the inter-electrode space. If there is a hole in the anode, the cathode rays can pass through the hole and keep moving in a straight path. The cathode rays emit light when they strike a fluorescent screen.

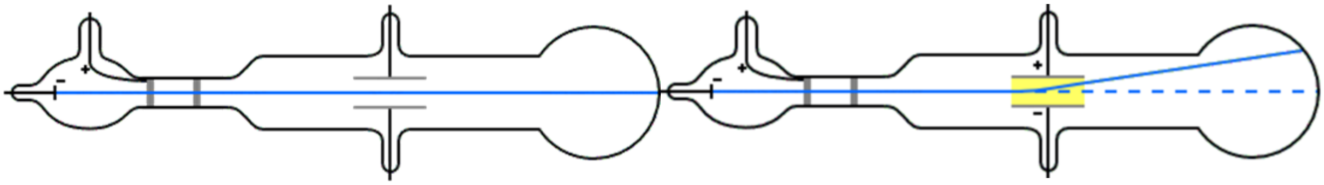


Figure 2.2.2: Cathode ray tube with cathode-ray shown deflected by an electric field. *Source: Kurzon / Public domain*

J.J Thomson's experiments -the discovery of electrons

J.J. Thomson studied the cathode rays and found that an electric field deflects the cathode rays towards the positive electrode. This observation indicates that the cathode rays were negative charges. Changing the cathode material did not change the properties of the cathode rays. J.J. Thomson concluded from these observations that the cathode rays were streams of particles, called **electrons**, that are present in the atoms of all elements.

Further discoveries revealed that the charge on the electrons is 1.602 x 10^{-19} C, and their mass is 9.10 x 10^{-28} g. The electrons are incredibly light, about two thousand times lighter than the lightest atom.

Plum Pudding Model of an atom

Based on the information from cathode ray experiments, J.J. Thomson concluded that there are –ve charge electrons and a +ve matter representing almost all the atom's mass. He proposed the plum-pudding model of atoms, i.e., the positive matter is like a diffused cloud or jelly that occupies the atom's space, and electrons are embedded in it like fruits in jelly in the case of the plum-pudding dessert dish as shown in Fig. 2.2.3.

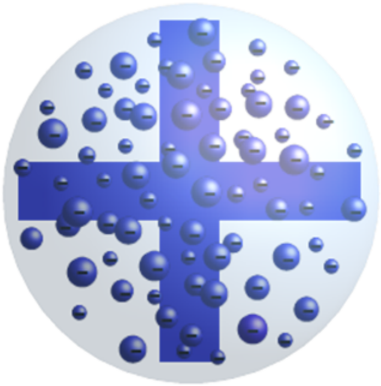


Figure 2.2.3: Plum pudding model of an atom. Atoms were initially thought to contain many hundreds or thousands of electrons as shown in this schematic representation of the plum pudding model. *Source: Tjlafave / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)*

The discovery of the nucleus of an atom

α-Rays

α-Rays, pronounced as alpha-rays, are high-energy radiations emitted from some radioactive sources. The α-rays are composed of α-particles that are helium atoms without any electrons.

Rutherford's gold foil experiment -the discovery of the nucleus

Rutherford tested the plum pudding model of the atom by bombarding α-rays on a thin gold foil. He expected that α-particles to pass through the gold foil un-deflected like bullets fired through a Styrofoam sheet. He observed that although most of the α-particles passed through the gold-foil un-deflected, one in ~20,000 deflected at larger angles, as illustrated in Fig. 2.2.4.

Since the plum-pudding model of an atom could not explain the deflection of the α-particles, Rutherford concluded that there was a tiny but very dense region in the center of an atom, now called the nucleus, that deflected the α-particles. Rutherford's gold foil experiment led to the discovery of the nucleus.

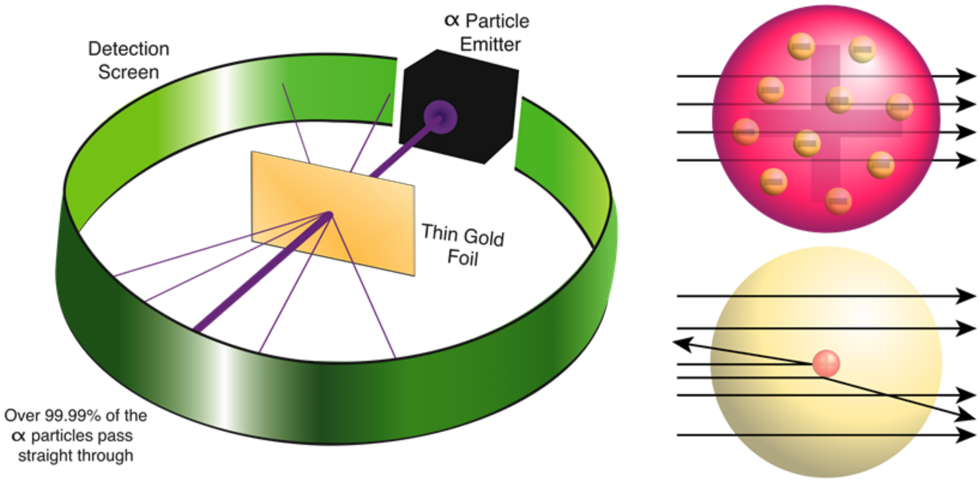


Figure 2.2.4: Illustration of Rutherford's gold foil experiment (left). Interpretation of the results – Almost all the atom's mass is in a tiny nucleus space. α-particles that come close to the atom's nucleus are deflected (right). Source: https://www.hiclipart.com/free-trans...xivja/download and https://www.hiclipart.com/free-trans...txlqr/download

The discovery of proton

Rutherford predicted that a positively charged fundamental particle of atoms should reside in the nucleus. Later on, Rutherford observed that shining α -rays on nitrogen gas produced positively charged particles called protons. The protons are about 20,000 times heavier than electrons but carry a +ve charge equal in magnitude to the –ve charge on an electron.

The discovery of the neutron

The mass of protons and electrons did not account for an atom's overall mass, which led to a search for another subatomic particle. James Chadwick discovered that bombarding α -rays on a beryllium target produced a highly penetrating radiation consisting of a beam of neutral particles, now called neutrons. The presence of neutrons in the nucleus accounts for the missing mass of atoms.

Other sub-atomic particles have been discovered, e.g., quarks that constitute protons and neutrons, but their knowledge is not critical for understanding basic chemistry.

Modern view of an atom

Protons and neutrons reside in the nucleus with a diameter of 10^{-15} m. Electrons occupy the region outside the nucleus with a diameter of 10^{-10} m, as illustrated in Fig. 2.2.5. If the nucleus is about the size of a marble, the atom would be about the size of a soccer field.

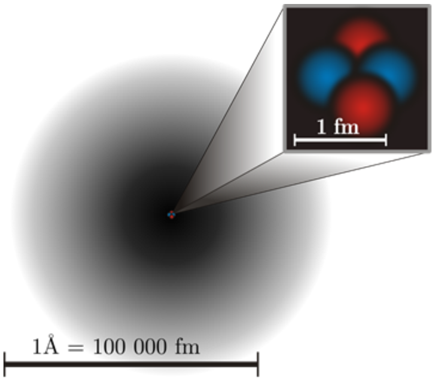


Figure 2.2.5: depiction of the atomic structure of the helium atom. The darkness of the electron cloud corresponds to the line-of-sight integral over the probability function of the 1s atomic orbital of the electron. The magnified nucleus is schematic, showing protons in pink and neutrons in purple. Source: User:Yzmo / CC BY-SA (http://creativecommons.org/licenses/by-sa/3.0/)

Properties of the subatomic particles

The basic SI units of mass, electric charge, and distance are too big for atomic-scale measurements. New units are defined for this purpose, i.e.:

Atomic mass unit (amu)

Atomic mass unit (amu) which is 1/12 of the mass of a single carbon atom that has 6 protons and 6 neutrons in it.

$$1 \text{ amu} = 1.660539606660(50) \times 10^{-27} \text{ kg}$$

Electron charge (e)

Charge on one electrons is electron charge (e).

$$1\ e = 1.602176634 \times 10^{-19} \text{ C}$$

Angstrom(Å)

$$1 \text{ Å} = 10^{-10} \text{ m}$$

These units are usually used for masses, charges, and diameters of atoms. Table 1 lists the basic properties of the subatomic particles.

Table 1: Basic properties of subatomic particles

Particle	Charge (e)	Mass (amu)
Proton	+1	1.0073

Particle	Charge (e)	Mass (amu)
Neutron	0	1.0078
Electron	-1	5.486×10^{-4}

How the subatomic particles are held in the atom

The gravitational force is negligible in the case of the behavior of subatomic particles in the atoms. Although electrons repel other electrons, they stay in a tiny space due to attraction towards the nucleus. Similarly, protons repel each other, but the electrical force is small compared to the strong nuclear force that holds protons and neutrons together in the nucleus.

2.3: Atoms of elements

Symbol of an element

Elements are represented by symbols, the first alphabet of their English or non-English name, written in capital letters. For example, C for carbon, N for nitrogen, and I for iodine. Usually, another alphabet is also chosen from the element's name and written as a small letter, e.g., Al for aluminum, Zn for zinc, and Ca for calcium. Some element symbols are derived from non-English names, e.g., Na for sodium from the Latin name *natium,* Cu for copper from Latin *cupurum*, and Ag for silver from Latin *argentum*.

Atoms of the same element have the same number of protons, and atoms of different elements have different numbers of protons. In other words, the number of protons in an atom defines the element. There are 118 elements known at this time; the number of protons in atoms varies from 1 for hydrogen to 118 for Oganesson (Og).

Atomic number

The number of protons in an atom is called the atomic number.

The atomic number defines the element. A subscript to the left of the symbol of an element represents the atomic number. For example, ${}_{1}\mathrm{H}$ shows one proton in a hydrogen atom, and ${}_{6}\mathrm{C}$ shows 6 protons in a carbon atom.

Mass number

The number of protons plus the number of neutrons in an atom is the mass number.

A superscript to the left of the symbol of an element represents the mass number. For example, ${}^{1}_{1}\mathrm{H}$ is a hydrogen atom with atomic number 1, mass number 1, and no neutrons, while ${}^{19}_{9}\mathrm{F}$ is a fluorine atom with 9 protons and 10 neutrons.

Number of electrons

The number of electrons in an atom equals the number of protons minus the charge on the atom.

The number of electrons is equal to the number of protons in the case of a neutral atom, as there is no charge on a neutral atom.

Cation

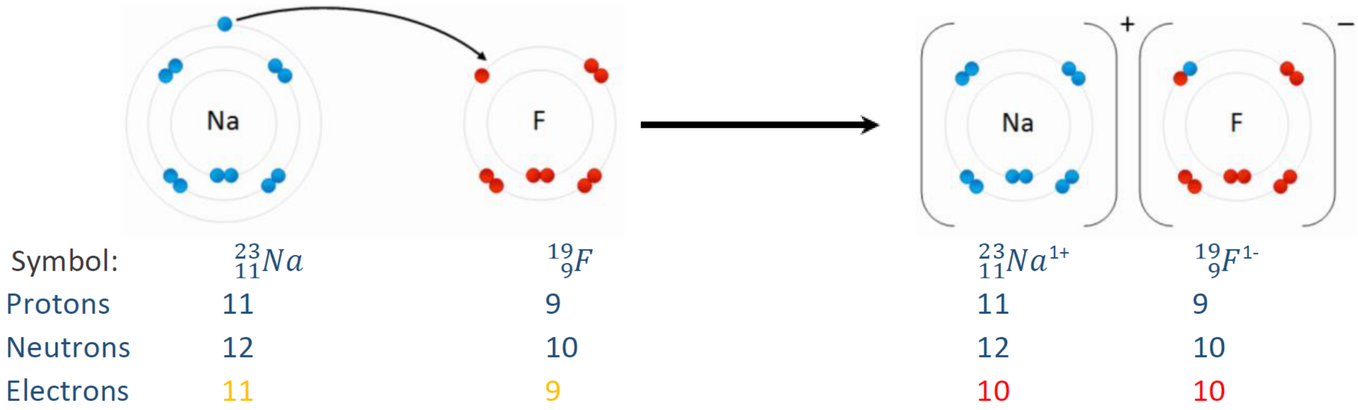
A neutral atom can lose some electrons and become a positively charged particle, called a **cation**.

The charge is represented as a superscript on the right side of the element symbol, e.g. ${}^{1}_{1}\mathrm{H}^{+}$ is hydrogen without any electron, i.e., 1 proton, 0 neutrons, and 0 electrons. ${}^{20}_{40}\mathrm{Ca}^{2+}$ is calcium with two fewer electrons than protons, i.e., 20 protons, 20 neutrons, and 18 electrons.

Anion

An atom can gain electrons and become a negatively charged particle, called an **anion**.

For example, ${}^{16}_{8}\mathrm{O}^{2-}$ is oxygen with two more electrons than protons on it, i.e., 8 protons, 8 neutrons, and 10 electrons. A ${}^{19}_{9}\mathrm{F}^{-}$ is fluorine with one more electron than protons on it, i.e., 9 protons, 10 neutrons, and 10 electrons. Fig. 2.3.1 illustrates the gain or loss of electrons from neutral atoms.



Symbol:	$^{23}_{11}Na$	$^{19}_{9}F$	$^{23}_{11}Na^{1+}$	$^{19}_{9}F^{1-}$
Protons	11	9	11	9
Neutrons	12	10	12	10
Electrons	11	9	10	10

Figure 2.3.1: Comparison of subatomic particles in neutral atoms and ions formed from them after the gain or loss of an electron. Source: modified from: Wdcf / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Calculating the number of protons, neutrons, and electrons

In general, an atom of a hypothetical element X is represented as $^{A}_{Z}X^{I\,charge}$ where Z is the atomic number, A is the mass number, and I is an integer equal to charge number and *charge* the sign of the charge number: + or -.The number of protons, neutrons, and electrons is calculated by using the following formulas:

$$\text{Number of protons} = A,$$

$$\text{Number of neutrons} = A - Z, \text{ and}$$

$$\text{Number of electrons} = Z - (charge\ I),$$

where a *charge* is a + or - sign of the charge number.

✓ Example 2.3.1

Calculate the number of protons, neutrons, and electrons in $^{16}_{8}O$, $^{16}_{8}O^{2-}$, and $^{16}_{8}O^{+}$?

Solution

$^{16}_{8}O$: number of protons = Z = 8, number of neutrons = $A - Z$ = 16-8 = 8,

and number of electrons = $Z - (charge\ I) = 8 - 0 = 8$.

$^{16}_{8}O^{2-}$: number of protons = Z = 8, number of neutrons = $A - Z$ = 16-8 = 8,

and number of electrons = $Z - (charge\ I) = 8 - (-2) = 8 + 2 = 10$.

$^{16}_{8}O^{1+}$: number of protons = Z = 8, number of neutrons = $A - Z$ = 16-8 = 8,

and number of electrons = $Z - (charge\ I) = 8 - (+1) = 8 - 1 = 9$.

Note

If charge number I is 1 in $^{A}_{Z}X^{I\,charge}$, it is usually not written, but a number more than one is written. For example, $^{16}_{8}O^{-}$ has change = -1, $^{16}_{8}O^{2-}$ has charge charge -2, and $^{16}_{8}O^{+}$ has charge = +1.

Isotopes

All atoms of the same element have the same number of protons but can have a different number of neutrons. For example, $^{1}_{1}H$, $^{2}_{1}H$, and $^{3}_{1}H$ have neutrons equal to 0, 1, and 2, respectively.

Atoms of the same element that have a different number of neutrons are called **isotopes**.

For examples, $^{1}_{1}H$, $^{2}_{1}H$, and $^{3}_{1}H$ are isotopes of hydrogen illustrated in Fig. 2.3.2. Another example is $^{6}_{3}Li$, and $^{7}_{3}Li$ are two isotopes of lithium. Natural samples of elements usually have almost constant ratios of isotopes. Table 1 lists some Isotopes of elements and their percent abundance in typical natural samples.

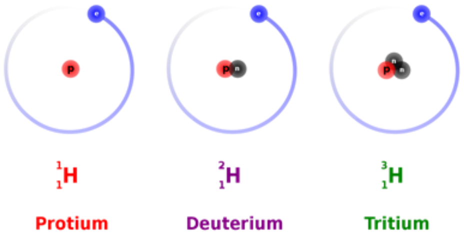


Figure 2.3.2: Isotopes of hydrogen. Source: Dirk Hünniger; Derivative work in english - Balajijagadesh / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Table 1: Some of the important isotopes of elements with abundance in typical natural samples

Element	Isotopes	Abundance (%)
Hydrogen	${}^{1}_{1}H$ ${}^{2}_{1}H$ ${}^{3}_{1}H$	99.99 0.01 Negligible
Lithium	${}^{6}_{3}Li$ ${}^{7}_{3}Li$	7.6 92.4
Carbon	${}^{12}_{6}C$ ${}^{13}_{6}C$ ${}^{14}_{6}C$	98.93 1.07 Negligible
Chlorine	${}^{35}_{17}Cl$ ${}^{37}_{17}Cl$	75.78 24.22
Bromine	${}^{79}_{35}Br$ ${}^{81}_{35}Br$	50.69 49.31
Uranium	${}^{235}_{92}U$ ${}^{238}_{92}U$	0.72 99.28

Atomic mass

> The **atomic mass** listed in the periodic table is the weighted average of the masses of the isotopes present in a natural sample of the element.

The following formula calculates the atomic mass:

$$\text{Atomic mass } = \sum[(\text{ mass of isotope }) \times (\text{ fractional abuncance of the isotope })$$

, where $\sum$ means summation over all isotopes of the element, the fractional abundance of the isotope is the % abundance divided by 100. Fig. 2.3.3. illustrates how the atomic mass is listed in a periodic table.

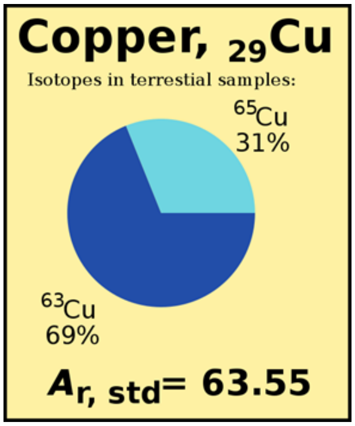


Figure 2.3.3: Two isotopes are present: copper-63 (62.9 amu) and copper-65 (64.9 amu), in abundances 69% + 31%. The standard atomic weight for copper is the average, weighted by their natural abundance. Source: DePiep / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

✓ **Example 2.3.2**

Calculate the atomic mass of chlorine with two isotopes in nature samples, i.e., $^{35}_{17}\mathrm{Cl}$ of mass 34.969 amu and % abundance 75.78% and $^{37}_{17}\mathrm{Cl}$ of mass 36.996 amu and % abundance 24.22%.

Solution

Formula: $\text{Atomic mass } = \sum[(\text{ mass of isotope }) \times (\text{ fractional abuncance of the isotope })$

Plug in the given values in the formula and calculate:

$$\left(34.969 \text{ amu} \times \frac{75.78}{100}\right)+\left(36.996 \text{ amu} \times \frac{24.22}{100}\right)=35.45 \text{ amu}$$

Note

1. Atomic masses of isotopes are close to but not the same as their mass numbers. For example, $^{35}_{17}\mathrm{Cl}$ has mass number mass = 35, but the atomic mass of this isotope is 34.969 amu as shown in the above example.
2. The weighted average atomic mass is usually closer to the mass number of the most abundant isotope, e.g., 35.45 amu in the above example is close to the mass number 35 of $^{35}_{17}\mathrm{Cl}$ isotope, which is the most abundant isotope.
3. The periodic table reports the atomic mass as calculated in the above example, i.e., the weighted average of the masses of the isotopes present in the natural sample of the element.

2.4: The periodic table

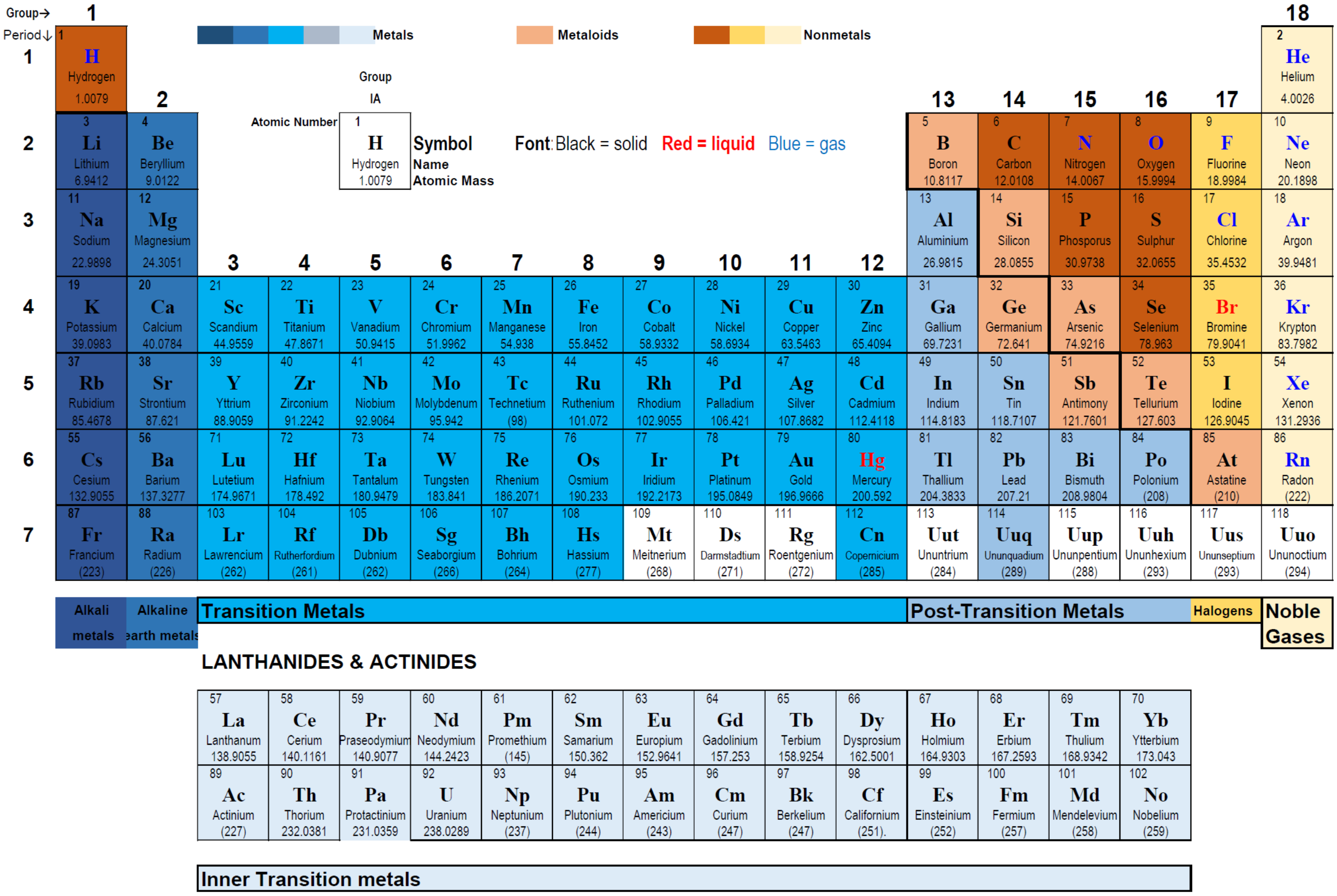
Early developments

The discoveries of elements happened over a long time. As the list of known elements grew, scientists tried to arrange them based on their properties. **Mendeleev** arranged elements in a table based on atomic masses. It resulted in elements having similar properties placed next to each other in most cases. There were gaps intentionally left in the table for the elements that were predicted based on the knowledge from the periodic table but not yet discovered.

Few exceptions were there observed where the properties of the elements did not agree with the group in which they were placed based on their atomic masses. **Mosely** developed a method to measure atomic numbers based on X-ray spectroscopy. The arrangement of the elements based on the atomic number instead of atomic masses removed the discrepancies in Mendeleev's periodic table.

The modern periodic table of elements

- The modern periodic table of elements arranges the elements according to the increasing order of the atomic number starting from atomic number 1 for H and ending with atomic number 118 for Og, as shown in Fig. 2.4.1.
- The elements are arranged in horizontal rows called **periods** and vertical columns called **groups**.



Period↓ / Group→	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H Hydrogen 1.0079																	2 He Helium 4.0026
2	3 Li Lithium 6.9412	4 Be Beryllium 9.0122											5 B Boron 10.8117	6 C Carbon 12.0108	7 N Nitrogen 14.0067	8 O Oxygen 15.9994	9 F Fluorine 18.9984	10 Ne Neon 20.1898
3	11 Na Sodium 22.9898	12 Mg Magnesium 24.3051											13 Al Aluminium 26.9815	14 Si Silicon 28.0855	15 P Phosporus 30.9738	16 S Sulphur 32.0655	17 Cl Chlorine 35.4532	18 Ar Argon 39.9481
4	19 K Potassium 39.0983	20 Ca Calcium 40.0784	21 Sc Scandium 44.9559	22 Ti Titanium 47.8671	23 V Vanadium 50.9415	24 Cr Chromium 51.9962	25 Mn Manganese 54.938	26 Fe Iron 55.8452	27 Co Cobalt 58.9332	28 Ni Nickel 58.6934	29 Cu Copper 63.5463	30 Zn Zinc 65.4094	31 Ga Gallium 69.7231	32 Ge Germanium 72.641	33 As Arsenic 74.9216	34 Se Selenium 78.963	35 Br Bromine 79.9041	36 Kr Krypton 83.7982
5	37 Rb Rubidium 85.4678	38 Sr Strontium 87.621	39 Y Yttrium 88.9059	40 Zr Zirconium 91.2242	41 Nb Niobium 92.9064	42 Mo Molybdenum 95.942	43 Tc Technetium (98)	44 Ru Ruthenium 101.072	45 Rh Rhodium 102.9055	46 Pd Palladium 106.421	47 Ag Silver 107.8682	48 Cd Cadmium 112.4118	49 In Indium 114.8183	50 Sn Tin 118.7107	51 Sb Antimony 121.7601	52 Te Tellurium 127.603	53 I Iodine 126.9045	54 Xe Xenon 131.2936
6	55 Cs Cesium 132.9055	56 Ba Barium 137.3277	71 Lu Lutetium 174.9671	72 Hf Hafnium 178.492	73 Ta Tantalum 180.9479	74 W Tungsten 183.841	75 Re Rhenium 186.2071	76 Os Osmium 190.233	77 Ir Iridium 192.2173	78 Pt Platinum 195.0849	79 Au Gold 196.9666	80 Hg Mercury 200.592	81 Tl Thallium 204.3833	82 Pb Lead 207.21	83 Bi Bismuth 208.9804	84 Po Polonium (208)	85 At Astatine (210)	86 Rn Radon (222)
7	87 Fr Francium (223)	88 Ra Radium (226)	103 Lr Lawrencium (262)	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (266)	107 Bh Bohrium (264)	108 Hs Hassium (277)	109 Mt Meitnerium (268)	110 Ds Darmstadtium (271)	111 Rg Roentgenium (272)	112 Cn Copernicium (285)	113 Uut Ununtrium (284)	114 Uuq Ununquadium (289)	115 Uup Ununpentium (288)	116 Uuh Ununhexium (293)	117 Uus Ununseptium (293)	118 Uuo Ununoctium (294)

57 La Lanthanum 138.9055	58 Ce Cerium 140.1161	59 Pr Praseodymium 140.9077	60 Nd Neodymium 144.2423	61 Pm Promethium (145)	62 Sm Samarium 150.362	63 Eu Europium 152.9641	64 Gd Gadolinium 157.253	65 Tb Terbium 158.9254	66 Dy Dysprosium 162.5001	67 Ho Holmium 164.9303	68 Er Erbium 167.2593	69 Tm Thulium 168.9342	70 Yb Ytterbium 173.043
89 Ac Actinium (227)	90 Th Thorium 232.0381	91 Pa Protactinium 231.0359	92 U Uranium 238.0289	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251).	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)

Figure 2.4.1: Periodic table of elements. Fort color of element symbols: blue are gases, red are liquids and black are solids at room temperature. Source: Modified from https://www.exceltemplates.org/category/academic)

Periods

The periodic table has seven horizontal rows called periods**.** The periods are numbered: 1 at the top to 7 at the bottom.

1. The 1st period has only two elements: hydrogen in group 1 and helium in group 18, with a gap from group 2 to group 17.

2. The 2nd and the 3rd periods have eight elements each, filling groups 1 and 2 followed by groups 13 to 18, leaving a gap from group 3 to group 12.
3. The periods 4th and 5th periods have eighteen elements that are filled successively from group 1 to group 18.
4. The periods 6th and 7th have 32 elements, each: the first two in groups 1 and 2, the next fourteen elements in separate rows below the table. These two rows of 14 elements each are called **Actinides** and **Lanthanoids**, respectively. Then the next sixteen elements fill the groups 3 to 18.

Groups

The periodic table has 18 vertical columns called groups or families. The groups are numbed starting from 1 on the leftmost and going through to 18 at the rightmost.

Alkali metals

The 1st group is called alkali metals. The alkali metals include lithium (Li), sodium (Na), potassium (K), rubidium (Rb), cesium (Cs), and francium (Fr), shown in Fig. 2.4.2. The alkali metals are the most reactive among the metals in the periodic table. They react vigorously with water, as shown in Fig. 2.4.3.

Figure 2.4.2: Alkali metals, from left to right: lithium, sodium, potassium, rubidium, and cesium. Source: Tomihahndorf at German Wikipedia, Dnn87 Contact email: Dnn87@yahoo.dk, and http://images-of-elements.com/potassium.php.

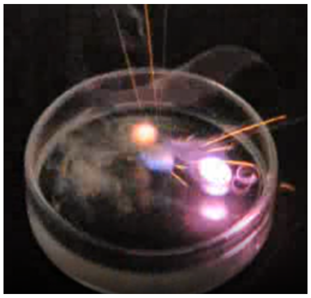


Figure 2.4.3: Potassium reacting with water. Source: Ozone aurora / Philip Evans / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Hydrogen

Hydrogen is in group 1 but is not included in alkaline earth metals. Hydrogen is a nonmetal and has properties quite different from alkali metals or any other group of elements.

Alkaline earth metals

The 2nd group is called alkaline earth metals. It includes beryllium (Be), magnesium (Mg), calcium (Ca), strontium (Sr), barium (Ba), and radium (Ra). They are reactive metals but less reactive than alkali metals. Alkaline earth metals impart characteristic color to a flame. Salts of alkali metals are used in firework formulation to give distinctive colors to the firework, as shown in Fig. 2.4.4.

Figure 2.4.4: New years eve fire works at Al Majaz waterfront, Sharjah UAE. Metal salts including alkali metals are used to give distinctive colors in fireworks. Source: Fariz Safarulla / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Transition metals

Groups 3 to 12 are called transition metals. They include precious metals like gold, silver, platinum, and construction metals like iron. Some make catalysts and are found in enzymes and other bio-molecules, like hemoglobin and chlorophyll.

Group 13 to 16

Group 13 to group 16 does not have a unique name. They comprise nonmetals at the top and metals at the bottom of each group called **post-transition metals**. Important nonmetals include carbon, nitrogen, oxygen, phosphorous, and sulfur.

Halogens

Group 17 elements are called halogens. The halogens include fluorine (F), chlorine (Cl), bromine, iodine (I), and astatine (At). The halogens are highly reactive nonmetals. Chlorine is gas, bromine is liquid, and iodine is solid at room temperature, as shown in Fig. 2.4.5.

Figure 2.4.5: From left to right: chlorine, bromine, and iodine. Source: W. Oelen / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Noble gases

Group 18 is called noble gases. They include helium (He), neon (Ne), argon (Ar), krypton (Kr), xenon (Xe), and radon (Rn). They are the least reactive of all the elements. Noble gases are used to create an inert atmosphere for chemical reactions. Noble gases are also used in the lighting system because of their chemically inert nature , as illustrated in Fig. 2.4.6.

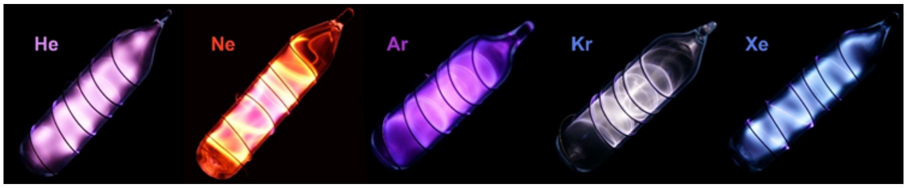


Figure 2.4.6: Glowing noble gases in glass vials with low pressure inside. Power supply: 5 kV, 20 mA, 25 kHz. Source: New work Alchemist-hp (talk) www.pse-mendelejew.de); original single images: Jurii, http://images-of-elements.com. / CC BY (https://creativecommons.org/licenses/by/3.0)

Metals, metalloids, and nonmetals

Metals

The elements towards the right-bottom corner of the periodic table are metals except for hydrogen, which is a nonmetal. Metals have common characteristics, including:

> 1. they are shiny,
> 2. solid at room temperature (except mercury which is liquid),
> 3. malleable (can be hammered into sheets) and ductile (can be drawn into wires),
> 4. good conductors of heat and electricity, and
> 5. tend to lose electrons and form ionic compounds when they react with nonmetals.
>
> The metals of group 1 are called alkali metals; group 2 are called alkaline earth metals, group 3 to group 13 are called transition metals, the two-row below transition metals in the periodic table are called **lanthanoids**, and **actinides** or **inner transition metals**, and metals in the group 13 to group 16 are called **post-transition metals**. Elements other than transition or inner-transition metals, i.e., the elements of groups 1 and 2 and groups 13 to 18, are collectively called **main group elements or representative elements**.

Metalloids

The dividing line between metals and nonmetals is a staircase line starting from $_5\text{B}$ and ending at $_{85}\text{At}$. The elements on the staircase line are metalloids except for aluminum and polonium, which are considered metals. Metalloids have properties in-between metals and nonmetals; e.g., they have moderate heat and electrical conductivity.

Nonmetals

Elements towards the top-right corner of the periodic table and hydrogen are called nonmetals.

> 1. The nonmetals usually have properties opposite to metals, e.g., they are not typically shiny, brittle if solid, and poor conductors of heat and electricity.
> 2. Nonmetals tend to make ionic compounds by accepting electrons from metals and making molecular compounds by reacting with each other.

Two groups in nonmetals also have unique names, i.e., group 17 is called halogens**,** and group 18 is called Noble gases.

> **The most reactive and nonreactive elements**
>
> Generally, alkali metals are the most reactive, followed by alkaline earth metals, and halogens are the most reactive nonmetals. Noble gases are the least reactive nonmetals, also called inert gases.

Fig. 2.4.7 shows examples of a metal, a metalloid, and a nonmetal.

Figure 2.4.7: Gold nugget –a metal, pure silicon –a metalloid, and sulfur –a nonmetal (from left to right). Source: Gold: Rob Lavinsky, iRocks.com – CC-BY-SA-3.0 / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0), Silicon: Enricoros at English Wikipedia / Public domain, Sulfur: Benjah-bmm27 / Public domain

Elements essential for life

The elements that are the main constituents of humans and other living organisms are oxygen, carbon, hydrogen, nitrogen, and sulfur. Phosphorous is present in bone, teeth, and DNA. Calcium and magnesium are the main constituents of bones and teeth and perform some other body functions. Sodium and potassium cations are the main electrolytes in body fluids, and chloride anion balances the charge. Iron is present in hemoglobin that carries oxygen to the cells. These elements are essential to life, and they are macronutrients. Besides these, several other elements are needed in a small amount. They are essential for life and called micronutrients. Fig. 2.4.8 shows the macronutrients in pink and micronutrients in blue color in a periodic table.

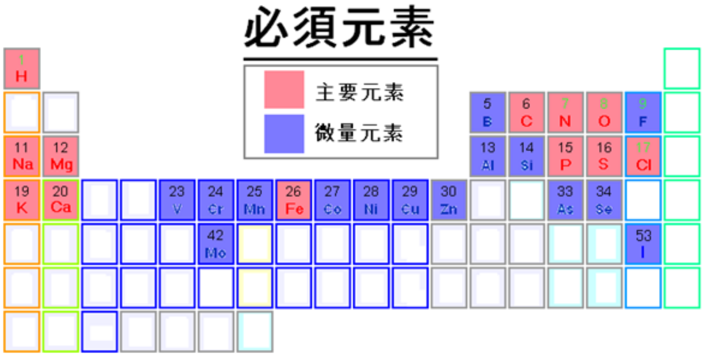


Figure 2.4.8: A table of elements important to human life. Pink elements are essential that are macroneutrients; blue elements are important that are microneutrients. Source: Tosaka / Public domain

Physical and chemical states of elements

Elements in gases state at ambient conditions

The term molecule is generally used for an electrically neutral group of two or more atoms held together by chemical bonds. In the kinetic molecular theory of gases, a **molecule** is the smallest particle of an element or compound with a stable and independent existence. Atoms of noble gases exist as independent species in the gas phase at room temperature, i.e., as **monoatomic molecules** like He, Ne, Ar, Kr, Xe, and Rn. Other elements that are gases at room temperature or **diatomic molecules**, i.e., H_2, N_2, O_2, $F_{2,}$ and Cl_2, are called dihydrogen, dinitrogen, dioxygen, and dichlorine, respectively. Note that usually prefix di is not used for the name of the element, i.e., these are usually called hydrogen, nitrogen, oxygen, fluorine, and chlorine, respectively. Monoatomic species of these elements, i.e., H, N, O, F, and Cl, exist, but they are very reactive species called free radicals, and they do not survive for a long time.

Elements in the liquid state at ambient conditions

Two elements exist as liquids at room temperature, i.e., mercury (Hg), a metal, and bromine (Br_2), a no metal that exists as diatomic molecules. Four elements, francium, cesium, gallium, and rubidium, are solid metals at 25 ^{o}C, but become liquid when the temperature is slightly warmer.

Elements in the solid-state at ambient conditions

All elements not mentioned in the previous two sections are solid at room temperature. They may be diatomic or polyatomic molecules, e.g., I_2, O_3, P_4, S_8, diiodine, ozone, tetraphosphorous, and octasulfur, with two or three, four, and eight atoms, respectively, in a molecule.

Allotropes

> Different forms of the same element in the same physical state are called allotropes.

The allotropes are different structural modifications of the element. For example, carbon exists in several allotropic forms; two of them are shown in Fig. 2.4.9. Another example is $O_{2,}$ and O_3 are gaseous forms of oxygen.

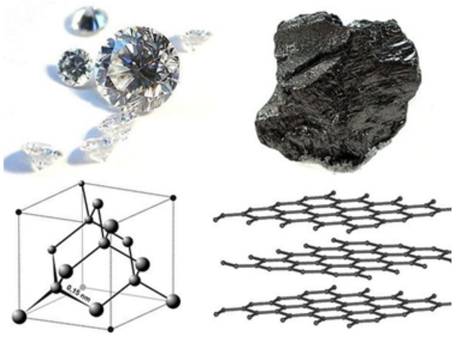


Figure 2.4.9: Diamond and graphite are two of the allotropes of carbon: pure forms of the same element that differ in structure. Source: Diamond_and_graphite.jpg: User:Itubderivative work: Materialscientist / CC BY-SA (http://creativecommons.org/licenses/by-sa/3.0/)

Elements that exist as giant molecules

Some elements exist as **giant molecules**, i.e., a collection of many atoms bonded with each other through a 3D network of bonds. For example, carbon is a giant molecule in several allotropic forms, including diamond, graphite, carbon nanotubes, and fullerenes. Fig. 2.4.9 shows the bonding in diamond and graphite allotropes. The whole piece of diamond is one molecule with carbon atoms interconnected in a 3D network of bonds.

Metals also exist as a collection of many atoms bonded together by metallic bonds. The metal atoms exist as +ions arranged in a well-defined 3D arrangement called crystal lattice with some of the outermost electrons roaming around in the whole piece of the metal, forming a sea of electrons around the metal atoms, as illustrated in Fig. 2.4.10.

The elements in giant molecules and metals are represented by element symbols without any subscript, e.g., C is carbon, Fe is iron, Au is gold, etc.

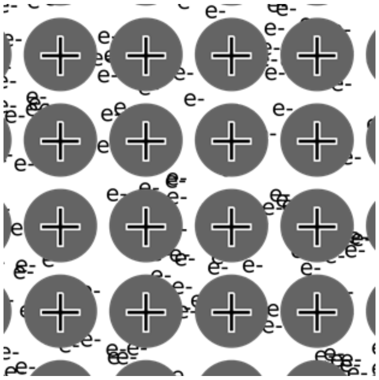


Figure 2.4.10: Metal ions in a sea of electrons. Source: Steven Legg (Sjlegg) / *Public domain*

2.5: Electrons in atoms

The electronic structure of an atom determines the properties of the element. Knowledge of electromagnetic radiation is described first as it plays an essential role in understanding the electronic structure of atoms.

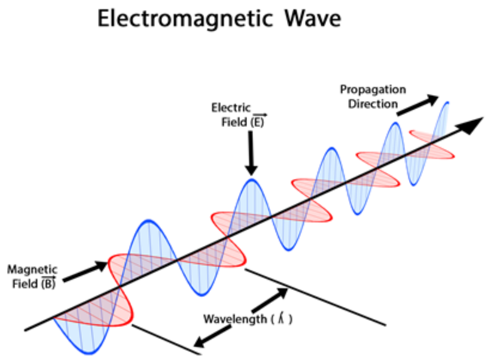


Figure 2.5.1: Illustration of electric field, magnetic field, propagation direction and wavelength of an electromagnetic wave. Source: DECHAMMAKL / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

Electromagnetic radiations

Electromagnetic radiations are waves that are oscillating electric and magnetic fields. The wave propagates in one direction, e.g., along the x-axis. The electric field oscillates perpendicular to it, e.g., along the y-axis. The magnetic field oscillates perpendicular to both, e.g., along the z-axis, as illustrated in Fig. 2.5.1. The distance between two consecutive maxima or between any two consecutive same phase points along the wave is called **wavelength** (λ, pronounced ‘lambda’). The number of waves that pass a reference point in one second is called **frequency** (ν, pronounced ‘nu’). The speed of electromagnetic radiation is called the speed of light (c). The speed of light is the product wavelength and frequency, i.e.,

$$c=\lambda\nu$$

The speed of light (c) is 3.00 x 10^8 m/s in a vacuum. The **energy** (E) of electromagnetic radiation is directly proportional to frequency, i.e.,

$$E=h\nu$$

, where h is a constant, called plank’s constant. Replacing ν with $\frac{c}{\lambda}$ shows that the energy is inversely proportional to the wavelength.

$$E=\frac{hc}{\lambda}$$

Fig. 2.5.2 illustrates the range of electromagnetic radiations that differ from each other concerning wavelength, frequency, or energy. The separation of the radiations based on their wavelength gives a **spectrum**. Visible light is a small portion of the spectrum of electromagnetic radiations, as illustrated in Fig. 2.5.2.

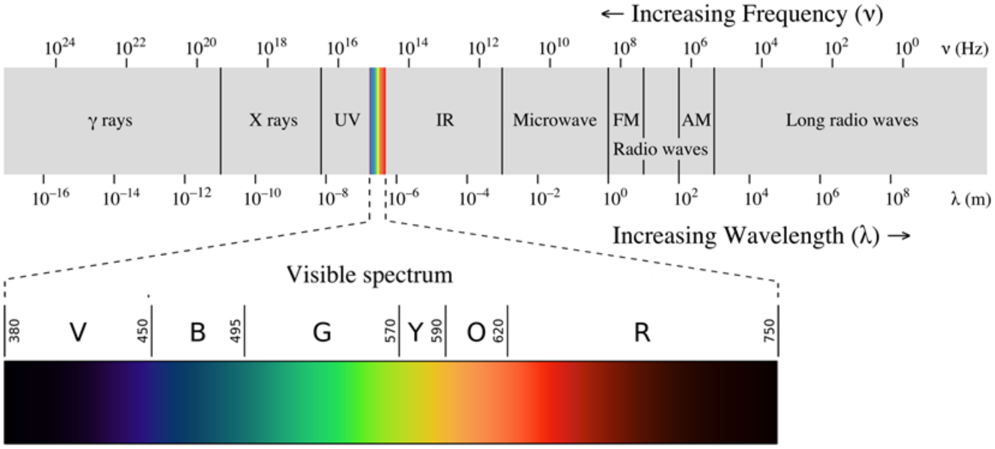


Figure 2.5.2: A spectrum of electromagnetic radiations. The visible range of the spectrum is expanded with the wavelength shown in nm units. Source: Philip Ronan, Gringer / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Continuous and line spectrum

The spectrum of sunlight contains radiations of all wavelengths within the visible range. The spectrum that contains all wavelengths in the range is called a continuous spectrum. Spectrum from sodium lamps or emissions from other atoms contains only some discrete wavelengths. The spectrum that contains discrete wavelengths is called the line spectrum. For example, as illustrated in Fig. 2.5.3, the emission from the hydrogen atom is a line spectrum.

Figure 2.5.3: Continues spectrum of visible light (400-700 nm range, top) and line spectrum from hydrogen (bottom). Source: it:Utente:Sassospicco / Public domain and Merikanto, Adrignola / CC0

Energy levels of electrons in an atom

The question is why the atomic emission has a discrete wavelength or discrete energy. The answer to this question came from the discoveries that concluded that the electron in an atom does not have continuous energy values; they have discrete energy values called shells and subshells.

The shell

Quantum numbers determine the allowed energy values of an electron in an atom.

- Principal quantum number (n) can have any integer value starting from 1, i.e., 1, 2, 3, 4, and so on.
- The smaller the n, the lower is the energy state, and the closer the electron is to the nucleus, the more tightly held the electron is by the nucleus.
- The value of n defines the shell, i.e., 1st shell has n = 1, 2nd shell has n = 2, 3rd shell has n =3, and so on.

Bohr introduced this concept of quantization of electronic energy levels. Fig. 2.5.4 illustrates Bohr's atomic model.

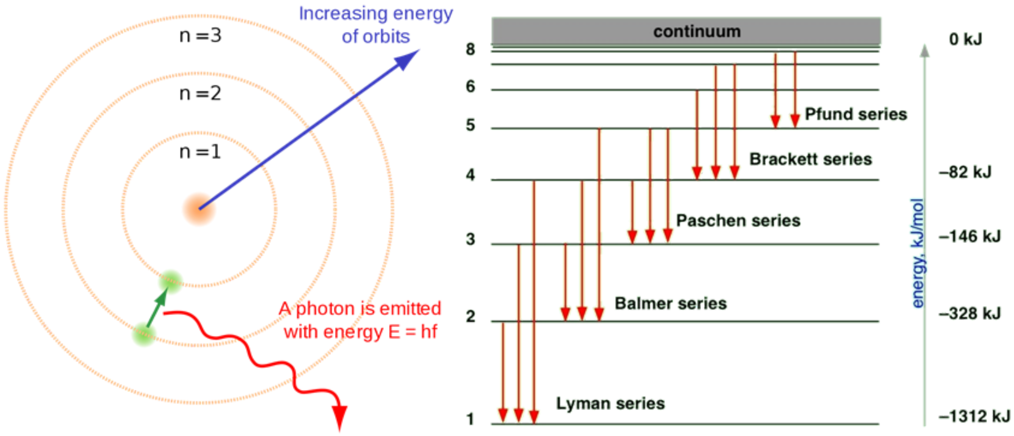


Figure 2.5.4: Bohr model of the atom generalized (left), and electron energy levels of a hydrogen atom with energy values and spectral emission series. Source: Brighterorange / CC BY-SA (http://creativecommons.org/licenses/by-sa/3.0/), and https://www.hiclipart.com/free-trans...cnxhb/download

- When an electron jumps from a lower shell to a higher shell, it absorbs electromagnetic radiation of energy equal to the energy gap between the initial and the final shell.
- When an electron jumps from a higher shell to a lower shell, it emits radiation equal to the energy gap between the initial and the final shell.

Fig. 2.5.3 illustrates the emission of radiation from atoms –it is a line spectrum because only discrete energy levels, called shells, are allowed to electrons in an atom.

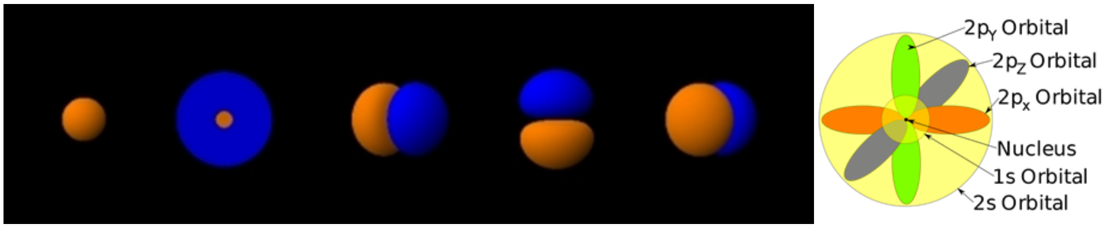


Figure 2.5.5: The shapes of the first five atomic orbitals are: (from left to right) 1s, 2s, $2p_x$, $2p_y$, $2p_z$, and of the five togather with the nucleus at the center. Source: Neon_orbitals.JPG, public domain, and John Trombley / CC BY (https://creativecommons.org/licenses/by/4.0)

The subshell

A second quantum number, called Azimuthal quantum number (*l*) defines subshells within a shell.

The subshells are usually designated as s, p, d, f, ...

Each shell has subshells equal to the shell number. For example, 1st shall have only one subshell, i.e., s. It is designated 1s, where the number is the principal quantum number, and the letter is the subshell. The 2nd shell has two subshells 2s and 2p; the 3rd shell has three subshells 3s, 3p, and 3d; and the 4th shell has four subshells 4s, 4p, 4d, and 4f.

The energy order of subshells is 1s<2s<2p<3s<3p<4s and so on.

Fig. 2.5.6 helps in remembering the order. This figure is drawn by placing the orbitals in columns and shell numbers in rows in increasing order of n from top to bottom, starting from 1s orbitals in the first column and first row, p orbitals in the second, d in the third, and f in the fourth. The filling of electrons follows arrows going from corner to corner, starting from the top left corner of the topmost cell, as described in more detail in a later section.

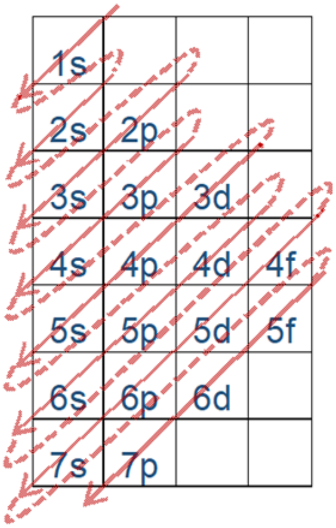


Figure 2.5.6: Order of filling of electrons in subshells. Start from the top and follow the arrows.

Orbital

The orbital is the region in space around the nucleus of an atom where electrons are most likely found.

Each subshell has a certain number of orbitals in them. The orbitals have a specific shape and orientation. The s subshell has only one orbital spherically symmetrical, like a ball with a nucleus at the center. The 1s orbital is smaller than 2s, and 2s is smaller than 3s, but they all have a spherically symmetrical shape, as illustrated in Fig. 2.5.5. The p subshell has three orbitals. Each p orbital is a dumbbell shape with two lobes, i.e., p_x oriented along the x-axis, p_y along the y-axis, and p_z along the z-axis, as illustrated in Fig. 2.5.5.

Degenerate orbitals

A set of orbitals having the same energy is called degenerate orbitals.

All the three p orbitals in the same shell have the same energy, i,e, $2p_x$, $2p_y$, and $2p_z$ is a set of degenerate orbitals. The d subshell has five degenerate orbitals, and f subshell has seven degenerate orbitals, as shown in Fig. 2.5.7. Their shapes and orientations are more complex and not shown here.

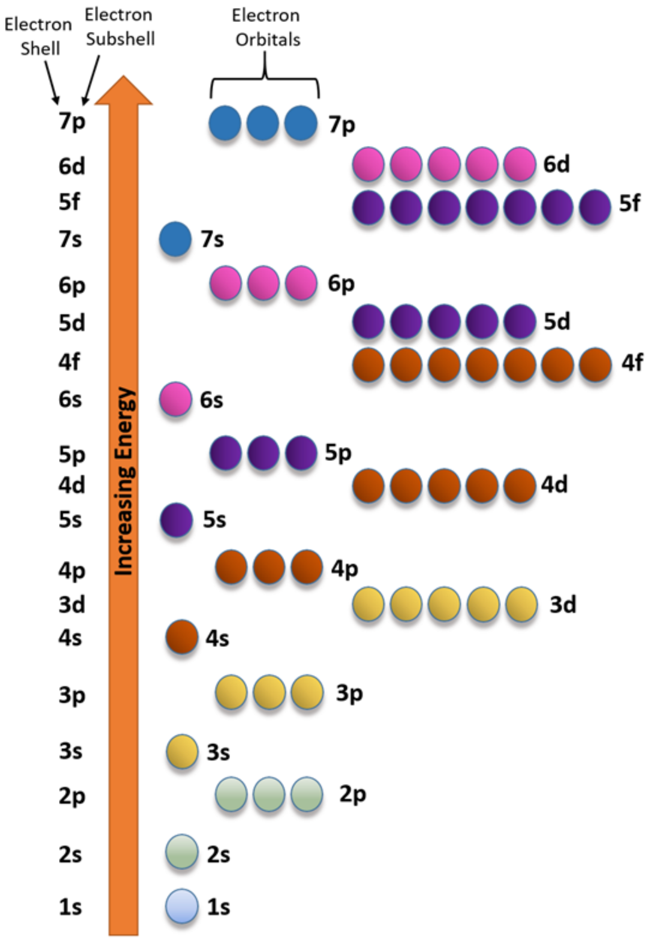


Figure 2.5.7: Relative energies of shells, subshells, and orbitals in multi-electron atoms. Source: https://www.hiclipart.com/free-trans...yfbwx/download

The electron configuration of atoms

The electron configuration is the distribution of electrons in the atom's orbitals.

Rules for distributing electrons in atom's orbitals

1. Each orbital can take a maximum of two electrons.
2. The orbitals are filled in the order of increasing energy: the lowest energy orbital is filled with electrons before the next higher energy orbital starts filling up.

The energy order of orbitals is 1s<2s<2p<3s<3p<4s and so on, as shown in Fig. 2.5.6 and Fig. 2.5.7.

The electron configuration of 1st-row elements

The hydrogen atom has one electron, and it occupies 1s orbital, i.e., $1s^1$ represents the electron configuration of the hydrogen atom. The superscript in $1s^1$ shows the number of electrons in the sub-shell. A helium atom has two electrons, and both occupy 1s orbital, giving helium the electron configuration of $1s^2$. Hydrogen and helium are in the 1st-row of the periodic table and have the 1st-shell containing electrons.

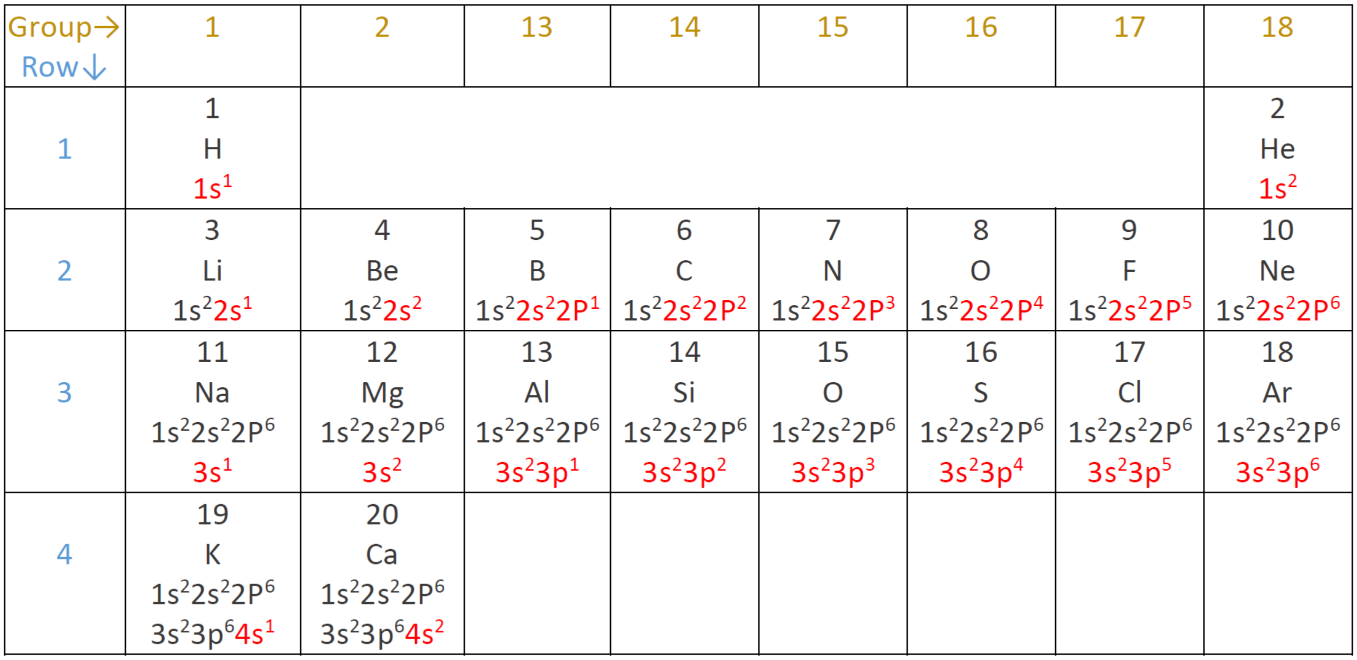
The electron configuration of 2nd-row elements

The 2nd row starts from lithium with 3 electrons: the first two occupy 1s, and the third occupy 2s giving lithium the electron configuration $1s^2\ 2s^1$. The next element is beryllium with 4 electrons with the configuration $1s^2\ 2s^2$. The next element is a boron with 5 electrons and the electron configuration $1s^2\ 2s^2\ 2p^1$. Carbon has 6 electrons with the electron configuration $1s^2\ 2s^2\ 2p^2$. Remember that the s subshell has one orbital and can take a maximum of two electrons, but the p subshell has three orbitals and can take a maximum of six electrons, i.e., two per orbital. Nitrogen, oxygen, fluorine and neon have 7, 8, 9, and 10 electrons and have the electron configuration $1s^22s^22p^3$, $1s^22s^22p^4$, $1s^22s^22p^5$, and $1s^22s^22p^6$, respectively. Atomic number 3 to 10, i.e., lithium to neon, completes the 2nd-row.

> **Valence electrons and core electrons**
>
> The outermost shell is called the valence shell, and electrons in the valence shell are called valence electrons. 1st shell is the valence shell for 1st-row elements hydrogen and helium. 2nd-row elements have an inner shell with configuration $1s^{2,}$ and a valence shell containing 2s and 2p being filled. The inner shell is also called the core-shell, and the electrons in the core-shell are called the core electrons.

The electron configuration of 3rd-row and 4th-row elements

The 3rd-row starts with sodium atomic number 11 and ends with argon atomic number 18. The electron configuration of the 3rd-row elements repeats the pattern of the 2nd-row, i.e., a set of full core-shells $1s^22s^22p^6$, and a valence shell having 3s or 3p being filled. The first two elements of the 4th-row are potassium and calcium with atomic numbers 19 and 20 having configurations $1s^22s^22p^63s^23p^64s^1$ and $1s^22s^22p^63s^23p^64s^2$, respectively. The electron configuration of elements with atomic numbers beyond 20 is more complicated, involving d and f subshell, and they are out of the scope of this book. Fig. 2.5.8 shows the electron configuration of the first twenty elements described above.



Group→ Row↓	1	2	13	14	15	16	17	18
1	1 H $1s^1$							2 He $1s^2$
2	3 Li $1s^22s^1$	4 Be $1s^22s^2$	5 B $1s^22s^22P^1$	6 C $1s^22s^22P^2$	7 N $1s^22s^22P^3$	8 O $1s^22s^22P^4$	9 F $1s^22s^22P^5$	10 Ne $1s^22s^22P^6$
3	11 Na $1s^22s^22P^6$ $3s^1$	12 Mg $1s^22s^22P^6$ $3s^2$	13 Al $1s^22s^22P^6$ $3s^23p^1$	14 Si $1s^22s^22P^6$ $3s^23p^2$	15 O $1s^22s^22P^6$ $3s^23p^3$	16 S $1s^22s^22P^6$ $3s^23p^4$	17 Cl $1s^22s^22P^6$ $3s^23p^5$	18 Ar $1s^22s^22P^6$ $3s^23p^6$
4	19 K $1s^22s^22P^6$ $3s^23p^64s^1$	20 Ca $1s^22s^22P^6$ $3s^23p^64s^2$						

Figure 2.5.8: The electron configuration of the first twenty elements in the periodic table of elements. Valence electrons are shown in red color fonts.

2.6: The periodic trends in properties of the elements

Properties of elements generally show a periodic trend that correlates with their position in the periodic table. The properties and their periodic trends are described below.

Valence electrons

Electrons in the outermost shell are the valence electrons. Fig. 2.5.8 shows the valence electrons of the first twenty elements in red fonts.

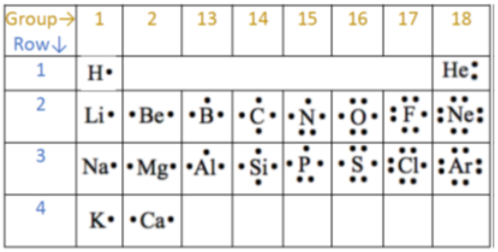
> **Periodic trend of valence electrons**
>
> All elements in a group have the same number of valence electrons equal to the first digit of their group number. For example, 1st group of hydrogen and alkali metals has one valence electron, 2nd group of alkali metals has two valence electrons, halogens in 17th group have seven valence electrons, and noble gases in 18th group have eight valence electrons.

> **Caution**
>
> The transition metals in groups 3 to 12, and inner-transition metals, i.e., lanthanoids and actinoids -the two rows of elements placed below the periodic table, are the exception to the general trend of valence electrons described above. Valence electron configurations of transition metals and inner-transition metals are not described here; it is beyond the scope of this book.

The valence electrons mainly determine the chemical properties of the elements. The elements in the same group have similar chemical properties because they have the same valence shell electron configuration. The elements in a row show a gradual change in chemical properties because their valence shell electron configuration changes gradually along the row.

Lewis symbols

> 1. Lewis symbols show the valence electrons as dots around the symbol of an element. One dot represents one valence electron, e.g., H•.
> 2. The dots are shown on any of the four sides of the symbol.
> 3. A single dot on the top, bottom, left, or right is shown four valence electrons. Then start pairing the dots beyond four valence electrons, as shown in Fig. 2.6.1 for the first twenty elements.
> 4. Helium is an exception that has only two valence electrons, but they are shown paired.

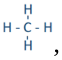
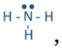


Group→ Row↓	1	2	13	14	15	16	17	18
1	H•							He:
2	Li•	•Be•	•B•	•C•	•N•	•O•	:F•	:Ne:
3	Na•	•Mg•	•Al•	•Si•	•P•	•S•	:Cl•	:Ar:
4	K•	•Ca•						

Figure 2.6.1: Lewis symbols or electron-dot symbols of the first twenty elements in the periodic table.

The electron dots in the Lewis structure are a convenient way to determine how many bonds an atom of an element can make.

> Generally, each unpaired dot can make one bond.

For example, a hydrogen atom with one unaired dot can make one bond as in H-H. A bond is represented by a line between the bonded atoms. A bond is formed by sharing unpaired valence electrons. It is called a covalent bond. Carbon, nitrogen, oxygen, and fluorine with 4, 3, 2, and 1 unpaired dot can make 4, 3, 2, and 1 bond, e.g., in the following molecules: , , , and .

> - Each line in these molecules represents a **bonding electron pair**, and
> - the pair of dots represent valence electrons that are not involved in bonding, called **lone pair of electrons**.

Atomic size

Electrons exist around the nucleus in a cloud-like appearance with no clearly defined boundaries. Therefore, the atomic size generally refers to the **covalent radius** of an atom that is one-half of the distance between the nuclei covalently bonded in a homonuclear molecule, like Cl_2, I_2, H_2, as illustrated in Fig. 2.6.2.

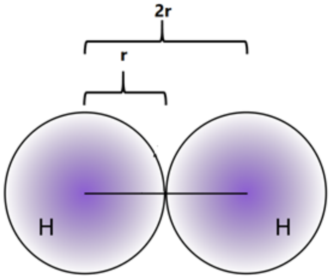


Figure 2.6.2: Diagram showing the atomic radius of H_2. Source: modified from CK-12 Foundation / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Periodic trend of atomic sizes

1. The atomic size generally increases from top to bottom in a group because the valence electrons add in the higher shell in each consecutive member of a group down the column.
2. The atomic size generally decreases from left to right in a row because the valence electrons are in the same shell while more protons add to the nucleus, increasing the pull on the valence electrons, as illustrated in Fig. 2.6.3.

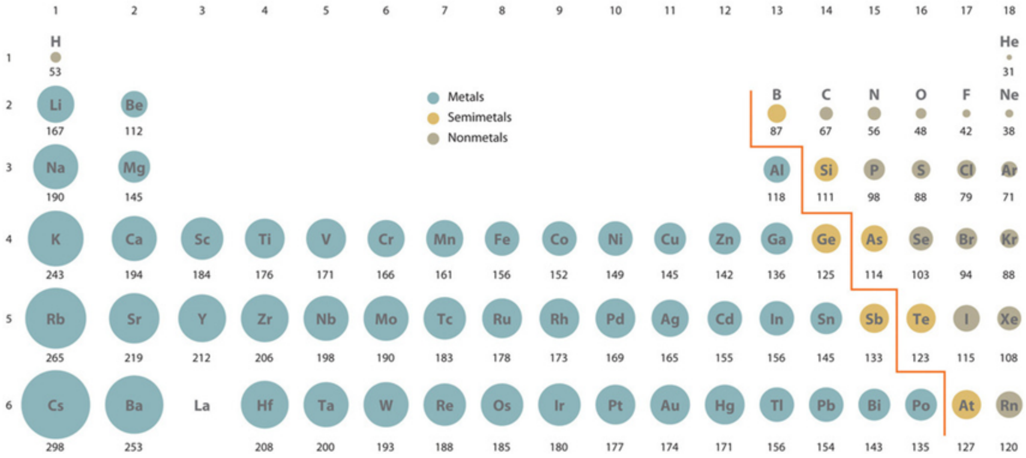


Figure 2.6.3: Illustration of the periodic trend of atomic sizes, Calculated Atomic Radii (in Picometers). Source: https://chem.libretexts.org/@api/dek...jpg?revision=1

Ionization energy

The positively charged nucleus attracts the negatively charged electrons. Therefore removal of an electron from the atom requires energy. The ionization produces a cation with fewer electrons than the parent neutral atom, i.e., cations.

Ionization energy

Ionization energy is the energy needed to remove an electron from a neutral atom, as in the following reaction.

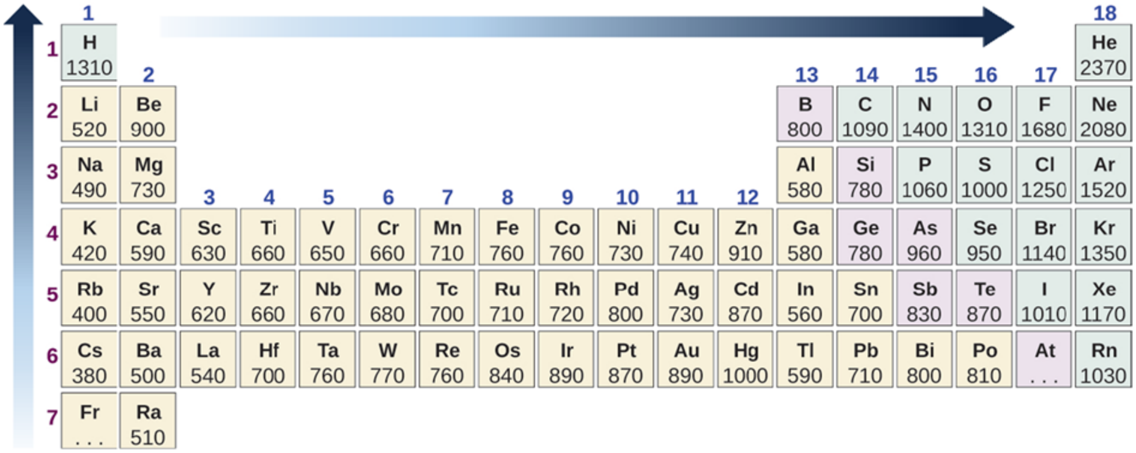
$$\mathrm{Na} + \text{ ionization energy } \rightarrow \mathrm{Na}^{1+} + \mathrm{e}^{-}$$

Periodic trend in ionization energy

1. The ionization energy generally decreases from top to bottom in a column because the valence electrons are further away and experience less pull to the nucleus down the column.

2. The ionization energy generally increases from left to right in a row because the valence electrons are in the same shell while more protons add to the nucleus, which increases the pull on the valence electrons.

Fig. 2.6.4 illustrates the periodic trend in the ionization energy.



	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H 1310																	He 2370
2	Li 520	Be 900											B 800	C 1090	N 1400	O 1310	F 1680	Ne 2080
3	Na 490	Mg 730											Al 580	Si 780	P 1060	S 1000	Cl 1250	Ar 1520
4	K 420	Ca 590	Sc 630	Ti 660	V 650	Cr 660	Mn 710	Fe 760	Co 760	Ni 730	Cu 740	Zn 910	Ga 580	Ge 780	As 960	Se 950	Br 1140	Kr 1350
5	Rb 400	Sr 550	Y 620	Zr 660	Nb 670	Mo 680	Tc 700	Ru 710	Rh 720	Pd 800	Ag 730	Cd 870	In 560	Sn 700	Sb 830	Te 870	I 1010	Xe 1170
6	Cs 380	Ba 500	La 540	Hf 700	Ta 760	W 770	Re 760	Os 840	Ir 890	Pt 870	Au 890	Hg 1000	Tl 590	Pb 710	Bi 800	Po 810	At . . .	Rn 1030
7	Fr . . .	Ra 510																

Figure 2.6.4: The 1st ionization energy in kJ/mol. Source: Download for free at https://openstax.org/details/books/chemistry

Electronegativity

Definition: Electronegativity

Electronegativity is the ability of an atom in a compound to attract the bonding electron pair to itself. Electropositivity is the opposite of electronegativity. Electronegativity is a property of an atom in a compound, i.e., a bonded atom, not a feature of an individual atom.

There are several electronegativity scales. The most commonly used is the Pauling electronegativity scale. Fig. 2.6.5 shows the electronegativities values on Pauling's electronegativity scale.

Group → ↓ Period	1	2	3		4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H 2.20																		He
2	Li 0.98	Be 1.57												B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne
3	Na 0.93	Mg 1.31												Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar
4	K 0.82	Ca 1.00	Sc 1.36		Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00
5	Rb 0.82	Sr 0.95	Y 1.22		Zr 1.33	Nb 1.6	Mo 2.16	Tc 1.9	Ru 2.2	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.1	I 2.66	Xe 2.60
6	Cs 0.79	Ba 0.89	La 1.1	*	Hf 1.3	Ta 1.5	W 2.36	Re 1.9	Os 2.2	Ir 2.20	Pt 2.28	Au 2.54	Hg 2.00	Tl 1.62	Pb 1.87	Bi 2.02	Po 2.0	At 2.2	Rn 2.2
7	Fr >0.79[en 1]	Ra 0.9	Ac 1.1	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og
				*	Ce 1.12	Pr 1.13	Nd 1.14	Pm 1.13	Sm 1.17	Eu 1.2	Gd 1.2	Tb 1.1	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb 1.1	Lu 1.27	
				**	Th 1.3	Pa 1.5	U 1.38	Np 1.36	Pu 1.28	Am 1.13	Cm 1.28	Bk 1.3	Cf 1.3	Es 1.3	Fm 1.3	Md 1.3	No 1.3	Lr 1.3[en 2]	

Values are given for the elements in their most common and stable oxidation states.

Figure 2.6.5: Periodic table of elements by Pauling scale. Source: https://en.Wikipedia.org/wiki/Electronegativity

Periodic trend in electronegativity

1. The electronegativity generally decreases from top to bottom in a column because the atomic size increases down the column making the nucleus less effective in pulling the bonding electrons.
2. The electronegative generally increases from left to right in a row because the atomic size decrease from left to right in a row, making the nucleus more effective in pulling the bonding electron pair to itself.

Metallic character

The metallic character relates to the ease of losing an electron in a chemical reaction. The metallic character trend is opposite to the trend of ionization energy.

Periodic trend in metallic character

1. The metallic character generally increases from top to bottom in a column because the atomic size increases down the column, making the valence electrons less tightly held and easier to remove.
2. The metallic character generally decreases from left to right in a row because the atomic size decreases from left to right, making the valence electrons more tightly held and difficult to remove.

Summary of the periodic trends

The ionization energy and the electronegativity generally increase from left to right in a row and from bottom to top in a column. The atomic size and the metallic character are opposite, i.e., they increase from right to left in a row and from top to bottom in a column. Fig. 2.6.6 summarizes the periodic trend in the properties of the elements.

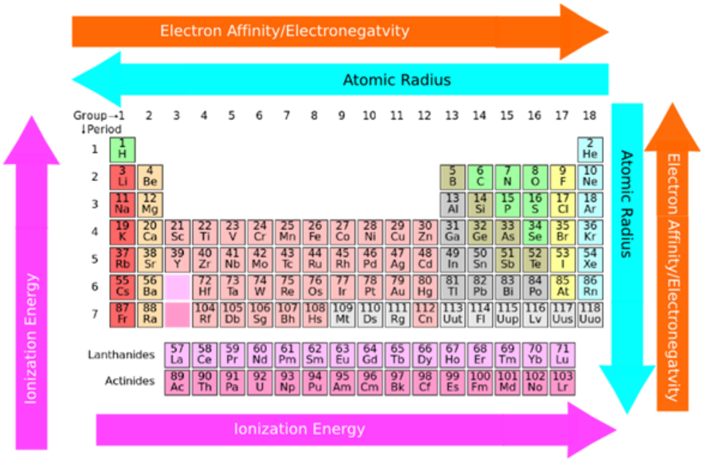


Figure 2.6.6: Summary of the periodic trend in the properties of elements. Source: https://www.hiclipart.com/free-trans...ntzga/download

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CHAPTER OVERVIEW

3: Compounds

3.1: Bonding in compounds

Chemical bonds

What is a compound?

Compounds are a pure form of matter formed by atoms of more than one element combined in a constant whole number ratio.

The bonds connect the atoms in the compounds. Sharing or transferring some valance electrons from one atom to the other makes the bonds. Noble gases have a full valence shell of eight valence electrons, except helium which has a full valence shell of two valence electrons. The noble gases are the least reactive, i.e., the most inert group of elements.

Octet rule

The octet rule states that atoms of all elements other than noble gases tend to share, lose, or gain valence electrons to acquire the electron configuration of the nearest noble gas having eight valence electrons.

Covalent bonds

A bond formed by sharing electrons is a covalent bond.

When a nonmetal atom combines with another nonmetal atom, they usually make a covalent bond. A covalent bond is a pair of shared electrons, called a **bonding pair** of electrons, where each bonded atom contributes one electron. For example, chlorine has seven valence electrons and needs one more to complete its octet. Hydrogen has one valence electron and requires one more to acquire the electron configuration of helium, i.e., **duet** instead of the octet. Hydrogen and chlorine combine by sharing one electron to make the compound HCl. Similarly, oxygen, nitrogen, and carbon make 2, 3, and 4 covalent bonds with hydrogen to complete their octet and make compounds H_2O, NH_3, and CH_4, respectively, as illustrated in Fig. 3.1.1.

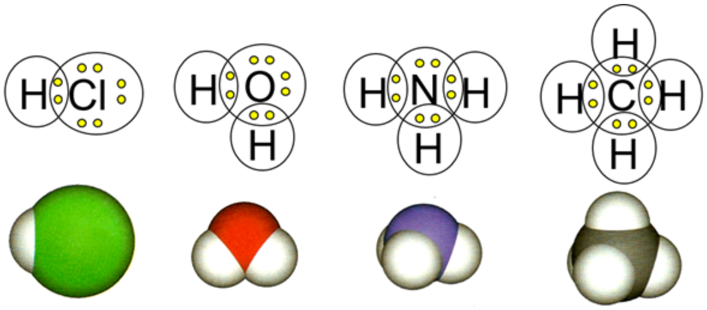


Figure 3.1.1: Examples of covalent bonds where Cl, O, N, and C acquire octet by sharing 1, 2, 3, and 4 electrons, respectively. Hydrogen shares one electron and acquires a duet, i.e., the electron configuration of helium. 2nd row is the space-filling model of the molecule where the white sphere is hydrogen, and the colored is the other atom. Source: "File:Kovalentne veze.png" by Drago Karlo CC BY-SA 4.0

Two atoms can share one, two, or three electrons to make a single, a double, or a triple covalent bond. For example, H_2 has a single bond (H-H), O_2 has a double bond (O=O), and N_2 has a triple bond (N≡N), where each line between the atoms represent one covalent bond. Fig. 3.1.2 illustrates the formation of three covalent bonds in N_2. A valence electron pair that is not involved in bonding is called a **nonbonding pair**. One nonbonding pair and three bonding pairs complete the octet of each nitrogen atom in the N_2 molecule, as shown in Fig. 3.1.2.

Note

The bonding pair of electrons counts towards the total valence electrons of each bonded atom., i.e., in H-H each hydrogen atom has two valence electrons, and in **:**N≡N**:** each nitrogen has eight valence electrons; two in the nonbonding pair and six in three bonding pairs.

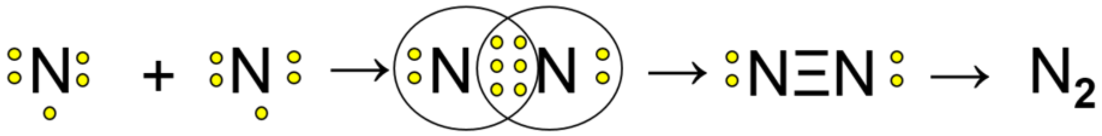


Figure 3.1.2: Illustration of three covalent bond formations between two nitrogen atoms. Source: File:Kovakentna veza dušika.png" by Drago Karlo is licensed under CC BY-SA 4.0

The formula of a covalent compound

A compound is represented by a chemical formula that combines the symbols of its constituent elements. More electropositive elements are usually written first, e.g., HF, NO, CO. Some exceptions to this rule, e.g., NH_3 and CH_4, have more electronegative elements written first. The majority of the covalent compounds exist as discrete molecules. A subscript to the right of the element's symbol represents the number of atoms of the component of the molecule. For example, H_2O has two hydrogen atoms and one oxygen atom in a water molecule. Note that subscript 1 is not written, i.e., the symbol of an element alone represents one atom.

A few covalently bonded compounds are giant molecules where the atoms are held together by a 3D network of bonds. The formula of these compounds shows the simplest whole-number ratio of elements in the compound. For example, Fig. 3.1.3 shows SiO_2 present in high-purity sand and quartz, a giant molecule.

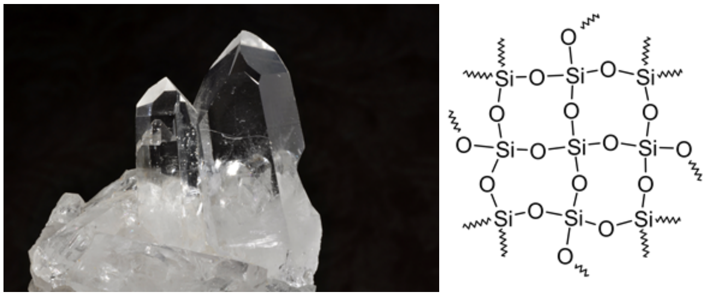


Figure 3.1.3: Quartz crystal composed of SiO_2, and an illustration of covalent bonds in a giant molecule of SiO_2. Source: Parent Géry, Public domain, via Wikimedia Commons, and Roland Mattern / Public domain

Ionic bond

> A bond formed by the transfer of electrons from one atom to the other atoms is an ionic bond.

A compound that has ionic bonds is an ionic compound. Usually, metal atoms lose electrons and become cations, and nonmetal atoms gain electrons to become anions. The electrostatic attraction between the opposite charges holds the ions together in the ionic compound. For example, sodium (Na) loses one electron, and fluorine (F) gains one electron to make a compound sodium fluoride (NaF), as illustrated in Fig. 3.1.4.

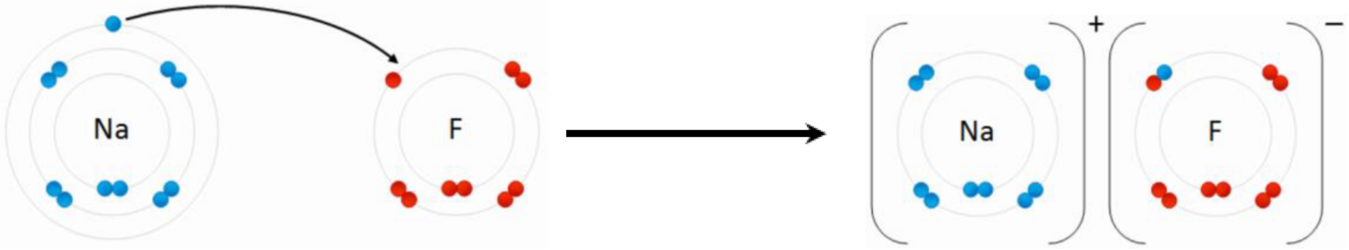


Figure 3.1.4: An example of ionic bond formation between Na and F. Source: modified from: Wdcf / CC BY-SA.

Ionic compounds

Table salt, i.e., NaCl is an example of an ionic compound. The Na completes its octet by losing one electron and becoming Na^+ cation. Losing electrons reduces the electron-electron repulsion, but the electron-nucleus attraction remains the same. Consequently, the electron cloud around the nucleus shrinks. Similarly, the chlorine atom has seven valence electrons. After gaining one electron, it becomes Cl^- anion with its octet complete. Gaining electrons increases the electron-electron repulsion, but the electron-nucleus attraction remains the same. Consequently, the electron cloud around the nucleus expands. Fig. 3.1.5 illustrates the formation of an ionic bond and the accompanying changes in the total number of electrons and sizes relative to the parent neutral atoms in the case of NaCl formation.

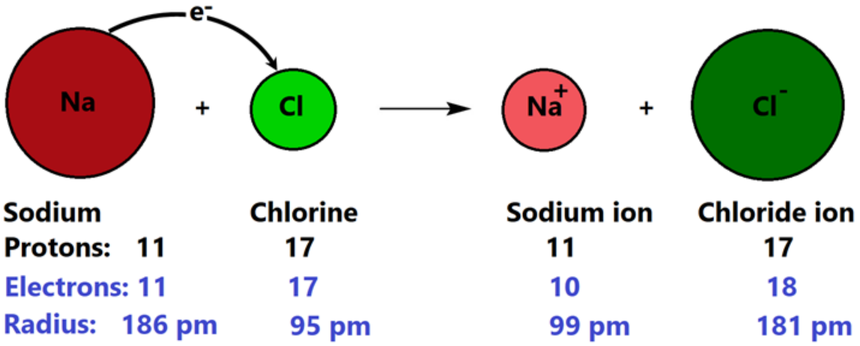


Figure 3.1.5: Illustration of an ionic compound formation by electron transfer from sodium (Na) to chlorine (Cl) making Na$^+$ cation with one less electron and Cl$^-$ anion with one more electron than their parent neutral atoms. The Na$^+$ cation is smaller than Na, and the Cl$^-$ anion is large than Cl atom.

The ionic bond is not localized or unidirectional. The electrostatic force is all around the ions. Therefore, the cations surround the anions, and the anion surrounds the cations in a regular array in a 3D crystal lattice. Fig 3.1.6 illustrates the structure of NaCl.

Note

1. The formula of the ionic compounds represents the simplest whole-number ratio of the atoms of the constituent elements.
2. A cation is always smaller in size than its parent neutral atom.
3. An anion is always larger than its parent neutral atom.

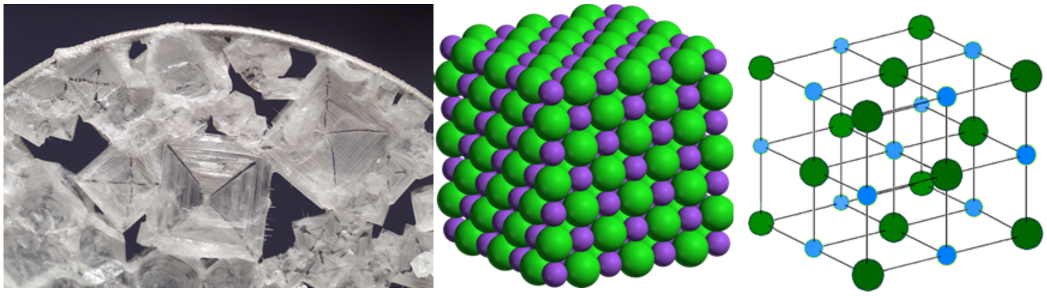


Figure 3.1.6: Sodium Chloride from left: actual crystals in a water bubble within a 50 mm metal loop, model, and crystal lattice. Na$^+$ is purple or blue, and Cl$^-$ is green in the models. Source: Photograph by the NASA Expedition 6 crew, Public domain, via Wikimedia Commons, Benjah-bmm27 (talk · contribs) / Public domain, and File: H Padleckas / Public domain

Criteria to distinguish between ionic and covalent bond

Usually, a metal and a nonmetal bond is ionic, and the bond between two nonmetals is covalent. Better criteria are based on the difference in electronegativities of the bonded atoms. Electronegativity is the ability of an atom to attract a pair of bonded electrons to itself. If the electronegativity difference is significant, the bonding electrons completely transfer to the more electronegative atom, and the bond is ionic. There is no single value of electronegativity difference to separate ionic and covalent bonds, but usually, the electronegativity difference of more than 1.8 results in an ionic bond. Otherwise, a covalent bond, but the bonding electrons are more towards the more electronegative atom, making it a polar covalent bond. An electronegativity difference less than 0.5 is considered a noncovalent bond, but a true noncovalent bond forms when the bonded atoms are the same element.

Properties of compounds

The properties of the compounds are usually altogether different from the properties of their constituent elements. For example, hydrogen (H_2) is a gas that burns in oxygen, oxygen (O_2) is a gas that assists combustion, but water (H_2O) is a liquid that extinguishes fire. Similarly, sodium (Na) is a soft metal that melts at 97.79 ^{o}C, chlorine (Cl_2) is yellowish color gas, but sodium chloride (NaCl) is a transparent crystal that melts at 801 ^{o}C.

The intermolecular interactions in covalent molecules are weak to moderate relative to the strength of covalent bonds or ionic bonds. Therefore, the covalent molecules are usually gases like O_2, NH_3, CH_4, liquids like H_2O, or soft and low melting solids like waxes, glucose ($C_6H_{12}O_6$, mp 146^{o}C).

Ions in the ionic compounds are held together by strong ionic bonds in a 3D array of crystal lattices. Therefore, ionic compounds are usually hard solids with high melting points. For example, NaCl melts at 801 ^{o}C. Covalent compounds that exist as a 3D network of covalent bonds, i.e., as giant molecules, are usually hard materials having a higher melting point than ionic compounds. For example, SiO_2 present in sand and quartz is a hard solid that melts at 1,710 ^{o}C. Diamond –the hardest known substance, is a giant molecule of carbon atoms held together in a 3D network of covalent bonds that melts around 4,027 ^{o}C.

3.2: Naming binary ionic compounds

Binary ionic compounds are compounds composed of monoatomic cations and monoatomic anions. For example, NaCl is a binary ionic compound composed of monoatomic cations Na^+ and monoatomic anions Cl^-. Another example is $CaCl_2$ composed of monoatomic cations Ca^{2+} and monoatomic anions Cl^-.

Charge on monoatomic ions

Nonmetals and metalloids of group 14 to group 17 usually form monoatomic anions. The charge on the anions is equal to the group number minus eighteen. For example, halogens in group 17 have charge: 17-18 = -1, oxygen in group 16 has charge: 16-18 = -2, and nitrogen in group 15 has charge: 15-18 = -3. Metals usually form cations: metals of group 1 from +1, metals of group 2 form +2, and aluminum of group 13 form +3 charge on cations, as shown in Fig. 3.2.1. Other metals have variable charges in compounds. The charge of the metals having variable charge can be calculated from the compound's chemical formula because the total –ve charge should be equal to the total +ve charge to make the compound neutral.

Example 3.2.1

calculate the charge of iron ion in $FeCl_2$?

Solution

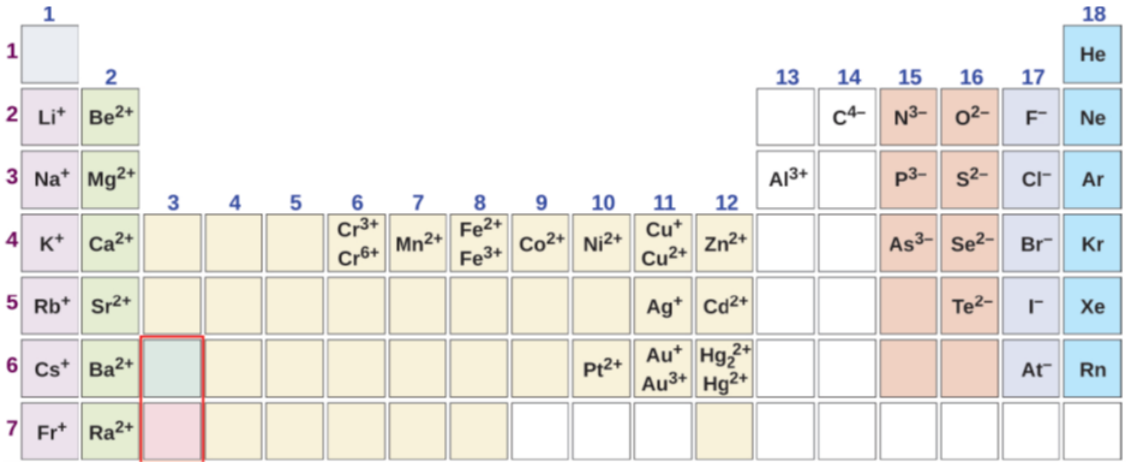
Three are two chloride anions, each with a -1 charge, making a total of -2. So the charge on cation has to be +2 to balance the negative charge. Answer: Fe^{2+}.

Example 3.2.2

Calculate the charge on an iron ion in Fe_2O_3?

Solution

There are three oxygen anions, each with a -2 charge, making -6. So the total charge on two iron atoms should be +6, i.e., the charge on iron atoms is +3. Answer: Fe^{3+}.



	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1																		He
2	Li^+	Be^{2+}												C^{4-}	N^{3-}	O^{2-}	F^-	Ne
3	Na^+	Mg^{2+}											Al^{3+}		P^{3-}	S^{2-}	Cl^-	Ar
4	K^+	Ca^{2+}				Cr^{3+} Cr^{6+}	Mn^{2+}	Fe^{2+} Fe^{3+}	Co^{2+}	Ni^{2+}	Cu^+ Cu^{2+}	Zn^{2+}			As^{3-}	Se^{2-}	Br^-	Kr
5	Rb^+	Sr^{2+}									Ag^+	Cd^{2+}				Te^{2-}	I^-	Xe
6	Cs^+	Ba^{2+}								Pt^{2+}	Au^+ Au^{3+}	Hg_2^{2+} Hg^{2+}					At^-	Rn
7	Fr^+	Ra^{2+}																

Figure 3.2.1: The charges on common ions. Download for free at https://openstax.org/details/books/chemistry.

Names of monoatomic ions

Name of a monoatomic anion

The name of a monoatomic anion is the element's name with the last syllable replaced with –ide ion. For example, Cl^- is a chloride ion, O^{2-} is an oxide ion, N^{3-} is a nitride ion, S^{2-} is sulfide ion, and C^{4-} is a carbide ion, derived from the element names chlorine, oxygen, nitrogen, sulfur, and carbon, respectively.

Name of a monoatomic cation having a fixed charge

Alkali metals have +1, alkaline earth metals have +2, and aluminum has +3 charge. Their name is the name of the element ending with ion. For example, Na^+ is a sodium ion, Ca^{2+} is a calcium ion, and Al^{3+} is an aluminum ion.

Name of a monoatomic cation having a variable charge

The names of the cations that have a variable charge is the name of the element followed by charge in roman numeral enclosed in small bracts and ending with ion. For example, Fe^{2+} is an iron(II) ion, and Fe^{3+} is an iron(III) ion, Cu^+ is a copper(I) ion, and Cu^{2+} is a copper(II) ion.

Ions in body fluids

The ions that are important in body fluids include sodium ion (Na^+), potassium ion (K^+), calcium ion (Ca^{2+}), magnesium ion (Mg^{2+}), and chloride ion (Cl^-), as shown in Fig. 3.2.2. Na^+ is present in fluids inside the cells. It regulates and controls body fluids. K^+ is present in fluids outside the cells and regulates body fluids and cell functions. Ca^{2+} and Ma^{2+} are present in the body fluids outside the cells, where Ca^{2+} is needed for muscle contraction, Mg^{2+} is needed for muscle contraction, nerve control, and enzymes. Cl^- is primarily present to balance the charge of the cations in the body fluids.

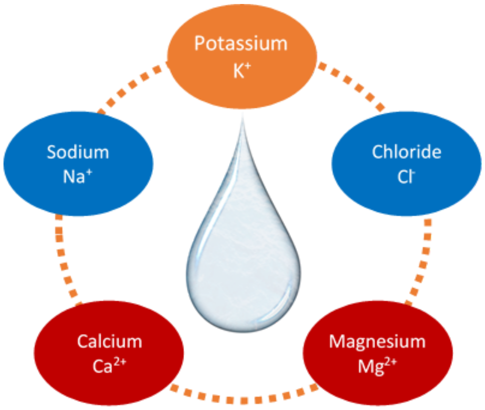


Figure 3.2.2: Electrolytes usually found in body fluids.

Writing the formula of a binary ionic compounds

The formula of an ionic compound is the symbol of the cation element with a subscript number followed by the symbol of the anion element with a subscript number. The formula shows the simplest whole-number ratio of the constituent elements in the subscripts, such that the total positive charge is equal to the total negative charge.script on the right of the symbols tell the number if they're more than one atom of the element.

Rules of writing the formula of a binary ionic compound

The rules are illustrated in Fig. 3.2.3:

1. Write cation followed by anion with charges,
2. swap the charge as a subscript of the opposite ion,
3. simplify the subscript to the simplest whole-number ratio,
4. use the simplified subscript in the final formula, and
5. do not write the subscript if it is one.

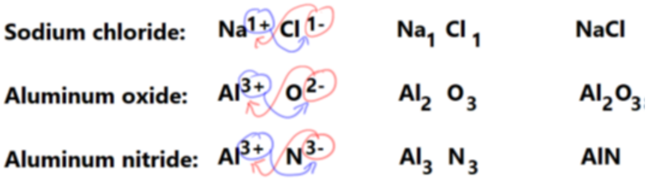


Figure 3.2.3: Rules to write the formula of the binary ionic compounds.

Writing the names of an ionic compound from the formula

Writing the name of ionic compounds of cations with fixed charge

If the cation has a fixed charge in compounds, the name starts with the name of the element of the cation, followed by the name of the anion without the world ion at the end. For example, KI is potassium iodide, and $CaCl_2$ is calcium chloride.

Writing the name of ionic compounds of cations with variable charge

Write the name of the cation, including the charge in roman numerals enclosed in small brackets but without the word ion at the end, followed by the name of the anion, without ion at the end. For example, $FeCl_2$ is iron(II) chloride, and Fe_2O_3 is iron(III) oxide. Additional examples are given in Table 1.

Transition metals with fixed charge

Silver, zinc, and cadmium cations have fixed changes: Ag^+, Zn^{2+}, and Cd^{2+}. Names of these cations are the names of the element with or without charge shown in roman numerals, both ways it is correct.

Table 1: Examples of writing names from the formulae of binary ionic compounds

Example#	Formula	Name of the cation	Name of the anion	Name of the compound
1	NaCl	Sodium ion	Chloride ion	Sodium chloride
2	Al_2O_3	Aluminum ion	Oxide ion	Aluminum oxide
3	$FeCl_3$	Iron(III) ion	Chloride ion	Iron(III) chloride
4	CuO	Copper(II) ion	Oxide ion	Copper(II) oxide
5	AgCl	Silver(I) ion, or Silver ion	Chloride ion	Silver(I) chloride, or Silver chloride

---

3.3: Polyatomic ions and their compounds

Polyatomic ions

Polyatomic ions are molecular ions composed of two or more atoms bonded by covalent bonds and acting as a single unit, but unlike molecules, they have a net charge on them.

The examples include cations like ammonium ion (NH_4^+), and hydronium ion (H_3O^+); and anions like hydroxide ion (OH^-), and cyanide ion (CN^-). Usually, the name of polyatomic cations ends with –ium, and the name of polyatomic anions end with –ide, except for oxyanions that have separate rules for their nomenclature.

Oxyanion

The oxyanions are oxides of nonmetals that are molecular ions. Examples include carbonate (CO_3^{2-}) , nitrate (NO_3^{2-}), phosphate (PO_4^{3-}), and sulfate (SO_4^{2-}). The following guidelines will help remember the names and charges of oxyanions in most cases.

Oxyanions having elements from groups 14, 15, and 16

1. the 2nd-row elements C, and N have three oxygen, and 3-row elements P, and S have four oxygen, i.e., one oxygen more than the row number,
2. the name of the polyatomic anion is the name of the atom other than oxygen with the last syllable replaced with –ate, and
3. the charge on these oxyanions equals the number of valence electrons on the non-oxygen atom minus twice the number of oxygen atoms. For example: in (PO_4^{3-}), phosphorous has 5 valence electrons and there are 4 oxygen atoms, so the charge = valence elections in the central atom -2 x number of oxygen atoms = 5-(2x4) = -3; in (SO_4^{2-}), sulfur has 6 valence electrons and there are 4 oxygen atoms, so the charge = 6-(2x4) = -2; in (CO_3^{2-}), carbon has 4 valence electrons and there are 3 oxygen atoms, so the charge = 4-(2x3) = -2; and in (NO_3^-), nitrogen 6 valence electrons and there are 3 oxygen atoms, so the charge = 6-(2x3) = -1.
4. There is a 2nd set of oxyanions of the elements mentioned above with one less oxygen but the same charge and the last syllable of the name changed from -ate to -ite. For example: (NO_3^-) is nitrate and (NO_2^-) is nitrite; (PO_4^{3-}) is phosphate and (PO_3^{3-}) is phosphite; and (SO_4^{2-}) sulfate and (SO_3^{2-}) is sulfite.

Oxyanions of halogens

Oxyanins of chlorine, bromine, and iodine are also common oxyanions with the following in common.

1. They have -1 charge,
2. a halogen with four oxygen is named by adding prefix "per-" to the name of the halogen with last syllable replaced with -ate, for example; (ClO_4^-) is perchlorate, (BrO_4^-) is perbromate, and (IO_4^-) is periodate.
3. a halogen with three oxygen is named as name of the halogen with last syllable replaced with -ate, for example; (ClO_3^-) is chlorate, (BrO_3^-) is bromate, and (IO_3^-) is iodate,
4. a halogen with two oxygen is named as name of the halogen with last syllable replaced with -ite; for example, (ClO_2^-) is chlorite,(BrO_2^-) is bromite, and (IO_2^-) is iodite,
5. a halogen with one oxygen is named by adding prefix "hypo-" to the name of the halogen with last syllable replaced with -ite; for example, (ClO^-) is hypochlorite, (BrO^-) is hypobromite, and (IO_3^-) is hypoiodaite.

Acids of oxyanions

Oxyanions are acids when their charge in neutralized with protons (H^+). Names of the acids are the names of oxyanions with -ate replaced with -ic acid and -ite replaced with -ous acid. For example: (HNO_3) is nitric acid and (HNO_2) is nitrous acid; (H_3PO_4) is phosphoric acid and (H_3PO_3) is phosphorous acid; and (H_2SO_4) sulfuric acid and (H_2SO_3) is sulfurus acid.

The prefixes "per-" and "hypo-" in the cases of oxyanions of halogens remain in the acid name. For example: ($HClO_4$) is perchloric acid; ($HClO_3$) is chloric acid; ($HClO_2$) is chlorous acid; and ($HClO$) is hypochlorous acid.

Oxyanions with one proton attached but charge one them not fully neutralized, i.e., they are still polyatomic anion are named beginning with hydrogen and ending with the name of the oxyanion. For example: (HSO_4^-) is hydrogen sulfate; (HSO_3^-) is

> hydrogen sulfite; and (HPO_4^{2-}) is hydrogen phosphate.
>
> Oxyanions with two protons attached but charge one them not fully neutralized, i.e., they are still polyatomic anion are named beginning with dihydrogen and ending with the name of the oxyanion. For example, ($H_2PO_4^-$) is dihydrogen phosphate

fTwo oxyanions containing a transition metal as the central atom in common use as reagents are in chemistry are chromate (CrO_4^{2-}) and permanganate (MnO_4^-). Table 3.3.1 lists the formulas and names of some of the common polyatomic ions.

Table 1: Names of some of the common polyatomic ions

Formula	Name	Formula	Name
(NH_4^+)	Ammonium	(MnO_4^-)	Permanganate
(H_3O^+)	Hydronium	(BrO_4^-)	Perbromate
(HO^-)	Hydorxide	(IO_4^-)	Periodate
(CN^-)	Cynide	(CrO_4^{2-})	Chromate
(CO_3^{2-})	Carbonate	(CO_2^{2-})	Carbonite
(NO_3^-)	Nitrate	(NO_2^-)	Nitrite
(PO_4^{3-})	Phosphate	(PO_3^{3-})	Phosphite
(SO_4^{2-})	Sulfate	(SO_3^{2-})	Sulfite
(HCO_3^-)	Hydrogen carbonate	(ClO_4^-)	Perchlorate
(HSO_4^-)	Hydrogne sulfate	(ClO_3^-)	Chlorate
(HPO_4^{2-})	Hydrogenphosphate	(ClO_2^-)	Chlorite
($H_2PO_4^-$)	Dihydrogenphosphate	(ClO^-)	Hypochlorite

Names of compounds containing polyatomic ions

Rules for naming ionic compounds containing polyatomic ions are the same as binary ionic compounds. That is, write the name of the cation followed by the name of the anion. For cations with variable charge, keep the roman numeral in the compound's name. For example, $NaNO_3$ is sodium nitrate, $CaCO_3$ is calcium carbonate, $FeCO_3$ is iron(II) carbonate, NH4Cl is ammonium chloride.

Writing formulae of compounds containing polyatomic ions

The polyatomic ion acts as a single unit, i.e., they are molecular ions. The writing formula of compounds containing polyatomic ions is the same as writing the formula of a binary ionic compound, except that the polyatomic ions must remain intact as a unit. If a subscript is needed for the anion, place the polyatomic ion within small brackets and write the subscript outside the bracket. Just like the subscript to the right of the monoatomic anion tells how many atoms of the anions are there, the subscript to the right of the small bracket around a polyatomic anion tells how many polyatomic anions are there in the compound. For example, iron(III) nitrate is $Fe(NO_3)_3$; sodium carbonate is Na_2CO_3; ammonium phosphate is $(NH_4)_3PO_4$; potassium permanganate is $KMnO_4$; and calcium phosphate is $Ca_3(PO_4)_2$. Note that in $Fe(NO_3)_3$, there are three nitrate ions, i.e., one iron atom, three nitrogen atoms, and nine oxygen atoms, in the formula unit of the compound.

3.4: Naming acids

Acids donate produce protons and anions when dissolved in water. The naming is different for acids that have oxyanions and the others.

Naming acid that does not contain oxyanion

There are two nomenclatures, first as ionic compounds and second as acids.

Naming acids as ionic compounds

Wright the name of the cation element, i.e., hydrogen, followed by the name of anion without ion at the end. For example, HCl is hydrogen chloride, and HCN is hydrogen cyanide. The ionic name is preferred when the compound is not acting as an acid, e.g., pure HCl in the gas phase.

Naming as acids

Add prefix hydro- to the name of anion and replace the last syllable from –ide to –ic acid. For example, HCl is hydrochloric acid, HCN is hydrocyanic acid, HI is hydroiodic acid. The acid name is preferred when the compound acts as an acid, particularly when it is in solution form in water.

Naming acid that contains oxyanion

Begin the name with the name of oxyanion and change the last syllable from -ate to -ic acid or from -ite to -ous acid. If there is prefix per- or hypo to the name of the oxyanion, it stays in the acid name. For example: $(\mathrm{NO_3^-})$ is nitrate and $(\mathrm{HNO_3})$ is nitric acid ; $(\mathrm{NO_2^-})$ is nitrite and $(\mathrm{HNO_2})$ is nitrous acid; $(\mathrm{SO_4^{2-}})$ is sulfate and {H2SO4}\)) sulfuric acid; $(\mathrm{ClO_4^-})$ is perchlorate and ($\mathrm{HClO_4}$) is perchloric acid; and $(\mathrm{ClO^-})$ is hypochlorite and (HClO) is hypochlorous acid.

One of the commonly encountered oxyacid is acetic acid. Acetic acid is an organic acid with the formula CH_3COOH, where the last hydrogen attached with oxygen is the acidic proton, and the other three oxygen attached with carbon are not acidic. The anion from acetic acid is called acetate ion that has a formula CH_3COO^- which may also be written as $C_2H_3O_2^-$.

3.5: Naming binary covalent compounds

What is a binary covalent compound?

Binary covalent compounds are atoms of two different elements held together by covalent bonds. Usually, they are composed of nonmetals elements, e.g., laughing gas NO, acid rain causing gas SO_2, etc.

Writing formulae of binary covalent compounds.

The molecular formula of a binary covalent compound shows the symbols of constituent elements, followed by a subscript showing how many atoms of the element are in the molecule. Usually, the symbol of an element closer to metals in a period or a group is written first, followed by the symbol of the other element. For example, CO_2, NO, P_2O_5, where carbon, nitrogen, and phosphorous are nearer to the metals in the periodic table than the other element. An exception occurs when the compound contains oxygen combined with chlorine, bromine, or iodine, where oxygen is closer to metals but is second in the formula, e.g., ClO_2.

Writing the names of binary covalent compounds

The name of binary covalent compounds contains prefixes, listed in Table 1, to indicate the number of atoms followed by the name of the elements according to the following rules:

1. name of the first element in the formula with a prefix showing the number of atoms, followed by,
2. the name of the second element with a prefix showing the number of atoms and its last syllable replaced with –ide.
3. Do not write mono- if it applies to the first element in the formula, but write mono- if it applies to the second element. Write all other prefixes.
4. If the prefix ends with a vowel and the element name begins with a vowel, drop the ending vowel of the prefix.

Table 3.5.1 lists the prefixes used to represent the number of atoms from 1 to 10. Examples of the names are: NO is nitrogen monoxide, CO_2 is carbon dioxide, PCl_3 is phosphorous trichloride, P_2O_5 is diphosphorus pentoxide, SiO_2 is silicon dioxide. Trivial names are well known for some molecular compounds and they are often used in the place of systematic names, e.g., water for H_2O and ammonia for NH_3.

Table 1: Prefixes used in naming binary covalent compounds

Prefix	Means
Mono-	1
di-	2
Tri-	3
tetra-	4
penta-	5
hexa-	6
hepta-	7
octa-	8
nona-	9
deca-	10

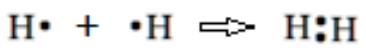
3.6: Lewis structures of molecules

Lewis symbols of elements

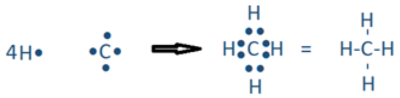
Lewis symbol of element shows the symbol of element with valence electrons shown as dots placed on top, bottom, left, and right sides of the symbol. Valence electrons up to four are shown as a single dot on either side of the symbol. The 5th, 6th, 7th, and 8th valence electron dots are paired with any of the first four dots. For example,  represent hydrogen, beryllium, boron, carbon, nitrogen, fluorine, and neon with 1, 2, 3, 4, 5, 6, 7, and 10 valence electrons, respectively. Lewis symbols of first twenty elements are shown in section 2.6, Table 1.

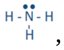
Lewis structures of simple molecules

An unpaired dot in the Lewis symbol of an element can make one bond by sharing it with an unpaired dot of another atom. The shared pair of dots represents a pair of bonding electrons, a covalent bond. For example, as shown below, a Hydrogen atom has one unpaired valence electron and makes a covalent bond with another hydrogen atom.



The covalent bond is usually represented by a single line between the bonded atoms, e.g., the H_2 molecule shown in the above equation is generally shown as H-H. An example is a reaction between hydrogen having one valence electron and carbon having four valence electrons react to form CH_4 molecule.



Similarly, hydrogen reacts with nitrogen, oxygen, and fluorine to form the following molecules: , , and . Each line in these molecules represents a **bonding electron pair**, and the pair of dots represent valence electrons that are not involved in bonding, called **lone pair of electrons**. The lone pair is usually omitted from the Lewis structure unless it is needed to emphasize their presence for some reason.

Procedure for writing Lewis structures of molecules

A systematic approach for writing the Lewis structure of molecules is explained with the help of the following example.

✓ Example 3.6.1

Draw the Lewis structures of CH_4, PCl_3, CO_2, and HCN

Solution

Step 1: Add the valence electrons of all the molecules' atoms:

- CH_4 has 4 valence electrons in C, and 1 in each of the four H: = 4 + 1x4 = 8 valence electrons
- PCl_3 has 5 valence electros in P and 7 in each of the three Cl: = 5 + 7x3 = 26 valence electrons
- CO_2 has 4 valence electrons in C and 6 in each of the two O: = 4 + 6x2 = 16 valence electrons
- HCN has 1 valence electron in H, 4 in C, and 5 in N: = 1 + 4 + 5 = 10 valence electrons

Step 2: Place the element symbol with more valances, i.e., having more unpaired dots in its Lewis structure, in the center and the rest of the atoms on four sides:

Step 3: Draw a line between the outer atom and the central atom to represent a single covalent bond:

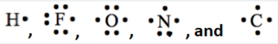
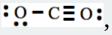
Step 4: Every single bond consumes two valence electrons. Subtract the total number of valence electrons consumed in all the bonds from the total valence electrons initially present in step 1:

- CH_4: 4 bond = 8 electrons consumed. 8 – 8 = 0 electrons left
- PCl_3: 3 bond = 6 electrons consumed. 26 – 6 = 20 electrons left
- CO_2: 2 bond = 4 electrons consumed. 16 – 4 = 12 electrons left
- HCN: 2 bond = 4 electrons consumed. 10 – 4 = 6 electrons left

Step 5: Distribute the remaining electrons as lone pairs, first to the outer atoms to complete their octet (duet in the case of hydrogen) and then to the central atom to complete its octet

Step 6: Check that the octet of each atom is complete (duet for hydrogen). If yes, the Lewis structure is complete, e.g., as in the cases of CH_4 and PCl_3 in the present examples. If not, move one of the lone pair of electrons from a neighboring atom to make a double bond, as shown by the red color arrows in the figure in the previous step. If the octet is still not complete, move one more lone pair of electrons from a neighboring atom: from the same atom to make a triple bond, as in the case of HCN above, or from another neighboring atom to make two double bonds, as in the case of CO_2 above. The result is Lewis structures shown below.

Note

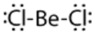
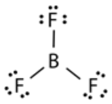
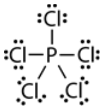
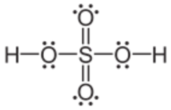
To draw the Lewis structure of the most stable form, try to keep covalent bonds with an atom equal to the number of unpaired dots in the Lewis symbol of the atoms. For example,  have 1, 1, 2, 3, and 4 unpaired electrons. So, hydrogen makes one, fluorine one, oxygen two, nitrogen 3, and carbon four covalent bonds in the stable molecules. When pulling a lone pair from neighboring atoms is needed to result in a double or triple bond, it is preferable to keep the resulting number of covalent bonds equal to the number of unpaired electrons in the Lewis symbol of the atom. For example, in the case of CO_2 molecule, if both lone pairs were pulled from the same oxygen in step 6 above, the resulting Lewis structure would have been , which is technically correct Lewis structure but not the most stable form of this molecule. Note that the latter structure has one covalent bond in one oxygen and three covalent bonds in the other instead of two covalent bonds needed for oxygen.

Exceptions to the octet rule

The octet rule generally applies in most cases, but there are exceptions in a few cases:

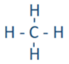
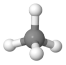
1. Atoms of hydrogen, lithium, and beryllium tend to share, lose, or gain valence electrons to acquire the electron configuration of the nearest noble gas helium having two valence electrons. This is called the **duet rule**.
2. Sometimes the atoms may end up in compounds with less than eight valence electrons. This often happens in the case of boron compounds and aluminum compounds of group 13. For example, boron has three valence electrons resulting in compounds like BF_3 with three covalent bonds and six instead of eight valence electrons around boron.
3. Atoms of elements in period three and beyond sometimes end up in compounds with more than eight valence electrons. For example, PCl_3 has octet complete, but PCl_5 has 10 valence electrons. Similarly, sulfur has its octet complete in H_2S but has 12 valence electrons in H_2SO_4. This happens because atoms in period thee and beyond have larger sizes and they have valence electrons in d or f orbitals in addition to the valence s and p orbitals. Table 1 lists some examples of exceptions to the octet rule.

Table 1: Some examples of exceptions to the octet rule.

Structure	H:H				

Name	Hydrogen	Beryllium dichloride	Boron trifluoride	Phosphorous pentafluoride	Sulfuric acid
Valence electrons on the central atom	2	4	6	10	12

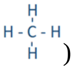
3.7: Molecular shapes –Valence shell electron pair repulsion (VSEPR) theory

The Lewis structure tells the connection between atoms and any lone pair present, but it does not tell the exact angles of bonds around the central atom or the actual shape of the molecule. The conventional way of presenting a Lewis structure of a molecule shows it as a planer, e.g., CH_4 as  which implies the molecule to be planar and H-C-H bond angles to be either 90^o or 180^o. The actual CH_4 molecule is nonplanar as  with all H-C-H bond angles 109.5^o. the following theory helps explain the actual shapes of molecules.

Valence shell electron pair repulsion (VSERP) theory

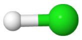
The valence shell electron pair repulsion theory predicts the shape of the molecule and bond angles based on the fact that valence shell electrons around the central atom in a molecule are grouped. The electron groups repel each other and go as far apart from each other as possible.

Electron groups

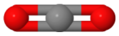
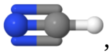
A lone pair, a single bond, a double bond, and a triple bond, each of these is one electron group. This is because two elections of single bond, four electrons of a double bond, and six electrons of a triple bond are located in the region along the axis of the bond, i.e., they are grouped together. Similarly, a lone pair is located in a defined space around the atom. For example, carbon in methane () has four electron groups that are the four single bonds (C-H bonds) around the carbon. Carbon in carbon dioxide (O=C=O) has two electron groups that are the two double bonds around the carbon, and in H-C≡N has two electron groups that are a single bond (C-H bond) and a triple bond (C≡N bond).

Molecular shapes and bond angles based on VSEPR theory

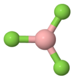
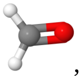
One electron group

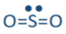
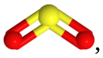
One electron group between two atoms is always a linear molecule. For example, H-H ,O=O, N≡N, and H-Cl , are linear molecules, where hydrogen is white and chlorine is green in the H-Cl model.

Two-electron groups

Two-electron groups are farthest apart in a **linear geometry** with the central atom in the middle of the line and the bond angles of 180^o around the central atom. The examples include CO_2  and HCN , where the central carbon atom is gray, hydrogen is white, nitrogen is blue, and oxygen is red.

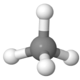
Three-electron groups

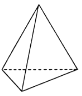
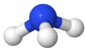
Three-electron groups are farthest apart when they are at the corners of a triangle in a **planar trigonal geometry** with the central atom in the middle of the triangle and the bond angles of 120^o around the central atom. Examples include BF_3 , and H_2CO , where boron is pink, F is green, carbon is gray, oxygen is red, and hydrogen is white.

If one of the electron domains is a lone pair, the electron domain geometry remains the same, but the geometry of the atoms in the molecule, i.e., **molecule geometry,** is **bent**. For example,  has three electron domains and trigonal planar electron domain geometry, but there is one lone pair. So, the molecule geometry is **bent** as , where sulfur is yellow, and oxygen is red (lone pair in not shown).

Four-electron groups

Four-electron groups are farthest apart when they are at the corners of a tetrahedron in a **tetrahedral geometry** with the central atom at the center of the tetrahedron and the bond angles of 109.5^o around the central atom as: . An example is methane CH_4

, where carbon is gray, and hydrogens are white.

If one of the electron domains is a lone pair, the electron domain geometry is still tetrahedral, but the molecule geometry is **trigonal pyramidal** as  with three pereferal atoms at the corners of the triangel and the central atom raised to the top of the pyramid. An example is ammonia (:NH_3) , where nitrogen is blue, and hydrogens are white.

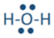
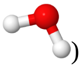
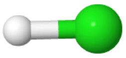
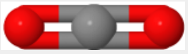
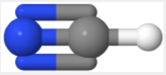
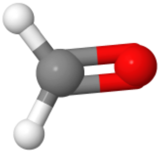
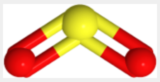
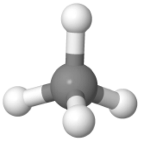
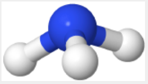
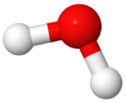
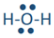
If two electron domains are lone pairs, the electron domains geometry is still tetrahedral, but the molecule geometry is bent. An example is water ( ), where oxygen is red, and hydrogens are white.

Table 1 is the summary of the electron domain geometries and the corresponding molecular geometries.

Table 1: Common molecular geometries around the central atom

Electron domain	**Lone pair**	**Electron domain geometry**	**Molecule geometry**	**Bond angles**	**Examples**
1	0	Linear	Linear	-	HCl 
2	0	Linear	Linear	180^{o}	CO_2  HCN 
3	0	Trigonal pyramidal	Trigonal pyramidal	120^{o}	H_2CO 
3	2	Trigonal pyramidal	Bent	120^{o}	 
4	0	Tetrahedral	Tetrahedral	109.5^{o}	 CH_4
4	1	Tetrahedral	Trigonal pyramidal	109.5^{o}	:NH_3 
4	2	Tetrahedral	Bent	109.5^{o}	 

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3.8: Polarity of molecules

The polarity of an atom

The negative charge of electrons balances the positive charge of protons in an atom. The electrons symmetrically distributed around the nucleus leave no negative or positive end. The atoms are nonpolar. Fig. 3.8.1 illustrates the polarity of a hydrogen atom with color codes.

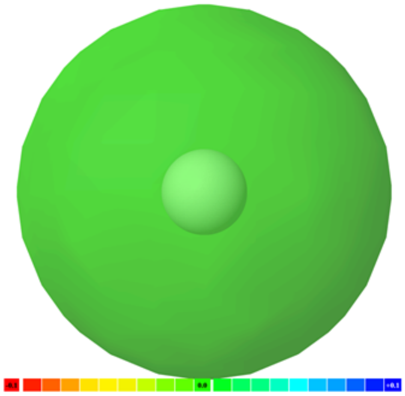

Figure 3.8.1: Electrostatic potential map of hydrogen atom, shown nonpolar by green color code. Source: drawn using free software https://chemagic.org/molecules/amini.html

The polarity of a covalent bond

When atoms of one element combine to make a covalent bond, e.g., H-H and F-F, the positive and negative charges are still symmetrical, and the bond is **nonpolar**, i.e., no negative end separated from a positive end. However, when atoms of different elements combine to make a covalent bond, the more electronegative atom attracts the bonding electron pair towards itself stronger than the other atom. The separation of positive and negative charges happens as the electrons shift more towards the electronegative atom. The bond becomes **polar** with a partially positive (δ+) end on the electropositive atom and a partially negative (δ-) end on the electronegative atom. For example, fluorine is more electronegative than hydrogen. Consequently, fluorine pulls the bonding electron pair towards itself in the H-F molecule, creating a partial negative charge (δ-) on fluorine and a partial positive charge (δ+) on hydrogen. The H-F bond is polar. Fig. 3.8.2 illustrates the polarity in H-F with color codes.

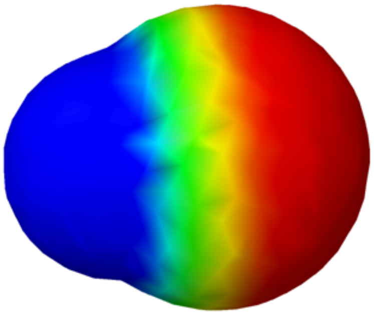

Figure 3.8.2: H-F molecule showing δ+ end in blue, δ- end in red and neutral part in green. Source: drawn using free software http://molview.org/?cid=14917

Bond polarity is a vector that has a magnitude and direction and can be represented by an arrow, like other vectors, as shown in Fig. 3.8.3 for the case of a water molecule.

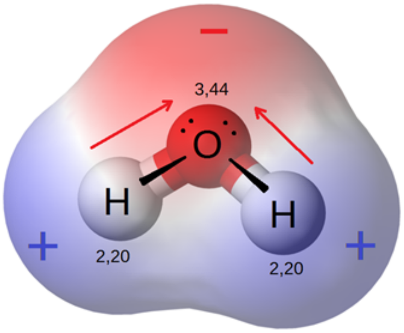

Figure 3.8.3: The water molecule is made up of oxygen and hydrogen, with respective electronegativities of 3.44 and 2.20. The electronegativity difference polarizes each H–O bond, shifting its electrons towards the oxygen (illustrated by red arrows). These effects add as vectors to make the overall molecule polar. Source: Riccardo Rovinetti / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

A bond is categorized as a nonpolar covalent, polar covalent, or an ionic bond based on the following convention: nonpolar covalent if the electronegative difference of the bonded atom is less than 0.5, a polar covalent if the electronegativity difference is between 0.5 to 1.9, and an ionic if the electronegativity difference is more than 1.9.

The polarity of a Molecule

The molecules fall into the following categories concerning molecular polarity.

The molecule is nonpolar if there is no polar bond in it, e.g., H-H, F-F, and CH_4 are nonpolar molecules. Fig. 3.8.4 illustrates CH_4 molecules with green color electron clouds that represent a nonpolar molecule.

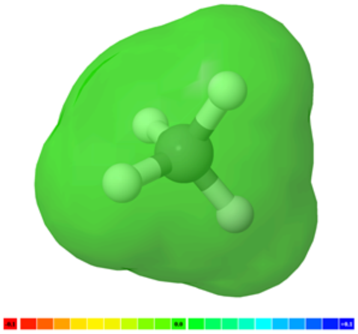

Figure 3.8.4: Methane (CH_4) with no polar bond is nonpolar. Source: drawn using free software https://chemagic.org/molecules/amini.html

If there is only one polar bond in a molecule, then the molecule is polar, e.g., the H-F molecule shown in Fig. 3.8.2.

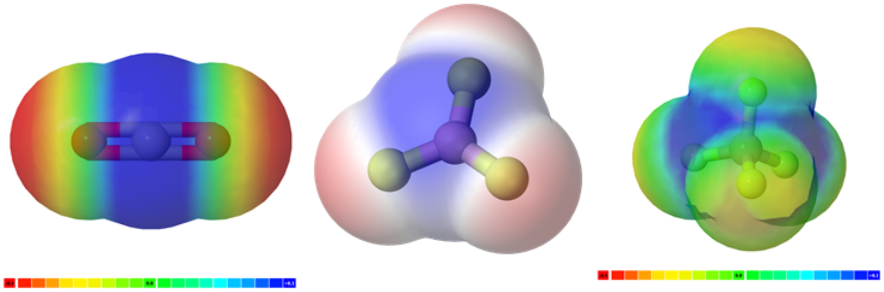

Figure 3.8.5: Examples of symmetric molecules with all polar bonds but the molecule as a whole is nonpolar. The examples are (from left to right) carbon dioxide CO_2, boron trifluoride BF_3, and carbon tetrafluoride CF_4.

If there is more than one polar bond in a molecule, the molecule may be polar or may be nonpolar, depending on the symmetry of the molecule: a) Polarity vector of individual bonds cancel out in symmetric molecules making the molecule nonpolar. For example, symmetric molecules, like CO_2, BF_3, and CCl_4, are nonpolar, although each bond in them is polar. Fig. 3.8.5 illustrates the symmetric molecules that have polar bonds, but the polarity of bonds cancels each other, making the molecule nonpolar. b) If a molecule has polar bonds and it is not symmetric, the polarity vectors do not cancel out, and the molecule is polar. Examples of polar molecules include $CHCl_3$, NH_3, and H_2O, as illustrated in Fig. 3.8.6.

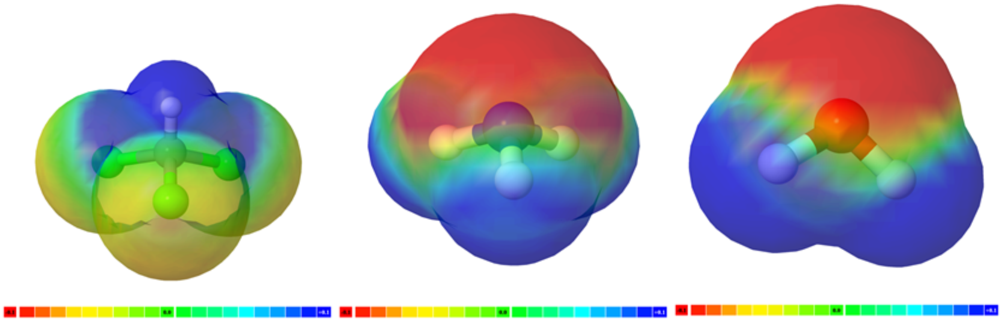

Figure 3.8.6: Non-symmetric molecules with polar bonds are polar molecules with a net δ+ end in red color and δ- ends in blue color. The examples are (from left to right) chloroform ($CHCl_3$), ammonia (NH_3), and water (H_2O).

3.9: Intramolecular forces and intermolecular forces

There are electrostatic interaction between charges or partial charges, i.e., the same charges attract each other, and opposite charges repel each other, as illustrated in Fig. 3.9.1.There are two types of electrostatic forces in compounds or molecules, intramolecular forces that exist between the bonded atoms of a compound or a molecule, and intermolecular forces that exist between molecules as described below.

Figure 3.9.1: Like charges repel each other and opposite charges attract each other.

Intramolecular forces

Intramolecular forces are the chemical bonds holding the atoms together in the molecules. The three major types of chemical bonds are the metallic bond, the ionic bond, and the covalent bond.

Metallic bond

Metals exist as a collection of many atoms as +ions arranged in a well-defined 3D arrangement called crystal lattice with some of the outermost electrons roaming around in the whole piece of the metal, forming a sea of electrons around the metal atoms, as illustrated in Fig. 3.9.2. The attraction between +ions and the sea of free moving electrons is the metallic bond that holds the atoms together in a piece of metal. The metallic bond is usually the strongest type of chemical bond.

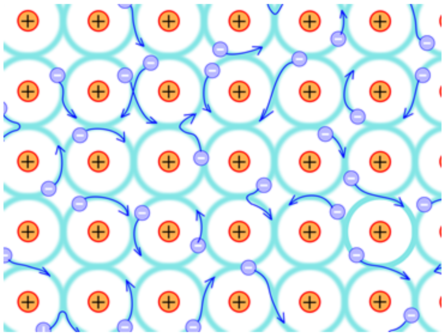

Figure 3.9.2: A model of metallic bond. Source: https://commons.wikimedia.org/wiki/F...bond_model.svg, Public domain

Ionic bond

When the electronegativity difference between bonded atoms is large, i.e., more than 1.9 in most cases, the bonding electrons completely transfer from a more electropositive atom to a more electronegative atom creating a cation and an anion, respectively. There is the electrostatic interaction between cation and anion, i.e., the same charges attract each other, and opposite charges repel each other, as illustrated in Fig. 3.9.1. The cations and anions orient themselves in a 3D crystal lattice in such a way that attractive interactions maximize and the repulsive interactions minimize, as illustrated in Fig. 3.9.3. Ionic bonds are usually weaker than metallic bonds but stronger there the other types of bonds.

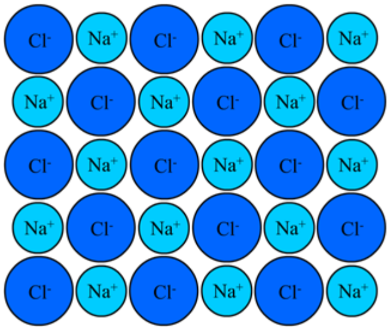

Figure 3.9.3: Illustration of an ionic bond: the ions in ionic crystals orient in such a way to optimize the attractive forces between opposite charges. Part of one layer of a crystal lattice is shown in this illustration, the 3D crystal lattice is illustrated in Fig. 3.1.6. Source: Eyal Bairey / Public domain

Covalent bond

When the electronegativity difference between bonded atoms is moderate to zero, i.e., usually less than 1.9, the bonding electrons are shared between the bonded atoms, as illustrated in Fig. 3.9.4. The attractive force between the bonding electrons and the nuclei is the covalent bond that holds the atoms together in the molecules. The covalent bond is usually weaker than the metallic and the ionic bonds but much stronger than the intermolecular forces.

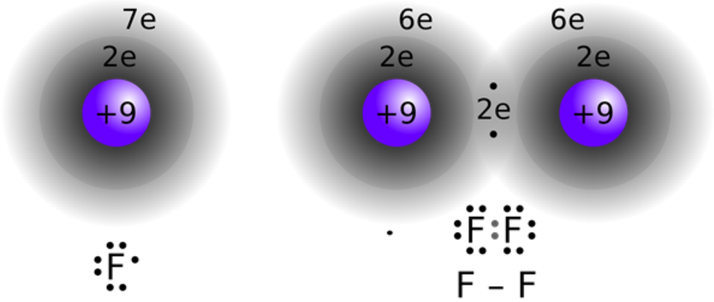

Figure 3.9.4: Illustration of a covalent bond in fluorine molecule: Jacek FH, CC BY-SA 3.0 <https://creativecommons.org/licenses/by-sa/3.0>, via Wikimedia Commons

Criteria to predict the type of chemical bond

Metals tend to have lower electronegativity and nonmetals have higher electronegativity. When the electronegativity difference between the bonded atoms is large, usually more than 1.9, the bond is ionic. Generally, a bond between a metal and a nonmetal is ionic. When the electronegativity difference is low, usually less than 1.9, the bond is either metallic or covalent. Nonmetals tend to make a covalent bond with each other. Nonmetals also have higher electronegativities. So, when the average electronegativity of the bonded atom is high and the electronegativity difference between them is low, they tend to make a covalent bond. Metals tend to make the metallic bond with each other. Metals also tend to have lower electronegativity values. So, when the average electronegativity of the bonded atom is low and the electronegativity difference between them is also low, they tend to make a metallic bond. Fig. 3.9.5 illustrates the criteria to predict the type of chemical bond based on the electronegativity difference. Keep in mind that there is no sharp boundary between metallic, ionic, and covalent bonds based on the electronegativity differences or the average electronegativity values.

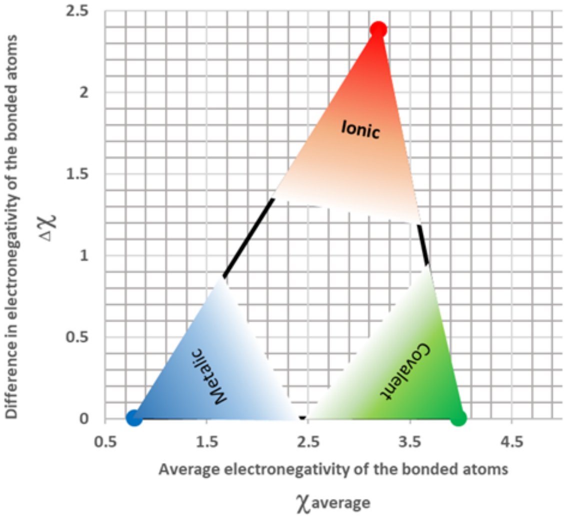

Figure 3.9.5: van Arkel-Ketelaar Triangle: plot of the difference in electronegativity ($\Delta\chi$) versus the average electronegativity in a bond ($\chi_{average}$). The top corner is mostly ionic, the lower left is metallic, and the lower right is covalent.

Intermolecular forces

Intermolecular forces are the electrostatic interactions between molecules. The intermolecular forces are usually much weaker than the intramolecular forces, but still, they play important role in determining the properties of the compounds. The major intermolecular forces include dipole-dipole interaction, hydrogen bonding, and London dispersion forces.

Dipole-dipole interactions

Polar molecules have permanent dipoles, one end of the molecule is partial positive (δ+) and the other is partial negative (δ-). The polar molecules have electrostatic interactions with each other through their δ+ and δ- ends called dipole-dipole interactions, though these interactions are weaker than ionic bonds. The polar molecules orient in a way to maximize the attractive forces between the opposite charges and minimize the repulsive forces between the same charges, as illustrated in Fig. 3.9.6.

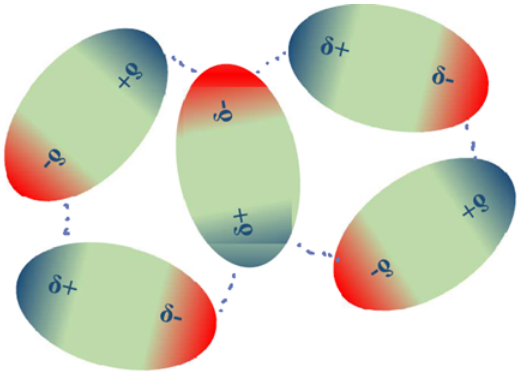

Figure 3.9.6: Illustration of dipole-dipole interactions by dotted liens in polar molecules.

Hydrogen bonds

Hydrogen bonding is a dipole-dipole interaction when the dipole is a hydrogen bond to O, N, or F, e.g. in water molecules as illustrated in Fig. 3.9.7. Although hydrogen bond is a dipole-dipole interaction, it is distinguished from the usual dipole-dipole interactions because of the following special features.

1. The electronegativity difference between H and O, N, or F is usually more than other polar bonds.
2. The charge density on hydrogen is higher than the δ+ ends of the rest of the dipoles because of the smaller size of hydrogen.
3. The δ+ Hydrogen can penetrate in less accessible spaces to interact with the δ- O, N, or F of the other molecule because of its small size.

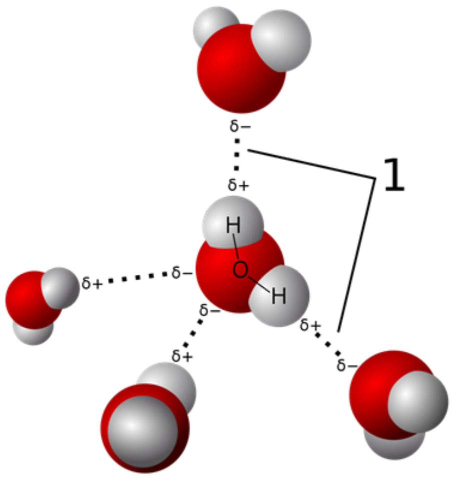

Figure 3.9.7: Illustration of hydrogen bonds by dotted lines in water molecules. Red balls are oxygen and white balls are hydrogen atoms. Source: User Qwerter at Czech Wikipedia: Qwerter. Transferred from cs.Wikipedia to Commons by sevela.p. Translated to english by by Michal Maňas (User:snek01). Vectorized by Magasjukur2 / Public domain

A hydrogen bond is usually stronger than the usual dipole-dipole interactions. Hydrogen bonding is the most common and essential intermolecular interaction in biomolecules. For example, two strands of DNA molecules are held together through hydrogen bonding, as illustrated in Fig. 3.9.8. Proteins also acquire structural features needed for their functions mainly through hydrogen bonding.

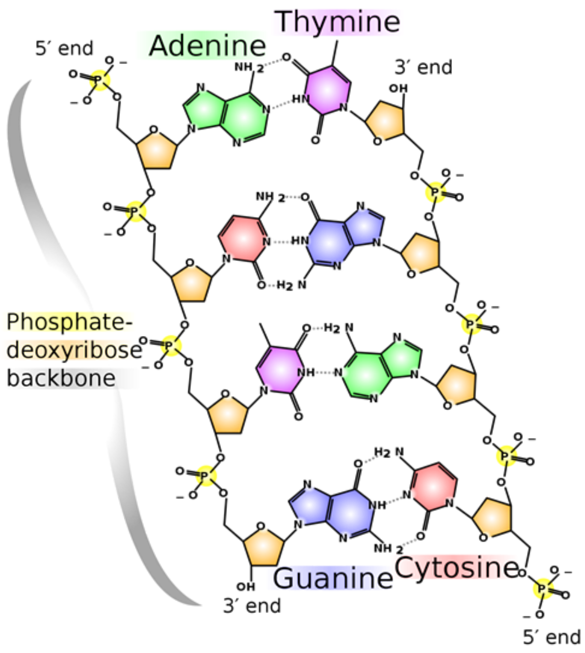

Figure 3.9.8: Chemical structure of DNA, with a colored label identifying the four bases as well as the phosphate and deoxyribose components of the backbone. Dotted lines are the hydrogen bonds holding the two strands of DNA together. Source: Madprime (talk · contribs) / CC0

London dispersion forces

It may appear that the nonpolar molecules should not have intermolecular interactions. Practically, there are intermolecular interactions called London dispersion forces, in all the molecules, including the nonpolar molecules. The electron cloud around atoms is not all the time symmetrical around the nuclei. It temporarily sways to one side or the other, generating a **transient dipole**. The transient dipole induces a dipole in the neighboring. A transient dipole-induced dipole interaction, called **London dispersion force** or **wander Wall’s force**, is established between the neighboring molecules as illustrated in Fig. 3.9.9. Although London dispersion forces are transient, they keep re-appearing randomly distributed in space and time. London dispersion forces are not unique to nonpolar molecules, they are present in all types of molecules, but these are the only intramolecular forces present in the nonpolar molecules.

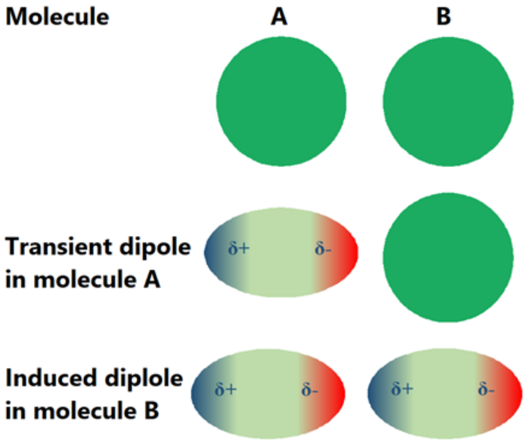

Figure 3.9.9: Illustration of transient dipole-induced dipole, i.e., London dispersion forces.

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CHAPTER OVERVIEW

4: Stoichiometry –the quantification of chemical reactions

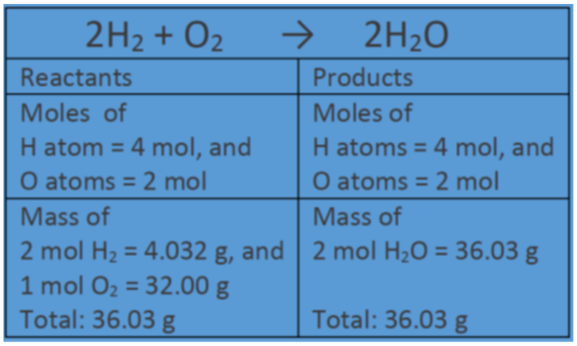
4.1: Stoichiometry

What is Stoichiometry

> Stoichiometry (stoi·chi·om·e·try /ˌstɔɪkiˈɒmɪtri/) is the study of the quantities of substances and energy consumed and produced in chemical reactions.

The basis of the stoichiometric calculations is the law of conservation of mass which states that the mass is neither created nor destroyed in a chemical reaction. Another form of the law states that atoms are neither created nor destroyed in a chemical reaction. It is the basis of stoichiometric calculations that are described in this chapter.

It can be concluded from the law of mass action that atoms of each element and their masses are the same in reactants and products. A balanced chemical equation shows atoms of each element and the total mass of reactants equal to that in the product, as illustrated in Fig. 4.1.1. The number of atoms and molecules is related to their quantity in moles through Avogadro's number. The mole, in turn, is related to the mass of the substance through molar mass in grams. These relationships are described in the next sections.



$2H_2 + O_2$	$\rightarrow$ $2H_2O$
Reactants	Products
Moles of H atom = 4 mol, and O atoms = 2 mol	Moles of H atoms = 4 mol, and O atoms = 2 mol
Mass of 2 mol H_2 = 4.032 g, and 1 mol O_2 = 32.00 g Total: 36.03 g	Mass of 2 mol H_2O = 36.03 g Total: 36.03 g

Figure 4.1.1: Stoichiometry of water formation from hydrogen and oxygen.

Atomic mass

Atomic mass is the weighted average of the masses of the isotopes present in a natural sample of the element, as explained with an example calculation in section 2.3. The mass of a single atom or molecule is expressed in the atomic mass unit (amu), which is equal to $\frac{1}{2}$th of the mass of $^{12}_{6}\mathrm{C}$ isotope of carbon that is unbound.

Atomic mass is listed in a periodic table as a number below the symbol and name of the element, as illustrated in Fig. 4.1.2. Atomic mass is listed as a number without a unit because it is the mass of an atom in amu and it is also the mass of one mole (molar mass) of the atom in grams. Molar mass is often used in stoichiometry calculation as explained in the next sections.

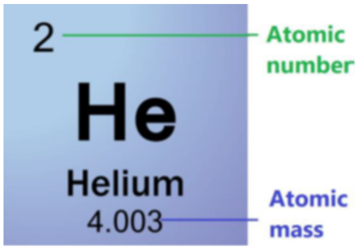


Figure 4.1.2: Copy and Paste Caption here. (Copyright; author via source)Atomic number and atomic mass in a periodic table for Helium

4.2: The mole

Avogadro’s number and mole

The Avogadro's number

The Avogadro's number is equal to 6.02214076 x 10^{23} exact.

Just like the dozen is equal to 12, the Avogadro's number 6.02214076 x 10^{32} is exact by definition, but usually, 6.022 x 10^{23} is used in calculations with 4 significant figures.

Mole (mol)

The mole is a SI unit of the amount of a substance that is equal to 6.02214076 x 10^{23} particles of the substance.

The particle of a substance are usually atoms, ions, or molecules. For example, 6.02214076 x 10^{23} atoms of ${}^{12}_{6}\mathrm{C}$ isotope is one mole of ${}^{12}_{6}\mathrm{C}$. The number 6.02214076 x 10^{32} is exact by definition, but usually, 6.022 x 10^{23} is used with 4 significant figures.

One mole of a substance is equal to one Avogadro’s number of atoms, molecules, or formula units of the substance. i.e.,

$$1 \text{ Avogadro's number of particles } = 1 \text{ mol} = 6.022 \times 10^{23} \text{ particles}$$

, where particles are atoms, molecules, or formula units in chemistry.

The equality between Avogadro's number and mole gives two conversion factor:

$$\frac{6.022 \times 10^{23} \text{ particles}}{1 \text{ mol}} \quad \text{and} \quad \frac{1 \text{ mol}}{6.022 \times 10^{23} \text{ particles}}$$

, where the first factor is used to convert a number of moles to a number of particles and the second for a number of particles to number moles conversions, as explained in the following examples.

Example 4.2.1

How many aspirin ($C_9H_8O_4$ molecules are in 0.0139 mol of aspirin?

Solution

Step 1. Write the given quantity and the desired quantity.

Given: 0.0139 mol ($C_9H_8O_4$, Desired: ? molecules of ($C_9H_8O_4$

Step 2. Write the two conversion factors from equality between the given and the desired quantity.

$$\frac{6.022 \times 10^{23} \text{ particles}}{1 \text{ mol}} \quad \text{and} \quad \frac{1 \text{ mol}}{6.022 \times 10^{23} \text{ particles}}$$

Step 3. Multiply the given quantity with the conversion factor that cancels the given unit and leaves the desired unit in the answer.

$$0.0139 \;\; \cancel{\text{mol } C_9H_8O_4} \times \frac{6.022 \times 10^{23} \text{ molecules } C_9H_8O_4}{1 \;\; \cancel{\text{mol } C_9H_8O_4}} = 8.37 \times 10^{21} \text{ molecules } C_9H_8O_4$$

Example 4.2.2

How many moles of aspirin (($C_9H_8O_4$) are in 9.50 x 10^{25} molecules of aspirin?

Solution

Step 1. Write the given quantity and the desired quantity.

Given: 9.50×10^{25} molecules of aspirin, Desired: ? mol of aspirin

Step 2. Write the two conversion factors from equality between the given and the desired quantity.

$$\frac{6.022 \times 10^{23} \text{ particles}}{1 \text{ mol}} \quad \text{and} \quad \frac{1 \text{ mol}}{6.022 \times 10^{23} \text{ particles}}$$

Step 3. Multiply the given quantity with the conversion factor that cancels the given unit and leaves the desired unit in the answer.

$$9.50 \times 10^{25} \text{ molecules } \cancel{C_9H_8O_4} \times \frac{1 \text{ mol } C_9H_8O_4}{6.022 \times 10^{23} \text{ molecules } \cancel{C_9H_8O_4}} = 158 \text{ mol } C_9H_8O_4$$

Moles of elements in a mole of a compound

Moles of an element in a mole of a compound is equivalent to atoms of the element in a molecule or formula unit of the compound. For example in 1 mole of glucose ($C_6H_{12}O_6$) there are 6 moles of carbon, 12 moles of hydrogen, and 6 moles of oxygen. Each of these equalities between a mole of a substance and the moles of the element in it gives two conversion factors for the calculations.

✓ Example 4.2.3

How many moles of hydrogen are in 3.0 moles of glucose ($C_6H_{12}O_6$)?

Solution

Step 1. Write the given quantity and the desired quantity.

Given: 3.0 moles of ($C_6H_{12}O_6$), Desired: ? mol of H

Step 2. Write the two conversion factors from equality between the given and the desired quantity.

$$\frac{12\ mol\ H}{1\ mol\ C_6H_{12}O_6} \quad \text{and} \quad \frac{12\ mol\ C_6H_{12}O_6}{1\ mol\ H}$$

Step 3. Multiply the given quantity with the conversion factor that cancels the given unit and leaves the desired unit in the answer.

$$3.0 \text{ mol } \cancel{C_6H_{12}O_6} \times \frac{12 \text{ mol H}}{1 \text{ mol } \cancel{C_6H_{12}O_6}} = 36\ mol\ H$$

✓ Example 4.2.4

Calculate the moles of oxygen are in 0.50 mole of $Ca(NO_3)_2$?

Solution

Step 1. Write the given quantity and the desired quantity.

Given: 0.50 moles of $Ca(NO_3)_2$, Desired: ? mol of O

Step 2. Write the two conversion factors from equality between the given and the desired quantity. Note that NO_3^- is polyatomic ion that has three oxygen atoms in it. There are two NO_3^- in the formula unit as shown by subscript 2 outside the bracket enclosing the polyatomic anion (\ce{NO3^-}\). So, the equality is:

$$1 \text{ mole } Ca(NO_3)_2 = 6 \text{ mole O},$$

and the two conversion factors from the equality are:

$$\frac{1\ mol\ Ca(NO_3)_2}{6\ mol\ O} \quad \text{and} \quad \frac{6\ mol\ O}{1\ mol\ Ca(NO_3)_2}$$

Step 3. Multiply the given quantity with the conversion factor that cancels the given unit and leaves the desired unit in the answer.

$$0.50\ mol\ \cancel{\mathrm{Ca(NO_3)_2}} \times \frac{6\ mol\ O}{1\ mol\ \cancel{\mathrm{Ca(NO_3)_2}}} = 3.0\ mol\ O$$

Molar mass

The mass of one mole of a substance, in $\frac{g}{mol}$, is called the molar mass.

Recall that one mole = 1 Avogadro's number, i.e., 6.022×10^{23} atoms, molecules, or formula units of a substance. Fig. 4.2.1 helps in visualizing the molar masses of aluminum, copper, and carbon. The molar mass of an element or a compound is a reasonable quantity to be measured on an analytical balance commonly available in laboratories, while the mass of an individual atom or molecule is too small to be easily measured. That is why the mole is commonly used in stoichiometric calculations.

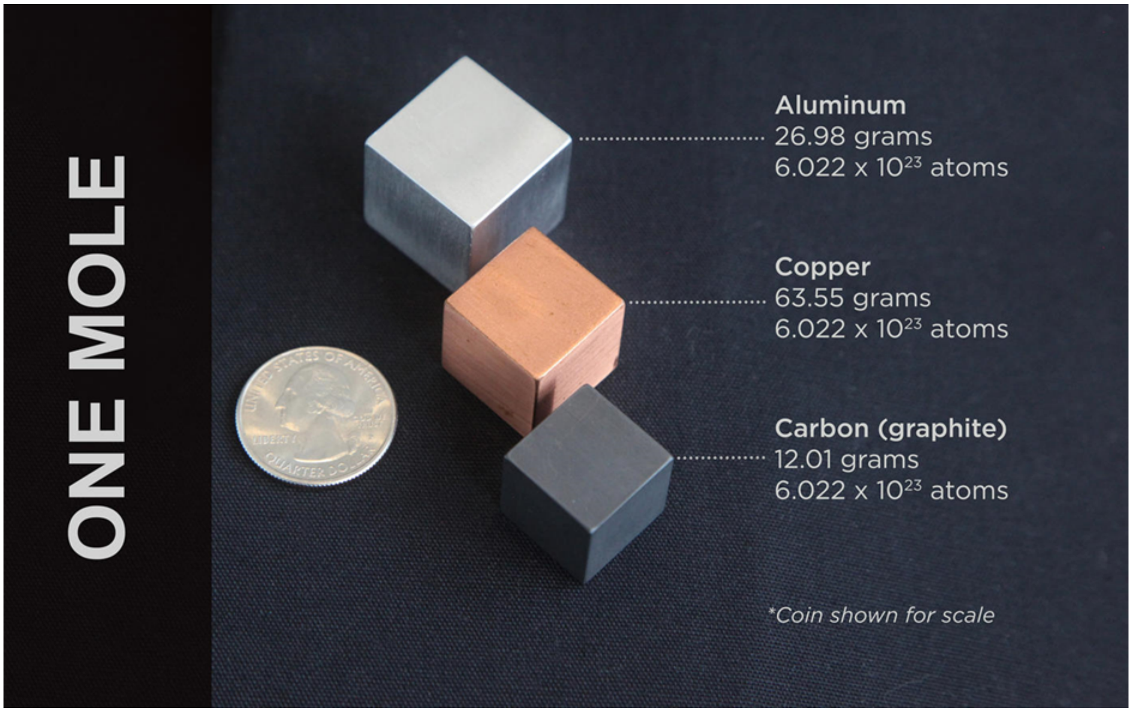


Figure 4.2.1: A mole of aluminum, copper, and carbon visualized. Source: photo: R. Press/NIST; graphic design: N. Hanacek/NIST

The molar mass of atoms of an element

The atomic mass listed in the periodic table is the molar mass of atoms of the element in $\frac{g}{mol}$. For example, the atomic mass of H listed in the periodic table is 1.008, so the molar mass of H is 1.008 $\frac{g}{mol}$. Similarly, the atomic mass of O listed in the periodic table is 15.999, and the molar mass of O is 15.999 $\frac{g}{mol}$.

The molar mass of molecules of an element

The molar mass of molecules of an element is the sum of atomic mass of atoms in the molecule expressed in $\frac{g}{mol}$. For example, the molar mass of H_2 is 1.008 $\frac{g}{mol}$ + 1.008 $\frac{g}{mol}$ = 2.016 $\frac{g}{mol}$.

The molar mass of a compound

The molar mass of a compound is the sum of the atomic masses of all the atoms in the molecular formula or formula unit of the compound. For example, the molar mass of water (H_2O) is the sum of the molar mass of two hydrogen atoms + the molar mass of one oxygen atom, i.e., 2x1.008 $\frac{g}{mol}$ H + 15.999 $\frac{g}{mol}$ O = 18.02 $\frac{g}{mol}$ H_2O. In other words, to calculate the molar mass of a compound, take the atomic masses of the constituent elements from a periodic table, multiply them with the number of atoms of the element in the formula of the compound, and then add these numbers, as explained in the following examples. Note that the unit $\frac{g}{mol}$ can also be written as: $g.mol^{-1}$.

✓ Example 4.2.5

Calculate the molar mass of NaOH?

Solution

Step 1. Find the atomic masses of the constituent elements from the periodic table.

Na = 22.990 g.mol^{-1}, O = 15.999 g.mol^{-1}, H = 1.008 g.mol^{-1}.

Step 2. Multiply the atomic masses with the number of atoms in the fourmula.

1x22.990 g.mol^{-1} Na, 1x15.999 g.mol^{-1}O, 1x1.008 g.mol^{-1} H.

Step 3. Add all the numbers from step 2.

1x22.990 g.mol^{-1} Na + 1x15.999 g.mol^{-1}O + 1x1.008 g.mol^{-1} H = 39.997 g.mol^{-1} NaOH

✓ Example 4.2.6

Calculate the molar mass of $Ca(NO_3)_2$?

Solution

Step 1. Find the atomic masses of the constituent elements from the periodic table.

Ca = 40.078 g.mol^{-1}, N = 14.007 g.mol^{-1}, O = 15.999 g.mol^{-1}.

Step 2. Multiply the atomic masses with the number of atoms in the formula. (Note that there are two NO_3 units in $(NO_3)_2$?, To get the total number of atoms, multiply the subscript outside the bracket with the subscript to the element symbol inside the bracket to get the total number of atoms. That is, there are 1x2 = 2 N and 3x2 = 6 O in this compound.

1x40.078 g.mol^{-1} Ca, 2x14.007 g.mol^{-1} N, 6x15.999 g.mol^{-1} O.

Step 3. Add all the numbers from step 2.

1x40.078 g.mol^{-1} Ca + 2x14.007 g.mol^{-1}N + 6x15.999 g.mol^{-1} O = 164.008 g.mol^{-1} $Ca(NO_3)_2$.

Conversion from grams to moles and moles to grams of a substance

The molar mass in $\frac{g}{mol}$ is a conversion factor converting the amount of a substance in moles to the mass of the substance in grams. Reciprocal of the molar mass in $\frac{mol}{g}$ is a conversion factor converting the mass of a substance in grams to the amount of the substance in moles. The conversions are explained in the following examples.

✓ Example 4.2.7

How many grams of water are in 2.50 moles of water?

Solution

Step 1. Write the given quantity and the desired quantity.

Given: 2.50 moles H_2O, Desired: ? g H_2O

Step 2. Calculate the molar mass of the substance.

2x1.008 g.mol^{-1} H + 15.999 g.mol^{-1} O = 18.02 g.mol^{-1} H_2O.

Step 3. Write the molar mass of the substance, and it's reciprocal as the two conversion factors.

$$\frac{18.02\ g\ \mathrm{H_2O}}{1\ \mathrm{mol\ H_2O}} \text{ and } \frac{1\ \mathrm{mol\ H_2O}}{18.02\ g\ \mathrm{H_2O}}$$

Step 4. Multiply the given quantity with the conversion factor that cancels the given unit and leaves the desired unit in the answer.

$$2.50 \ \text{mol} \ \cancel{H_2O} \times \frac{18.02 \ g \ H_2O}{1 \ \text{mol} \ \cancel{H_2O}} = 45.1 \ g \ H_2O$$

✓ Example 4.2.8

How many moles are present in 2.50 g of aspirin? (Aspirin $C_9H_8O_4$, molar mass 180.2 g.mol^{-1})

Solution

Step 1. Write the given quantity and the desired quantity.

Given: 2.50 g $C_9H_8O_4$, Molar mass of $C_9H_8O_4$ = 180 g.mol^{-1}, Desired: ? g H_2O

Step 2. Calculate the molar mass of the substance.: given 180.2 g.mol^{-1}

Step 3. Write the molar mass of the substance, and it's reciprocal as the two conversion factors.

$$\frac{180 \ g \ C_9H_8O_4}{1 \ mol \ C_9H_8O_4} \quad \text{and} \quad \frac{1 \ mol \ C_9H_8O_4}{180 \ g \ C_9H_8O_4}$$

Step 4. Multiply the given quantity with the conversion factor that cancels the given unit and leaves the desired unit in the answer.

$$2.5 \ \ g \ \cancel{C_9H_8O_4} \times \frac{1 \ mol \ C_9H_8O_4}{180 \ \ g \ \cancel{C_9H_8O_4}} = 0.0193 \ mol \ C_9H_8O_4$$

✓ Example 4.2.9

How many moles of NaOH are in 10.0 g of NaOH?

Solution

Step 1. Write the given quantity and the desired quantity.

Given: 10.0 g NaOH, Desired: ?mol NaOH

Step 2. Calculate the molar mass of the substance.

22.99 g.mol^{-1} Na + 16.00 g.mol^{-1} O + 1.01 g.mol^{-1} H = 40.00 g.mol^{-1} NaOH.

Step 3. Write the molar mass of the substance and it's reciprocal as the two conversion factors.

$$\frac{40.00 \ g \ NaOH}{1 \ mol \ NaOH} \quad \text{and} \quad \frac{1 \ mol \ NaOH}{40.00 \ g \ NaOH}$$

Step 4. Multiply the given quantity with the conversion factor that cancels the given unit and leaves the desired unit in the answer.

$$10.0 \ \ g \ \cancel{NaOH} \times \frac{1 \ mol \ NaOH}{40.00 \ \ g \ \cancel{NaOH}} = 0.250 \ \text{mol NaOH}$$

4.3: Chemical reaction

What is a chemical reaction?

A chemical reaction is a combination, separation, or rearrangement of atoms in a substance.

Atoms are healed together in a substance by chemical bonds. The combination makes bonds, separation breaks bonds, and rearrangement breaks some of the old bonds and makes some new bonds in the substances during a chemical reaction. It results in new substances with a different composition of elements than the starting substances. The starting substances are called reactants and the new substances formed are called products.

When a chemical bond is broken energy is required and when a chemical bond is formed energy is released. The amount of energy depended on the chemical bond, but for the same bond, the energy that needs to break is the same energy released to make the bond. Therefore, energy is released in some chemical reactions and absorbed in others.

Examples of chemical reactions are photosynthesis which converts carbon dioxide and water into glucose in the green leaves of plants using energy from sunlight. Digestion of food is a chemical reaction that releases the energy needed for the functioning of living things. The burning of a candle is a chemical reaction that converts the organic compounds in the fule to carbon dioxide, water, and heat energy. Rusting iron is another chemical reaction that converts the element iron to compound iron oxide.

Indications of a chemical reaction

A chemical reaction is usually accompanied by some physical changes that can be observed. The changes include color change, flame, heat, light, the evolution of a gas, formation of a precipitate, etc., as illustrated in Fig. 4.3.1

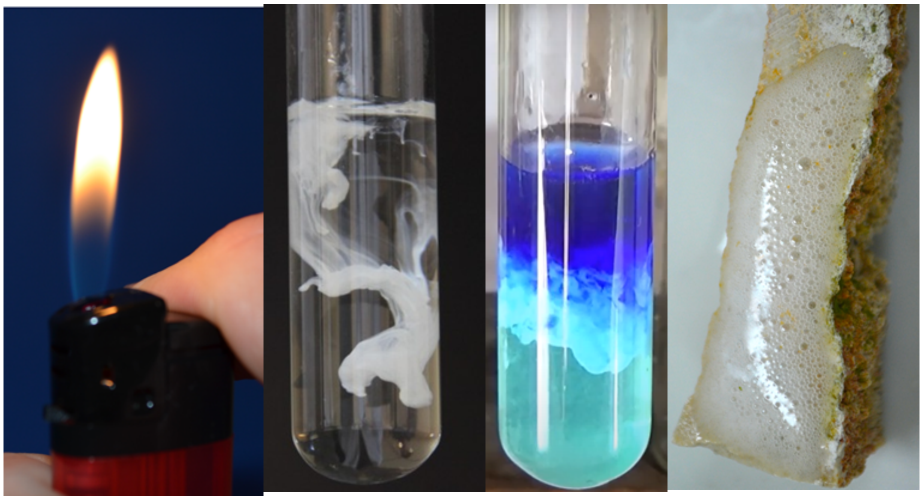


Figure 4.3.1: Examples of indications of chemical reactions: from left a) butane burning with flame and light, b) Silver chloride formation with precipitation, c) copper ammonia complex formation with a color change to greenish to dark blue, and d) Reaction of limestone with HCl with carbon dioxide gas formation. Source: a) Renate90 / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0) , b) Luisbrudna / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0), c) https://www.youtube.com/watch?v=7TIIOj-SHkw&t=102s, d) Alessandro e Damiano / CC BY (https://creativecommons.org/licenses/by/4.0)

Representing a chemical reaction- a chemical equation

Chemical equaitron

A chemical equation represents a chemical reaction.

1. The formulas of the reactants are written on the left side separated by a + sign.
2. Formulas of the products are written on the right-side separated by a + sign.
3. An arrow pointing in the direction of products separates the reactants from the products.

Fig. 4.3.2 illustrates the photosynthesis reaction between carbon dioxide (CO_2 and water (H_2O producing glucose ($C_6H_{12}O_6$ and oxygen (O_2:

$$6\,CO_2 + 6\,H_2O \xrightarrow{sunlight} C_6H_{12}O_6 + 6\,O_2$$

Writing a chemical equation

1. First correct formulas of reactants and products are written, separated by plus signs and arrows.
2. Then the number of species is adjusted by adding a number, called a coefficient, at the beginning of a formula. The coefficients are needed to make atoms of each element equal on both sides of the equation because atoms are neither created nor destroyed in a chemical reaction.
3. Subscripts within the formulas can not be changed as they represent the composition of the substance that is constant.
4. The coefficient is not written if it is one.

For example, Fig. 4.3.2 shows coefficients 6 for carbon dioxide, water, and oxygen, but no coefficient for glucose means the coefficient is actually one for glucose in a balanced chemical equation for photosynthesis reaction.

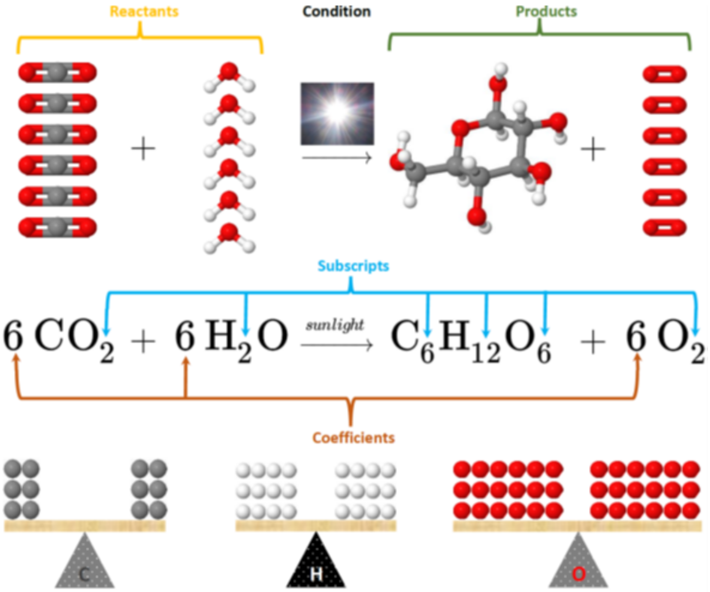


Figure 4.3.2: Model and components of a balanced chemical equation with the example of photosynthesis reaction.

Symbols in a chemical equation

Sometimes the physical state of the substances is shown by symbols in small brackets next to the formula.

1. The symbols for the physical state are: (s) for solid, (l) for liquid, (g) for gas, and (aq) for a substance dissolved in water. The symbol (aq) stands for aqueous, i.e., water.
2. If a gas evolves, it can be shown by an up-arrow (↑), and if a precipitate forms, it is shown by a down-arrow (↓).

For example, combustion of butane ($ceC4H10$ in lighter shown in Fig. 4.3.1. can be represented as:

$$2\,C_4H_{10}(g) + 13\,O_2(g) \longrightarrow 8\,CO_2(g) + 10\,H_{26}O(g)$$

, where all the reactants and products are in the gas phase. Reaction of NaCl and $AgNO_3$ in the water that results in a precipitate, as shown in Fig. 4.3.1 is:

$$NaCl(aq) + AgNO_3(aq) \longrightarrow AgCl(s)\downarrow + NaNO_3(aq)$$

, where NaCl, $AgNO_{3,}$ and $NaNO_3$ are in the water, and AgCl precipitates out as white solid. The reaction of limestone with HCl, shown in Fig. 4.3.1 is:

$$CaCO_3(s) + 2\,HCl(aq) \longrightarrow CaCl_2(aq) + H_2O(l) + CO_2(g)\uparrow$$

Reaction conditions, catalysts, or heat can be written above or below the arrow. Heat can also be represented by Δ symbol, e.g.,

$$\mathrm{CaCO_3(s) + CaO(s) \xrightarrow{\Delta} CO_2(g)\uparrow}$$

A two way arrows $\rightleftharpoons$ or $\leftrightarrows$ represents a two ways reaction, e.g.,

$$\mathrm{2\,NO_2(g) \rightleftharpoons N_2O_4(g)}$$

Balancing a chemical equation

The first step is wright correct formulas of reactants and products separated by plus signs and an arrow. For example, the initial equation for burning hydrogen burns in oxygen and producing water would be:

$$\mathrm{H_2 + O_2 \longrightarrow H_2O}$$

Note that hydrogen is written as H_2 (not H) and oxygen as O_2 (not O) because these reactants usually exist as molecules, not as atoms.

The next step is to add coefficients to balance atoms of each element on the two sides of the equation. For example, in the above equation hydrogen is balanced but oxygen is not. Balance oxygen by changing the coefficient of water from 1 to 2:

$$\mathrm{H_2 + O_2 \longrightarrow 2\,H_2O}$$

Caution

Subscripts in the formulae can not be changed, as they are constant. For example, if O_2 is changed to O in the above equation to balance the oxygen, it is incorrect as O_2 is molecular oxygen which is a different chemical than atomic oxygen O.

The coefficient is a multiplier of each subscript in the formula, i.e., in $2H_2O$ there are 2x2 = 4 hydrogen and 2x1 =2 oxygen. Now look for the other elements again: note that hydrogen atoms have changed to 4 on the right side. To balance hydrogen, change the coefficient of H_2 from 1 to 2:

$$\mathrm{2\,H_2 + O_2 \longrightarrow 2\,H_2O}$$

Check again: Now, the atoms of each element are the same on both sides, i.e., the equation is balanced, as illustrated in Fig. 4.3.3.

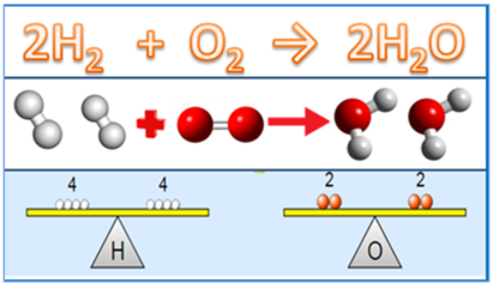


Figure 4.3.3: Illustration of a balanced chemical equation of water formation from hydrogen and oxygen. Atoms of each type are balanced. Source: Kvr.lohith / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

Rules to balance a chemical equation

The method described above to balance a chemical equation is called the hit and trial method. There are no hard and fast rules in this method. The general guidelines are:

1. if an element occurs only in one reactant and one product, balance it first,
2. if there is a free element in the reactants or products, balanced it last,
3. if there is a polyatomic ion in reactants and products, balance the number of polyatomic ions as a unit, i.e., add coefficient to but do not change the subscripts in the polyatomic ion or of any formula.
4. in some cases, a fractional coefficient is needed to balance the equation, in that case first use the fractional coefficient and when the equation is balanced, remove the fraction by multiplying all the coefficients with a common multiplier,
5. if the set of coefficients in the balanced equation is not in the simplest whole-number ratio, the equation is still balanced, but it is recommended to convert the set of coefficients to the simplest whole-number ratio.

The following examples explain the guidelines.

Figure 4.3.4: Propane torch being used to solder copper pipes for residential water mains. Source: Kevin L Neff / CC BY (https://creativecommons.org/licenses/by/2.0)

Example 4.3.1

Combustion of propane (C_3H_8) is used in gas welding, as shown in Fig. 4.3.4. The propane reacts with oxygen and produces carbon dioxide and water. Write and balance the chemical equation of the reaction?

Solution

Start with writing the correct formulae of reactants and products in a chemical equation form:

$$C_3H_8 + O_2 \longrightarrow CO_2 + H_2O$$

According to rule 1, look at carbon or hydrogen first. Both are not balanced. Balance the carbon by changing the coefficient of CO_2 from 1 to 3:

$$C_3H_8 + O_2 \longrightarrow 3\,CO_2 + H_2O$$

Balance the hydrogen by changing the coefficient of H_2O from 1 to 4:

$$C_3H_8 + O_2 \longrightarrow 3\,CO_2 + 4\,H_2O$$

Now, look at oxygen (rule 2) and balance it by changing the coefficient of O_2 from 1 to 5:

$$C_3H_8 + 5\,O_2 \longrightarrow 3\,CO_2 + 4\,H_2O$$

The last equation is balanced, as illustrated in Fig. 4.3.5.

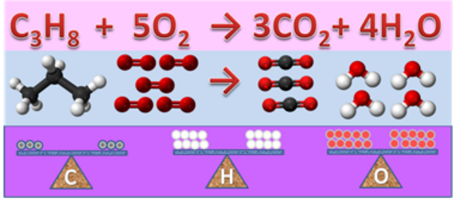


Figure 4.3.5: Illustration of a balanced chemical equation of propane combustion reaction. Source: Kvr.lohith / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

Example 4.3.2

The reaction between Aluminium metal powder and iron oxide, called thermite reaction, is highly exothermic that melts the ion. The thermite reaction is used for railroad welding as shown in Fig. 4.3.6. Wright and balance the reaction equation.

Solution

Start with writing the correct formulae of reactants and products in a chemical equation form:

$$Al + Fe_2O_3 \longrightarrow Fe + Al_2O_3$$

Rule 1 does not apply as all elements are in one reactant and one product. According to rule 2, look at either one of the compounds. Balance aluminum by changing the coefficient in the eactant from 1 to 2:

$$2\,\mathrm{Al} + \mathrm{Fe_2O_3} \longrightarrow \mathrm{Fe} + \mathrm{Al_2O_3}$$

Now balance iron by change its coefficient from 1 to 2 in the product:

$$2\,\mathrm{Al} + \mathrm{Fe_2O_3} \longrightarrow 2\,\mathrm{Fe} + \mathrm{Al_2O_3}$$

All atoms are balanced at this stage and coefficients are in the simplest whole-number ratio. So the equation is balanced.

Figure 4.3.1: Thermite reaction proceeding. Shortly after this, the liquid iron flows into the mold around the rail gap. Source: http://en.Wikipedia.org/wiki/Image:V...ewelding-1.jpg, Public domaine.

✓ Example 4.3.3

Methanol (CH_4O) reacts with oxygen and produces carbon dioxide and water. Write and balance the chemical reaction equation?

Solution

The starting equation with correct formulas is:

$$\mathrm{CH_4O} + \mathrm{O_2} \longrightarrow \mathrm{CO_2} + \mathrm{H_2O}$$

According to rule 1, look at carbon and hydrogen first. Carbon is already balanced. There are 4 hydrogens on the left but only two on the right side, so balance them by changing the coefficient of water from 1 to 2:

$$\mathrm{CH_4O} + \mathrm{O_2} \longrightarrow \mathrm{CO_2} + 2\,\mathrm{H_2O}$$

Now, look at oxygen (rule 2). There are three oxygen atoms on the right (one in methanol and two in free element oxygen) but four oxygen on the right, it is not balanced. Changing the coefficient of CH_4O from 1 to 2 balances the oxygen, but carbon and hydrogen go out of balance. Changing the coefficient of O_2 from 1 to 2 does not balance the oxygen. A fractional coefficient 3/2 for O_2 works at this stage (rule 4):

$$\mathrm{CH_4O} + \tfrac{3}{2}\mathrm{O_2} \longrightarrow \mathrm{CO_2} + 2\,\mathrm{H_2O}$$

All elements are balanced, i.e., the equation is balanced, but, according to rule 5, it is better to remove the fraction by multiplying each coefficient in the equation with 2:

$$2\,\mathrm{CH_4O} + 3\,\mathrm{O_2} \longrightarrow 2\,\mathrm{CO_2} + 4\,\mathrm{H_2O}$$

The set of coefficients in the balanced equation is already in the simplest whole-number ratio, so no further step is needed in this case.

✓ Example 4.3.4

Aluminum reacts sulfuric acid to produce aluminum sulfate and hydrogen gas. Wright a balanced chemical equation for the reaction.

Solution

The starting equation with correct formulas of reactants and products is:

$$Al + H_2SO_4 \longrightarrow Al_2(SO_4)_3 + H_2$$

All elements occur in one reactant and one product, so rule 1 do not apply. According to rule 2, leave aluminum till the end and, according to rule 3, balance the polyatomic ion (SO_4^{2-}) as a unit by changing the coefficient of sulfuric acid from 1 to 3:

$$Al + 3\,H_2SO_4 \longrightarrow Al_2(SO_4)_3 + H_2$$

Now balance the hydrogen by changing it coefficient from 1 to 3:

$$Al + 3\,H_2SO_4 \longrightarrow Al_2(SO_4)_3 + 3\,H_2$$

Finally balance aluminum by changing its coefficient from 1 to 2:

$$2\,Al + 3\,H_2SO_4 \longrightarrow Al_2(SO_4)_3 + 3\,H_2$$

Double-check at the end –All elements are balanced, and all the coefficients are in the simplest whole-number ratio. No further step is needed.

4.4: Patterns of chemical reactions

General types of chemical reactions

There are several ways to classify chemical reactions. The general types of chemical reactions fall in the categories of combination, decomposition, replacement, and combustion reactions, as illustrated in Fig. 4.4.1.

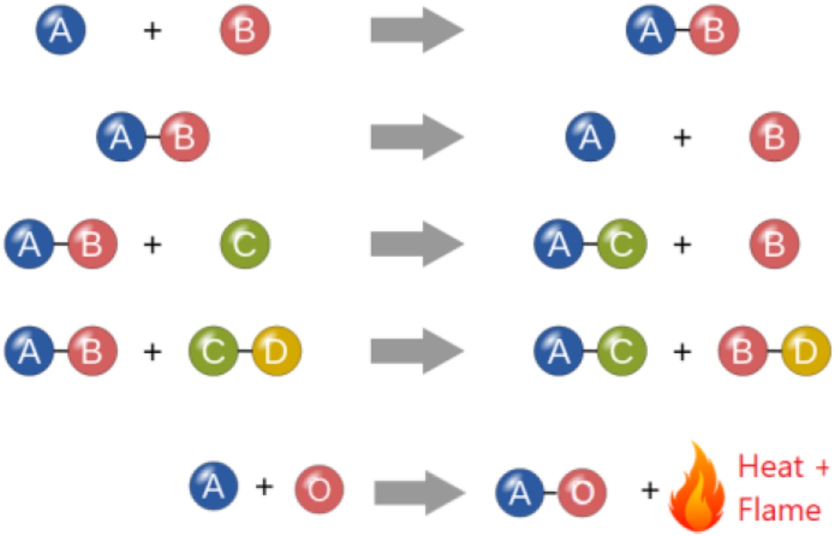


Figure 4.4.1: Illustration of four basic patterns of chemical reactions: combination, decomposition, single & double replacement, and combustion reactions. Source: https://www.hiclipart.com/free-trans...dunqu/download

Combination reactions

A compound is synthesized or formed from two or more substances, e.g.:

$$C + O_2 \longrightarrow CO_2$$

$$2\,H_2 + O_2 \longrightarrow 2\,H_2O$$

$$2\,Mg + O_2 \longrightarrow 2\,MgO$$

$$2\,Na + Cl_2 \longrightarrow 2\,NaCl$$

$$CaO + CO_2 \longrightarrow CaCO_3$$

Fig. 4.4.2 shows an example of a hydrogen with oxygen combination reaction that is being developed for use as a fuel in the future.

Figure 4.4.2: Berlin public bus using hydrogen as a fuel in an internal combustion engine (ICE). Hydrogen is stored in ten pressure cylinders of 50 kg of hydrogen at 350 bar. Reaction: \{\ce{2H2 + O2 -> 2H2O}\) + heat. Source: StralsundByzantion / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Decomposition reactions

The decomposition reactions are the reverse of the combination reaction, i.e., one compound splits apart into two or more substances, usually by heating, e.g.:

$$H_2CO_3 \longrightarrow H_2O + CO_2$$

$$\mathrm{CaCO_3} \xrightarrow{\Delta} \mathrm{CaO} + \mathrm{CO_2}$$

$$2\,\mathrm{KClO_3} \xrightarrow{\Delta} 2\,\mathrm{KCl} + 3\,\mathrm{O_2}$$

$$2\,\mathrm{H_2O(l)} \xrightarrow{Electrolyisis} 2\,\mathrm{H_2(g)} + \mathrm{O_2(g)}$$

Fig. 4.4.3 illustrates the last reaction, i.e., decomposition of water through electrolysis.

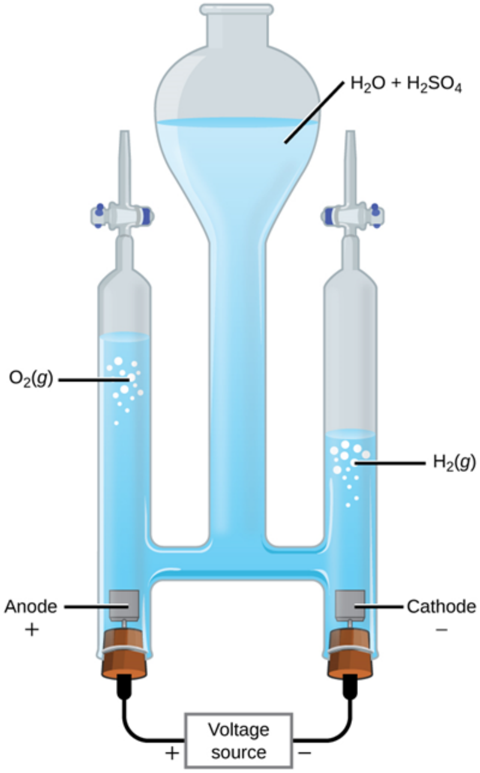


Figure 4.4.3: Decomposition of water through electrolysis $2\,\mathrm{H_2O(l)} \xrightarrow{Electrolyisis} 2\,\mathrm{H_2(g)} + \mathrm{O_2(g)}$. Source: OpenStax / CC BY (https://creativecommons.org/licenses/by/4.0)

Replacement or substitution reactions

There are two sub-classes of this category of reactions, i.e., single replacement and double replacement reaction.

Single replacement reactions involve one substance replacing a part of another, e.g.:

$$\mathrm{Zn(s)} + \mathrm{CuCl_2(aq)} \longrightarrow \mathrm{ZnCl_2(aq)} + \mathrm{Cu(s)}$$

$$2\,\mathrm{Al(s)} + 6\,\mathrm{HCl(aq)} \longrightarrow \mathrm{AlCl_3(aq)} + 3\,\mathrm{H_2(g)}$$

Fig. 4.4.4 shows an example of a single replacement reaction of magnesium resulting in hydrogen gas formation.

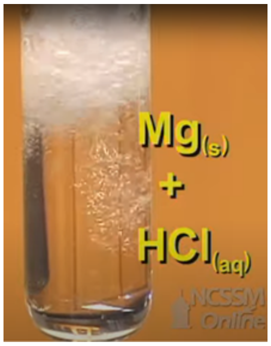


Figure 4.4.4: Single replacement reaction of magnesium with hydrochloric acid producing hydrogen gas: $Mg(s) + 2\,HCl(aq) \longrightarrow MgCl(aq) + H_2(g)\uparrow$ Source: taken form NCSSM online youtube video, 05/18/20, https://www.youtube.com/watch?v=OBdgeJFzSec

Double replacement reactions or metathesis involve the mutual exchange of partners between two substances, e.g. the following precipitation reactions:

$$NaCl(aq) + AgNO_3(aq) \longrightarrow AgCl(s)\downarrow + NaNO_3(aq)$$

$$Na_2CO_3(aq) + CaCl_2(aq) \longrightarrow CaCO_3(s)\downarrow + 2\,NaCl(aq)$$

Combustion reactions

Combustion is a reaction of a substance with oxygen, often with the formation of flame and release of much heat, e.g.:

$$C_8H_{16} + 12\,O_2 \longrightarrow 8\,CO_2 + 8\,H_2O + Heat$$

$$C + O_2 \longrightarrow CO_2 + Heat$$

$$2\,H_2 + O_2 \longrightarrow 2\,H_2O + Heat$$

$$2\,Mg + O_2 \longrightarrow 2\,MgO + Heat$$

Fig. 4.4.5 shows the above reaction, i.e., combustion of Mg in air.

Figure 4.4.5: An image of Ignited Magnesium burning in the air in normal conditions. Yannickcosta1, CC BY SA3, https://commons.wikimedia.org/wiki/File:Magburn1.jpg

Usually, combustion is considered as the reaction of a substance containing carbon and hydrogen with oxygen resulting in carbon dioxide, water, flame, and heat, e.g., burning methane on a kitchen stove:

$$CH_4 + 3\,O_2 \longrightarrow CO_2 + 2\,H_2O + Heat$$

Classification of chemical reaction

> The chemical reactions are generally classified based on what exchanges during the reaction. These include;
>
> 1. the transfer of electrons in oxidation-reduction reactions,
> 2. transfer of protons in acid-base reactions, and
> 3. a part of reactants mutually exchanges in precipitation reactions, as described below.

Oxidation-reduction reactions

The oxidation-reduction or **redox** reaction involves the exchange of electrons. For example, reactions between a metal and nonmetal involve the transfer of electrons from the metal to the nonmetal forming an ionic bond, as shown in Fig. 4.4.6.

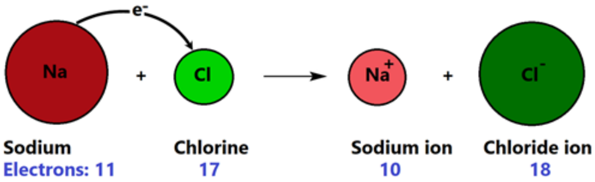


Figure 4.4.6: Illustration of an electron transfer in an oxidation-reduction reaction: $\mathrm{Na} + \mathrm{Cl} \longrightarrow \mathrm{Na}^{+} + \mathrm{Cl}^{-}$

Acid-base reactions

The acid-base reactions involve the transfer of protons from an acid to a base, as shown in Fig. 4.4.7.

Figure 4.4.7: Proton transfer from HCl to NH_3 is an example of an acid-base reaction: $\mathrm{HCl} + \mathrm{NH_3} \longrightarrow \mathrm{NH_4Cl}$. Hydrochloric acid (in beaker) reacts with ammonia fumes to produce ammonium chloride (white smoke). Source:
Walkerma, Public domain

Precipitation reactions

These are double displacement reactions in water that results in the precipitation of one of the products, as shown in Fig. 4.4.8.

Figure 4.4.8: Lead (II) iodide precipitates when potassium iodide is mixed with lead (II) nitrate: $\mathrm{Pb(NO_3)_2(aq)} + 2\,\mathrm{NaI(aq)} \longrightarrow 2\,\mathrm{NaNO_3(aq)} + \mathrm{PbI_2(s)}\downarrow$ Source: PRHaney / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

The precipitation reactions and the acid-base reactions are described in the later chapters. The oxidation-reduction reactions are discussed in the following section.

4.5: Oxidation-reduction reactions

What are Oxidation and Reduction?

The oxidation-reduction is defined in three ways:

1. **O**xidation **i**s the **l**oss of electrons and **r**eduction **i**s the **g**ain of electrons. The word **OIL RIG** helps in remembering this definition.
2. The addition of oxygen is oxidation, and the removal of oxygen is a reduction.
3. The removal of hydrogen is oxidation, and the addition of hydrogen is a reduction.

The oxidation-reduction or in short **redox** reaction is one of the most common types of chemical reactions happening in and around us. For example, rusting of metals, photosynthesis, digestion of food, and combustion of fuels are redox reactions.

Figure 4.5.1: Green patina on the statue of liberty is a result of the oxidation of copper. Source: https://www.hiclipart.com/free-trans...hybox/download

Oxidation-half and reduction-half reactions

The oxidation-reduction reactions happen in a pair because one thing loses electrons and is oxidized; the other thing gains the electrons and is reduced. That is why it is commonly called redox reaction, where red- represents reduction and –ox represents oxidation.

The green patina on the statue of liberty, shown in Fig. 4.5.1, is a result of the oxidation of copper:

$$2\,\mathrm{Cu(s)} + \mathrm{O_2(g)} \longrightarrow \mathrm{CuO(s)}$$

The transfer of electrons becomes apparent when the reaction is split into the oxidation-half and reduction-half. The oxidation-half is:

$$\mathrm{Cu} \longrightarrow \mathrm{Cu}^{2+} + 2\,\mathrm{e}^-$$

copper lost electrtons, so copper is oxides. The reduction half is:

$$\mathrm{O}_2 + 4\,\mathrm{e}^- \longrightarrow 2\,\mathrm{O}^{2-}$$

Oxygen gained electrons, so oxygen is reduced.

Oxidizing agent and reducing agent

- The substance that oxidizes another substance is an **oxidizing agent**. Oxygen is an oxidizing agent in the above reaction, as it oxidizes copper.
- The substance that reduces another substance is a **reducing agent**. Copper is a reducing agent in the above reaction, as it reduces oxygen.

The electrons lost in an oxidation-half must be equal to the electrons gained by the accompanying reduction-half. Multiplying the oxidation-half with 2 makes the electrons lost equal to the electrons gained in the reduction half in the above reaction. Then adding the oxidation and the reduction half gives the overall reaction:

$$2\,\mathrm{Cu} \longrightarrow 2\,\mathrm{Cu}^{2+} + \ 4\,\cancel{\mathrm{e}-}$$

$$\mathrm{O}_2 + \ 4\,\cancel{\mathrm{e}-} \longrightarrow 2\,\mathrm{O}^{2-}$$

$$\text{Overall reaction: } 2\,\mathrm{Cu(s)} + \mathrm{O}_2\mathrm{(g)} \longrightarrow \mathrm{CuO(s)}$$

Manipulating a chemical equation

The chemical equations can be manipulated like algebraic equations, i.e., they can be multiplied or divided by a constant, added, and subtracted, as demonstrated in the example of the copper redox-half reactions above. Note that electrons on one side of the equation canceled the electrons on the other side of the equation during the addition operation.

A silver color zinc strip dipped in copper nitrate solution becomes coated with a layer of reddish color copper, as shown in Fig. 4.5.2. The molecular equation of the reaction, that shows formula units of compounds in the reactants and products, is:

$$\mathrm{Zn(s)} + \mathrm{Cu(NO_3)_2(aq)} \longrightarrow \mathrm{Cu(s)} + \mathrm{Zn(NO_3)_2(aq)}$$

The complete ionic equation for the reaction is obtained by showing the dissolved ionic compounds as ions, e.g.:

$$\mathrm{Zn(s)} + \mathrm{Cu}^{2+}\mathrm{(aq)} + 2\,\mathrm{NO}_3^-\mathrm{(aq)} \longrightarrow \mathrm{Cu(s)} + \mathrm{Zn}^{2+}\mathrm{(aq)} + 2\,\mathrm{NO}_3^-\mathrm{(aq)}$$

The oxidation-half of the reaction is:

$$\mathrm{Zn(s)} \longrightarrow \mathrm{Zn}^{2+}\mathrm{(aq)} + 2\,\mathrm{e}^-$$

The reduction-half of the reaction is:

$$\mathrm{Cu}^{2+}\mathrm{(aq)} + 2\,\mathrm{e}- \longrightarrow \mathrm{Cu(s)}$$

The net ionic equation that is the addition of the oxidation-half and the reduction-half is:

$$\mathrm{Zn(s)} + \mathrm{Cu}^{2+}\mathrm{(aq)} \longrightarrow \mathrm{Cu(s)} + \mathrm{Zn}^{2+}\mathrm{(aq)}$$

Note that NO_3^- was on both sides of the complete ionic equation and has been canceled out in the net ionic equation:

$$\mathrm{Zn(s)} + \mathrm{Cu}^{2+}\mathrm{(aq)} + \ 2\,\cancel{\mathrm{NO}_3^-\mathrm{(aq)}} \longrightarrow \mathrm{Cu(s)} + \mathrm{Zn}^{2+}\mathrm{(aq)} + \ 2\,\cancel{\mathrm{NO}_3^-\mathrm{(aq)}}$$

Ions that do not participate in the chemical reaction are called spectator ions, and they appear on both sides of the molecular equation, like NO_3^- in this case.

Biological oxidation and reduction reactions

In the redox reactions involving metal species, the transfer of electrons is usually evident through the oxidation-half and the reduction-half reactions, as in the above examples. In the organic and biochemical redox reactions, the transfer of electrons is usually not so obvious, but the transfer of hydrogen or oxygen is usually apparent. For example, the metabolism of methanol $H_3C{-}OH$ starts with oxidation through the loss of hydrogen:

$$H_3C{-}OH \longrightarrow H_2C{=}O + 2\,H$$

Metanol is oxidized to formaldehyde $H_2C{=}O$. Formaldehyde oxidizes further by gaining oxygen:

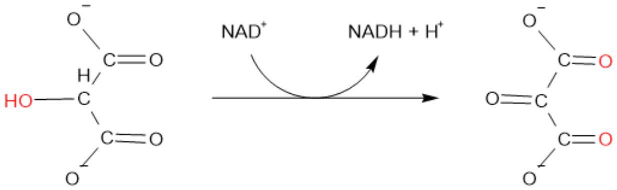
$$H_2C{=}O \longrightarrow HCOOH$$

Finally, the formic acid (HCOOH) is oxidized by gaining oxygen and forming carbon dioxide and water:

$$2\,HCOOH \longrightarrow 2\,O{=}C{=}O + 2\,H_2O$$

The increase in the C-O bond from a single bond in methanol to two double bonds (four C-O bonds) in carbon dioxide is a clear indication of the oxidation of the carbon.

Removal of hydrogen is also oxidation, e.g., hydroxymalonate is oxidized to oxomalonate by an enzyme hydroxymalonate dehydrogenase:



The reverse of these, i.e., removal of oxygen and addition of hydrogen is reduction.

4.6: Energetics of chemical reactions

Energetics deals with the energies involved in chemical reactions. There are two types of energies: the first is related to thermodynamics which is the energy released or absorbed when the reactants convert to the products, and the second is related to the kinetics of the reaction, i.e., the energy that the reacting molecules must possess to surpass the energy barrier for conversion to the products.

Reaction coordinate diagram

The progress of the reaction versus energy graph is shown in Fig. 4.7.1.

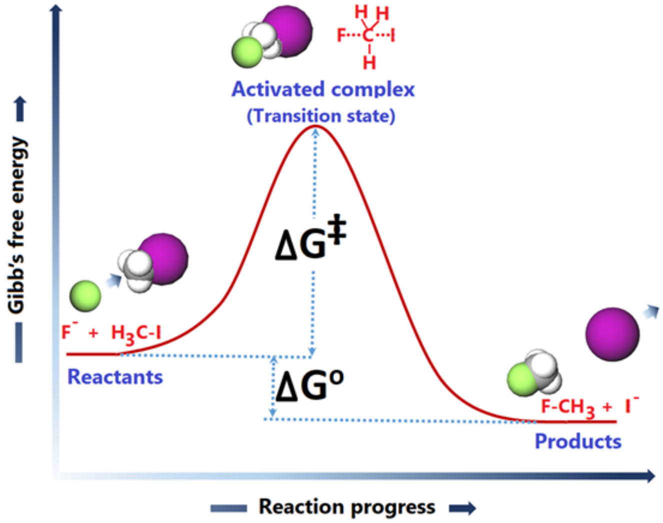


Figure 4.6.1: A reaction coordinate diagram for the reaction: $F^- + H_3C{-}I \longrightarrow F{-}CH_3 + I^-$. The green sphere is F^-, purple is I^-, gray is C, and white is H. $\Delta G^‡$ is the activation energy, and ΔG^o is the overall energy released or absorbed in a chemical reaction.

The starting point shows the energy level of reactants. Remember that every substance has internal energy which is manifested as temperature. The molecules are moving around due to the internal energy and collied with other molecules. The collision between the reactants is usually the first requirement for the reaction to proceed.

The F^- ion in this example collides with the target H_3C-I from the side opposite to the C-I bond. The collision at an angle other than 180^o to the C-I bond is less effective or ineffective in initiating the C-I bond breaking. So, the proper orientation of the reacting molecules at the time of the collision is the second requirement.

After a properly oriented collision, the C-I bond starts breaking, the F-C bond starts making, and the energy of the system rises to a maximum level where the bond breaking and making are about halfway. The specie at the maxima of the energy curve is called **activated complex** or a **transition state**. The difference in energy between the reactants and the transition state is called activation energy ($\Delta G^‡$). The reactants must have enough kinetic energy to surpass the activation energy barrier, which is the third requirement for the reaction to happen. A summary of the basic requirements of a chemical reaction to happen is the following.

Requirement of a chemical reaction

1. The reacting molecules collide with each other –the more frequent the collision, the faster the reaction.
2. The molecules should have proper orientation at the time of the collision –this factor varies from reaction to reaction.
3. The colliding molecules must have energy, in addition to the potential chemical energy, equal to or higher than the energy of activation –the lower the activation energy, the faster the reaction.

The activated complex forms if the basic requirements are fulfilled. The activated complex rolls down the hill on the energy scale and settles at the energy level of the products where the old bonds are entirely broken, and the new bonds are fully formed. The graph of the reaction progress versus the energy, as in Fig. 4.7.1 is called the **reaction coordinate diagram**.

Exothermic and endothermic reactions

The energy absorbed or released in the form of heat at constant pressure conditions is called enthalpy change (ΔH), which is almost the same as the internal energy absorbed or released (ΔG) in most of the reactions.

> A chemical reaction that releases heat is exothermic. A chemical reaction that absorbs heat is an endothermic reaction.
>
> Bond-forming is always exothermic, and bond-breaking is the opposite, i.e., endothermic, as illustrated in Fig. 4.7.2.

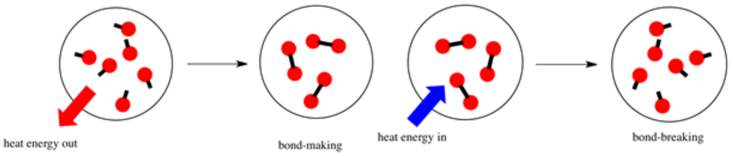


Figure 4.6.2: Bond forming releases heat, i.e., exothermic, and breaking the same bond absorbed the same energy, i.e., endothermic. Source: https://www.hiclipart.com/free-trans...alsen/download

In a chemical reaction, some bonds break, and some bonds form. If the bond-breaking absorbs less heat than the heat released in the new bond making, the reaction is exothermic. The products are lower in energy than the reactants, and the ΔH is negative for exothermic reactions. The opposite is true for an endothermic reaction, i.e., the bond-breaking absorbs more heat than the bond-forming; the products are higher in energy than the reactants, and ΔH is positive, as illustrated in Fig. 4.8.3.

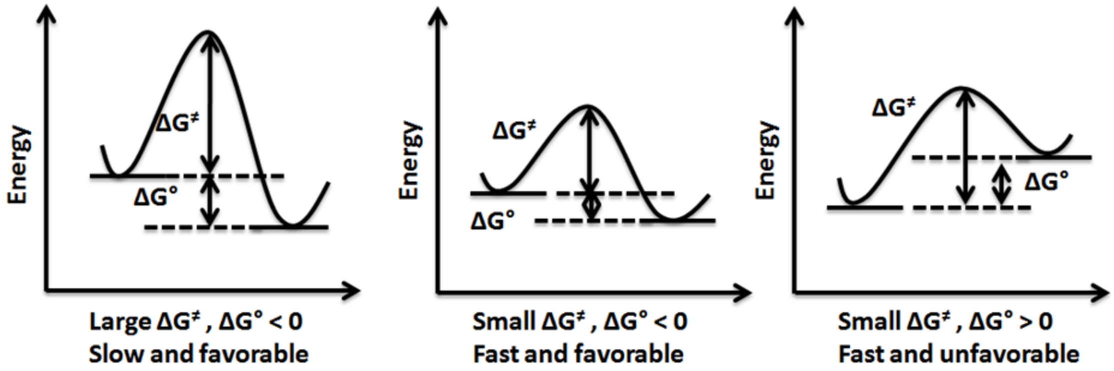


Figure 4.6.3: Reaction Coordinate Diagrams showing exothermic with products lower in energy than the reactants (left and middle) and endothermic with products higher in energy than the reactant (right) reaction. It also shows that the reaction on the left is the slowest due to the highest activation energy ($\Delta G^{\ddagger}$), and the reaction in the middle is the fastest due to the lowest activation energy ($\Delta G^{\ddagger}$). Source: AimNature / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

An example of an exothermic reaction is the combustion of methane that releases heat used for cooking.

$$\mathrm{CH_4 + 2\,O_2 \longrightarrow CO_2 + 2\,H_2O \quad \Delta H^{o} = -891\,kJ}$$

An example of an endothermic reaction is photosynthesis.

$$\mathrm{6\,CO_2 + 6\,H_2O \longrightarrow C_6H_{12}O_6 + 6\,O_2 \quad \Delta H^{o} = +2800\,kJ}$$

Note that the sign of ΔH is –ve for exothermic and +ve for an endothermic reaction. Sometimes, the energy is shown as a product for exothermic reaction, and as reactant for edothermic reaction. For example, the above two creations may be written as:

$$\mathrm{CH_4 + 2\,O_2 \longrightarrow CO_2 + 2\,H_2O + 891\,kJ}$$

$$\mathrm{6\,CO_2 + 6\,H_2O + 2800\,kJ \longrightarrow C_6H_{12}O_6 + 6\,O_2}$$

Figure 4.6.4: Cold Hot Pack used for medication. Source: Mamun2a, CC BY-SA 4.0 <https://creativecommons.org/licenses/by-sa/4.0>, via Wikimedia Commons

The instant hot or cold packs used in hospitals are based on the heat of dissolution of salts in water, as shown in Fig. 4.7.4. The salt and the water are in separate pockets in the pack. When the seal is ruptured, the salt dissolves in water and releases or absorbs heat. The dissolution of $CaCl_2$ salt in water is an exothermic process that is the source of heat in a hot pack:

$$\mathrm{CaCl_2(s)} \longrightarrow \mathrm{CaCl_2(aq)} \quad \Delta H^o = -82\,\mathrm{kJ}$$

The dissolution of NH_4NO_3 salt in water is an endothermic process that is utilized to absorb heat in a cold-pack.

$$\mathrm{NH_4NO_3(s)} \longrightarrow \mathrm{NH_4NO_3(aq)} \quad \Delta H^o = -26\,\mathrm{kJ}$$

Factors that affect the rate of a chemical reaction

The rate of a chemical reaction, i.e., the amount of a reactant consumed or the amount of a product formed per unit time, is dependent on the energy of activation of the reaction —the higher the activation energy, the slower the rate of a reaction and vice versa. A reaction requires collision between the reactant molecules, with proper orientation, and sufficient energy to surpass the activation energy barrier.

> Any factor that increases the rate of collisions, enhances the proper orientation or increases the kinetic energy of the molecules causes an increase in the rate of reaction. The factors include concentration, temperature, and catalysts.

Effect of concentration of reactants

> The higher the concentration, the more frequent the collisions, and the faster the reaction, as illustrated in Fig. 4.7.5.

In the breathing process, oxygen (O_2) binds with hemoglobin (Hb) in the lungs.

$\mathrm{Hb(aq)} + \mathrm{O_2(g)} \rightarrow \mathrm{HbO_2(aq)}$

Patients having breathing problems are given breathing masks with a higher concentration of oxygen than in the atmosphere to increase the rate of oxygen binding with the hemoglobin.

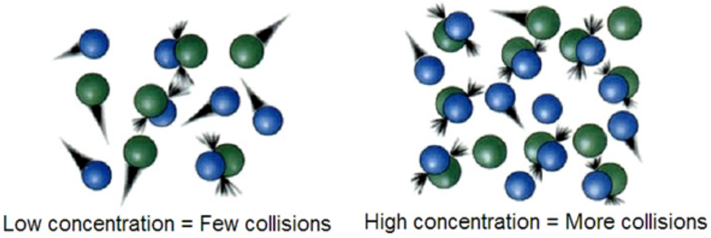


Figure 4.6.5: Illustration of higher the concentration, the more frequent the collisions leading to faster reaction. Source: Sadi Carnot / Public domain

Effect of temperature

The kinetic energy of molecules at a given temperature follows Boltzman distribution, as illustrated in Fig. 4.8.6. Increased temperature increases the average kinetic energy of the molecules which increases the fraction of molecules with more than the activation energy.

> An increase In temperature increases the rate of chemical reactions—generally, a 10 ^{o}C increase in temperature doubles the rate of a chemical reaction.

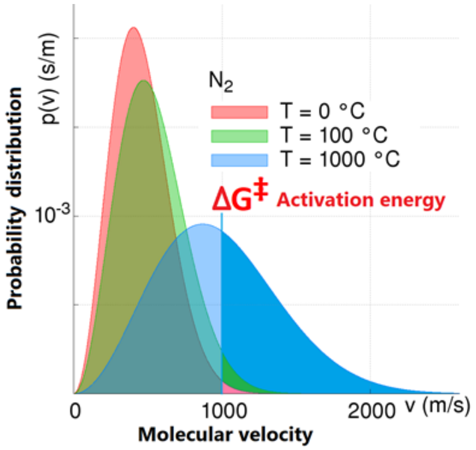


Figure 4.6.6: Illustrating increased temperature increases the average kinetic energy of the molecules that increases the fraction of molecules with more than the activation energy barrier ($\Delta G^{\ddagger}$). Source: modified from "TDF / CC0"

Some practical examples of the use of this principle are the following. Storing foods in refrigerators at lower temperatures decreases the rate of reactions resulting in longer life of the foods. Cooking foods in a pressure cooker increases the temperature resulting in faster cooking than in an open pan. In some cardiac surgeries, the body temperature is lowered to 28 ^{o}C to decrease the rate of metabolism which decreases the oxygen demand so that the heart may be stopped temporarily for the surgery.

Effect of catalysts and enzymes

> The catalysts and enzymes increase the rate of reaction by decreasing the energy of activation of the reaction through an alternate route, as illustrated in Fig. 4.7.7.

The catalysts and the enzymes do not consume in the reaction -they regenerate and repeat the action. Enzymes are the catalysts in biochemical reactions. Enzymes also increase the rate of reaction by binding with the reactants and properly orienting them for the reaction.

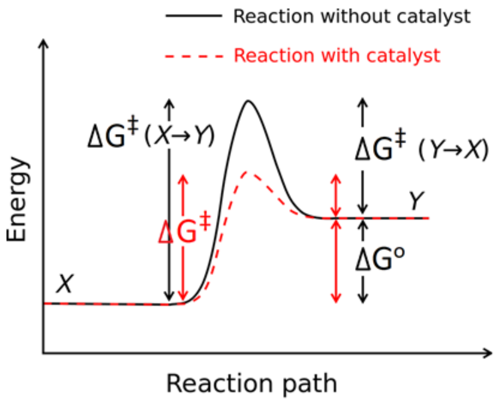


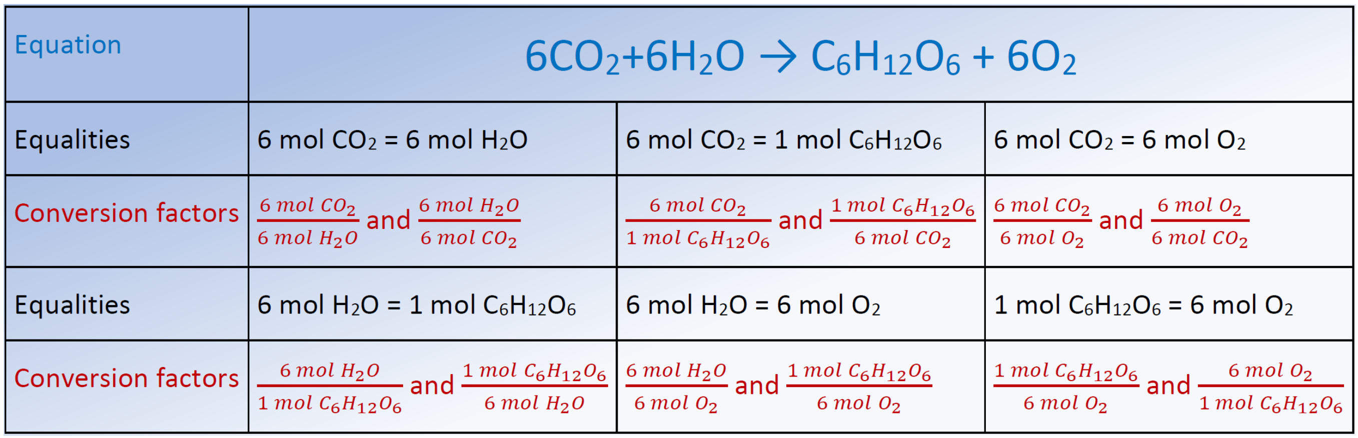
Figure 4.6.1: Effect of catalysts –When the catalyst is added, the activation energy $\Delta G^{\ddagger}$ decreases. However, the energy absorbed or released, i.e., ΔG^{o} remains constant. Source: Bkell, Public domain.

4.7: Stoichiometric calculations

Conversion factors from a chemical equation

Stoichiometry pronounced as “stɔɪkiˈɒmɪtri” is the calculation of the amount of reactants and products in a chemical reaction. It is based on the fact that a balanced chemical equation is also a set of mole-to-mole equalities between the reactants and the products. Each equality gives two conversion factors that allow calculating the mole of one substance from the given mole of any other substance in the equation.

Fig. 4.6.1 lists the chemical equation for photosynthesis reaction, the mole-to-mole equalities from the equation, and the two conversion factors from each of the equality, as an example. The conversion factors are used to calculate the unknown quantity in the mole from the known quantity in the mole of any other reactant or product in the same chemical equation, as explained in the following examples.



Equation	$6CO_2 + 6H_2O \rightarrow C_6H_{12}O_6 + 6O_2$		
Equalities	6 mol CO_2 = 6 mol H_2O	6 mol CO_2 = 1 mol $C_6H_{12}O_6$	6 mol CO_2 = 6 mol O_2
Conversion factors	$\frac{6\ mol\ CO_2}{6\ mol\ H_2O}$ and $\frac{6\ mol\ H_2O}{6\ mol\ CO_2}$	$\frac{6\ mol\ CO_2}{1\ mol\ C_6H_{12}O_6}$ and $\frac{1\ mol\ C_6H_{12}O_6}{6\ mol\ CO_2}$	$\frac{6\ mol\ CO_2}{6\ mol\ O_2}$ and $\frac{6\ mol\ O_2}{6\ mol\ CO_2}$
Equalities	6 mol H_2O = 1 mol $C_6H_{12}O_6$	6 mol H_2O = 6 mol O_2	1 mol $C_6H_{12}O_6$ = 6 mol O_2
Conversion factors	$\frac{6\ mol\ H_2O}{1\ mol\ C_6H_{12}O_6}$ and $\frac{1\ mol\ C_6H_{12}O_6}{6\ mol\ H_2O}$	$\frac{6\ mol\ H_2O}{6\ mol\ O_2}$ and $\frac{1\ mol\ C_6H_{12}O_6}{6\ mol\ O_2}$	$\frac{1\ mol\ C_6H_{12}O_6}{6\ mol\ O_2}$ and $\frac{6\ mol\ O_2}{1\ mol\ C_6H_{12}O_6}$

Figure 4.7.1: Balanced chemical equation of the photosynthesis reaction, mol-to-mol equalities, and conversion factors derived from the equation.

Mole-to-mole conversion from a chemical equation

Calculation of the mole of the desired substance from the given mole of any reactant or product needs one conversion factor. The steps are:

1. write the given quantity and the desired quantity,
2. write the balanced chemical equation,
3. write the equality between the given and the desired substances,
4. right the conversion factor that has the given substance in the denominator and the desired substance in the numerator,
5. multiply the given quantity with the conversion factor. Double-check to make sure that it cancels the given substance and leaves the desired substance in the answer.

Example 4.7.1

Calculate the moles of glucose produced from 3.0 moles of carbon dioxide in the photosynthesis reaction?

Solution

i. Given: 3.0 mole CO_2, Desired: ? moles of $C_6H_{12}O_6$

ii. Chemical equation: $6\,CO_2 + 6\,H_2O \longrightarrow C_6H_{12}O_6 + 6\,O_2$

iii. The desired equality: 6 mol CO_2 = 1 mol $C_6H_{12}O_6$,

iv. Desired conversion factor: $\frac{1\text{ mol }C_6H_{12}O_6}{6\text{ mol }CO_2}$

v. Calculations:

$$3.0\ \text{mol}\ \cancel{CO_2} \times \frac{1\ \text{mol}\ C_6H_{12}O_6}{6\ \text{mol}\ \cancel{CO_2}} = 0.50\ \text{mol}\ C_6H_{12}O_6$$

✓ Example 4.7.2

Magnesium reacts with HCl by this reaction: $Mg(s) + 2\,HCl(aq) \longrightarrow MgCl_2(aq) + H_2(g)\uparrow$. Calculate the moles of Mg needed to produce 3 moles of H_2?

Solution

i. Given: 3 mol of H_2. Desired: ? Moles of Mg.

ii. The chemical equation is given.

iii. The desired equality: 1 mol Mg = 1 mol H_2.

iv. The desired conversion factor: $\frac{1\ mol\ Mg}{1\ mol\ H_2}$

v. Calculation:

$$3\ \text{mol}\ \cancel{H_2} \times \frac{1\ \text{mol Mg}}{1\ \text{mol}\ \cancel{H_2}} = 3\ \text{mol}\ Mg$$

Mole-to-mass conversion from a chemical equation

Calculations described in the previous two examples show calculating moles of the desired substance from the moles of the given substance using a conversion factor from a chemical equation. The molar mass is a conversion factor from a mole-to-gram of the substance. So, add a molar mass of the desired substance as a second conversion factor, as explained in the following examples. Double-check that all the units cancel out, leaving the mass unit of the desired substance in the final answer.

✓ Example 4.7.3

Calculate grams of AgCl precipitate formed from 2.0 moles of $CaCl_2$ consumed in the following reaction:

$$2\,AgNO_3 + CaCl_2 \longrightarrow Ca(NO_3)_2 + 2\,AgCl(s)\downarrow$$

Solution

i. Given: 2.0 moles of $CaCl_2$. Desired: ? g AgCl

ii. Molar mass of AgCl = 1x107.87 g Ag.mol^{-1} + 1x35.45 g C.mol^{-1} = 143.3 g AgCl.mol^{-1}

iii. The chemical equation is given.

iv. The desired equality: 1 mol $CaCl_2$ = 2 mol AgCl, and 1 mol AgCl =143.3 g AgCl.

v. The desired conversion factors:

$$\frac{2\ \text{mol AgCl}}{1\ \text{mol}\ CaCl_2} \quad \text{and} \quad \frac{143.3\ \text{g AgCl}}{1\ \text{mol AgCl}}$$

vi. Calculation:

$$2.0\ \text{mol}\ \cancel{CaCl_2} \times \frac{2\ \text{mol}\ \cancel{AgCl}}{1\ \text{mol}\ \cancel{CaCl_2}} \times \frac{143.3\ \text{g AgCl}}{1\ \text{mol}\ \cancel{AgCl}} = 573.3\ \text{g AgCl}$$

✓ Example 4.7.4

How many grams of carbon dioxide are needed to react with 2 moles of water in the photosynthesis reaction?

Solution

i. Given: 2.0 moles of H_2O Desired: ? g CO_2.

ii. Molar mass of CO_2 = 1x12.011 g C.mol^{-1} + 2x15.999 g O.mol^{-1} = 44.009 g CO_2.mol^{-1}

iii. The chemical equation: : $6CO_2 + 6\ H_2O \rightarrow C_6H_{12}O_6 + 6O_2$.

iv. The desired equality: 6 mol CO_2 = 6 mol H_2O, and 1 mol CO_2 = = 44.009 g CO_2.

v. The desired conversion factors:

$$\frac{6\text{ mol }CO_2}{6\text{ mol }H_2}O \quad \text{and} \quad \frac{44.009\text{ g }CO_2}{1\text{ mol }CO_2}$$

vi. Calculation:

$$2.0\ \text{mol}\ \cancel{H_2O} \times \frac{6\ \text{mol}\ \cancel{CO_2}}{6\ \text{mol}\ \cancel{H_2O}} \times \frac{44.009\text{ g }CO_2}{1\ \text{mol}\ \cancel{CO_2}} = 88\text{ g }CO_2$$

Mass-to-mass conversion from a chemical equation

A chemical equation gives a mole-to-mole conversion factor. If the given substance is in grams and the desired substance is also in grams, then two additional conversion factors based on the molar masses are needed. That is, the following conversions are needed:

> Mass of given substance⇒mole of the given substance⇒mole of the desired substance⇒grams of the desired substance.

The reciprocal molar mass of the given substance is the first conversion factor, the mole to mole conversion factor from the chemical equation is the second conversion factor, and the molar mass of the desired substance is the third conversion factor needed. Make sure that each conversion factor cancels the denominator unit of its multiplier to the right, and the desired unit is left in the answer. The following examples explain these calculations.

✓ Example 4.7.5

How many grams of Mg are needed to produce 1.01 g of H_2 gas in this reaction:

$$Mg(s) + 2\,HCl(aq) \longrightarrow MgCl_2(aq) + H_2(g)\uparrow$$

Solution

i. Given: 1.01 g H_2 Desired: ? g Mg.

ii. Molar mass of H_2 = 2 x1.008 g H.mol^{-1} = 2.016 g H_2.mol^{-1}, and molar mass = 24.305 g Mg.mol^{-1}.

iii. The chemical equation is given in the problem.

iv. The desired equalities : 1 mol Mg = 1 mol H_2, 1 mol H_2 = 2.016g H_2, 1 mol Mg = 24.305 g Mg

v. Calculate by multiplying the given quantity consecutively with the three desired conversion factors from the equalities:

$$1.01\ \text{g}\ \cancel{H_2} \times \frac{1\ \text{mol}\ \cancel{H_2}}{2.016\ \text{g}\ \cancel{H_2}} \times \frac{1\ \text{mol}\ \cancel{Mg}}{1\ \text{mol}\ \cancel{H_2}} \times \frac{24.305\text{ g Mg}}{1\ \text{mol}\ \cancel{Mg}} = 11.9\text{ g Mg}$$

✓ Example 4.7.6

How many grams of glucose are produced if 22.0 g of carbon dioxide is consumed in the photosynthesis reaction?

Solution

i. Given: 22.0 g CO_2 Desired: ? g $C_6H_{12}O_6$.

ii. Molar masses: of CO_2 = 1x12.011 g C.mol^{-1} + 2x15.999 g O.mol^{-1} = 44.009 g CO_2.mol^{-1}, and molar mass of $C_6H_{12}O_6$ = 6x12.011 g C.mol^{-1} + 12x1.008 g H.mol^{-1} + 6x15.999 g O.mol^{-1} = 180.156 g $C_6H_{12}O_6$.mol^{-1} .

iii. The chemical equation: $6\,CO_2 + 6\,H_2O \longrightarrow C_6H_{12}O_6 + 6\,O_2$

iv. The desired equalities: 6 mol CO_2 = 1 mol $C_6H_{12}O_6$, 1 mol CO_2 = 44.009 g CO_2, 1 mol $C_6H_{12}O_6$ = 180.156 g $C_6H_{12}O_6$.

v. Calculate by multiplying the given quantity consecutively with the three desired conversion factors from the equalities:

$$22.0\ \text{g}\ \cancel{\text{CO}_2} \times \frac{1\ \text{mol}\ \cancel{\text{CO}_2}}{44.009\ \text{g}\ \cancel{\text{CO}_2}} \times \frac{1\ \text{mol}\ \cancel{\text{C}_6\text{H}_{12}\text{O}_6}}{6\ \text{mol}\ \cancel{\text{CO}_2}} \times \frac{180.156\ \text{g}\ \text{C}_6\text{H}_{12}\text{O}_6}{1\ \text{mol}\ \cancel{\text{C}_6\text{H}_{12}\text{O}_6}} = 15.0\ \text{g}\ \text{C}_6\text{H}_{12}\text{O}_6$$

Fig. 4.6.2 illustrates what each conversion factor does in the case of the above example number 4.6.5

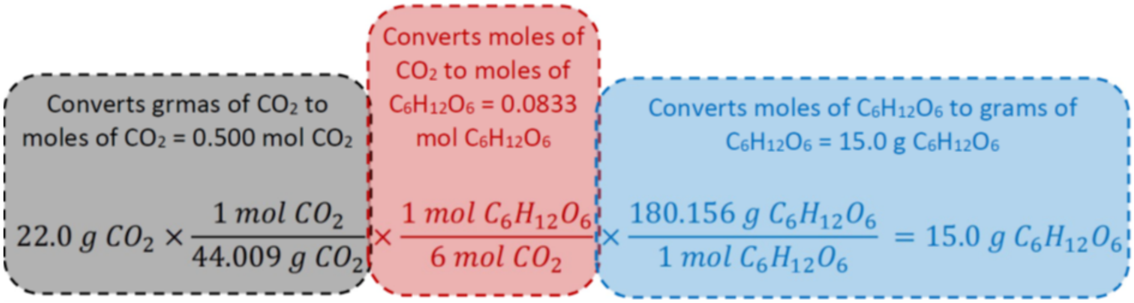


Figure 4.7.2: Illustration of the operation of conversion factors in a mass-to-mass calculation based on a balanced chemical equation of example 4..6.6 for question: "calculate grams of $C_6H_{12}O_6$ produced from 22.0 g CO_2 in photosynthesis reaction $6\,CO_2 + 6\,H_2O \longrightarrow C_6H_{12}O_6 + 6\,O_2$ ".

CHAPTER OVERVIEW

5: Solutions

5.1: Introduction to solution

Solutions are all around us, e.g., air, seawater, body fluids, metal alloys are solutions. Fig. 5.1.1 illustrates that air is a mixture of nitrogen, oxygen, carbon dioxide, and some other gases; Fig. 5.1.2 illustrates that seawater is a mixture of water, chloride, sodium, sulfate, magnesium, and some other ions, and Fig. 5.1.3. illustrates that about 60% of the human body is composed of solutions called body fluids.

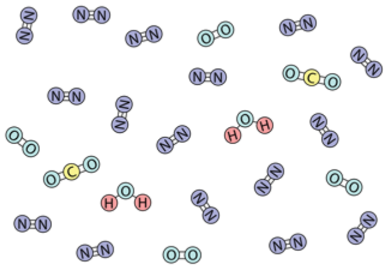


Figure 5.1.1: Air is a solution of nitrogen (N_2), oxygen (O_2), carbon dioxide (CO_2), and some other gases . Source: RoRo / CC0

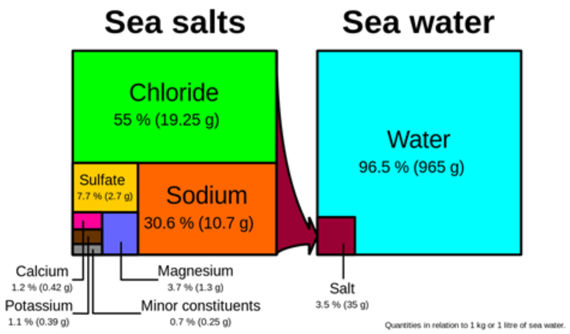


Figure 5.1.2: Seawater is a solution of water and several ions, expressed in wt/wt%. Source: derivative work: Tcncv (talk)Sea_salt-e_hg.svg: Hannes Grobe, Alfred Wegener Institute for Polar and Marine Research, Bremerhaven, Germany; SVG version by Stefan Majewsky / CC BY-SA (https://creativecommons.org/licenses/by-sa/2.5)

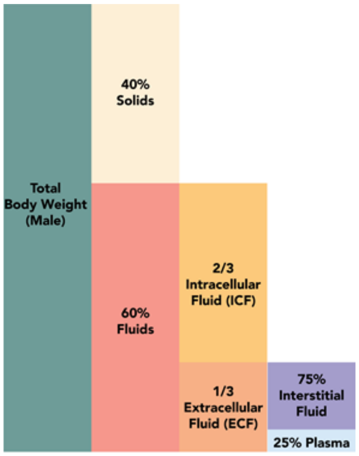


Figure 5.1.3: This schematic shows the relative volumes of the different fluid compartments in an adult male. Source: Alan Sved and David Walsh / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

What is a solution?

- A solution is a homogeneous mixture of two or more pure substances.
- The substance that is in a large amount in the solution is called the **solvent**.
- The substance that is in smaller amounts in a solution is called the **solute**.

For example, the air is a solution in which nitrogen is the solvent, and water is the solvent in seawater and body fluids. Oxygen, carbon dioxide, and water vapors are solutes in the air; and sodium, chloride, sulfate, magnesium, and some other ions are solutes in seawater.

Types of solution

The solutions are generally classified in two ways: i) based on the physical state of the solution and the solute, and ii) based on the particle size of the solute.

Types of solution based on the physical state of the solution and the solute

The solutions can be classified based on the physical state of the solution, solvent, and solute. For example, the air is gas in a gas solution; carbonated water is a gas in a liquid solution; vinegar is a liquid in a liquid solution; metal alloys are solid in solid solutions. Table 5.1.1 lists the major types of solutions, solvents, and primary solutes in them.

Table 1: Examples of main types of solutions and solvent and major solute in them.

Type	Example	solvent	Primary solute
Gas in gas	Air	Nitrogen	Oxygen
Gas in liquid	Carbonated water	Water	Carbon dioxide
Liquid in liquid	Vinegar	Water	Acetic acid
Solid in liquid	Seawater	Water	Sodium chloride
Solid in solid	Brass	Copper	Zinc

Types of solutions based on the particle size of the solute

Solution

A solution is a homogeneous mixture comprising smaller component/s called solute/s of small molecules or ions comparable in size to the molecules of a larger component called the solvent.

For example, NaCl dissolved in water is a solution. The solute is almost uniformly distributed in the solvent, making a homogeneous mixture. The solute does not separate by filtration or by a semipermeable membrane but can be separated by some other physical process. For example, the distillation process separates a solid in a liquid or a liquid into a liquid solution. The solution is transparent, though it may be colored. A light passing through a solution is not visible, as shown in Fig. 5.1.4.

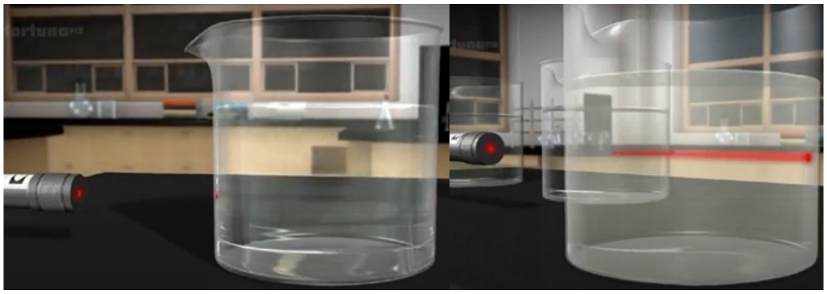


Figure 5.1.4: Demonstration of Tyndall effect: a red-laser bean passing through a solution is not visible (left), but visible when passing through a colloid (right). Source: https://youtu.be/8Xcpq6e8pBY, Creative Commons Attribution license (reuse allowed)

Suspension

A suspension is a heterogeneous mixture of solvent and solute particles of larger than 10,000 Å.

For example, muddy water is a suspension. If the suspension is allowed to stand, the suspended particles settle down and separate. The suspended particles can be filtered out. Some medicines, e.g., milk of magnesia, are suspensions. It is instructed to shake just before administering medicine to re-suspend the settled suspension.

Colloid

A colloid falls between a solution and a suspension. The colloidal particles are larger molecules like proteins or groups of molecules or ions.

Unlike a suspension, the colloids usually do not settle if allowed to stand. The colloidal particles can not be filtered but can be separated by a semipermeable membrane. When a light beam passes through a colloid, it scatters by the colloid particles, called the Tyndall effect, and becomes visible, as shown in Fig. 5.1.4.

Examples of colloids include:

1. fog and clouds that are liquid water droplets dispersed in air;
2. smoke that is solid carbon particles dispersed in air;
3. whipped cream that is air dispersed in a liquid;
4. styrofoam is a gas dispersed in a solid; and
5. ager medium that is liquid dispersed in a solid medium.
6.

Water –a universal solvent

Water (H_2O) is an essential substance for life. It covers more than 70% of the earth's surface (Fig. 5.1.5), and it comprises more than 60% of the human body (5.1.3). In addition to being the most abundant solvent, water is a universal solvent because it is a polar molecule with a partial negative charge on oxygen and a partial positive charge on hydrogen atoms as shown in Fig. 5.1.6. The polarity of water molecules allows them to interact with other water molecules as well as with other polar compounds through dipole-dipole interactions and with other ions through ion-dipole interactions. These interactions help to dissolve a lot of polar and ionic compounds that are in and around us.

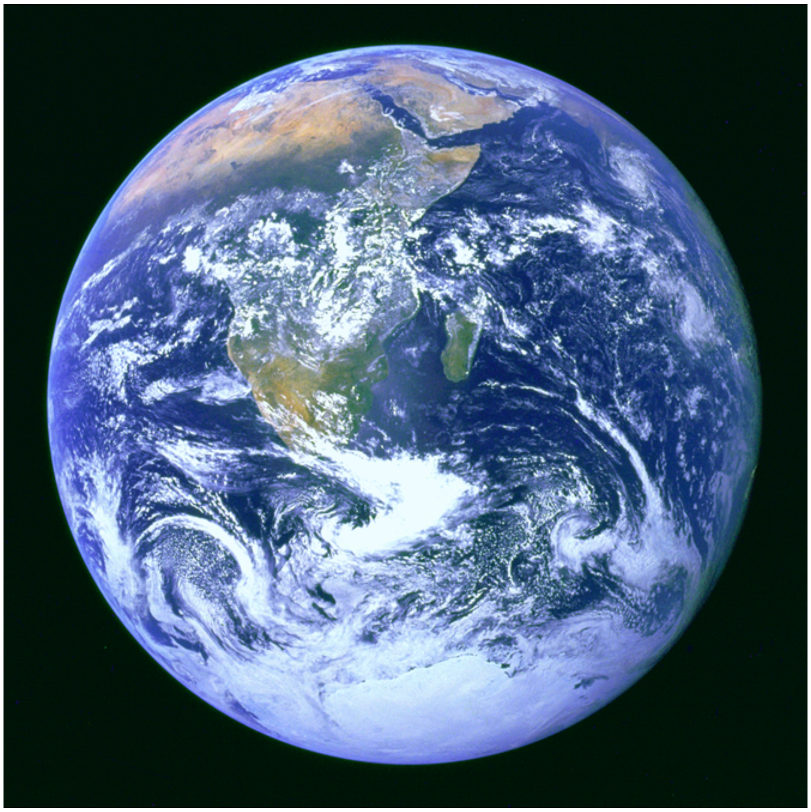


Figure 5.1.5: the image of the earth showing saltwater in the sea, fresh water on the Antarctic ice sheet, and clouds. Source: by NASA mission AS17. Public domain.

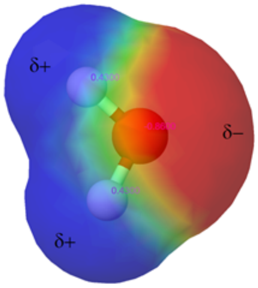


Figure 5.1.6: A model of water molecule showing oxygen in red and hydrogen in white color balls overplayed with an electrostatic potential map showing the partial positive (+d) region in red and the partial negative (-d) region in blue, drawn using a free web app **https://molview.org**

How does water dissolves polar and ionic compounds?

Water molecules establish electrostatic interaction, called hydrogen bonding, through the partial +ve end of one molecule with a partial –ve end of a neighboring molecule. These interactions impart unique properties to water, like its relatively higher boiling point and melting point compared to other substances of similar molecular weight. Other polar substances have similar interactions, e.g., ethanol has hydrogen bonding similar to water as illustrated in Fig. 5.1.7.

Dissolution of polar substance in water

When water mixes with other polar substances, like ethanol, some of the hydrogen bonding between water molecules replace with similar hydrogen bonding with ethanol molecules. Since the electrostatic potential energy is similar, the natural tendency to go towards more dispersion drives the dispersion of ethanol molecules uniformly in water resulting in the solution.

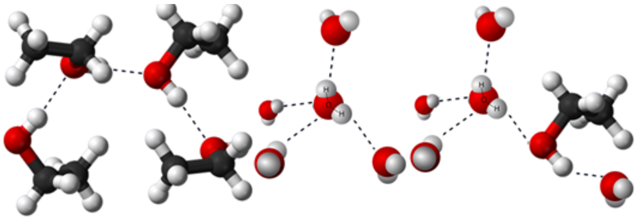


Figure 5.1.7: Models showing hydrogen bonding in ethanol (left), water (middle), and ethanol water solution (right). Source: modified from Benjah-bmm27, and snek01. Public domain

Ionic compounds are held together by electrostatic forces between opposite ions, i.e., ionic bonds. When an ionic compound is added to water, water molecules surround the cation and establish ion-dipole interaction by orienting their partial -ve end to the cation. Similarly, water molecules establish ion-dipole interaction with anions by orienting their partial +ev end towards the anion, as illustrated in Fig. 5.1.8

Dissolution of ionic compounds in water

The ion-dipole interactions, along with nature's tendency to disperse the particles, are usually strong enough to overcome the ionic bonds, dissociate the compounds into ions, and disperse them almost uniformly in the water.

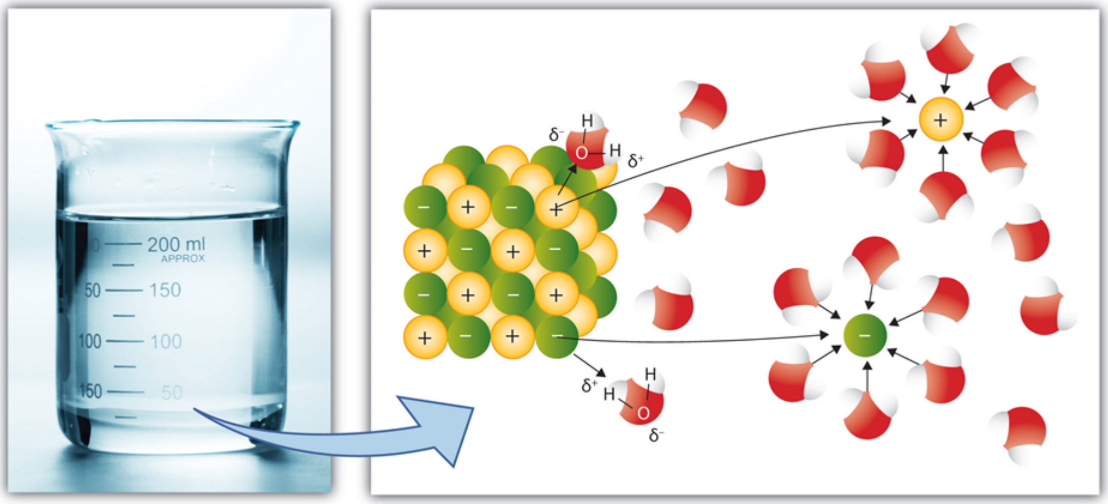


Figure 5.1.8: Dissolution of sodium chloride in water through dissociation into ions and dispersion in water driven by ion-dipole interactions and nature’s tendency to disperse particles. Source: Andy Schmitz / CC BY (https://creativecommons.org/licenses/by/3.0)

The separation of the cations from the anions of the ionic compound is called dissociation.

The formation of a layer of water molecules around ions, driven by ion-dipole interactions, is called hydration.

Non-polar substances, like vegetable oil or gasoline, do not dissolve in water. The molecules in non-polar substances have only London dispersion forces. They easily dissolve in non-polar solvents like hexane or carbon tetrachloride that have similar London dispersion forces among their molecules.

The fact that ionic and polar substances dissolve in polar solvents and non-polar substances dissolve in non-polar solvents of similar intermolecular interactions is called “**like dissolves like**.”

5.2: Solubility

Solubility and its related terminologies

The majority of solutes do not dissolve in water or other solvents in all proportions.

> ### What is solubility
>
> The maximum proportion of the solute that can dissolve in a given amount of the solvent, usually expressed in grams of solute in 100 grams of solvent, is called the **solubility** of the solute in the solvent.

1. Substances that make a solution when mixed in any proportion are called **miscible**. For example, ethanol and water are miscible.
2. Some substances make a solution when mixed in some proportion but not in all proportions; these are called **partially miscible**. For example, n-butanol can mix in water up to 7.3 g n-butanol/100 ml water.
3. Substances that almost do not dissolve in each other are called **immiscible**. For example, n-Hexane is immiscible in water.
4. The solution that has not yet reached its solubility limits and can dissolve more solute added is called an **unsaturated solution**.
5. The solution that has reached its solubility limits and can not dissolve if more solute is added to it is called a **saturated solution**.

When a solute is added to a saturated solution, it does dissolve, but, at the same time, the dissociated components recombine to form the crystals of the solute, i.e., recrystallize, at the same rate, so that there is no net dissolution, as illustrated in Fig. 5.2.1.

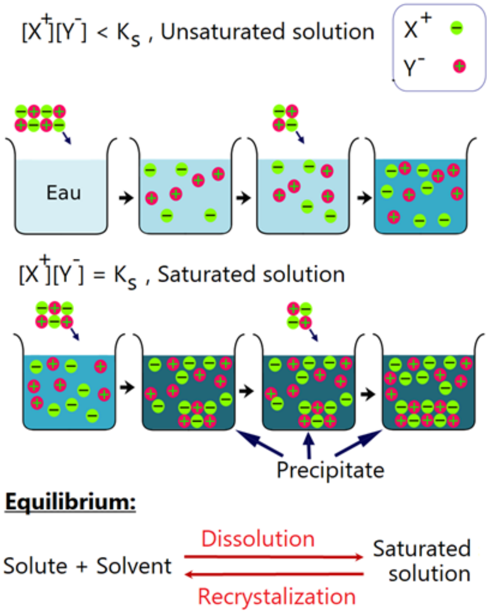


Figure 5.2.1: Illustration of unsaturated and saturated solution and the dynamic equilibrium between dissolution and recrystallization in the saturated solution. Source: No machine-readable author provided. Romary assumed (based on copyright claims). / CC BY-SA (http://creativecommons.org/licenses/by-sa/3.0/)

Effect of temperature on solubility

> The solubility of most of the solids and liquids increases as the temperature increases.

For example, when a saturated solution of sugar in water is heated, it can dissolve more sugar. Fig 5.2.2 show the solubility vs temperature curves for some compounds.

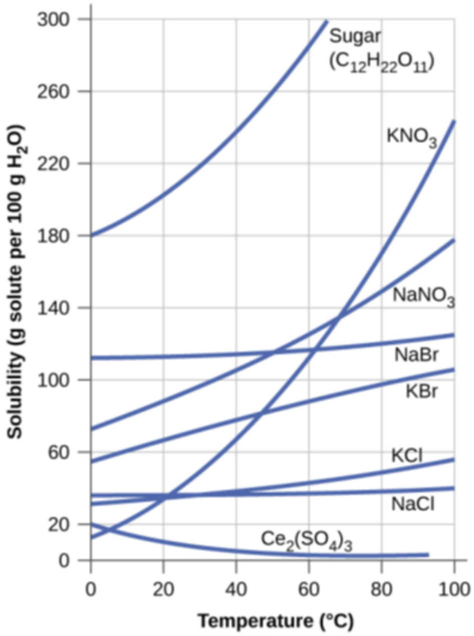


Figure 5.2.2: Solubility of some ionic and polar molecular compounds in water as a function of temperature. Download for free at https://openstax.org/details/books/chemistry.

When a hot saturated solution is cooled, the concentration of solute in the solution becomes above the solubility limits, making a **supersaturated solution**.

The supersaturated solution is unstable and ultimately crystallizes out the excess solute leaving any impurities in the solution, as illustrated in Fig. 5.2.3. This process is called re-crystallization, which is used to purify the solutes.

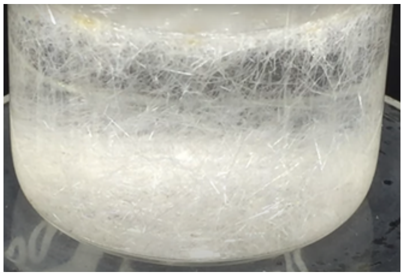


Figure 5.2.3: Salicylic acid recrystallized in water. Source: https://www.youtube.com/watch?v=QwqvzfPneUo

Medical issues related with solubility

The crystallization of excess solute from a supersaturated solution is responsible for some medical problems like gout and kidney stone. Gout is the crystallization of uric acid in the cartilage, tendons, and soft tissues when the concentration of the uric acid in blood plasms exceeds its solubility limit of ~7 mg/100 mL at 37 ^{o}C. It causes redness, swelling, and pain in the affected area, as illustrated in Fig. 5.2.4. Kidney stones are solid materials formed in the urinary tubes, as illustrated in Fig. 5.2.5. Kidney stones are the result of the crystallization of excess calcium phosphate, calcium oxalate, or uric acid in the urine.

Figure 5.2.4: Illustration of gout as a result of the recrystallization of uric acid in the cartilage, tendons, and soft, causes swelling, joint stiffness, and aching around the joint in the foot. Source: www.scientificanimations.com/ / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

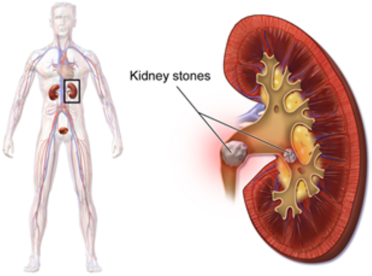


Figure 5.2.5: Kidney Stones illustrated. Source: Blausen.com staff (2014). "Medical gallery of Blausen Medical 2014". WikiJournal of Medicine 1 (2). DOI:10.15347/wjm/2014.010. ISSN 2002-4436/ CC BY (https://creativecommons.org/licenses/by/3.0)

Opposite to the solids and liquids, the solubility of gases generally decreases with an increase in temperature.

That is why the carbonated water releases dissolved gas when heated, causing pressure increase, which, in turn, causes the bursting of the soda can

Effect of pressure on solubility

The pressure has almost no effect on the solubility of solids and liquids but has a strong effect on the solubility of gases.

Henry's law

The solubility of gases in liquids is directly proportional to the pressure of the gas above the liquid.

An increase in pressure causes a decrease in the gas volume that increases the gas concentration. More frequent collision of the gas molecules with the gas-liquid boundary in a concentrated solution causes an increase in the rate of dissolution of the gas in the liquid, as illustrated in Fig 5.2.6. The opposite happens when the gas pressure decreases. For example, carbon dioxide starts bubbling out when a soda can is open because the gas escapes resulting in a decrease in the gas pressure above the liquid and a decrease in the solubility of the gas in water.

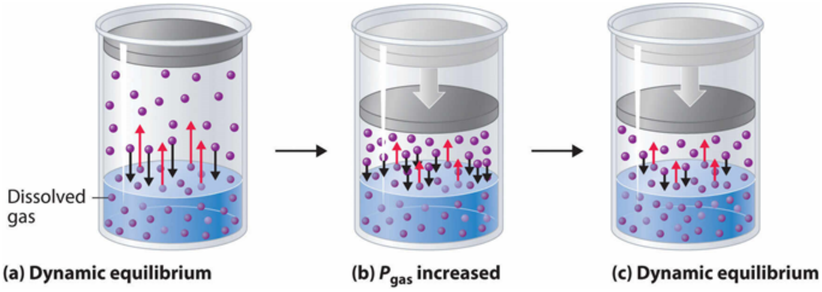


Figure 5.2.6: The Solubility of a gas increases as the partial pressure increases at a constant temperature. Source: Abozenadah, H., Bishop, A., Bittner, S. and Flatt, P.M. (2017) Preparatory Chemistry. CC BY-NC-SA. Available at: https://wou.edu/chemistry/courses/on...ory-chemistry/

Solubility guidelines for dissolution of ionic compounds in water

> If the solubility of a compound is less than 0.01 mol/L, it is considered **insoluble**.

The solubility of ionic compounds in water depends on the nature of the compound. For example, lead(II)iodide (PbI_2) and silver chloride (AgCl) are insoluble in water because the solubility of PbI_2 is 0.0016 mol/L of the solution and the solubility of AgCl is about 1.3 x 10^{-5} mol/L of solution. Potassium iodide (KI) and $Pb(NO_3)_2$ are soluble in water. When aqueous solutions of KI and $Pb(NO_3)_2$ are mixed, the concentration of PbI_2 in the mixture goes above its solubility limits, and it precipitates out, as illustrated in Fig. 5.2.7.

Figure 5.2.7: Precipitation reaction: $\mathrm{Pb(NO_3)_2(aq) + 2\,KI(aq) \longrightarrow PbI_2(s)\!\downarrow + 2\,KNO_3(aq)}$. source: PRHaney [CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)]

There are no fail-proof guidelines for predicting the solubility of ionic compounds in water. However, the following guideline can predict the solubility of most ionic compounds.

Soluble ions

1. Salts of alkali metals (Li^{1+}, Na^{1+}, K^{1+}, Rb^{1+}, Cs^{1+}) and ammonia (NH_4^{1+}) are soluble. No exceptions.
2. Salts of nitrate (NO_3^{1-}), acetate (CH_3COO^{1-}), and perchlorate (ClO_4^{1-}) are soluble. No exceptions.
3. Salts of chloride (Cl^{1-}), bromide (Br^{1-}), and Iodide (I^{1-}) are soluble, except when the cation is Pb^{2+}, Hg_2^{2-}, or Ag^{1+}. (Remember the acronym “LMS” based on the first letter of the element name, or phrase ‘Let Me See” to recall Lead, Mercury, and Silver.)
4. Sulfates (SO_4^{2-}) are soluble except when the cation Pb^{2+}, Hg_2^{2-}, Ag^{1+}, or a heavy alkaline earth metal ions: calcium (Ca^{2+}), barium (Ba^{2+}), or strontium (Sr^{2+}). ((recall “Let Me See” for Lead, Mercury, and Silver. Remember the acronym “CBS” based on the first letter of the element name, or the phrase “Come By Soon” to recall calcium, barium, and strontium.)

Insoluble ions

1. Hydroxide (OH^{1-}) and sulfides (S^{2-}) are insoluble except when the cation is an alkali metal, ammonia, or a heavy alkaline earth metal ions: Ca^{2+}, Ba^{2+}, and Sr^{2+}. (Recall the phrase “Come By Soon” to recall calcium, barium, and strontium.)
2. Carbonates (CO_3^{2-}), phosphates (PO_4^{3-}), and oxide (O^{2-}) are insoluble except when the cation is an alkali metal, ammonia
3. If there is a conflict between the two guidelines, then the guideline listed first has priority. For example, the salts of insoluble ions become soluble when the cation is an alkali metal, ammonia (rule#1).

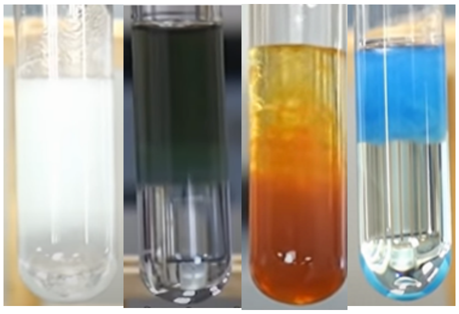


Figure 5.2.8: The precipitates of some insoluble ionic compounds formed by mixing the aqueous solution of appropriate soluble ionic compounds. The precipitates are from the left: white Calcium sulfate ($CaSO_4$), black Iron(II) hydroxide ($Fe(OH)_2$, brown Iron(III) hydroxide ($Fe(OH)_3$), and blue Copper(II) hydroxide ($Cu(OH)_2$). Source: https://youtu.be/jltLlzZ6FqU

Fig. 5.2.8 shows precipitates of some insoluble ionic compounds formed by mixing aqueous solutions of appropriate soluble ionic compounds. The precipitation can be predicted, as illustrated in Fig. 5.2.9. List the ions of the soluble ionic compounds and then cross-combine the cations of one with the anion of the other to make the potential products. If any of the potential products is an insoluble ionic compound, it precipitates out.

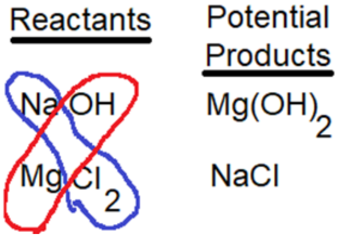


Figure 5.2.9: Cross-combine the cation-anion in the reactants. If any of the cross-combination is an insoluble salt, it will precipitate out, e.g: $\mathrm{NaOH(aq)} + \mathrm{MgCl_2(aq)} \rightarrow \mathrm{Mg(OH)_2(\,s)} \downarrow + \mathrm{NaCl(aq)}$

5.3: Electrolytes

What is an electrolyte?

Electric current is defined as the movement of electric charges. The substances through which an electric current can flow are called electrical conductors, and the others are electrical nonconductors. Metals are electrical conductors because valence electrons of metal atoms can move around in a piece of metal. Ionic compounds are composed of cations and anions, but the ions in a solid can not move around. Therefore, solid ionic compounds are electrical nonconductors. Pure water does not have a sufficient concentration of ions in it and is an electrical nonconductor. The ionic compounds dissociate into ions when dissolved in water. The solution of ionic compounds in water is an electrical conductor because the ions can move around in the solution, as illustrated in Fig. 5.3.1.

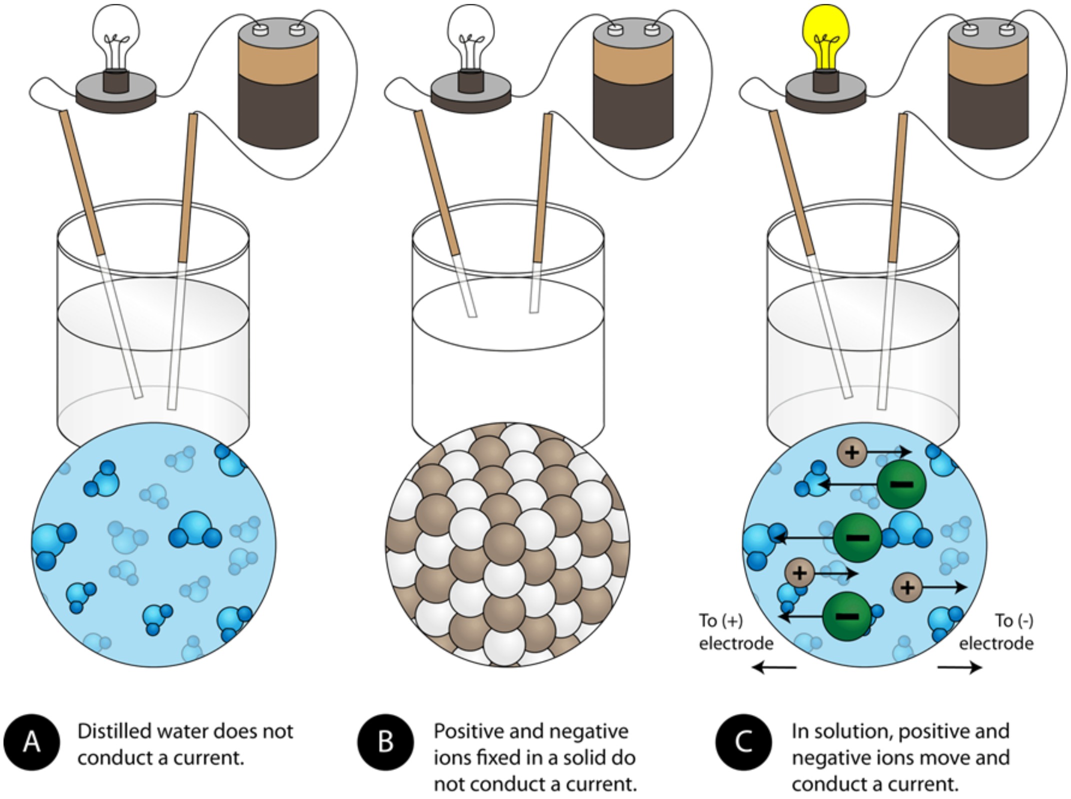


Figure 5.3.1: Pure water (A) and solid ionic compounds (B) are electrical nonconductors, but the solution of ionic compounds in water is an electrical conductor. Source: https://www.hiclipart.com/free-trans...cmeih/download

> Substances that produce electrically conducting solution when dissolved in water (or in another polar solvent) are called **electrolytes**.

All ionic compounds, acids, and bases produce ions in water and are classified are electrolytes.

> Substances that produce an electrically nonconducting solution when dissolved in water are called **nonelectrolytes**.

Molecular compounds other than acids and bases, such as methanol, acetone, sugar, and glucose, remain neutral molecules when dissolved in water. The molecular solutes, other than acids and bases, are nonelectrolytes.

Strong and weak electrolytes

> Substances that almost 100% dissociate into ions when dissolved in water are **strong electrolytes**.
>
> 1. All ionic compounds that are soluble in water are strong electrolytes.
> 2. Strong acids are strong electrolytes.
> 3. Strong bases are ionic compounds and strong electrolytes.

A strong electrolyte does not mean that it is necessarily highly soluble in water. It means that the portion of the solute that dissolves, it also dissociates 100% into ions in water, e.g., all ionic compounds. The solubility $Ca(OH)_2$ is only 0.16 g $Ca(OH)_2$/100 g water at 20 ^{o}C, but all the dissolved $Ca(OH)_2$ dissociates into Ca^{2+} and OH^{-} ions.

Strong bases are hydroxides of alkali metals, i.e., LiOH, NaOH, KOH, RbOH, and CsOH, and hydroxides of heavy alkaline earth metals, i.e., $Ca(OH)_2$, $Sr(OH)_2$ and $Ba(OH)_2$, which are strong electrolytes. Strong acids, i.e., HCl, HBr, HI, $HClO_4$, $HNO_{3,}$ and $H_2SO_{4,}$ are molecular compounds but are strong electrolytes because they dissociate almost 100% into ions when dissolved in water. For example, HCl almost wholly dissociates into ions when dissolved in water.

$$\mathrm{HCl(g) + H_2O(l) \rightarrow H_3O^{1+}(aq) + Cl^{1-}(aq)}$$

> Substances that partially dissociate into ions when dissolved in water are **weak electrolytes**. Weak acids and weak bases are weak electrolytes.

Week acids and week bases, like acetic acid (CH_3COOH) and ammonia (NH_3), are soluble in water, but partially dissociate into ions. For example, if 1-mole acetic acid or 1-mole of ammonia is dissolved in 1 liter of water at room temperature, they establish the following equilibrium between dissolved molecules and dissociated ions:

$$\mathrm{CH_3COOH(l) \xrightarrow{Water} CH_3COOH(aq) + H_2O(l) \rightleftharpoons CH_3COO^{1-}(aq) + H_3O^{1+}(aq),}$$
$$\mathrm{NH_3(\,g) \xrightarrow{Water} NH_3(aq) + H_2O(l) \rightleftharpoons NH_4{}^{1+}(aq) + OH^{1-}(aq),}$$

where only about 0.4% of the dissolved molecules dissociate into ions, the remaining about 99.6% of molecules remain neutral. Weak acids and weak bases are weak electrolytes.

Fig. 5.3.2 illustrates the difference between nonelectrolytes, strong electrolytes, and weak electrolytes.

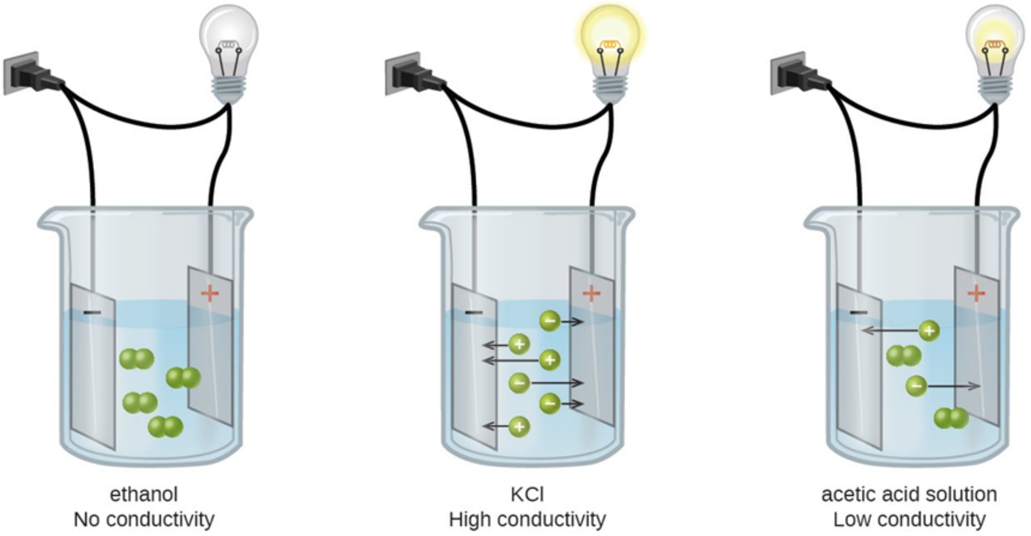


Figure 5.3.2: Illustration of a nonelectrolyte that does not conduct electricity, a strong electrolyte that has high electrical conductivity, and a weak electrolyte that has low electrical conductivity. Source: Karishma50/ (https;//creativecommons.org/licences/by-sa/4.0)

Equivalent

The amount of molecules and atoms is usually measured in moles. Ionic compounds are composed of ions but are overall neutral because the +ve charge is balanced by the –ve charge. Therefore, the mole ratio of cations to anions is not always one to one. For example, NaCl has a one-to-one mole ratio of Na^{+} and Cl^{-}, but $CaCl_2$ has a one-to-two ratio of Ca^{2+} and Cl^{-}. A new unit, called equivalent (officially abbreviated as Equiv but commonly abbreviated as Eq), is introduced, to differentiate between a mole of ion and a mole of charge on the ion.

> The *equivalent* is the amount of a substance needed to react with or supply one mole of hydrogen ions (H^+) in an acid-base reaction, or react with or supply one mole of electrons in a redox reaction. In other words, the number of equivalents of a given ion in a solution is equal to the number of moles of that ion multiplied by its valence.

$$1\text{ mol Na}^+ = 1\text{ Eq Na}^+\text{, but}\quad 1\text{ mol Ca}^{2+} = 2\text{ Eq Ca}^{2+}\text{, and }1\text{ mol Al}^{3+} = 3\text{ Ea Al}^{3+}$$

Similarly,

$$1\text{ mol Cl}^- = 1\text{ Eq Cl}^-\text{, but}\quad 1\text{ mol CO}_3{}^{2-} = 2\text{ Eq CO}_3{}^{2-}\text{ and }1\text{ mol PO}_4{}^{3-} = 3\text{ Ea PO}_4{}^{3-}$$

> The solutions of electrolytes are overall electrically neutral, i.e., the number of equivalents of cations is equal to the number of equivalents of anions in the solution.

For example, if 1 mole of NaCl is dissolved in water, there is 1 Eq of Na^+ ions and 1 Eq of Cl^- ions in the solution. If one mole of $CaCl_2$ is dissolved in the water there is 2 Eq of Ca^{2+} ions and 2 Eq of Cl^- ions in the solution. Similarly, if 1 mole of NaCl and 1 mole of $AlCl_3$ are dissolved in the water there is 1 Eq of Na^+ ions, 3 Eq of Al^{3+} ions, and 4 Eq of Cl^- ions to balance cations in the water.

Equality gives two conversion factors. For example, the equality 1 mol Ca^{2+} = 2 Eq Ca^{2+} gives the following two conversion factors:

$$\frac{1\ \text{mol}\ Ca^{2+}}{2\ Eq\ Ca^{2+}}$$

and

$$\frac{2\ Ea\ Ca^{2+}}{1\ mol\ Ca^{2+}}$$

The first conversion factor converts the given amount in equivalents to moles, and the second converts the given amount in moles to equivalents of the ion as explained in the following examples.

✓ Example 5.3.1

a) Calculate mEq of Fe^{3+} in 0.0200 mol of Fe^{3+}? b) if chloride ion is the only anion in the solution, how many mEq of Cl^- are present in the solution?

Solution

a) Given 0.0200 mol Fe^{3+}. Desired mEq Fe^{3+}.

The equality: 1 mol Fe^{3+} = 3 Eq Fe^{3+} gives the conversion factor $\frac{3\ Eq\ Fe^{3+}}{1\ mol\ Fe^{3+}}$ that converts the given amount in moles to Eq of Fe^{3+}. Another equality: 1 Eq Fe^{3+} = 1000 mEq Fe^{3+} gives the conversion factor $\frac{1000\ mEq\ Fe^{3+}}{1\ Eq\ Fe^{3+}}$, that converts the Eq of Fe^{3+} to mEq of Fe^{3+}.

Calculations:

$$0.0200\ \text{mol}\ \cancel{Fe^{3+}} \times \frac{3\ \ Eq\ \cancel{Fe^{3+}}}{1\ \ mol\ \cancel{Fe^{3+}}} \times \frac{1000\ mEq\ Fe^{3+}}{1\ \ Eq\ \cancel{Fe^{3+}}} = 60\ mEq\ Fe^{3+}$$

✓ Example 5.3.2

An intervenous saline solution contains 145 mEq/L of Na^+. How many moles of Na^+ are in 0.500 L of the solution?

Solution

a) Given: 145 mEq Na^+ /L solution and 0.500 L solution, Desired: ? mol Na^+

Conversion factors needed: The concentration in mEq/L is the first factor for L to mEq conversion, the equality 1 mEq Na^+ = 1 mmol Na^+ givens the second conversion needed for mEq to mmol conversion, and the equality 1000 mmol Na^+ = 1 mol Na^+

given the third conversion factor needed needed for mEq to mol conversion. The three conversion factors are applied one after the other in a single row in the following calculation:

$$0.500\ \text{L}\ \cancel{\text{solution}}\times\frac{145\ \cancel{\text{mEq Na}}}{1\ \cancel{\text{L solution}}}\times\frac{1\ \cancel{\text{mmol Na}^{+}}}{1\ \cancel{\text{mEq Na}^{+}}}\times\frac{1\ \text{mol Na}^{+}}{1000\ \cancel{\text{mmol Na}^{+}}}=0.0725\ \text{mol Na}^{+}$$

Note how the units of the numerator in one fraction are canceled by the units of the denumerator of the following fraction leaving only the desired units uncancelled that become the units of the answer number.

Electrolytes in body fluids

Fig. 5.3.3 shows the electrolytes and their concentrations commonly found in body fluids. They play an essential role in cell and body functions. For example, sodium ions regulate the water content and play a role in electrical impulse transmission in the nervous system. Potassium ions play a role in maintaining a regular heartbeat and also play a part in electrical impulse transmission. Chloride ions are there to balance the charge. Carbonate ions are involved in maintaining the pH of the blood.

Concentrations of electrolytes in body fluids are not high enough to be reported in a mole or equivalent units. The electrolytes in the body fluids are usually reported in millimoles (mmol) or milliequivalent (mEq) units, where: $1000\ \text{mmol} = 1\ \text{mol}$ and $1000\ \text{mEq} = 1\ \text{Eq}$.

The overall concentration of electrolytes in intravenous fluids given to patients is about the same as of electrolytes in the body fluids. For example, Ringer's lactate solution contains about: 130 mEq/L Na^{+}, 4 mEq/L K^{+}, 3 mEq/L Ca^{2+}, 109 mEq/L Cl^{-} , and 28 mEq/L lactate^{-}. Note that the overall +ve charge (130+4+3= 137 mEq/L) is equal to the overall –ve charge (109+28 = 137 mEq/L).

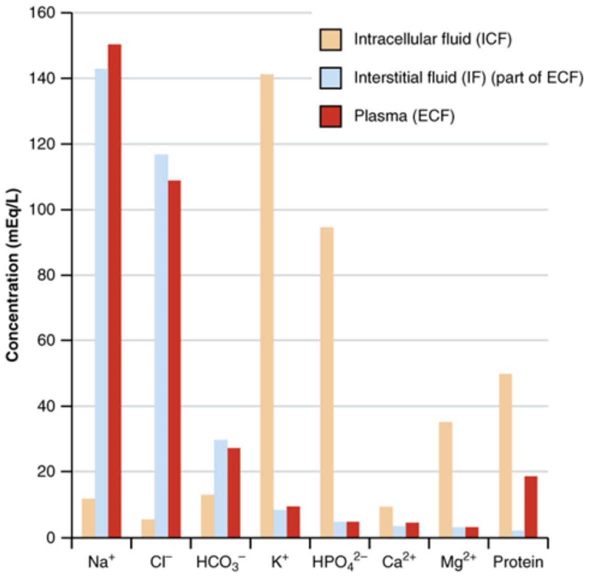


Figure 5.3.3: Concentrations of electrolytes in body fluids. Source: OpenStax College / CC BY (https://creativecommons.org/licenses/by/3.0)

5.4: Concentration of solutions

The concentration of a solution tells the amount of solute dissolved in a given amount of solution.

Making a solution of know concentration

A measured amount of solute is dissolved in enough solvent to make the desired volume of the solution, as illustrated in Fig. 5.4.1. The concentration of the solution can be expressed in different ways using mass, volume, or mole units, as explained in the following.

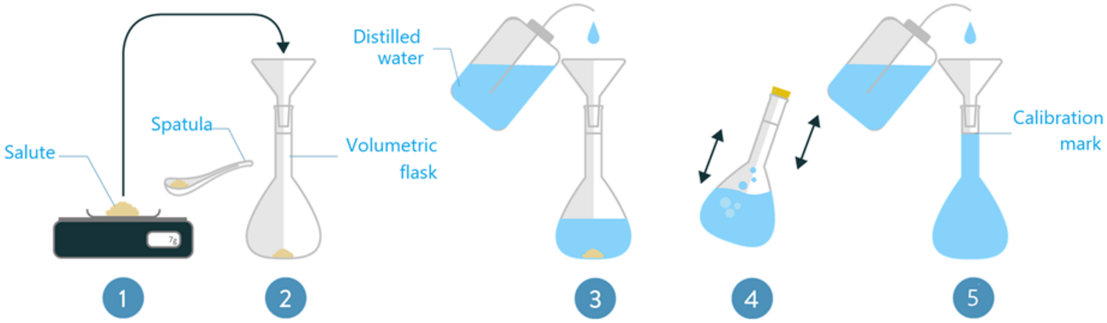


Figure 5.4.1: Making an aqueous solution: 1) measure the mass of the solute on an analytical balance, 2) pour the solute into a volumetric flask of know volume, 3) add distilled water (or solvent) to more than half fill the flask, 4) stopper the flask and shake it to dissolve the solute, 5) add more water to fill the flask to the calibration mark –measure from the lowest point of the water meniscus, 6) stopper the flask and shake again to make a homogeneous solution. Source: modified from https://www.hiclipart.com/free-trans...cvcrq/download

Concentration in percent (%)

What is percent (%)

Percentage (%) is a number or ratio that represent a fraction of 100.

For example, 5% means 5:100, where 5 is the part, and 100 is the total. The percentage is calculated as a hundred times of part by total, i.e.,

$$\text{Percentage }(\%) = \frac{\text{part}}{\text{Total}} \times 100.$$

Example 5.4.1

A 50.0 g NaCl is dissolved in water to make a 500 g solution. What is the percentage of NaCl in the solution?

Solution

Given part = 50.0 g NaCl, and total = 500 g solution. Desired: %NaCl in the solution?

Formula: $\text{Percentage }(\%) = \frac{\text{part}}{\text{Total}} \times 100.$

Calculations: $\text{Percentage }(\%) = \frac{50.0\mathit{cancel}\text{ g}}{500\mathit{cancel}\text{ g}} \times 100 = 10.0\ \%\text{NaCl}$

The units cancel in the fraction calculation part, and a % sign is added to the answer to tell that it is a fraction out of a hundred.

Mass percent (m/m)% concentration

The mass percent concentration expresses the mass units of solute in a hundred mass units of the solution.

$$\text{Mass}(\%) = \frac{\text{mass of solute }(g)}{\text{mass of solute }(g) + \text{mass of solvent }(g)} \times 100 = \frac{\text{mass of solute }(g)}{\text{mass of solution }(g)} \times 100$$

Note that the total is solute and solvent added together, i.e., solution.

Example 5.4.2

What is the mass % of NaOH in a solution prepared by dissolving 10.0 g NaOH in 100 g water?

Solution

Given solute = 10.0 g, and solvent = 100 g, Desired: Mass% NaOH?

Formula: $\text{Mass (\%)} = \frac{\text{mass of solute } (g)}{\text{mass of solute } (g) + \text{mass of solvent } (g)} \times 100$

Calculations: $\text{Mass (\%)} = \frac{10.0 \text{ gNaOH}}{(10.0 \text{ g} + 100 \text{ g}) \text{ solution}} \times 100 = 9.09\% \text{NaOH}$

Note that the mass% concentration and its reciprocal are two conversion factor: $\frac{\text{given } g \text{ solute}}{100 g \text{ solution}}$ and $\frac{100 g \text{ solution}}{\text{given g solute}}$

Example 5.4.3

Neosporin antibiotic is a 3.5% m/m neomycin solution. How many grams of neomycin are in 50 g of ointment?

Solution

Given: 3.5% neomycin $= \frac{3.5 \text{ g neomycin}}{100 \text{ g solution}}$, and Solution amount = 50 g, Desired: ? g neomycin

Calculations:

$$50 \text{ g } \cancel{\text{solution}} \times \frac{3.5 \text{ g neomycin}}{100 \text{ g } \cancel{\text{solution}}} = 1.8 \text{ g neomycin.}$$

Volume percent (v/v)% concentration

> The volume percent concentration expresses the volume units of solute in a hundred volume units of the solution.

The mathematical form of the v/v % is:

$$\text{Volume (\%)} = \frac{\text{volume of solute (mL)}}{\text{volume of solution (mL)}} \times 100$$

Fig. 5.4.2 shows the volume percent concentration ranges of different classes of fragrances.

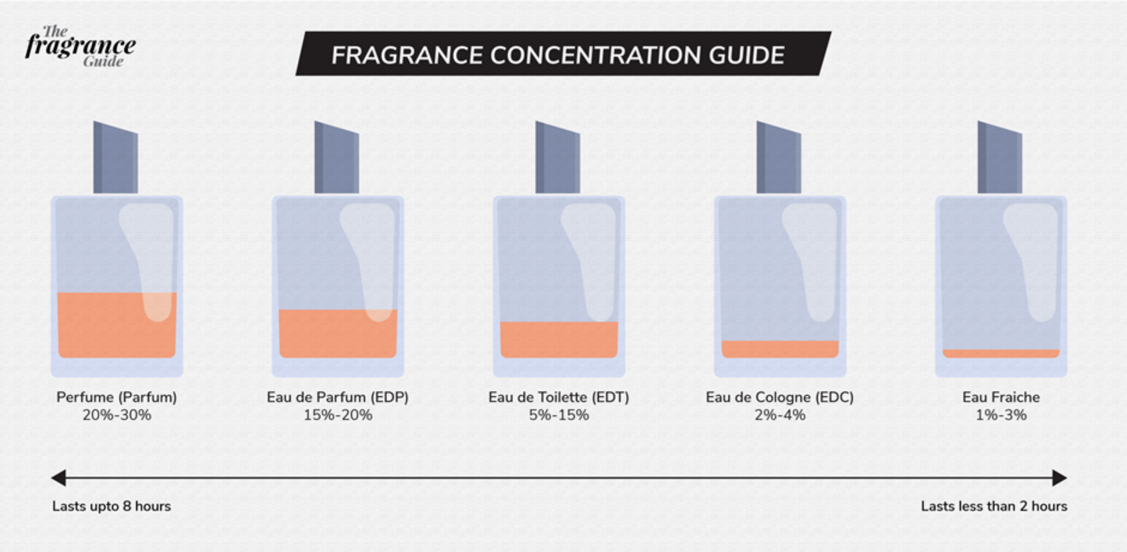


Figure 5.4.2: This info-graphic explains the differences between Parfums, Perfumes, Eau de Perfume, Eau de Parfum, Eau de Toilette, and Cologne. It also gives an approximate idea of how the concentration of Parfum oils vary as we move to lighter scents. Source: Nicole Smith / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

Example 5.4.4

What is the volume % of rose extract in a solution prepared by dissolving 14.0 mL rose extract in a solvent to make 200 mL of solution?

Solution

Given: Solute = 14.0 g, and solution = 200 g, Desired: Volume% rose solution?

Formula:

$$\text{Volume }(\%)=\frac{\text{volume of solute }(mL)}{\text{volume of solution }(mL)}\times 100$$

Calculations:

$$\text{Volume }(\%)=\frac{14\text{ mL rose extract}}{200\text{ mL solution}}\times 100=7.0\%\text{ rose solution}$$

The two conversion factors for v/v % concentration are:

$$\frac{\text{given mL solute}}{100\text{ mL solution}}\quad\text{, and}\quad\frac{100\text{ mL solution}}{\text{given mL solute}}$$

Example 5.4.5

What is the volume of bromine (Br_2) in 250 mL of 4.8% v/v of Br_2 solution in carbon tetrachloride?

Solution

Given: Concentration 4.8% v/v bromine = $\frac{4.8\,mL\text{ bromine}}{100\,mL\text{ solution}}$, volume of solution = 250 mL, Desired: Volume of solute, i.e., ? mL bromine.

Calculations:

$$250\text{ mL solution}\times\frac{4.8\text{ mL bromine}}{100\text{ mL solution.}}=12\text{ mL bromine.}$$

Mass/volume percent (m/v)% concentration

> The mass/volume percent concentration expresses the mass units of solute in a hundred volume units of solution.

Mathematical form of m/v % is:

$$\text{Mass/volume }(\%)=\frac{\text{mass of solute }(g)}{\text{volume of solution }(mL)}\times 100$$

Example 5.4.6

What is the mass/volume % of glucose solution prepared by dissolving 50 g glucose in enough water to make 1000 mL of solution?

Solution

Given: Solute = 50.0 g, and Solution = 1000 mL, Desired: Mass/volume % glucose solution?

Formula:

$$\text{Mass/volume }(\%)=\frac{\text{mass of solute }(g)}{\text{volume of solution }(mL)}\times 100$$

Calculations:

$$\frac{\text{Mass}}{\text{volume}}(\%)=\frac{50 \text{ g glucose}}{1000 \text{ mL solution}}\times 100=5.0\% \text{ glucose solution by } \frac{\text{m}}{\text{v}}.$$

The two conversion factors from ms/v % concentration are:

$$\frac{\text{given } g \text{ solute}}{100 \text{ mL solution}} \quad \text{and} \quad \frac{100 \text{ mL solution}}{\text{given g solute}}$$

✓ Example 5.4.7

How many grams of clindamycin antibiotics are in a 45 mL capsule of the 1.0% (m/v) clindamycin?

Solution

Given: % m/v concentration: 1.08 % m/v clindamycin $=\frac{1.0 \text{ g clindamycin}}{100 \text{ mL solution}}$, and volume of solution = 45 mL, Desired: ? g clindamycin?

Calculations:

$$45 \text{ mL solution } \times \frac{1.0 \text{ g clindamycin}}{100 \text{ mL solution}}=4.5 \text{ g clindamycin.}$$

Parts per million (ppm) and parts per billion (ppb) concentration

Parts per million (ppm) is a number or ratio expressed as a fraction of a million (10^6).

For example, 2 ppm means $\frac{2}{1{,}000{,}000}$ or 2:1,000,000, where 2 is the part, and 1,000,000 is the total. The concentration in ppm is calculated as a million times of part by total, i.e.:

$$\text{Concentration in ppm }=\frac{\textit{part}}{\text{Total}}\times 10^6$$

Parts per billion (ppb) is a number or ratio expressed as a fraction of billion (10^9).

That is:

$$\text{Concentration in ppb }=\frac{\text{part}}{\text{Total}}\times 10^9$$

Like percentage concentration, the ppm and ppb can be mass/mass (m/m), volume/volume (v/v) or mass/volume (m/v).

✓ Example 5.4.8

EPA’s action limit for copper is 1.3 mg/L in drinking water. What is this limit in ppm of copper m/v in the drinking water?

Solution

Given: 1.3 mg copper in 1L solution, Desired: ? ppm m/v of Copper in water

Formula: $\text{Concentration in ppm }=\frac{\text{solute(g)}}{\text{solution(mL)}}\times 10^6$

Calculations: First, convert the given units of mass and volume into the corresponding units that the formula takes, then plug the values in the formula and calculate.

$$\text{Solute }=1.3 \text{ mg}\times\frac{1 \text{ g}}{1000 \text{ mg}}=0.0013 \text{ g}$$

$$\text{Solution }=1 \text{ L}\times\frac{1000 \text{ mL}}{1 \text{ L}}=1000 \text{ mL}$$

$$\text{Concentration in ppm }=\frac{0.0013 \text{ g}}{1000 \text{ mL}}\times 10^6=1.3 \text{ ppm copper } v/\text{m}$$

✓ Example 5.4.9

EPA's action limit for lead is 0.015 mg/L in drinking water. What is this limit in ppb of lead m/v in the drinking water?

Solution

Given: 0.015 mg in 1L solution, Desired: ? ppb m/v of Lead in water

Formula: $\text{Concentration in ppb } = \frac{\text{solute}(g)}{\text{solution}(\text{mL})} \times 10^9$

Calculations: First, convert the given units of mass and volume into the corresponding units that the formula takes, then plug the values in the formula and calculate.

$$\text{Solute } = 0.015 \text{ mg} \times \frac{1 \text{ g}}{1000 \text{ mg}} = 0.000015 \text{ g}$$

$$\text{Solution } = 1 \text{ L} \times \frac{1000 \text{ mL}}{1 \text{ L}} = 1000 \text{ mL}$$

$$\text{Concentration in ppb } = \frac{0.000015 \text{ g}}{1000 \text{ mL}} \times 10^9 = 15 \text{ ppb lead v/m}$$

Molarity

Molarity (M) expresses the moles of solute in a liter of solution.

The most common solution concentration unit used in chemistry is molarity (M):

$$\text{Molarity } (M) = \frac{n \text{ (moles of solute)}}{V \text{ (Litters of solution)}}$$

✓ Example 5.4.10

What is the molarity (M) of a solution prepared by dissolving 50.0 g NaOH in enough water to make 250 mL solution?

Solution

Given: Solute = 50.0 g NaOH, Volume of solution = 250 mL, Desired: ? M NaOH solution?

Formula: $\text{Molarity } (M) = \frac{n \text{ (moles of solute)}}{V \text{ (Litters of solution)}}$

Calculations: First, convert the given units of mass and volume into the corresponding units that the formula takes, then plug the values in the formula and calculate.

$$\text{Solute } = 50.0 \text{ g NaOH} \times \frac{1 \text{ mol NaOH}}{40.00 \text{ g NaOH}} = 1.25 \text{ mol NaOH}$$

$$\text{Solution } = 250 \text{ mL} \times \frac{1 \text{ L}}{1000 \text{ mL}} = 0.250 \text{ L}$$

$$\text{Molarity } (M) = \frac{1.25 \text{ mol NaOH}}{0.250 \text{ L solution}} = 5.00 \text{ M NaOH}$$

The two conversion factor from molarity are the following:

$$\frac{n \text{ (moles of solute)}}{V \text{ (Litters of solution)}} \quad \text{and} \quad \frac{V \text{ (Litters of solution)}}{n \text{ (moles of solute)}}$$

✓ Example 5.4.11

How many litters of 0.211 M HCl solution are needed to provide 0.400 mol of HCl?

Solution

Given: amount of solute = 0.400 mol HCl, Concentration of solute = 0.211M = $\frac{0.211 \text{ mol HCl}}{1 L \text{ solution}}$

Calculations:

$$\text{Liters of solution needed } = 0.400 \text{ mol HCl} \times \frac{1 \text{ L soluton}}{0.211 \text{ mol HCl}} = 1.90 \text{ L solution}$$

Example 5.4.12

A 2.50 L of 1.12 M NaOH solution contains how many moles of NaOH?

Solution

Given: Volume of solution = 2.50 L solution, concentration of solution = $1.12 \text{ M NaOH} = \frac{1.12 \text{ mol NaOH}}{1 \text{ L solution}}$, Desired: ? moles of NaOH?

Calculations:

$$\text{Moles of NaOH in the solution } = 2.50 \text{ L solution } \times \frac{1.12 \text{ mol NaOH}}{1 \text{ L solution}} = 2.80 \text{ mol NaOH}$$

Dilution of solutions

Dilution of a solution is the addition of a solvent to decrease the solute concentration of the solute in the solution.

The product of concentration (C) and volume (V) is the amount of solute, i.e.,

$$\text{Amount of solute } = C \text{ in } \frac{\text{amount of solute}}{\text{volume of solution}} \times V \text{ in volume of solution.}$$

The amount of solute does not change by adding solvent. Therefore, the product of concentration and volume, i.e., CV, which is the amount of solute, is a constant, i.e.,

$$C_1 V_1 = C_2 V_2 = \text{ amount of solute}$$

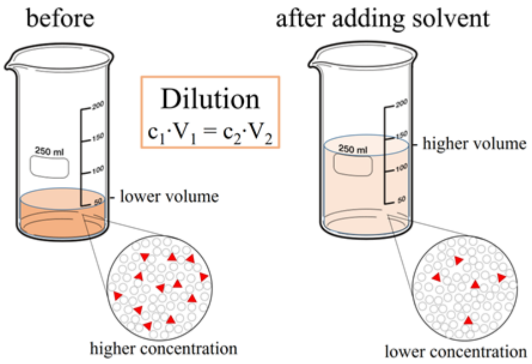


Figure 5.4.3: This image illustrates that when more solvent is mixed with the solution, the amount of solute remains the same, but its concentration decreases. Source: Theislikerice / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

Fig. 5.4.3 shows that if the initial concentration is C_1, the initial volume is V_1, and after dilution, the final concentration is C_2, the final volume is V_2, then $C_1V_1 = C_2V_2$ = amount of solute that is constant. If three of the four variables in this equation are known, the missing one can be calculated, as explained in the following example.

Caution

Keep in mind that the concentrations and volumes should be in the same units on both sides of the equation: $C_1V_1 = C_2V_2$. If they are not in the same units, convert them to the same units before plunging them in the formula.

✓ Example 5.4.13

how much volume of 11.3 M HCl is needed to prepare 250 mL of 2.00 M HCl?

Solution

Given: C_1 = 11.3 M HCl, C_2 = 2.00 M HCl, V_2 = 250 mL solution, Desired V_1 = ?

Formula: $C_1V_1 = C_2V_2$, rearrange it to isolate the desired parameter: $V_1 = \frac{C_2V_2}{C_1}$

Calculations:

$$V_1 = \frac{C_2V_2}{C_1} = \frac{2.00 \text{ M HCl} \times 250 \text{ mL solution}}{11.3 \text{ M HCl}} = 44.2 \text{ mL solution}$$

✓ Example 5.4.14

what is the molarity of the NaOH solution prepared by diluting 100 mL of 0.521 M NaOH solution to 500 mL?

Solution

Given C_1 = 0.521 M NaOH, V_1 = 100 mL solution, V_2 = 500 mL solution, Desired: Concentration of the final solution C_2 = ? M NaOH

Formula: $C_1V_1 = C_2V_2$, rearrange to isolate the desired parameter: $C_2 = \frac{C_1V_1}{V_2}$

Calculations:

$$C_2 = \frac{C_1V_1}{V_2} = \frac{0.521 \text{ M NaOH} \times 100 \text{ mL NaOH}}{500 \text{ mL NaOH}} = 0.104 \text{ M NaOH}$$

✓ Example 5.4.15

Dopamine is administered intravenously to a patient to increase blood pressure. How many milliliters (mL) of a 4.0% (m/v) dopamine solution is needed to prepare 250 mL of a 0.030% m/v) solution?

Solution

Given: C_1 = 4.0% (m/v), C_2 = 0.030% (m/v), V_2 = 250 mL solution, Desired V_1= ?

Formula: $C_1V_1 = C_2V_2$, rearrange to isolate the desired parameter: $V_1 = \frac{C_2V_2}{C_1}$

Calculations:

$$V_1 = \frac{C_2V_2}{C_1} = \frac{0.030\% \times 250 \text{ mL solution}}{4.0\%} = 5.0 \text{ mL of solution}$$

Logarithmic dilution

> Take a unit volume of a given solution and add enough solvent to increase the volume of the solution 10 times for a logarithmic diluiton.

A logarithmic dilution is ten times dilution, i.e., proven by the following formula:

$$C_2 = \frac{C_1V_1}{V_2} = \frac{1 \text{ mL} \times C_1}{10 \text{ mL}} = 0.1 \times C_1$$

Repeating the above step with the diluted solution results in 10x10 = 100-time dilution, and repeating third-time results in 10x10x10 = 1000-time dilution. This dilution of 10 times in each step is called logarithmic dilution. Fig. 5.4.4 shows that five steps of logarithmic dilution on a 10% initial solution results in a concentration of 10 ppm in the final solution.

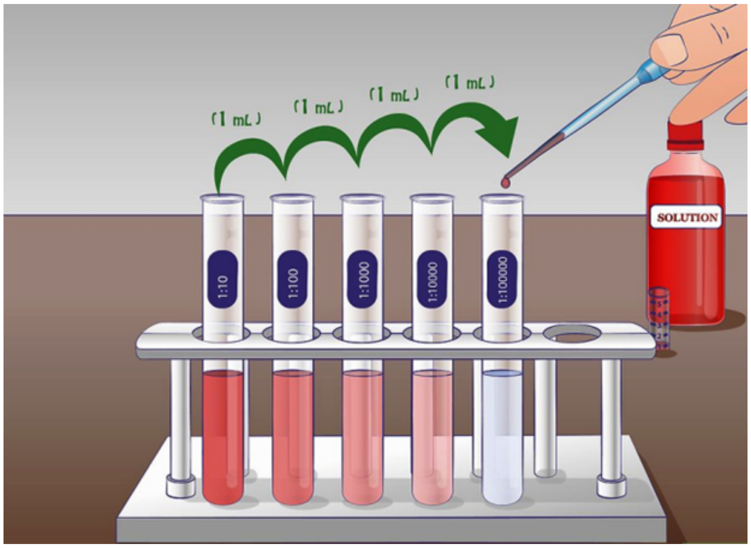


Figure 5.4.4: Logarithmic dilution: five steps of logarithmic dilution on a 10% initial solution results in a concentration of 10 ppm of the final solution. Source: Grasso Luigi / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

5.5: Osmosis

Semipermeable membranes surround living cells and organelles in the cells. The semipermeable membranes allow water and small molecules but do not allow the passage of large molecules and ions.

> Osmosis is the passage of water and small molecules across a semipermeable membrane with a net flow from a less concentrated solution to a more concentrated solution.

Osmosis helps in the absorption, retention, and flow of water, nutrients, and other molecules required in the biological systems. Fig. 5.5.1 illustrates the process of osmosis.

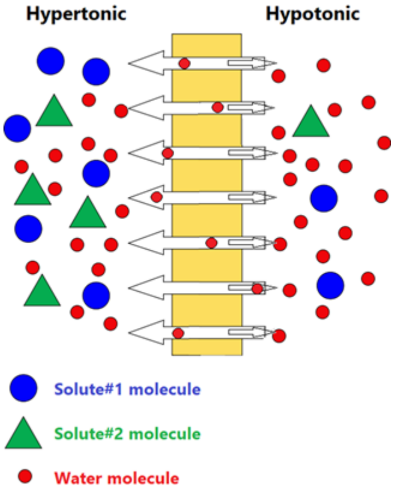


Figure 5.5.1: Illustration of osmosis. Osmosis is the passage of water and small molecules through a semipermeable membrane with a net flow from low solute concentration to high solute concentration. The larger molecules and ions cannot pass the semipermeable membrane.

Osmotic pressure

Osmosis causes net water flow from the less concentrated to the more concentrated solution across the semipermeable membrane. Consequently, the water level rises in the less concentrated solution compartment, as illustrated in Fig. 5.5.2. The difference in the height of water increases and applies pressure, pumping water back to the more concentrated side until the flow of water is equal on the two sides.

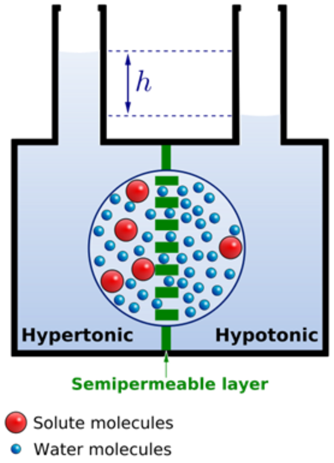


Figure 5.5.2: Osmotic pressure is the pressure, due to the difference in the height of water in this example, that prevents the excess flow of water from less concentrated to more concentrated solution side across the semipermeable membrane that separates the two solutions. Source: WYassineMrabetTalk✉ This W3C-unspecified vector image was created with Inkscape. / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

The pressure that prevents additional water flow to the more concentrated solution side of the semipermeable membrane is called osmotic pressure.

The osmotic pressure is proportional to the overall concentration of the solute particles. For example, 0.1 molar NaCl has osmotic pressure about twice that of 0.1 molar glucose because each mole of glucose adds one mole of solute particles, while each mole of NaCl produces two moles of particles, i.e., one-mole Na^+ and one-mole Cl^- ions in the solution.

Reverse Osmosis

Reverse osmosis is the net flow of water to the less concentrated or pure water across the semipermeable membrane by applying external pressure more than the osmotic pressure on the more concentrated solution side.

Reverse osmosis is the net flow of water to the less concentrated or pure water across the semipermeable membrane by applying external pressure more than the osmotic pressure. Note that solvent flow in reverse osmosis driven by external pressure is the opposite of regular osmosis. Reverse osmosis is used to produce drinking water from seawater sources, as illustrated in Fig. 5.5.3.

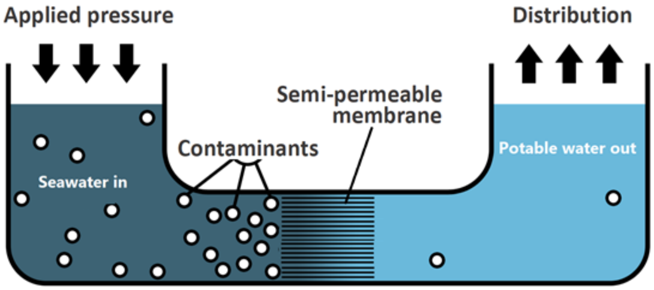


Figure 5.5.3: Illustration of reverse osmosis –used to produce drinking water from a seawater source. Source: Colby Fisher / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Isotonic, hypertonic, and hypotonic solutions

Cell membranes are semipermeable membranes that separate intracellular and extracellular fluids. The concentration difference across the membrane and the resulting osmotic pressure plays an essential role in cell functions. Intravenous solutions injected into patients must have the same osmotic pressure as the body fluids.

Solutions with the same solute particle concentration and osmotic pressure are called **isotonic**. If the two solutions across a semipermeable membrane do not have the same solute particle concentration, the solution with higher solute particle concentration and higher osmotic pressure is **hypertonic**, and the other has lower solute particle concentration and lower osmotic pressure is **hypotonic**.

Remember that hyper- means more and hypo-means less, concerning solute particle concentration in the case of osmosis.

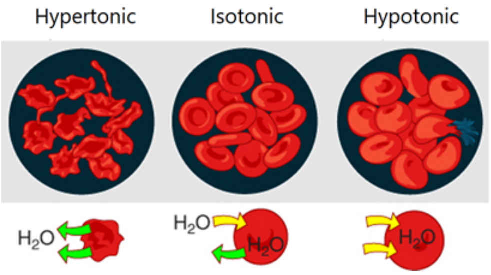


Figure 5.5.4: A hypertonic solution has a solute concentration higher than another solution. An isotonic solution has a solute concentration equal to another solution. A hypotonic solution has a solute concentration lower than another solution. Source: OpenStax / CC BY (https://creativecommons.org/licenses/by/3.0)

Cells placed in an external solution may retain their size, shrink, or swell depending on the relative osmotic pressure of fluid inside and outside of the cell, as illustrated in Fig. 5.5.4. For example, red blood cells placed in an isotonic solution retain their size because the flow of water into and out of the cell is the same.

- Typical isotonic solutions are 0.9% m/v NaCl solution in water or 5% m/v glucose solution in water.
- Red blood cells placed in a hypertonic solution shrink in size due to more flow of water out than into the cell –a process called **crenation**.
- Red blood cells placed in a hypotonic solution swell and burst due to more water flow into than out of the cells –a process called **hemolysis**.

A similar situation happens in plant cells that are placed in different environments concerning osmotic pressure, as illustrated In Fig. 5.5.5.

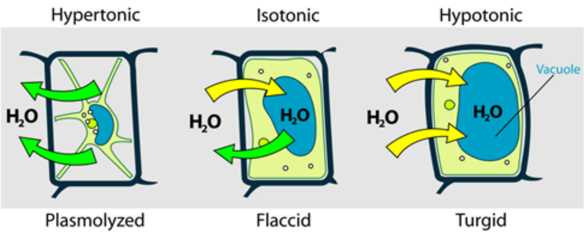


Figure 5.5.5: Plant cells under different environments concerning osmotic pressure. source: LadyofHats / Public domain

Dialysis

> Dialysis separates colloids from water, dissolved ions, and molecules of small dimention

Dialysis is similar to osmosis with the difference that in dialysis water, small molecules and ions can pass through a dialyzing membrane leaving behind collide particles like proteins and starch molecules, as illustrated in Fig. 5.5.6.

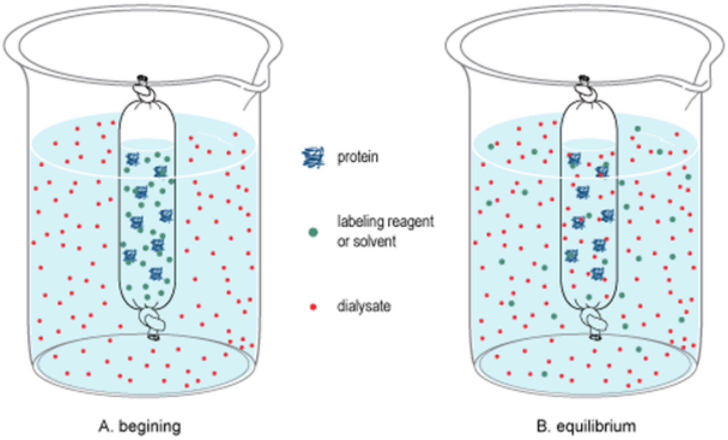


Figure 5.5.6: Dialysis separates colloidal particles like protein and starch from water, small molecules, and ions. Source: Potcherboy at English Wikipedia / CC BY (https://creativecommons.org/licenses/by/3.0)

Role of dialysis in the human body

Kidneys filter the blood by dialysis process. There are over a million tubular structures, called nephrons, in the kidney surrounded by dialyzing membranes. The nephrons filter the water, small molecules like glucose, amino acids, urea, and ions from the blood. Useful products and most of the water reabsorb later on, but urea and other waste products excrete through urine, as illustrated in Fig. 5.5.7.

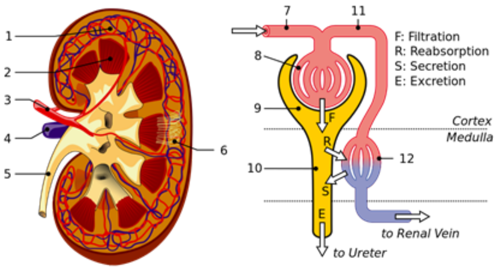


Figure 5.5.7: Schematics of dialysis for blood cleaning through kidney and nephron. 1: Renal cortex. 2: Medulla. 3: Renal artery. 4: Renal vein. 5: Ureter. 6: Nephrons. 7: Afferent arteriole. 8: Glomerulus. 9: Bowman's capsule. 10: Tubuli and loop of Henle. 11: Efferent arteriole. 12: Peritubular capillaries. Source: File:Physiology_of_Nephron.svg: Madhero88File:KidneyStructures_PioM.svg: Piotr Michał Jaworski; PioM EN DE PLderivative work: Daniel Sachse (Antares42) / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Hemodialysis

Hemodialysis is used to extract urea and other waste products from the blood when a person's kidney fails to remove them, as illustrated in Fig. 5.5.8. A hemodialysis system is a kind of artificial kidney in which the blood flows through long cellophane tubes placed in an isotonic solution containing NaCl, KCl, $NaHCO_3$, and glucose. Cellophane is a dialyzing membrane that does not let proteins, other large molecules, and blood pass through it, but urea excretes.

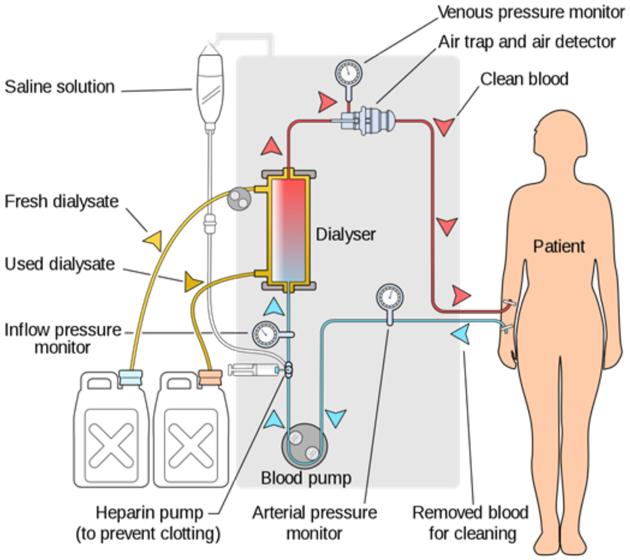


Figure 5.5.8: Simplified hemodialysis circuit. Source: GYassineMrabetTalk✉ This W3C-unspecified vector image was created with Inkscape. / CC BY (https://creativecommons.org/licenses/by/3.0)

CHAPTER OVERVIEW

6: Acids and bases

6.1: What is an Acid and a Base?

General Properties of Acids and Bases

We commonly encounter acids and bases in our foods –some foods are acidic, and others are basic (alkaline) as illustrated in Fig. 6.1.1.

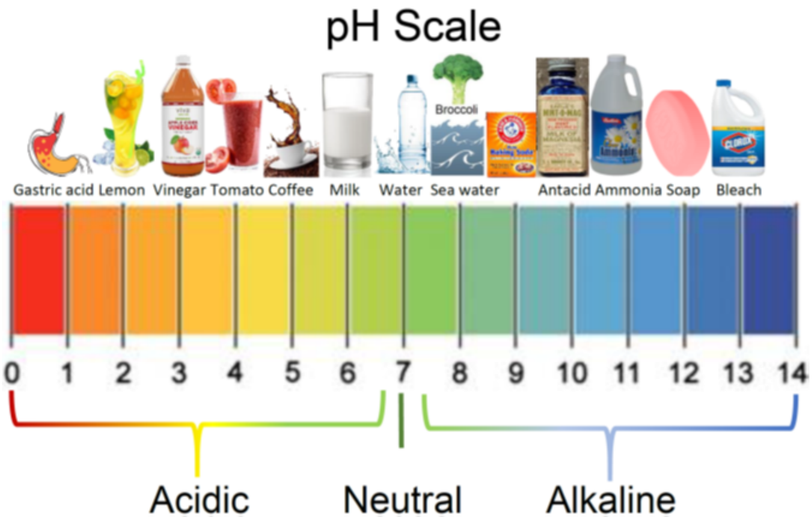


Figure 6.1.1: Acidic and alkaline foods along with a pH scale, Copyright; Public domain

The general properties of acids and bases are the following.

1. Acids taste sour, e.g., citrus fruits taste source because of citrus acid and ascorbic acid, i.e., vitamin C, in them. Basic (alkaline) substances, on the other hand, taste bitter.
2. Basic (alkaline) substances feel soupy, while acidic substances may sting.
3. The acids turn blue litmus paper to read but do not change the color of red litmus paper. Bases turn red litmus paper blue but do not change the color of blue litmus paper, as illustrated in Fig. 6.1.2.
4. Phenolphthalein indicator turns colorless in acid and turns pink in basic solution, as illustrated in Fig. 6.1.3.
5. Acids and bases neutralize each other. Hydrochloric acid is found in the stomach that helps digestion. Excess hydrochloric acid may cause acid burns—antacids like milk of magnesia are bases that help by neutralizing excess acid in the stomach.

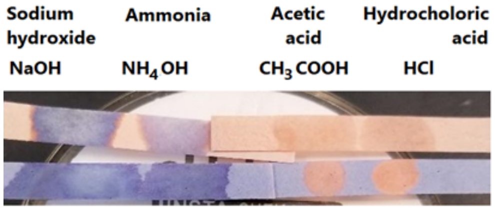


Figure 6.1.2: Demonstration of acids turn red litmus paper blue and bases turn blue litmus paper red - solution listed at the top of the image was spotted on the red litmus paper (top) or blue litmus paper (bottom).

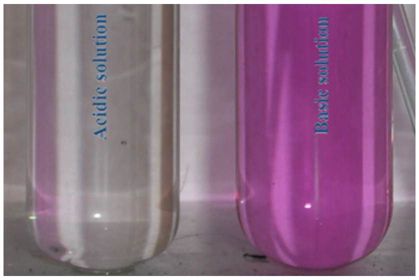


Figure 6.1.3: Colours of phenolphthalein in acid(left) and base (right) solutions. Source: User:Siegert / Public domain.

Arrhenius's Definition of Acids and Bases

The earliest definition of acids and bases is Arrhenius's definition which states that:

- An acid is a substance that forms hydrogen ions H^+ when dissolved in water, and
- A base is a substance that forms hydroxide ions OH^- when dissolved in water.

For example, hydrochloric acid (HCl) is an acid because it forms H^+ when it dissolves in water.

$$HCl(g) \xrightarrow{Water} H^+(aq) + Cl^-(aq)$$

Similarly, NaOH is a base because it forms OH^- when it dissolves in water.

$$NaOH(s) \xrightarrow{Water} Na^+(aq) + OH^-(aq)$$

Note that hydrogen ion H^+ does not exist in reality. It bonds with water molecules and exists as hydronium ion H_3O^+(aq).

$$H^+(aq) + H_2O \rightarrow H_3O^+(aq)$$

However, $H^+(aq)$ is often written in the place of (H_3O^+(aq).

Naming Arrhenius acids and bases

Table 1 lists the names and formulas of some of the common acids and their anions.

Rules for naming acids

1. The names end with the word "acid."
2. If the anion is not an oxyanion, then add the prefix hydro- to the name of the anion and change the last syllable of the anion name to –ic. For example, Cl^- is a chloride ion, and HCl is hydrochloric acid.
3. If the anion is an oxyanion with the last syllable –ate, change the last syllable with –ic. Do not use the prefix hydro-, but add the last word "acid." If there is a prefix per- in the name of the oxyanion, retain the prefix in the acid name. For example, NO_3^- is a nitrate, and HNO_3 is nitric acid. Another example, ClO_4^- is a perchlorate, and $HClO_3$ is perchloric acid.
4. If the anion is an oxyanion with the last syllable –ite, change the last syllable with –ous. Do not use the prefix hydro-, but add the last word "acid." If there is a prefix hypo- in the name of the oxyanion, retain the prefix in the acid name. For example, NO_2^- is nitrite, and HNO_2 is nitrous acid. Another example, ClO^- is hypochlorite, and HClO is hypochlorous acid.

Table 1: Names of some common acids and their anions.

Acid formula	Acid name	Anion	Anion name
HCl	Hydrochloric acid	Cl^-	Chloride
HBr	Hydrobromic acid	Br^-	Bromide
HI	Hydroiodic acid	I^-	Iodide
HCN	Hydrocyanic acid	CN^-	Cyanide
HNO_3	Nitric acid	NO_3^-	Nitrate
HNO_2	Nitrous acid	NO_2^-	Nitrite
H_2SO_4	Sulfuric acid	SO_4^{2-}	Sulfate
H_2SO_3	Sulfurous acid	SO_3^{2-}	Sulfite
H_2CO_3	Carbonic acid	CO_3^-	Carbonate
CH_3COOH	Acetic acid	CH_3COO^-	Acetate

Acid formula	Acid name	Anion	Anion name
H_3PO_4	Phosphoric acid	PO_4^{3-}	Phosphate
H_3PO_3	Phosphorous acid	PO_3^{3-}	Phosphite
$HClO_4$	Perchloric acid	ClO_4^-	Perchlorate
$HClO_3$	Chloric acid	ClO_3^-	Chlorate
$HClO_2$	Chlorous acid	ClO_2^-	Chlorite
$HClO$	Hypoclorous acid	ClO^-	Hypochlorite

Table 2 lists the names and formulas of some of the common Arrhenius bases.

Naming Arrhenius Bases

The Arrhenius bases are ionic compounds of metal and hydroxide ion, and their name starts with the name of the metal element followed by the name of the anion, i.e., hydroxide. For example, NaOH is sodium hydroxide.

Table 2: Names of some of the common Arrhenius bases

Formula	Name
$LiOH$	Lithium hydroxide
$NaOH$	Sodium hydroxide
KOH	Potassium hydroxide
$Ca(OH)_2$	Calcium hydroxide
$Sr(OH)_2$	Strontium hydroxide
$Ba(OH)_2$	Barium hydroxide

6.2: Brønsted–Lowry acids and bases

Some bases do not have hydroxide ions in their formula, yet they act as bases and neutralize acids. For example, ammonia (NH_3) and calcium carbonate ($CaCO_3$) do not contain hydroxide ions, but they neutralize acids. Further, Arrhenius's definition limits the acid-base reactions in the water medium. The acid-base reactions can take place in other mediums also, e.g., HCl –an acid, and NH_3 –a base can react with and neutralize each other in the gas phase also. The Brønsted–Lowry bordered the definition of acids and bases by including the bases mentioned above and also by including acid-base reactions in a non-aqueous medium.

Brønsted–Lowry's definition of acids and bases

Brønsted–Lowry's definition states that:

1. An acid is a proton donor, and
2. A base is a proton acceptor.

or example, HCl is an acid because it donates a proton to the water solvent.

$$\mathrm{HCl(g) + H_2O(l) \rightarrow Cl^{-}(aq) + H_3O^{+}(aq)}$$

Water is a base in the above reaction because it accepts a proton from the acid. In a reaction between HCl and NH_3:

$$\mathrm{HCl(g) + NH_3(\,g) \rightarrow NH_4Cl(s)}$$

HCl is an acid because it donates its proton to NH_3, and the NH_3 is a base because it accepts a proton, as shown in Fig. 6.2.1.

Figure 6.2.1: Proton transfer from HCl to NH_3 is an example of an acid-base reaction. Hydrochloric acid evaporates from liquid HCl in a beaker reacting with ammonia fumes coming from the test tube to produce ammonium chloride (white smoke). Source: Walkerma, Public domain.

Brønsted–Lowry's acids have ionizable protons that they donate to bases. Therefore, Brønsted–Lowry's acid is generally written as HA, where H^+ is the donatable proton, and A^- is the anion of the acid. Examples of acids are HCl, H_2SO_4, HNO_3, and CH_3COOH. Note that acetic acid has only one acidic proton that is attached to the O atom in the carboxylic acid group (–COOH). The rest of the protons attached to carbon atoms are not acidic. All organic acids have a carboxylic acid group (–COOH). Brønsted–Lowry's acid may have net +ve charge, no charge, or net –ve charge on it. For example, H_3O^+, HCl, and HSO_4^- are all acids because they can donate a proton to a base.

Mono-, di- and tri-protic acids

Acids that have only one acidic proton are mono-protic, e.g., **H**Cl, **H**NO_3, CH_3COO**H**, are mono-protic acids where the acid proton is shown in bold font. Some acids have two acidic protons –they are di-protic, e.g., $\mathbf{H_2}SO_4$ and $\mathbf{H_2}CO_3$ are di-protic. The acids with three acidic protons are tri-protic, e.g., $\mathbf{H_3}PO_3$ is a tri-protic acid. For example, phosphoric acid (H_3PO_4) can dissociate and donate three protons, as shown in chemical reactions below:

$$\mathrm{H_3PO_4 + H_2O \rightleftharpoons H_3O^{+} + H_2PO_4{}^{-}}$$
$$\mathrm{H_2PO_4{}^{-} + H_2O \rightleftharpoons H_3O^{+} + HPO_4{}^{2-}}$$
$$\mathrm{HPO_4{}^{2-} + H_2O \rightleftharpoons H_3O^{+} + PO_4{}^{3-}}$$

The base accepts proton by making a bond with it. The bond is a pair of bonded electrons. Since the proton is a hydrogen atom without an electron, both electrons in the bond come from the base. The base must have a lone pair of electrons on it. The base is usually represented as $:B$ to emphasize a lone pair of electrons on it that is shown as a pair of dots. For example, ammonia, water, and hydroxide ion ($:NH_3$, $H_2\ddot{O}:$, and $:\ddot{\underset{..}{O}}H^-$) are Brønsted–Lowry's bases, because each of these has an atom with lone pair or lone pairs of electrons on them.

Conjugate acid-base pairs

The acid-base reactions described above are one-way reactions, i.e., reactants go-to products almost 100%. However, the majority of the acid-base reactions are two ways, i.e., reactants form the products and the products react with each other and re-form the reactants. Double arrows between reactants and products represent the two ways reactions. For example, hydrofluoric acid (HF) is a weak electrolyte; it partially dissociates in water to form F^- and H_3O^+, and the products react to re-form the reactants, as shown in Fig. 6.2.2. In the reverse reaction, H_3O^+ is acting as an acid, and F^- is acting as a base. The acid and the base in the products are called conjugate acid and conjugate base, respectively. The acid HF becomes conjugate base F^- after removal of a proton, and the base H_2O becomes conjugate acid H_3O^+ after accepting a proton.

The conjugate acid-base pair

The conjugate acid-base pair is related to the loss and gain of H^+. For example, HF/F^- is a conjugate acid-base pair, and H_3O^+/H_2O is also a conjugate acid-base pair.

In other words, remove the acidic proton from an acid to get its conjugate base and add a proton to a base to get its conjugate acid.

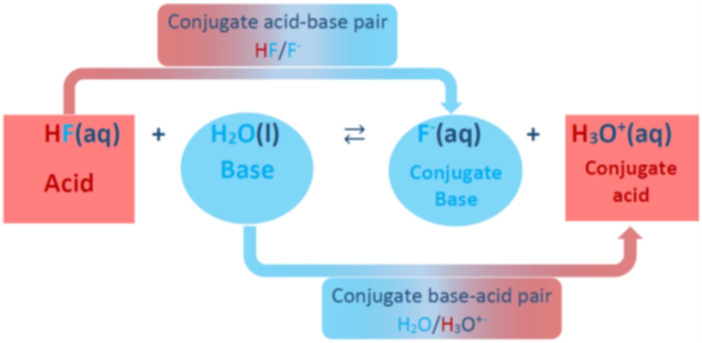


Figure 6.2.2: HF –an acid that loses a proton to form its conjugate base F^-, and water -acts as a base by accepting a proton to form its conjugate acid H_3O^+.

Another example is ammonia NH_3 which dissolves in water and accepts a proton to form its conjugate acid NH_4^+, as shown in Fig. 6.2.3. Water H_2O acts as an acid by donating a proton and forming its conjugate base OH^-. The two conjugate acid-base pairs in this reaction are NH_4^+ /NH_3 and H_2O/OH^- that are related by loss and gain or an H^+.

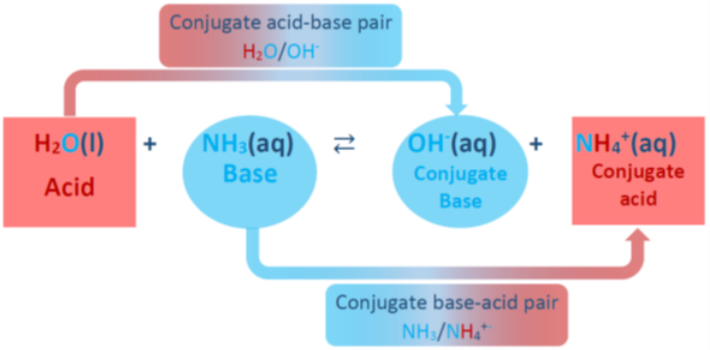


Figure 6.2.3: H_2O –acts as an acid that loses a proton to form its conjugate base OH^-, and NH_3 –a base accepts a proton to form its conjugate acid NH_4^+.

✓ Example 6.2.1

Identify the conjugate acid-base pairs in the following reaction?

$$H_3PO_4(aq) + NH_3(aq) \rightleftarrows H_2PO_4^- + NH_4^+$$

Solution

1. Identify the substance that has donated a proton in the reactants –it is an acid.
2. Remove a proton from the acid to form its conjugate base: $H_3PO_4/H_2PO_4^-$.
3. Identify the substance that has accepted a proton in the reactants –it is a base.
4. Add a proton to the base to form its conjugate acid: NH_3/NH_4^+.

Note

Note that loss of a proton from an acid forms its conjugated base with the charge decreased by one, e.g., $H_3PO_4/H_2PO_4^-$, HSO_4^-/SO_4^{2-}, and NH_4^+/NH_3. Similarly, the gain of a proton by a base forms its conjugate acid with the charge increased by one, e.g., $HPO_4^{2-}/H_2PO_4^-$, HCO_3^-/H_2CO_3, and NH_3/NH_4^+.

Amphoteric substances

Water acts as a base in some reactions, e.g., with HF, and as an acid in some reactions, e.g., with NH_3.

Substances like water that can act as an acid and also as a base are called amphoteric substances.

Other examples of amphoteric substances include HSO_4^-, HCO_3^-, and NH_3, as illustrated in Fig. 6.2.4.

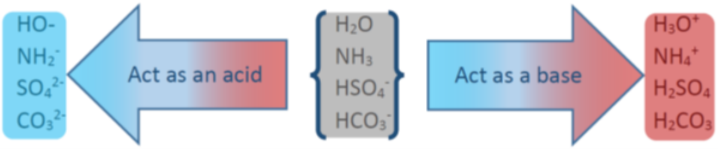


Figure 6.2.4: Examples of amphoteric substances that can act as an acid in some reactions and also as a base in other reactions.

6.3: Strength of acids and bases

The strength of acid HA is the extent to which the acid dissociates into H^+ and A^- ions, as illustrated in Fig. 6.3.1.

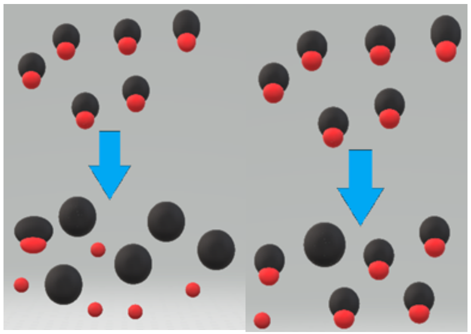


Figure 6.3.1: Image of strong acid mostly dissociating (left) and a weak acid partially dissociating into ions in water (right). Source: Cwszot / CC0

Strong acids

> Strong acids, like HCl, almost 100% dissociate into ions when they dissolve in water.

$$\mathrm{HCl(g) + H_2O(l) \rightarrow H_3O^+(aq) + Cl^-(aq)}$$

> One arrow is used to indicate that the reaction is nearly 100% complete.
>
> Strong acids include $HClO_4$, H_2SO_4, HI, HBr, HCl, and HNO_3

Weak acids

> Weak acids dissolve in water but partially dissociate into ions.

For example, acetic acid (CH_3COOH) is a weak acid, 1 M acetic acid dissolves in water, but only 0.4% of the dissolved molecules dissociate into ions, the remaining 99.6% remain undissociated, as illustrated in Fig. 6.3.2. and equation of the dissociation equilibrium below.

$$\mathrm{CH_3COOH(aq) + H_2O(I) \overset{\rightharpoonup}{\longleftarrow} H_3O^+(aq) + CH_3COO^-(aq)}$$

> Two arrows pointing in opposite directions are used for the dissociation of weak acids to indicate that the reaction is an equilibrium, i.e., two ways.

Often the arrows are not equal in size -the longer arrow points to acid-base pair that is weaker and present in a larger concentration at equilibrium than their conjugate pair.

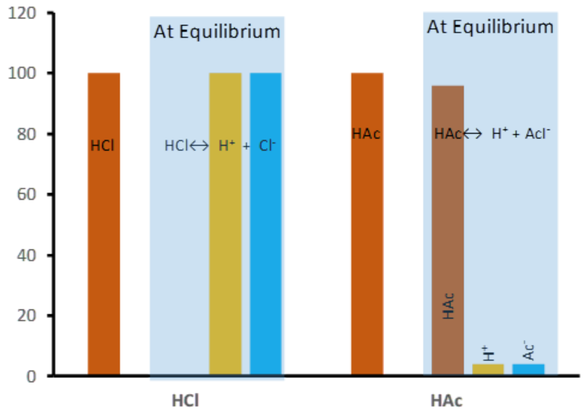


Figure 6.3.2: After dissolution in water. HCl –the strong acid is 100% dissociated into H^+ and Cl^- ions leaving no dissolved HCl molecules in water, but acetic acid (HAc) –the weak acid has a high concentration of HAc molecules and low concentration of H^+ and Ac^- ions.

Strong bases

Strong bases almost %100 dissociate into ions when dissolved in water. For example, NaOH is a strong base, and it dissociates almost 100% into ions in water.

Strong bases almost %100 dissociate into ions when dissolved in water. For example, NaOH is a strong base, and it dissociates almost 100% into ions in water.

$$NaOH(s) \xrightarrow{Water} Na^+(aq) + OH^-(aq)$$

One arrow is used for the dissolution of strong bases to indicate that the reaction is almost complete.

Strong bases include hydroxides of alkali metals, i.e., LiOH, NaOH, KOH, RbOH, CsOH, and hydroxides of heavy alkaline earth metals, i.e., $Ca(OH)_2$, $Sr(OH)_2$, and $Ba(OH)_2$.

The last three, i.e., the hydroxides of heavy alkaline earth metals, have low solubility in water, but the dissolved fraction exists as ions.

Weak bases

Weak bases partially dissociate into ions when dissolved in water.

For example, ammonia is a weak base –only 0.42% of the dissolved ammonia molecules dissociate into ammonium ions and hydroxide ions in water from a 1 M solution of ammonia.

$$NH_3(aq) + H_2O(I) \overset{\rightharpoonup}{\longleftarrow} NH_4{}^+(aq) + OH^-(aq)$$

Weak bases in household use include ammonia (NH_3) in window cleaners, NaClO in bleach, Na_2CO_3 and Na_3PO_4 in laundry detergent, $NaHCO_3$ in tooth past, Na_2CO_3 in baking powder, $CaCO_3$ for use in lawns, $Mg(OH)_2$ and $Al(OH)_3$ in antacids and laxatives.

The weak bases mentioned above are all ionic compounds except ammonia. Ionic compounds are strong electrolytes, i.e., they dissociate into ions almost 100% upon dissolution in water. It appears to contradict the fact that these ionic compounds are weak bases. It does not actually contradict, because the base properties do not refer to these ionic compounds, the base properties refer to the reactions of their polyatomic anions, i.e., ClO^-, $CO_3{}^{2-}$, and $PO_4{}^{3-}$ with water, as shown in the reactions below:

$$\begin{aligned} &ClO^- + H_2O \overset{\rightharpoonup}{\longleftarrow} HClO + OH^- \\ &CO_3^{2-} + 2H_2O \overset{\rightharpoonup}{\longleftarrow} H_2CO_3 + 2OH^-, \text{ and} \\ &PO_4{}^{3-} + 3H_2O \overset{\rightharpoonup}{\longleftarrow} H_3PO_4 + 3OH^- \end{aligned}$$

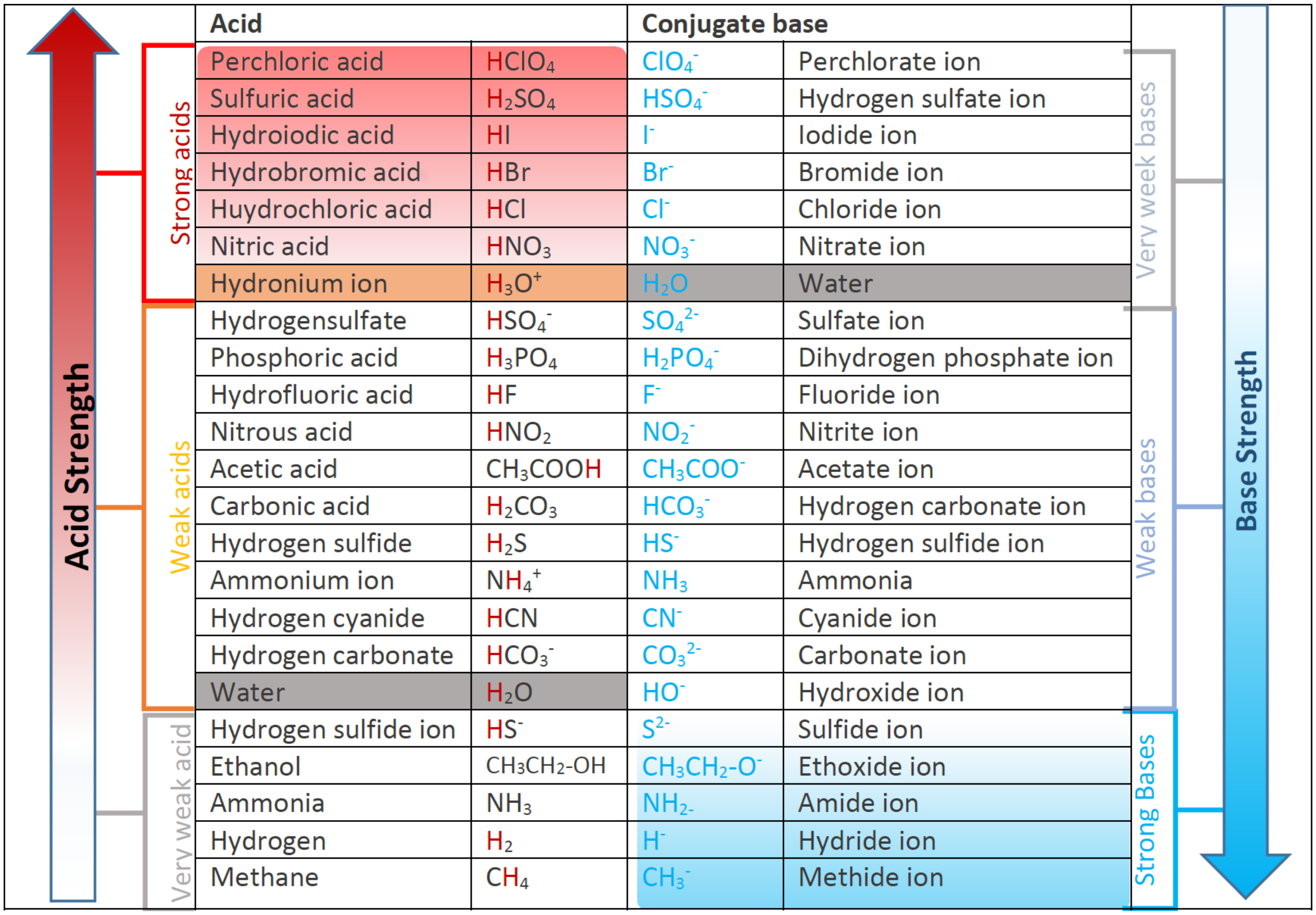
The above reactions are equilibrium reactions that are more favored in the revers than the forward direction, producing a small number of OH^- ions compared to the anion on the reactant sides. The last two examples, i.e., $Mg(OH)_2$ and $Al(OH)_2$ are classified as weak bases because they are considered insoluble in water. The solubility of $Mg(OH)_2$ is 0.00064 g/100 mL (25 °C), and the solubility of $Al(OH)_3$ is 0.0001 g/100 mL, which are in the range of insoluble ionic compounds.

> The solubility and the strength of acids and bases are two different things. A strong base may be less soluble, and a weak base may be more soluble or vice versa, but a dissolved strong base exists as ions only, and a dissolved weak base exists both as molecules and ions.

The relative strength of acid-conjugate base pair

> A general rule is that the stronger the acid, the weaker the conjugate base, and vice versa.

The conjugate bases of strong acids have negligible base strength, and the conjugate acids of strong basses have negligible acid strength. Fig. 6.3.3. illustrates the relative strengths of some acids and their conjugated bases.



Acid		Conjugate base	
Perchloric acid	$HClO_4$	ClO_4^-	Perchlorate ion
Sulfuric acid	H_2SO_4	HSO_4^-	Hydrogen sulfate ion
Hydroiodic acid	HI	I^-	Iodide ion
Hydrobromic acid	HBr	Br^-	Bromide ion
Huydrochloric acid	HCl	Cl^-	Chloride ion
Nitric acid	HNO_3	NO_3^-	Nitrate ion
Hydronium ion	H_3O^+	H_2O	Water
Hydrogensulfate	HSO_4^-	SO_4^{2-}	Sulfate ion
Phosphoric acid	H_3PO_4	$H_2PO_4^-$	Dihydrogen phosphate ion
Hydrofluoric acid	HF	F^-	Fluoride ion
Nitrous acid	HNO_2	NO_2^-	Nitrite ion
Acetic acid	CH_3COOH	CH_3COO^-	Acetate ion
Carbonic acid	H_2CO_3	HCO_3^-	Hydrogen carbonate ion
Hydrogen sulfide	H_2S	HS^-	Hydrogen sulfide ion
Ammonium ion	NH_4^+	NH_3	Ammonia
Hydrogen cyanide	HCN	CN^-	Cyanide ion
Hydrogen carbonate	HCO_3^-	CO_3^{2-}	Carbonate ion
Water	H_2O	HO^-	Hydroxide ion
Hydrogen sulfide ion	HS^-	S^{2-}	Sulfide ion
Ethanol	CH_3CH_2-OH	CH_3CH_2-O^-	Ethoxide ion
Ammonia	NH_3	NH_{2-}	Amide ion
Hydrogen	H_2	H^-	Hydride ion
Methane	CH_4	CH_3^-	Methide ion

Figure 6.3.3: Strength of acid-conjugate base pairs relative to water as a reference.

> **Direction of acid-base equilibrium**
>
> In any Brønsted–Lowry acid-base reaction, the general rule is that a stronger acid and a stronger base tend to form a weaker acid and a weaker base.

For example, a dissociation reaction between HCl and H_2O is almost 100% complete because HCl is a stronger acid than H_3O^+ and H_2O is a stronger base than Cl^-:

$$HCl + H_2O \rightarrow H_3O^+ + Cl^-$$

The dissolution of acetic acid (CH_3COOH) and ammonia (NH_3) are equilibrium reactions because all the acids, bases, and their conjugates are in the weak acids or weak bases category. However, acetic acid and water dominate over their conjugates H_3O^+ and CH_3COO^- by 99.6:0.4 ratio (in 1 M acetic acid solution) because the conjugate acid H_3O^+ is a stronger acid than CH_3COOH, and conjugate base CH_3COO^- is a stronger base than H_2O.

$$\mathrm{CH_3COOH(aq) + H_2O(l) \overset{\rightharpoonup}{\longleftarrow} H_3O^+(aq) + CH_3COO^-(aq)}$$

> The longer arrow, in the unbalanced equilibrium arrows, points to the acid-base pair in the reaction that exists in a higher concentration relative to their conjugates.

Similarly, ammonia (NH_3) and water (H_2O) dominate over their conjugates NH_4^+ and OH^- by ~99.6:0.4 ratio (1M ammonia solution) because the conjugate acid NH_4^+ is a stronger acid than H_2O and conjugate base OH^- is a stronger base than NH_3.

$$\mathrm{NH_3(aq) + H_2O(I)) \overset{\rightharpoonup}{\longleftarrow} NH_4^+(aq) + OH^-(aq)}$$

6.4: Acid-base equilibrium

Most of the acid-base reactions are equilibrium reactions, i.e., the reactants form the products, and the products react to re-form the reactants. The reaction is shown with double arrows to indicate that both the forward and the reverse reactions happen simultaneously.

Pre-equilibrium and equilibrium

Initially, there are only reactants present. The concentration of the reactants decreases over time as they convert to the products. The rate of the reaction is proportional to the concentration of the reactants. So, the rate of the forward reaction decreases over time. The products build up over time. The products react with each other to re-form the reactants, i.e., the reverse reaction. The rate of the reverse reaction increases over time as the concentration of the products increases, until the rate of reverse reaction becomes equal to the rate of the forward reaction, as illustrated in Fig. 6.4.1

- At the beginning of the equilibrium when the rate of the reverse reaction is slower than the rate of forward reaction is the pre-equilibrium phase.
- The equilibrium phaes starts at the point when the rate of reverse reaction becomes equal to the rate of the forward reaction

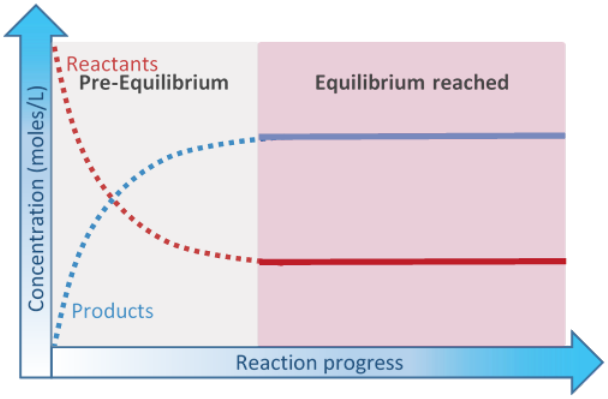


Figure 6.4.1: In pre-equilibrium, reactants react and their concentration, and, consequently, the rate of forward reaction decreases over time. The products build-up and the reverse reaction increases over time. When rate of forward reaction becomes equal to the rate of reverse reaction the equilibrium is reached and the concentration of reactants and products do not change.

At the point when the rate of reverse reaction becomes equal to the rate of the forward reaction, **equilibrium** has reached. The concentration of the reactants and products do not change at equilibrium because they are consumed and re-formed at the same rate –it is a dynamic equilibrium.

The equilibrium reactions are not limited to acid-base reactions; they are common in all types of chemical reactions. Fig. 6.4.2 illustrates the concentrations and rates of reactions changes in pre-equilibrium and equilibrium phases with the help of an actual chemical equilibrium reaction between a decomposition reaction of a colorless gas N_2O_4 and its reverse reaction, i.e., a combination reaction of brown color gas NO_2.

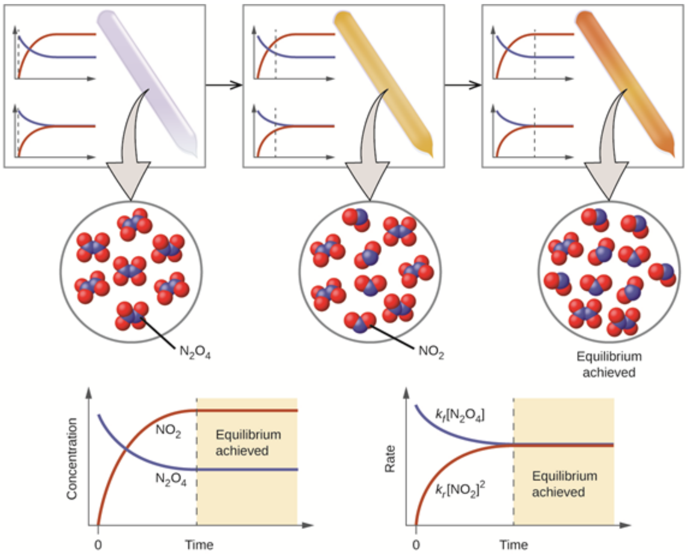


Figure 6.4.2: Top row: a sealed tube containing colorless gas N_2O_4 darkens as it decomposes to yield brown gas NO_2 by the reaction: $N_2O_4 \rightleftarrows 2NO_2$. The middle row: shows the models of the molecules at the timeline marked by the dotted lines in the graphs. Bottom row: shows concentration vs time (left graph); rate of forward reaction by blue curve and rate of reverse reaction by red curve (right graph). Source: OpenStax / CC BY (https://creativecommons.org/licenses/by/4.0)

What happens when a chemical equilibrium is disturbed?

The concentration of the reactants and products does not change in the mixture when the reaction is at equilibrium because the rate of the forward reaction is equal to the rate of the reverse reaction. Any change made at the equilibrium adds stress to the equilibrium. The system moves in a way to relieve the stress. For example, if one of the reactants is added to the mixture, the rate of forward reaction increases removing the added reactant until a new equilibrium establishes, i.e., the system relieves the stress by removing the added reactant.

Le Chatelier's principle

If a chemical equilibrium is disturbed, the rates of forward and reverse reactions change to relieve the stress and re-establish the equilibrium.

The stresses can be changes in the concentration, pressure, or temperature, as explained in the following section.

Effect of concentration on a chemical equilibrium

The following are the consequences of concentration changes on a chemical reaction at equilibrium.

1. If a reactant is added, the forward reaction increases to remove the reactant.
2. If a reactant is removed, the forward reaction decreases; consequently, the reverse reaction adds the reactant.
3. If a product is added, the reverse reaction increases to remove the product.
4. If a product is removed, the reverse reaction decreases; consequently, the forward reaction adds the product.

Fig. 6.4.3 illustrates the effects with the help of water level in two tanks connected through a conduit in the left tank representing reactants and in the right tank representing products.

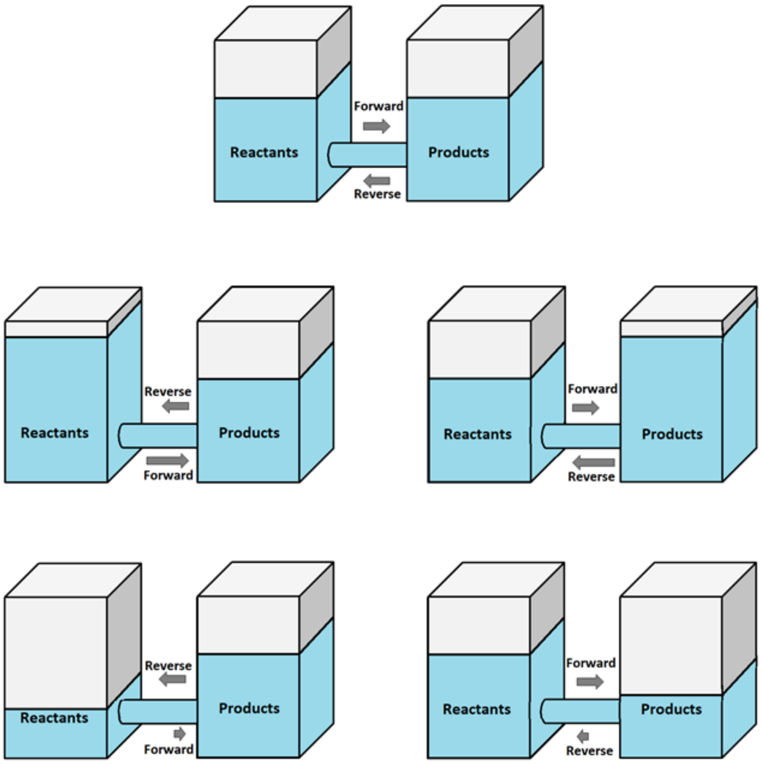


Figure 6.4.3: Illustration of Le Chatelier's principle using two water tanks connected through a conduit; 1) at equilibrium the rate of forward and reverse reactions are equal (the topmost), 2) when any reactant is increased the forward reaction rate increase (middle left), 3) when any product is increased the reverse reaction rate increases (middle right), 4) when any reactant is decreased the forward reaction rate decreases (bottom left), and 5) when any product is decreased the reverse reaction decreases (bottom right)

Fig 6.4.4 demonstrates the effect of concentration change on the chemical equilibrium between brown dichromate ions and yellow chromate ions:

Figure 6.4.4: Demonstration of effect of concentration change on chemical equilibrium: $Cr_2O_7^{2-}(aq,\ brown\ ) + H_2O(I) \rightleftarrows 2CrO_4^{2-}(aq, yellow\ ) + 2H^+(aq)$. Addition of H^+ to the tube on left by adding HNO_3 shifts the equilibrium to left making more of brown $Cr_2O_7^{2-}$ shown in the middle tube. Removal of H^+ by adding a base NaOH shift the reaction to the right making more of yellow CrO_4^{2-} shown in right most tube. Source: NCSSMDistanceEd / CC BY (https://creativecommons.org/licenses/by/3.0)

$$Cr_2O_7^{2-}(aq,\ brown\ ) + H_2O(I) \rightleftarrows 2CrO_4^{2-}(aq,\ yellow\ ) + 2H^+(aq)$$

The addition of acid to the test tube on the left increases H^+ in the system, increasing reverse reaction, which can be observed by the increased brown color in the middle test tube. Then, the addition of a base removes H^+ from the system by an acid-base reaction: $H^+ + OH^- \rightarrow H_2O$. The decrease in H^+ shifts the equilibrium to the product side, which can be observed by the increased yellow color in the test tube on the right.

A practical example of the effect of concentration on a chemical equilibrium is the binding of oxygen (O_2) with hemoglobin (Hb) during the breathing process.

$$\mathrm{Hb(aq)+O_2(\,g) \rightleftarrows HbO_2(aq)}$$

The concentration of oxygen is higher in the lunges that shift the equilibrium to the product side, binding more oxygen with the hemoglobin. When the blood arrives in tissues, the concentration of oxygen is lower in tissues, causing the equilibrium to shift to the reactant side, releasing the oxygen.

The oxygen concentration decreases as the altitude increases. The mountain climbers may experience hypoxia, i.e., inadequate supply of oxygen to the body because the lower level of oxygen at high altitude may shift the equilibrium to the right, resulting in less binding of oxygen with the hemoglobin in the lungs. The body reacts by producing more hemoglobin, but it takes about 10 days for the body to re-adjust the hemoglobin level in the blood. Peoples living at higher altitudes usually have a higher level of hemoglobin in their blood for the reasons described above.

Effect of pressure on a chemical equilibrium

Changes in pressure do not affect the concentration of solids and liquid. However, an increase in pressure decreases the volume, and, consequently, increases the concentration of gases, as illustrated in Fig. 6.4.5.

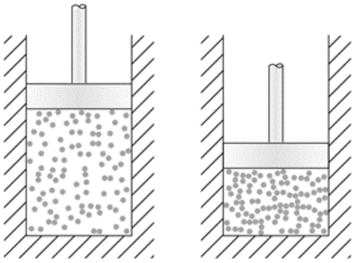


Figure 6.4.5: Illustration of increase in pressure causes decrease in the volume and increase in the concentration of gas molecules. Source: Olivier Cleynen / CC0

> If a chemical equilibrium involves gases, an increase in pressure has the same effect as increases in the gaseous reactant or product—the equilibrium shifts in the direction where there are fewer moles of gases.

Fig. 6.4.6 demonstrated this effect for the equilibrium between colorless N_2O_4 gas and brown color NO_2 gas:

$$\mathrm{N_2O_4(\,g,\ colorless\,) \rightleftarrows 2NO_2(\,g,\ brown\,)}$$

The color becomes light in going from a syringe on the right to the syringe in the middle. It can be explained based on the fact that the concentration of gases decreased upon an increase in volume as a result of a decrease in pressure. Then the color becomes darker over time, as shown by the syringe on the right. The darker color indicates that the equilibrium has shifted to the product side where there are more moles of gas, to relieve the stress.

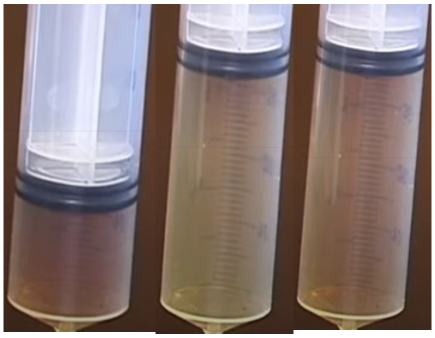


Figure 6.4.6: Decrease in pressure on the equilibrium: $\mathrm{N_2O_4(\,g,\ colorless\,) \rightleftarrows 2NO_2(\,g,\ brown\,)}$, Middle syringe → syringe on the right, increases the forward reaction to release the stress. Source: NCSSMDistanceEd / CC BY (https://creativecommons.org/licenses/by/3.0)

Effect of temperature on a chemical equilibrium

Exothermic reaction releases heat, i.e., heat is one of the products. If the forward reaction is exothermic, the reverse reaction must be endothermic by the same amount and vice versa.

> When a reversible reaction at equilibrium is disturbed by increasing temperature, the equilibrium shifts in the endothermic direction of the reaction to remove the heat and vice versa.

In the equilibrium between colorless N_2O_4 and brown color NO_2 gases, the reaction is endothermic in the forward direction:

$$\mathrm{N_2O_4}(g,\ \text{colorless}) + \text{Heat} \rightleftarrows 2\mathrm{NO_2}(g,\ \text{brown})$$

An increase in temperature shifts the equilibrium in the endothermic direction to relieve the stress, as demonstrated in Fig. 6.4.7.

Figure 6.4.7: Increase in temperature shifts the equilibrium in the endothermic direction producing more of the colored NO_2 in the following equilibrium: $\mathrm{N_2O_4}(g,\ \text{colorless}) + \text{Heat} \rightleftarrows 2\mathrm{NO_2}(g,\ \text{brown})$. An overlay of the same 99.9% pure NO_2/N_2O_4 sealed in an ampoule. From left to right -196 °C, 0 °C, 23 °C, 35 °C, 50 °C. Source: Eframgoldberg / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

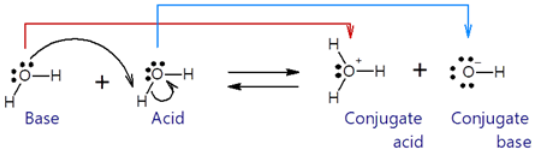
6.5: Dissociation of water

How do water molecules dissociate?

Water is an amphoteric substance, which means water can accept a proton acting as a base, and it can also donate A proton acting as an acid.

> About one water molecule in half a billion dissociates into an OH^- ion by losing a proton to another water molecule. The molecule that receives a proton becomes H_3O^+.

The dissociation of water is an equilibrium reaction in which one water molecule donates its proton to another water molecule.



The water molecule that receives proton is acting as a base, and it converts to conjugate acid H_3O^+. The other water molecule that donates a proton is acting as an acid, and it converts to conjugate base OH^-. The arrows in the reaction show that the base uses one of its lone pairs of electrons to make a bond with proton, and the previous bond pair of electrons turns into a third lone pair of electrons on the oxygen atom of the base. The reaction is reversible, i.e., the conjugate acid (H_3O^+) and the conjugate base (OH^-) react to re-form the two water molecules.

Water dissociation constant

The dissociation of water is an equilibrium reaction. It means the rate of the forward reaction is equal to the rate of the reverse reaction and the concentration of the reactants and products do not change at equilibrium. The molar concentration of H_3O^+ represented as $[H_3O^+]$ is equal to 10^{-7} M in a pure water sample at 25 ^oC, where M is in moles/Liter. The molar concentration of OH^- represented as $[OH^-]$ is equal to the molar concentration of H_3O^+ in pure water, i.e., $[H_3O^+] = [OH^-] = 10^{-7}$ M.

> The product of the molar concentration of H_3O^+ and OH^- in water is a constant called **water dissociation constant K_w** equal to 10^{-14} at 25 ^oC, i.e.:
>
> $$\mathbf{K_w = \left[H_3O^+\right]\left[OH^-\right] = \left(10^{-7}\right)\left(10^{-7}\right) = 10^{-14}} \tag{6.5.1}$$

Neutral, acidic, or basic aqueous solutions

> A solution that has an equal concentration of H_3O^+ and OH^-, each equal to 10^{-7} M, is a **neutral solution**.

An acidic solution has an acid dissolved in water. When an acid dissolves in water it dissociates adding more H_3O^+. The $[OH^-]$ must decrease to keep the K_w constant.

> A solution that has $[H_3O^+]$ more than 10^{-7}, and $[OH^-]$ less than 10^{-7} is an **acidic solution**.

A basic solution has a base dissolved in water. When a base dissolves in water it dissociates adding more OH^-. The $[H_3O^+]$ must decrease to keep the K_w constant.

> A solution that has $[H_3O^+]$ less than 10^{-7}, and $[OH^-]$ more than 10^{-7} is a **basic solution**.

Calculations of $[H_3O^+]$ and $[OH^-]$ based on K_w

The water dissociation constant remains the same whether the aqueous solution is neutral, acidic, or basic, i.e.:

$$\mathrm{K_w = \left[H_3O^+_-\right]\left[OH^-\right] = \left(10^{-7}\right)\left(10^{-7}\right) = 10^{-14}\ at\ 25^\circ C}$$

Therefore, if the molar concentration of hydronium ions $[H_3O^+]$ is known, the molar concentration of hydroxide ions $[OH^-]$ can be calculated using the following formula:

$$\left[\mathrm{H_3O^+}\right]=\frac{\mathrm{K}_w}{\left[\mathrm{OH^-}\right]}=\frac{10^{-14}}{\left[\mathrm{OH^-}\right]}$$

Similarly, if the molar concentration of hydroxide ions [OH^-] is known, the molar concentration of hydronium ions [OH^-] can be calculated using the following formula:

$$\left[\mathrm{OH^-}\right]=\frac{K_w}{\left[\mathrm{H_3O^+}\right]}=\frac{10^{-14}}{\left[\mathrm{H_3O^+}\right]}$$

When a strong acid like HCl dissolves in water, it dissociates ~100% into ions. Therefore, the [H_3O^+] is equal to the molar concentration of the acid. The amount H_3O^+ added by dissociation of water molecules is very small compared to that coming from the dissociation of a strong acid and can be neglected. Similarly, when a strong base like NaOH dissolves in water, it dissociates ~100% into ions. Therefore, the [OH^-] is equal to the molar concentration of the base.

Note

When a weak acid or a weak base dissolves in water, it partially dissociates into ions. Therefore, the [H_3O^+] or the [OH^-] in the cases of weak acids and weak bases has to be determined experimentally for the calculations.

Example 6.5.1

Calculate the concentration of OH^- ions in a 0.10 M HNO_3 solution?

Solution

The HNO_3 is a strong acid. Therefore, [HNO_3] = 0.10 M = [H_3O^+]. Desired [OH^-] = ?

Formula: $\left[\mathrm{OH^-}\right]=\frac{10^{-14}}{\left[\mathrm{H_3O^+}\right]}$

Plug in values an calculate: $\left[\mathrm{0H^-}\right]=\frac{10^{-14}}{0.10}=10^{-13}\ \mathrm{M}$

Example 6.5.2

A vinegar solution has [H_3O^+] = 2.0 x 10^{-3}. a) What is the hydroxide ion concentration in the vinegar solution? b) is the solution acidic, basic, or neutral?

Solution

a) Given [H_3O^+] = 2.0 x 10^{-3}. Desired [OH^-] = ?

Formula: $\left[\mathrm{OH^-}\right]=\frac{10^{-14}}{\left[\mathrm{H_3O^+}\right]}$

Plug in values and calculate: $\left[0H^-\right]=\frac{10^{-14}}{2.0\times10^{-3}}=5.0\times10^{-12}\mathrm{M}$

b) The solution is acidic because [H_3O^+] > [OH^-].

Example 6.5.3

Calculate the value of [H^3O^+] and [OH^-] in a 0.010 M NaOH solution?

Solution

The NaOH is a strong base. Therefore [NaOH] = 0.010 M = [OH^-]. Desired [H_3O^+] = ?

Formula: $\left[\mathrm{H_3O^+}\right]=\mathrm{K_w}/\left[\mathrm{OH^-}\right]=10^{-14}/\left[\mathrm{OH^-}\right]$

Calculations: $\left[\mathrm{H_3O^+}\right]=10^{-14}/0.010=10^{-12}\mathrm{M}$

✓ Example 6.5.4

a) Calculate the $[H_3O^+]$ in an ammonia solution that has $[OH^-] = 4.0 \times 10^{-4}$ M? b) Is the solution acidic, basic, or neutral?

Solution

a) Given $[OH^-] = 4.0 \times 10^{-4}$. Desired $[H_3O^+]$ = ?

Formula: $\left[\mathrm{H_3O^+}\right] = \mathrm{K_w} / \left[\mathrm{OH^-}\right] = 10^{-14} / \left[\mathrm{OH^-}\right]$

Calculations: $[0H^-] = \frac{10^{-14}}{4.0\times10^{-4}} = 2.5 \times 10^{-11}\mathrm{M}$

b) The solution is basic because $[H_3O^+] < [OH^-]$.

6.6: The pH

What is pH?

The acidity of an aqueous solution relates to H_3O^+ ion concentration, but there are two problems with it. The first problem is that the molar concentration of hydronium ion $[H_3O^+]$ varies over a wide range, usually from 1-to-0.00000000000001 which is not easy to comprehend. Log scale solves the problem, e.g., if a number increases from 1 to 1000, it increases from 0 to 3 on a log scale to the base 10. The second problem is that the $[H_3O^+]$ is usually a small number between 0 and 1. The log of a number that is between 0 and 1 is a negative number that is not easy to grasp mentally. If a number is between 0 and 1, its reciprocal is more than 1, and its log is a +ve number.

> The **pH** is defined as a log of reciprocal of the molar concentration of hydronium ions $[H_3O^+]$. It can also be stated that the pH is a negative log of the molar concentration of hydronium ion $[H_3O^+]$. The mathematical form of the pH is the following.
>
> $$pH = \log \frac{1}{\left[\mathrm{H_3O^+}\right]} = -\log\left[\mathrm{H_3O^+}\right]$$

A pH is usually a positive number between 0 to 14.

Calculating pH

First, determine the molar concentration of hydronium ion $[H_3O^+]$. Than take log base 10 of $[H_3O^+]$ and change the sign of the answer, i.e.:

$$pH = -\log\left[\mathrm{H_3O^+}\right]$$

✓ Example 6.6.1

Calculate the pH of neutral water that has $[H_3O^+] = 10^{-7}$M?

Solution

Given $[H_3O^+] = 10^{-7}$ M, desired pH = ?

Formula: $pH = -\log\left[\mathrm{H_3O^+}\right]$

Plug in values and calculate: $pH = -\log\left(10^{-7}\right) = 7.0$

The keys-sequence for the calculation on a Microsoft Window’s scientific calculator is (the last box is the output of the keys-sequence):

negate(log(10^(-7)))

7

Significant figures in pH value

The given number in scientific notation is **1** x 10^{-7} which has one significant figure shown by the coefficient part of the number in bold font. **The number of decimal places in the pH number shows the significant figures**, i.e., 7.**0** has one decimal place shown in bold font, which means it has one significant figure.

✓ Example 6.6.2

Calculate the pH of the 0.010 M HCl solution?

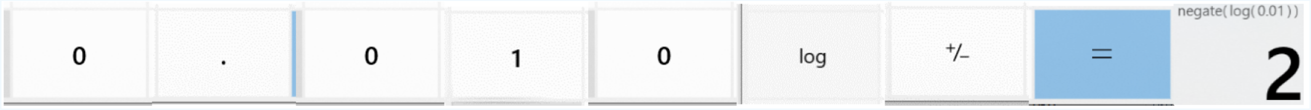
Solution

Given [HCl] = 0.010 M = $[H_3O^+]$, desired pH = ?

Formula: $pH = -\log\left[\mathrm{H_3O^+}\right]$

Plug in values and calculate: $pH = -\log(0.010) = 2.00$

The keys-sequence for the calculation on a Microsoft Window’s scientific calculator is (the last box is the output of the keys-sequence):



negate(log(0.01))

2

Note that the given number 0.0**10** M has two significant figures shown in bold fonts. So, the answer pH 2.**00** also has two significant figures shown in bold fonts.

Example 6.6.3

Calculate the pH of 0.10 M HCl solution?

Solution

Given [HCl] = 0.10 M = [H_3O^+], desired pH = ?

Formula: $pH = -\log\left[\mathrm{H_3O^+}\right]$

Calculations: $pH = -\log(0.10) = 1.00$

As the acid 0.01M and 0.10M is gradually added to increase the acid from neutral water in example 1 to 0.01M in example 2 to 0.10 M in example 3, , the pH gradually decreased from 7 to 2 to 1.

The pH of the acidic solution is less than 7. The more acidic the solution, the lower the pH.

The pH decreases as the [H3O+] increases because the reciprocal of [H3O+] is used in the pH calculation. The larger the given number, the smaller the reciprocal; it translates to “the more acidic the solution, the lower the pH.

Example 6.6.4

Calculate the pH of 0.010 M NaOH solution?

Solution

Given [NaOH] = 0.010 M = [OH^-], desired pH = ?

First, calculate [H_3O^+] from the give [OH^-]: $\left[\mathrm{H_3O^+}\right] = 10^{-14}/\left[\mathrm{OH^-}\right] = 10^{-14}/0.010 = 1.0 \times 10^{-12}$

Than calculate the pH: $pH = -\log\left[\mathrm{H_3O^+}\right] = -\log\left(1.0 \times 10^{-12}\right) = 12.00$

Note that the given number 0.0**10** M has two significant figures shown in bold fonts. So, the answer pH 12.**00** also has two significant figures shown in bold fonts.

Example 6.6.5

Calculate the pH of 0.10 M NaOH solution?

Solution

Given [NaOH] = 0.10 M = [OH^-], desired pH = ?

First, calculate [H_3O^+] from the give [OH^-]: $10^{-14}/\left[\mathrm{OH^-}\right] = 10^{-14}/0.10 = 1.0 \times 10^{-13}$

Formula: [H_3O^+] = 10^{-14}/[OH^-] = 10^{-14}/0.10 = 1.0 x 10^{-13}.

Than calculate the pH: $pH = -\log\left[\mathrm{H_3O^+}\right] = -\log\left(1.0 \times 10^{-13}\right) = 13.00$

As the base, 0.010M and 0.10M are gradually added in the previous two exams to the neutral water at pH 7, the pH increases from 7 to 12 to 13.

> The pH of the basic solution is more than 7. The more basic the solution, the higher the pH.

pH measurement

The pH is usually measured in laboratories by digital pH meters. The electrode of the pH meter is first calibrated with solutions of know pH values, and then the electrode is dipped in the test solution to read its pH value. Universal pH indicator papers are available that turn to a specific color when placed in the solution. The pH is read by matching the color of the test paper with the color on the chart. Fig. 6.6.1 shows a digital pH meter and two universal pH indicating papers commonly used for pH measurements in laboratories.

Figure 6.6.1: pH/Ion Meter (left) and universal pH indicator papers (middle and right). Source: Datamax / Public domain; Bordercolliez / CC0; Fredquintao~commonswiki, CC-BY-SA-2.5.

The pH indicators are weak acids or weak bases that change color in a specific pH range. A few drops of the solution of a pH indicator paper are added to the test solution in which pH is changed by adding acid or base. The change in the color of the solution indicates the pH range in which the indicator changes the color. Figure 6.6.2 shows the colors and the color transition ranges of some of the common pH indicators.

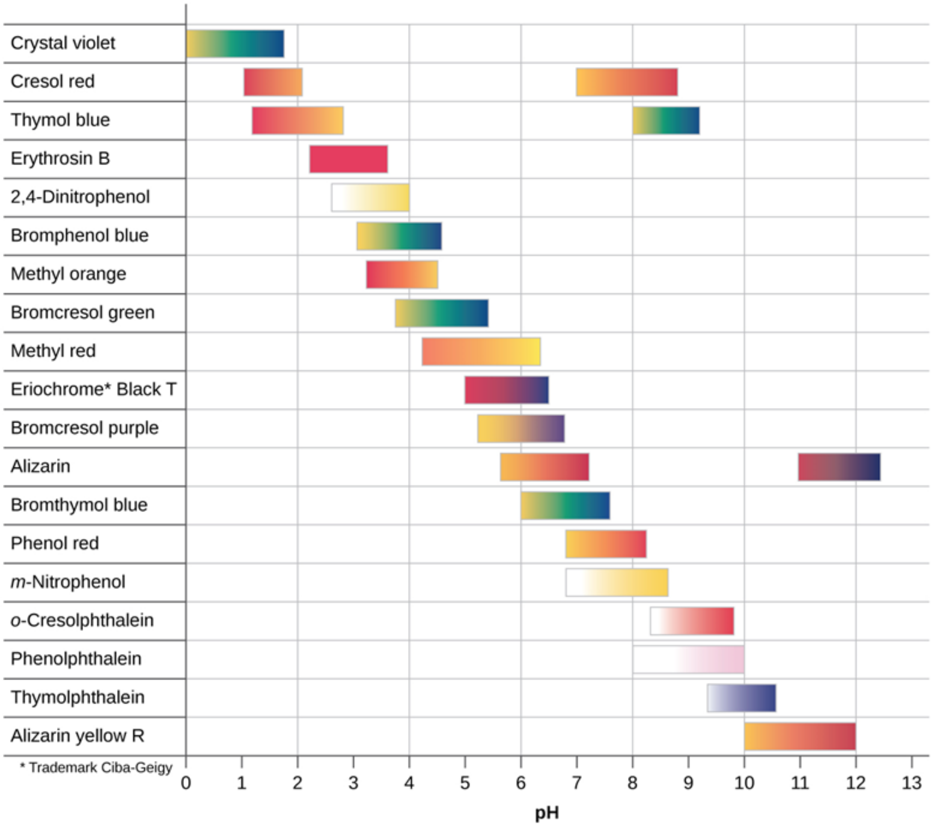


Figure 6.6.2: The colors and the pH ranges of color transition of some of the common pH indicators. Source: OpenStax / CC BY (https://creativecommons.org/licenses/by/4.0)

Calculating hydronium ion concentration from pH

The formula for calculating the molar concentration of hydronium ions $[H_3O^+]$ is obtained by rearranging the pH formula. $pH = -\log\left[\mathrm{H_3O^+}\right]$, re-arranges to: $\left[\mathrm{H_3O^+}\right] = \text{antilog}(-pH) = 10^{-pH}$.

Example 6.6.6

Calculate $[H_3O^+]$ of a urine sample that has pH 7.56?

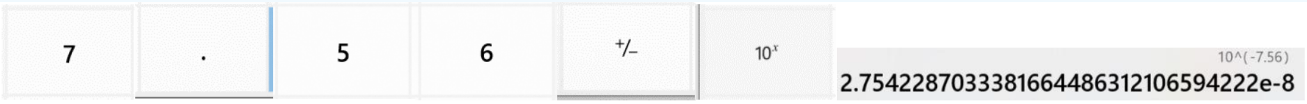
Solution

Given: pH = 7.56, Desired: $[H_3O^+]$ = ?

Formula: $\left[\mathrm{H_3O^+}\right] = 10^{-pH}$.

Plug in the values and calculate: $[H_3O^+] = 10^{-pH} = 10^{-(7.56)} = 2.8 \times 10^{-8}\,M$

The keys-sequence for the calculation on a Microsoft Window’s scientific calculator is (the last box is the output of the keys-sequence):



10^(-7.56)

2.7542287033381664486312106594222e-8

> The calculated answer in the above example is a lengthy number, but it is rounded to two significant figures shown in bold font in $\mathbf{2.8}\times 10^{-8}\,M$, because the given number pH 7.**56** has two significant figures shown in bold font.

Significance of pH Scale

The pH scale varies from ~0 to ~14. The pH of 7 is neutral, pH more than 7 is basic, and pH less than 7 is acidic, as illustrated in Fig. 6.6.3. Different foods have different pH values, as shown in Fig. 6.1.1. Similarly, several of the acids and bases in household use have a specific pH range, as shown in Fig. 6.6.3.

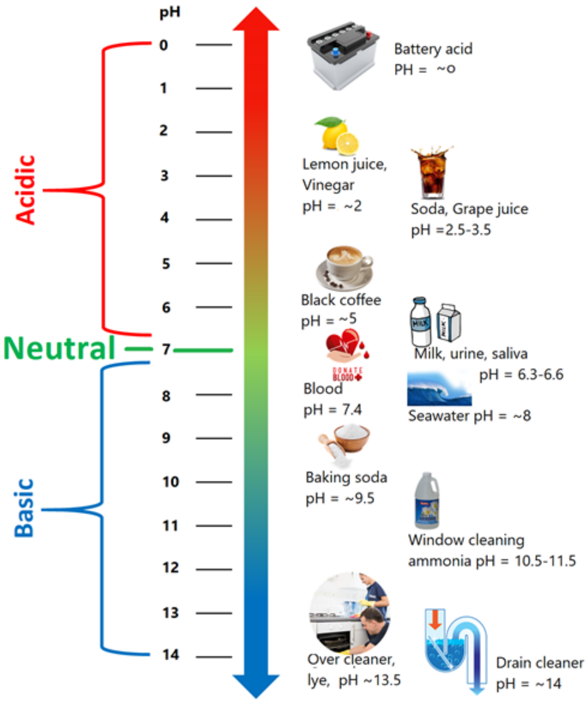


Figure 6.6.3: pH scale and pH of some common substances. pH 7 is neutral, pH less than 7 is acidic, and pH more than 7 is basic.

The control of pH is essential in the proper functioning of biological systems. Plants thrive if the soil does not have too acidic or too basic a pH. Lacks and revers have a specific range of pH in which the aquatic life can survive. US natural water has a pH in the range of 6.5 to 8.5 range. Seawater has a specific narrow range of pH 7.5 to pH 8.4 in which the life in the sea can function correctly.

The pH of body fluids

Human body fluids vary in pH, as shown in Fig. 6.6.4. Saliva in the mouth is slightly acidic, but the stomach has the lowest pH in the body. The strongly acidic pH in the stomach helps in digesting some foods, and it also helps in killing bacteria that may enter the stomach through the foods. When the food enters the large intestine, the pH changes to basic which helps in digesting the foods that could not be digested in the acidic environment of the stomach. The pH changes to more basic in the small intestine.

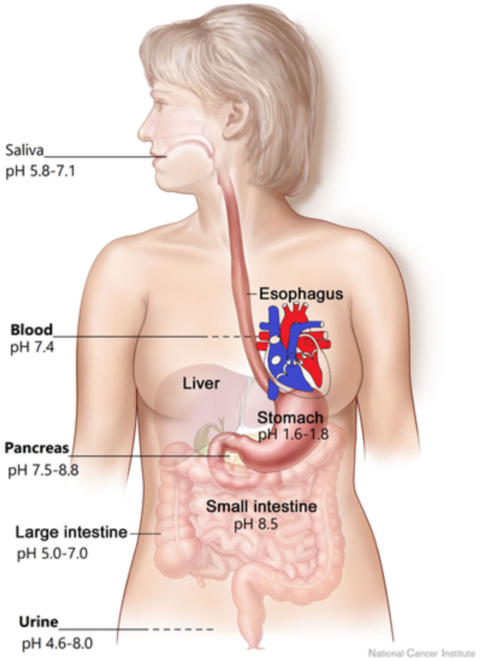


Figure 6.6.4: The pH in various human body fluids is shown. Source: Modified from National Cancer Institute / Public domain

The blood has a pH of 7.4, and it can vary in a small range of 7.35 to 7.45. If the blood pH goes outside of the 7.35 to 7.45 range it can result in medical problems. Enzymes in the body need a specific pH range because hydrogen bonding plays a vital role in the structures needed for proper functioning. pH changes affect the hydrogen bonding and can make the enzymes less active or may inactivate them. The pH of blood is maintained by a complex action of buffers that are described in the later sections. The pH of urine can vary over a broad range from 4.6 to 8, depending on the recent diet and exercises.

Acid rain

Acidic gases like NO, NO_2, N_2O_4, SO_2 are released into the environment primarily during the combustion of fossil fuels. These gases dissolve in the rainwater and make the rain acidic. For example, sulfur dioxide dissolves in water and makes sulfurous acid:

$$\mathrm{SO_2(g) + H_2O(I) \rightleftarrows H_2SO_3(aq)}$$

The acid rain damages the environment by making the soil, river water, and lack-water acidic. The acidic soil and water, in turn, affect the plants and aquatic life. The acid water also reacts with calcium carbonate and corrodes metals that are responsible for damage to the sculpture and other structures, as illustrated in Fig. 6.6.5, Fig. 6.6.6, and Fig. 6.6.7.

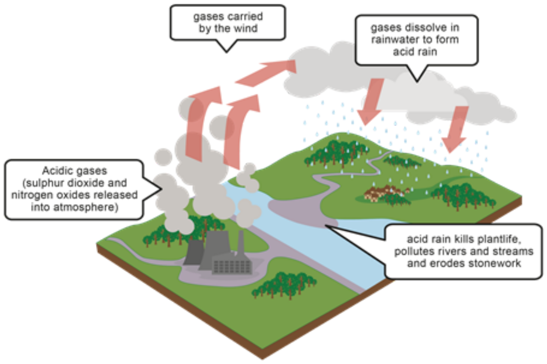


Figure 6.6.5: Illustration of acid rain. Source: https://www.hiclipart.com/free-trans...bacyp/download

Figure 6.6.6: Effect of acid rain on forest . Source: Lovecz / Public domain.

Figure 6.6.7: PEffect of acid rain on monuments. Source: Nino Barbieri / CC BY-SA (http://creativecommons.org/licenses/by-sa/3.0/)

6.7: Acid-base reactions

Acid-base reactions are chemical reactions that involve the transfer of a proton (H^+). Examples include the reactions of acids with metals, carbonates, and Arrhenius bases, described in the following.

Reactions of acids with metals

Metals tend to give out an electron and become cations. The majority of the metals, called reactive metals, give out electrons to protons in the acids and release H_2 gas. For example, Fig. 6.7.1 shows magnesium reacting with hydrochloric acid by the following reaction:

$$\mathrm{Mg(s)+2HCl\rightarrow MgCl_2(aq)+H_2(g)}\uparrow$$

Figure 6.7.1: Mg reacting with HCl and H_2 gas bubbling out. Source: https://youtu.be/cpy_Zh-8sKA, CC BY

Alkali metals like Na give out one electron, alkaline earth metals like Mg give out two electrons, and aluminum gives out three electrons. A proton can accept one electron. Therefore, the number of acidic protons should be equal to the number of electrons given out to balance the electron transfer in these reactions.

Note

Noble metals or jewelry metals like gold, silver, platinum, copper are exceptions –they do not react with acids.

Example 6.7.1

write a balanced equation for the reaction of aluminum with HBr?

Solution

Step 1) write the equation with the correct formulas of reactants and products.

$$\mathrm{Al(s)+HBr(aq)\rightarrow AlBr_3(aq)+H_2(g)}$$

Note that Al gives out three electrons to make Al^{3+}; that is why three Br^- are attached to it in the product to balance the charge.

Step 2) balance the electrons lost by the metal with the number of acidic protons.

$$\mathrm{Al(s)+3HBr(aq)\rightarrow AlBr_3(aq)+H_2(g)}$$

Step 3) Balance the rest of the elements by the hit and trial method. There are 3 hydrogen atoms on the left, balance them by adding 3/2 coefficient to the hydrogen on the right.

$$\mathrm{Al(s)+3HBr(aq)\rightarrow AlBr_3(aq)+\frac{3}{2}H_2(g)}$$

Step 4. Although the equation is balanced, it is recommended to remove the fraction by multiplying the coefficients in the whole equation with the highest common factor to obtain the final balanced equation.

$$\mathrm{2Al(s)+6HBr(aq)\rightarrow 2AlBr_3(aq)+3H_2(g)}$$

Reactions of acids with carbonates and hydrogen carbonates

Carbonic acid (H_2CO_3) is a weak acid found in carbonated water. The H_2CO_3 is a product of carbon dioxide (CO_2) and water (H_2O) by the following equilibrium reaction.

$$CO_2(aq) + H_2O(l) \rightleftharpoons H_2CO_3(aq)$$

Hydrogen carbonate (HCO_3^-) and carbonate (CO_3^{2-}) are one and two hydrogen less, respectively than carbonic acid. The salts containing HCO_3^- and CO_3^{2-} accept one and two protons, respectively, from acids to make H_2CO_3. The H_2CO_3 decomposes to carbon dioxide and water by the reverse reaction shown above. Fig. 6.7.2 shows the reaction of sodium hydrogen carbonate with hydrochloric acid.

$$\mathrm{NaHCO_3(\,s) + HCl(aq) \rightarrow NaCl(aq) + H_2O(I) + CO_2(\,g)\uparrow}$$

Figure 6.7.2: The reaction of sodium carbonate with HCl. Before and after HCl addition. Carbon dioxide bubbles out after HCl addition. Source: NCSSM, 05/18/20, https://youtu.be/TJYOxGHNTzg, CC BY 3.0

Similarly, calcium carbonate found in limestone reacts with acids. For example, sulfuric acid is one of the components in acid rain that reacts with calcium carbonate and damages sculptures made of stone.

$$\mathrm{CaCO_3(\,s) + H_2SO_4(aq) \rightarrow CaSO_4(aq) + H_2O(l) + CO_2(\,g)\uparrow}$$

Reactions of acids with Arrhenius bases

Acids release proton (H^+) and Arrhenius bases release hydroxide ions (OH^-) in solution. When an acid mix with the Arrhenius base, H^+ and OH^- ions react with each other and produce water molecules.

$$\mathrm{H^+(aq) + OH^-(aq) \rightarrow H_2O(l)}$$

This is the net ionic equation of a reaction of an acid with an Arrhenius base. The cation of the base and the anion of the acid do not react –they are spectator ions. The reaction equation for an acid-base reaction is written in various ways explained below.

Molecular equation

The molecular equation shows the formulas of the substances. For example, the molecular equation of the reaction of HCl with NaOH is the following.

$$\mathrm{HCl(aq) + NaOH}(aq) \rightarrow \mathrm{NaCl}(aq) + \mathrm{H_2O(l)}$$

Complete ionic equation

The complete ionic equation shows the electrolytes dissociated into ions as they actually exist in the water phase, i.e., as aqueous ions. The complete ionic equation of the reaction of HCl with NaOH is the following.

$$\mathrm{H^+(aq) + Cl^-(aq) + Na^+(aq) + OH^-(aq) \rightarrow H_2O(l) + Na^+(aq) + Cl^-(aq)}$$

It is evident that Na^+ and Cl^- do not react –they are the spectator ions.

Net ionic equation

The spectator ions are present on both sides of the equation in equal numbers. The spectator ions can be canceled out, like the terms in an algebraic equation.

$$\mathrm{H^+(aq)} + \mathrm{Cl^-}\cancel{\mathrm{(aq)}} + \mathrm{Na^+}\cancel{\mathrm{(aq)}} + \mathrm{OH^-(aq)} \rightarrow \mathrm{H_2O(l)} + \mathrm{Na^+}\cancel{\mathrm{(aq)}} + \mathrm{Cl^-}\cancel{\mathrm{(aq)}}$$

The **net ionic equation** shows the substances that are not spectator ions after canceling out the spectator ions from the complete ionic equation. The net ionic equation of the reaction of HCl with NaOH is the following.

$$\mathrm{H^+(aq)} + \mathrm{OH^-(aq)} \rightarrow \mathrm{H_2O(l)}$$

Note

All of the reactions of the strong acids with strong Arrhenius bases have the same net ionic equation.

Writing a balanced chemical equation of the reaction of acids with Arrhenius bases

The following example shows the steps needed to write the balanced equation of the reaction of an acid with an Arrhenius base.

Example 6.7.2

Write a balanced chemical equation of a reaction between HCl and $Ca(OH)_2$?

Solution

Step 1) Write the formula of acid and base in the reactants and salt and water in the products. All the strong electrolytes dissolve in water, so use (aq) to represent their state.

$$\mathrm{HCl(aq)} + \mathrm{Ca(OH)_2(aq)} \rightarrow \ \mathrm{Salt(aq)}\ + \mathrm{H_2O(l)}$$

Step 2) Balance the H^+ in the acid with the OH^- in the base.

$$\mathrm{2HCl(aq)} + \mathrm{Ca(OH)_2(aq)} \rightarrow \mathrm{Salt(aq)} + \mathrm{H_2O(l)}$$

Step 3) Balance the H_2O with the H^+ in the acid, or with the OH^- in the base.

$$\mathrm{2HCl(aq)} + \mathrm{Ca(OH)_2(aq)} \rightarrow \ \mathrm{Salt\ (aq)} + \mathrm{2H_2O(I)}$$

Step 4) Write the salt by combing the cations from the base and the anions from the acid. Make sure the charges are balanced in the salt to make it a neutral substance.

$$\mathrm{2HCl(aq)} + \mathrm{Ca(OH)_2(aq)} \rightarrow \mathrm{CaCl_2(aq)} + \mathrm{2H_2O(I)} \tag{6.7.1}$$

Example 6.7.3

Write a balanced chemical equation of a reaction between H_2SO_4 and $Ba(OH)_2$?

Solution

Step 1) Write the formula of acid and base in the reactants and salt and water in the products. All the strong electrolytes dissolve in water, so use (aq) to represent their state.

$$\mathrm{H_2SO_4(aq)} + \mathrm{Ba(OH)_2(aq)} \rightarrow \mathrm{Salt(aq)} + \mathrm{H_2O(l)}$$

Step 2) Balance the H^+ in the acid with the OH^- in the base. They are already balanced in the above equation.

Step 3) Balance the H_2O with the H^+ in the acid, or with the OH^- in the base.

$$\mathrm{H_2SO_4(aq)} + \mathrm{Ba(OH)_2(aq)} \rightarrow \mathrm{Salt(aq)} + \mathrm{2H_2O(l)}$$

Step 4) Write the salt by combing the cations from the base and the anions from the acid. Make sure the charges are balanced in the salt to make it a neutral substance.

$$\mathrm{H_2SO_4(aq)} + \mathrm{Ba(OH)_2(aq)} \rightarrow \mathrm{BaSO_4(aq)} + \mathrm{2H_2O(l)}$$

Antacids

The stomach sometimes produces excess HCl that may cause heartburn.

> Antacids are the substances used to neutralize the excess HCl in the stomach.

Figure 6.7.3: Bottle of Antacid tablets. Source: Midnightcomm / CC BY-SA (http://creativecommons.org/licenses/by-sa/3.0/).

Fig. 6.7.3 shows antacid tablets. The antacids include Arrhenius bases with very low solubility in water, like Al(OH)_3, and Mg(OH)_2, or weak bases like CaCO_2, and NaHCO_3. that react with and neutralize the acid:

$$
\begin{aligned}
&\mathrm{Al(OH)_3(\,s) + 3HCl(aq) \rightarrow AlCl_3(aq) + 3H_2O(l)} \\
&\mathrm{Mg(OH)_2(\,s) + 2HCl(aq) \rightarrow MgCl_2(aq) + 2H_2O(l)} \\
&\mathrm{CaCO_3(\,s) + 2HCl(aq) \rightarrow CaCl_2(aq) + H_2O(I) + CO_2(\,g)} \\
&\mathrm{NaHCO_3(\,s) + HCl(aq) \rightarrow NaCl(aq) + H_2O(I) + CO_2}(g)
\end{aligned}
$$

Side effects of the antacids

The antacids have side effects, e.g., aluminum and calcium-containing antacids may cause constipation. Magnesium-containing antacids have a laxative effect. Some formulations use a mixture of aluminum and magnesium-containing antacids to cancel out the side effect of each other. The calcium-containing antacid is not recommended for persons who tend to develop kidney stones, because the kidney stone is usually a salt of calcium. Sodium-containing antacids may increase the sodium level in the body fluid and may raise the blood pH.

Acid-base titration

> The acid-base titration is an analytical process of determining the concentration of acid, called **analyte**, by neutralizing it with a base of know concentration, called the **standard**, or vice versa.

Usually, the base is in a burette and added drop by drop to a known volume of the acid in an Erlenmeyer flask, as illustrated in Fig. 6.7.4. A few drops of an acid-base indicator are mixed with the acid. The indicator changes color at a specific narrow pH range.

> - The point when the stoichiometric amount of the base has been added to the acid is called the **equivalence point.**
> - The point when the indicator changes color is the **end-point**.

Usually, the equivalence point is almost the same as the end-point.

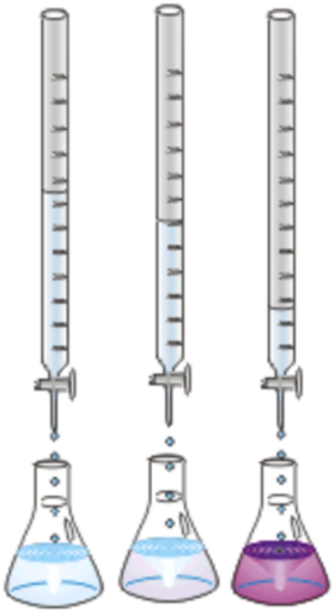


Figure 6.7.4: Acid-base titration set-up. The analyte color due to the indicator before, at the endpoint, and after being shown by the images on the left, middle, and right, respectively. *Source: Taken from Luigi Chiesa / Public domain.*

The calculation steps after the titration are usually the following.

Steps in acid-base titration calculations

1. The amount, in moles, of the standard is calculated by multiplying the amount in liters with the molarity of the standard.
2. Then, the amount, in moles, of the analyte, is calculated by using the mol-to-mol conversion factor from the balanced chemical equation of the reaction.
3. Finally, the molarity of the analyte is calculated by dividing moles by the volume in liters of the analyte.

✓ Example 6.7.4

What is the molarity of the HCl solution if 50.0 mL of the HCl solution requires 42.0 mL of 0.123 M NaOH solution in the titration?

Solution

Step 1) Given:

$$[\mathrm{NaOH}] = 0.123\ \mathrm{M} = \frac{0.123\ \mathrm{mol}\ NaOH}{1\ \mathrm{NaOH}}$$

$$\text{Volume of standard} = 42.0\ \mathrm{mL.} = 42.0\ \mathrm{mL\ NaOH} \times \frac{1\ \mathrm{L\ NaOH}}{1000\ \mathrm{mL\ NaOH}} = 0.0420\ L\ \mathrm{NaOH}$$

$$\text{Vol. analyte} = 50.0\ \mathrm{mL} = 50.0\ \mathrm{mL\ HCl} \times \frac{1\ \mathrm{L\ HCl}}{1000\ \mathrm{mL\ HCl}} = 0.0500\ \mathrm{L\ HCl}$$

Step 2) Calculate the moles of the standard from the volume and the molarity product.

$$\text{Moles of NaOH\textasciitilde consumed} = 0.0420\ \mathrm{L\ NaOH} \times \frac{0.123\ \mathrm{mol\ NaOH}}{1\ \mathrm{L\ NaOH}} = 0.00517\ \mathrm{mol\ NaOH}$$

Step 3) write the balanced chemical equation of the reaction.

$$\mathrm{HCl(aq)} + \mathrm{NaOH(aq)} \rightarrow \mathrm{NaCl(aq)} + \mathrm{H_2O(l)}$$

Step 4) write the conversion factor for mole of standard to mole of analyte calculation from the equation.

$$\frac{1 \text{mol HCl}}{1 \text{ mol NaOH}}$$

Step 5) Calculate the moles of the analyte by multiplying the moles of the standard and the conversion factor.

$$0.00517 \text{ mol NaOH} \times \frac{1 \text{ mol HCl}}{1 \text{ mol NaOH}} = 0.00517 \text{ mol HCl}$$

Step 6) Calculate the molarity of the analyte by dividing the moles with the volume in liters of the analyte.

$$0.00517 \text{ mol NaOH} \times \frac{1 \text{ mol HCl}}{1 \text{ mol NaOH}} = 0.00517 \text{ mol HCl}$$

After learning the steps thoroughly, the calculations can be done in a few steps, as shown in the following.

Calculations:

$$42.0 \text{ mL NaOH} \times \frac{1 \text{ L NaOH}}{1000 \text{ mL NaOH}} \times \frac{0.123 \text{ mol NaOH}}{1 \text{ L NaOH}} \times \frac{1 \text{ mol HCl}}{1 \text{ mol NaOH}} = 0.00517 \text{ mol HCl}$$

Molarity of HCl:

$$M = \frac{n(\text{mol})}{V(L)} = \frac{0.00517 \text{ mol HCl}}{50.0 \text{ mL HCl}} \times \frac{1000 \text{ mL HCl}}{1 \text{ L HCl}} = 0.103 \text{ M HCl}$$

Example 6.7.5

What is the molarity of the H_2SO_4 solution if 50.0 mL of the H_2SO_4 solution requires 32.3 mL of 0.201 M NaOH solution in the titration?

Solution

Step 1) Given:

$$[\text{NaOH}] = 0.201 \text{ M} = \frac{0.201 \text{ mol NaOH}}{1 \text{ L NaOH}}$$

$$\text{Vol. standard } = 42.0 \text{ mL} = 32.3 \text{ mL NaOH} \times \frac{1 \text{ L NaOH}}{1000 \text{ mL NaOH}} = 0.0323 \text{ L NaOH}$$

$$\text{Vol. analyte } = 50.0 \text{ mL} = 50.0 \text{ mL HCl} \times \frac{1 \text{ L HCl}}{1000 \text{ mL HCl}} = 0.0500 \text{ L HCl}$$

Step 2) Calculate the moles of the standard from the volume and the molarity product.

$$\text{Moles of NaOH consumed } = 0.0323 \text{ N NaOH} \times \frac{0.201 \text{ mol NaOH}}{1 \text{ L NaOH}} = 0.00649 \text{~mol } NaOH$$

Step 3) write the balanced chemical equation of the reaction.

$$\text{H}_2\text{SO}_4(\text{aq}) + 2\text{NaOH}(\text{aq}) \rightarrow \text{Na}_2\text{SO}_4(\text{aq}) + 2\text{H}_2\text{O}(\text{l})$$

Step 4) write the conversion factor for the moles of standard to mole of analyte calculation from the equation.

$$\frac{1 \text{ mol H}_2\text{SO}_4}{2 \text{ mol NaOH}}$$

Step 5) Calculate the moles of the analyte by multiplying the moles of the standard and the conversion factor.

$$0.00649 \text{ mol NaOH} \times \frac{1 \text{ mol H}_2\text{SO}_4}{2 \text{ mol NaOH}} = 0.00325 \text{ mol H}_2SO_4$$

Step 6) Calculate the molarity of the analyte by dividing the moles with the volume in liters of the analyte.

$$\text{Concentration of H}_2\text{SO}_4 = \frac{0.00325 \text{ mol H}_2\text{SO}_4}{0.0500 \text{ L H}_2\text{SO}_4} = 0.0649 \text{ M } H_2SO_4$$

The same calculation in a summary form is in the following.

$$\text{Concentration of } \mathrm{H_2SO_4} = \frac{0.00325 \text{ mol } \mathrm{H_2SO_4}}{0.0500 \text{ L } \mathrm{H_2SO_4}} = 0.0649 \text{ M } \mathrm{H_2SO_4}$$

$$\begin{aligned}\text{Moles of } \mathrm{H_2SO_4} = \quad & 32.3 \text{ mL NaOH} \times \frac{1 \text{ L NaOH}}{1000 \text{ mL NaOH}} \times \frac{0.201 \text{ mol NaOH}}{1 \text{ L NaOH}} \times \frac{1 \text{ mol } \mathrm{H_2SO_4}}{2 \text{ mol NaOH}} \\ & = 0.00326 \text{ mol } \mathrm{H_2SO_4}\end{aligned}$$

$$\text{Molarity of } \mathrm{H_2SO_4}: \quad M = \frac{n(\text{ mol})}{V(L)} = \frac{0.00326 \text{ mol } \mathrm{H_2SO_4}}{50.0 \text{ mL } \mathrm{H_2SO_4}} \times \frac{1000 \text{ mL } \mathrm{H_2SO_4}}{1 \text{ L } \mathrm{H_2SO_4}} = 0.0649 \text{ M } \mathrm{H_2SO_4}$$

6.8: pH Buffers

What is a pH buffer?

> A pH buffer is an aqueous solution consisting of a weak acid and its conjugate base or vice versa that lets the pH change to be minimal when a small amount of a strong acid or a strong base adds to it.

For example, the addition of 0.020 mol HCl into 1 L of water changes pH from 7 to 1.7, i.e., about an 80% change in pH. The addition of 0.020 mol NaOH to the same water changes pH from 7 to 12.3, i.e., again, about an 80% change in pH. In contrast to pure water, 1 L of buffer solution containing 0.50 mol acetic acid (CH_3COOH) and 0.50 mol CH_3COO^- -the conjugate of the acetic acid, changes pH from 4.74 to 4.70 by the addition of the same 0.020 mol HCl and from 4.74 to 4.77 by the addition of 0.020 mol NaOH, i.e., about 1% change in pH, as illustrated in Fig. 6.8.1.

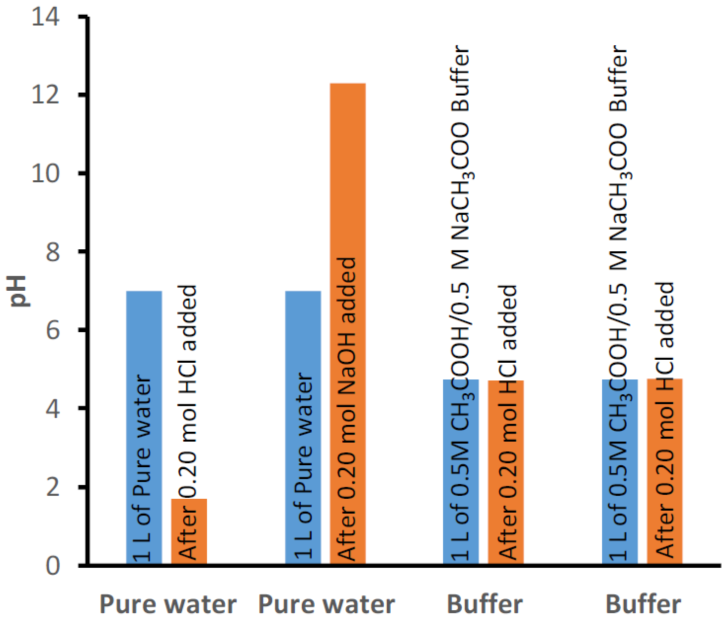


Figure 6.8.1: Effect acid and base addition on pH change of pure water at pH 7.00 and on acetic acid/sodium acetate buffer at pH 4.74.

Buffers of different initial pH values can be prepared, e.g., by varying the ratio of the weak acid to its conjugate base or by using a different set of a weak acid and its conjugate base. One example is a buffer of initial pH 4.74 comprising 0.5 M acetic acid and 0.5 M sodium acetate shown in Fig. 6.8.1. Another example is a buffer comprising 0.1M dihydrogen phosphate and 0.1M hydrogen phosphate that has an initial pH of 7.21, as shown in Fig. 6.8.2.

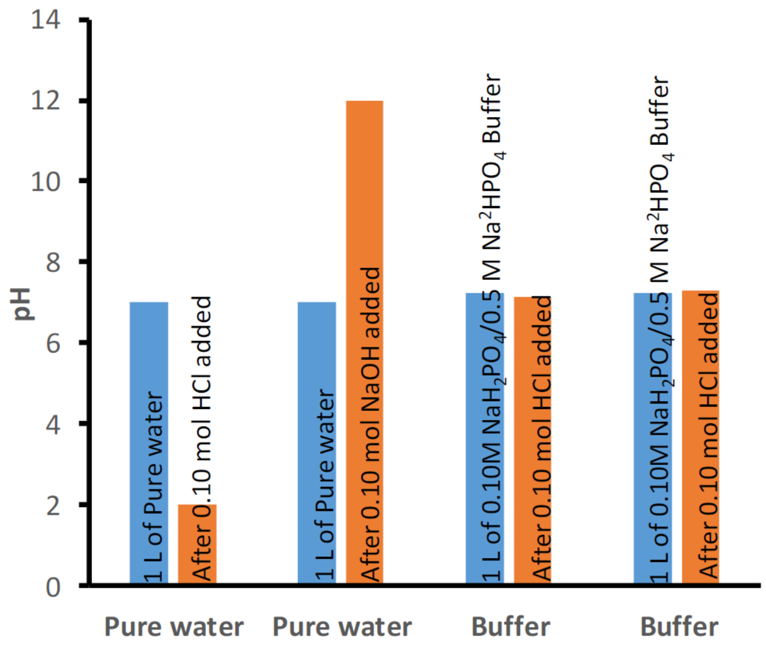


Figure 6.8.2: Effect of acid and base addition on pH change of pure water at pH 7.00 and on Na_2HPO_4/NaH_2PO_4 buffer of pH 7.21.

Buffer capacity

Buffer capacity refers to how much amount of a strong acid or a strong base the buffer can handle before a drastic change in pH happens.

Higher the amount of weak acid/conjugate base higher the buffer capacity. The buffer has an equal amount of weak acid and its conjugate base has a higher buffer capacity than the same buffer that has an unequal ratio of the acid and its conjugate base.

Caution

Strong acid and its conjugate base or a strong base and its conjugate acid do not make a buffer solution.

Mechanism of buffer action

The buffer contains a weak acid and its conjugate base in equilibrium. For example, acetic acid/sodium acetate buffer has the following equilibrium.

$$\mathrm{CH_3COOH} \rightleftarrows \mathrm{H^+} + \mathrm{CH_3COO^-}$$

The molar concentration of hydrogen ions [H^+] defines the pH of the solution. The conjugate base consumes any strong acid added.

$$\mathrm{HA} + \mathrm{CH_3COO^-} \rightarrow \mathrm{CH_3COOH} + \mathrm{A^-}$$

, where HA is any strong acid and A^- is its conjugate base. The concentration of CH_3COOH increases and CH_3COO^- decrease, but pH decreases small because [H^+] increases only a little. Similarly, the weak acid consumes any strong base added.

$$\mathrm{MOH} + \mathrm{CH_3COOH} \rightarrow \mathrm{CH_3COO^-} + \mathrm{M^+} + \mathrm{H_2O}$$

Where MOH is any strong base, and M^+ is its conjugate acid. Fig. 6.8.3 illustrates the mechanism of buffer action.

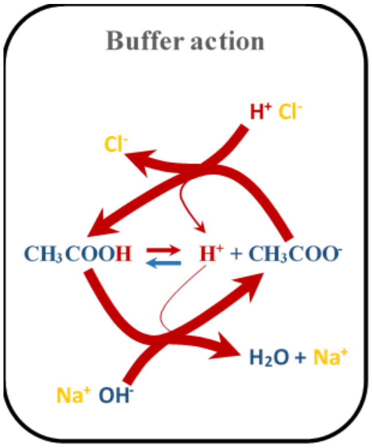


Figure 6.8.3: Mechanism of blood buffer action: The main blood buffer is H_2CO_3/HCO_3^-. Added acid is consumed by reacting with the HCO_3^- and added base is consumed by consumed by reacting with H_2CO_3, maintaining the pH ~7.4. Longs regulate the pH by regulating the rate of CO_2 exhale and kidney regulates the pH by regulating the HCO_3^- in the buffer system.

Note

Strong acid and its conjugate base mixture have no buffer action because the acid dissociates almost 100%, leaving no acid behind for the buffer action. The conjugate base of a strong acid is a very weak base that does not react with the added acids. The same explanation applies to a strong base and its conjugate acid mixture having no buffer action.

Buffers in the blood

The blood maintains its pH of ~7.4 primarily by the carbonic acid/hydrogen carbonate buffer system. The blood pH in the range of 7.45 to 7.35 is considered healthy, but outside of this range causes medical problems. If the blood pH decreases to 6.8 or increases to 8.0, death may occur. It is critical to maintain the blood pH in a narrow range for the cells to function correctly. Specifically, the enzymes and other proteins have secondary, tertiary, and quaternary structures needed for their proper functions. Hydrogen bonding plays a crucial role in defining the protein’s structure. pH changes alter the hydrogen bonding making the proteins less effective or ineffective in their functions.

Buffer systems regulate the blood pH. The primary blood buffer system is carbonic acid/hydrogen carbonate, as illustrated in Fig. 6.8.4. Metabolic processes in the cells produce carbon dioxide (CO_2) that enters the bloodstream and produces carbonic acid (H_2CO_3) by reacting with water. Kidneys supply the hydrogen carbonate (HCO_3^-) –the conjugate base of the carbonic acid and also keep a reservoir of the HCO_3^-. The H_2CO_3 consumes any base added and the HCO_3^- consumes any acid added, thus minimizing the pH change due to the added acids and bases.

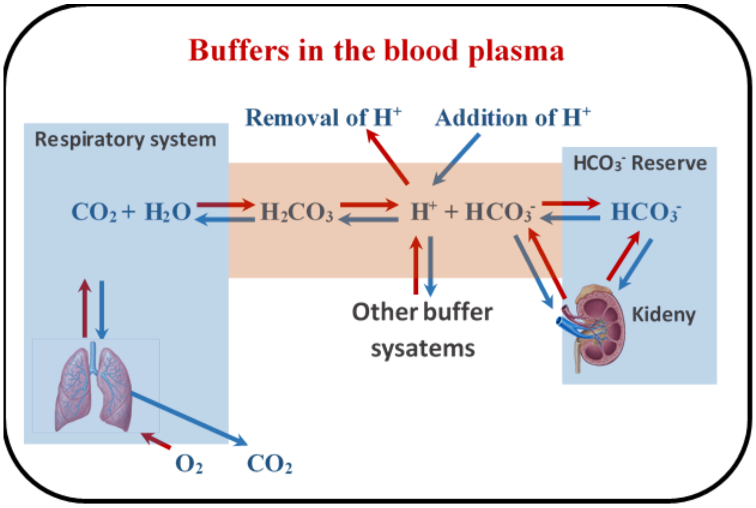


Figure 6.8.4: Mechanism of blood buffer action: The main blood buffer is H_2CO_3/HCO_3^-. Added acid is consumed by reacting with the HCO_3^- and the added base is consumed by reacting with H_2CO_3, maintaining the pH ~7.4. Longs regulate the pH by regulating the rate of CO_2 exhale and the kidney regulates the pH by regulating the HCO_3^- in the buffer system.

The primary mechanism for pH regulation by the H_2CO_3/HCO_3^- buffer in the blood is through the lungs. When the blood pH is acidic compared to the average, the breathing rate increases exhaling more CO_2 that decreases the concentration of H^+, following the blue arrows in Fig. 6.8.4, increasing the pH. The decrease in the breathing rate has the opposite effect. Kidneys also regulate the blood pH by adding or removing HCO_3^-, but the kidney's response is delayed compared to the response of the lungs.

CHAPTER OVERVIEW

7: Gases

7.1: Characteristics of gases

What is a gas

Gas is one of the four states of matter that falls between the liquid and the plasma state. The air around us is a gas composed of ~78% nitrogen (N_2), ~21% oxygen, and the remaining ~1% are other gases, including carbon dioxide, water vapors, argon, etc., as illustrated in Fig. 7.1.1.

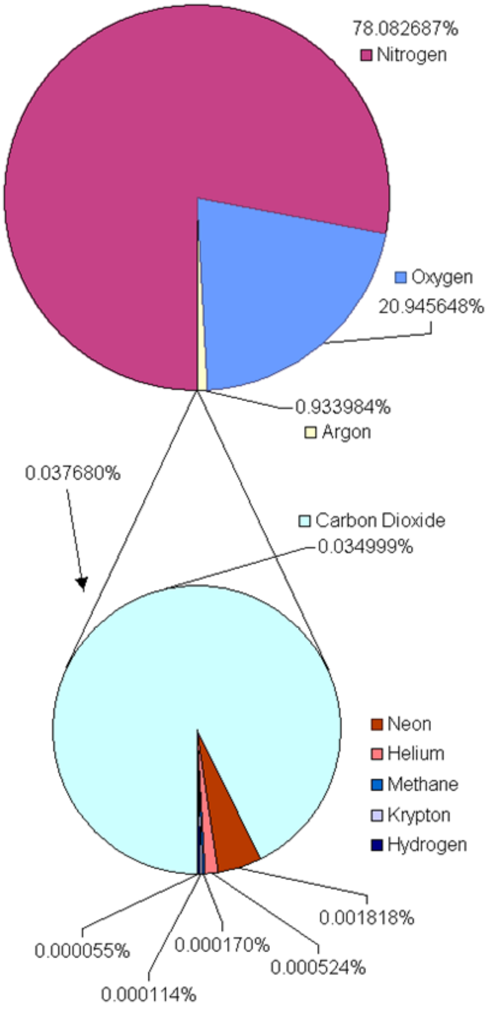


Figure 7.1.1: Depictions of the composition of the Earth's atmosphere; the lower pie represents the least common gasses that compose 0.037680% of the atmosphere. Source: Brockert at English Wikipedia / Public domain

Elements that exist as gases at room temperature and atmospheric pressure include noble gases which are monoatomic molecules including helium (He), neon (Ne), argon (Ar), krypton (Kr), xenon (Xe), and radon (Rn), and diatomic elemental molecules that include hydrogen (H_2), nitrogen (N_2), oxygen (O_2), and two halogens: fluorine (F_2) and chlorine (Cl_2). Several molecular compounds exist as gases at room temperature, e.g., carbon dioxide (CO_2), carbon monoxide (CO), methane (CH_4), nitrogen dioxide (NO_2), sulfur dioxide (SO_2), hydrogen sulfide (H_2S), ammonia (NH_3).

The properties of gases are defined by their amount in moles (n), volume (V), temperature (T), and pressure (P). These parameters are described in the following.

The amount of a gas

The amount of gas is measured in moles (n), i.e., 6.022 x 10^{23} molecules of a gas is one mole of the gas. The gas has mass and can be measured in mass units like grams or kilograms, but the mass needs to be divided by the molar mass of the gas to obtain the amount in moles for calculations.

Note

The amount of gas in moles is needed in gas laws because the properties of gases are proportional to the number of molecules, not to the masses of the molecules.

Example 7.1.1

How many moles are in 10.0 g of oxygen gas?

Solution

Step 1. Given: Mass = 10.0 g O_2, Desired: ? moles of O_2.

Step 2. Equality between the given and the desired units: 1 mole of O_2 = 32.00 g O_2.

Step 3. The conversion factors from the equality: $\frac{1\,mol\,O_2}{32.00\,g\,O_2}$ and $\frac{32.00\,g\,O_2}{1\,mol\,O_2}$

Step 4. Multiply the given quantity with the conversion factor that cancels the given and leaves the desired unit in the answer:

$$10.0\ \cancel{g\,O_2)} \times \frac{1\,mol\,O_2}{32.00\ \cancel{g\,O_2}} = 0.312\,g\,O_2$$

The volume of a gas

Volume (*V*) is the space a substance occupies. The SI unit of volume is a meter cube (m^3), i.e., the space inside of a 1m x 1m x 1m cube.

Usually, the volume is reported in liters (L), which is dm^3, or milliliter (mL), which is cm^3. The relationship between the volume units is the following.

$$1\ \mathrm{m}^3 = 1000\ \mathrm{L}$$

$$1\ \mathrm{L} = 1000\ \mathrm{mL}$$

The gases do not have a fixed shape or volume. The gases acquire the shape of the container. The gases expand or contract to fill the available space in a container.

The temperature of a gas

The temperature (*T*) is a measure of how hot or cold an object is.

The temperature is a manifestation of the thermal energy of a substance. Thermal energy is a source of heat. Heat is the flow of energy from a hot to a cold object. The SI unit of temperature is Kelvin (K) which has a value of 273.15 K at the freezing point of water and 375.15 K at the boiling point of water. The zero of the kelvin scale is called the absolute zero at which no more energy can flow out of a substance as heat. There is no negative number on the kelvin scale of temperature.

Other commonly used units of temperature are Celsius (^oC) which has a value of 0 ^oC at the freezing point of water and 100 ^oC at the boiling point of water. The relationship between temperature in kelvin (T_K) and the temperature in Celsius (T_C) is the following.

$$T_K = T_C + 273.15$$

Fahrenheit is a temperature scale used in the English system of measurement that has a value of 32 ^oF at the freezing point of water and 212 ^oF at the boiling point of water. The relationship between the temperature in Fahrenheit (T_F) and the temperature in Celsius (T_C) is the following.

$$T_F = \frac{9}{5}T_C + 32$$

Note

The temperature in Kelvin (K) is used in the gas law calculations.

The pressure of a gas

Pressure (P) is the force (F) per unit area (A), i.e., $P=\frac{F}{A}$.

The matter has mass and applies a force, which is the weight due to gravitational pull. For example, a column 1 m x 1m at sea level and height equal to the earth's atmosphere, as illustrated in Fig. 7.1.2 has a mass of ~10,000 kg. Mercury (Hg) filled in a column of 1 m x 1m and height 0.760 m has the same mass as the mass of air of 1 m x 1 m column extending from the sea level to the entire atmosphere of the earth.

Figure 7.1.2: Illustration of an air column of 1m x 1m base and height covering the entire atmosphere of the earth. Modified from: http://wikimapia.org/8706099/Norfolk.../photo/1606686

A column of air extending from sea level to the entire atmosphere applied pressure equal to one atmosphere (atm), where atm is the pressure unit. One atmosphere (atm) is equal to 760 millimeter of mercury (mmHg), where mmHg is another unit of pressure. One mmHg is also called Torr. The relationship between atm, mmHg, and Torr is the following.

$$1\text{ atm}=760\text{ mmHg}=760\text{ Torr}$$

Pascal (Pa)

The SI unit of pressure is pascal (Pa), which is pressure (P) applied by a force (F) of one newton (N) on an area of one meter square (m^2). Mathematical form of the unit is: $1\ Pascal=\frac{1\ Newton}{1\ meter-square}$ or $Pa=\frac{N}{m^2}$

Kilopascal is 1000 Pa, and kilopascal is also called the bar. The English system unit of pressure is pound-force per square inch (psi). The relationship between different units of pressure mentioned above is the following.

$$1\text{ atm}=760\text{ mmHg}=760\text{ Torr}=1.01325\times10^5\text{ Pa}=1.01325\times10^2\text{ kP}=1.01325\text{ bar}=14.7\text{ psi}$$

These relationships are changed to conversion factors that allow conversion from one to another pressure unit, as explained in the following examples.

Example 7.1.2

Express 51 mm Hg in a) atm and b) in Pa.

Solution

Given: Pressure = 51 mm Hg. Required: pressure in atm and Pa

Relationship between mm Hg and atm: $1\text{ atm}=760\text{ mmHg}$

The conversion factors from the equality: $\frac{1\text{ atm}}{760\text{ mmHg}}$ and $\frac{760\text{ mmHg}}{1\text{ atm}}$

Calculations: multiply the given quantity with the conversion factor that cancels the given unit and leaves the desired unit in the answer.

$$51\ \cancel{\text{mmHg}}\times\frac{1\text{ atm}}{760\ \cancel{\text{mmHg}}}=6.7\times10^{-2}\text{ atm}$$

Similarly, the relationship between mm Hg and Pa: $760\text{ mmHg}=1.01325\times10^{5}\text{ Pa}$

The conversion factors from the equality: $\frac{760\text{ mmHg}}{1.01325\times10^{5}\text{ Pa}}$ and $\frac{1.01325\times10^{5}\text{ Pa}}{760\text{ mmHg}}$

Calculations: multiply the given quantity with the conversion factor that cancels the given unit and leaves the desired unit in the answer.

$$51\ \cancel{\text{mmHg}}\times\frac{1.01325\times10^{5}\text{ Pa}}{760\ \cancel{\text{mmHg}}}=6.8\times10^{3}\text{ Pa}$$

Measurement of gas pressure

> The instrument used to measure the atmospheric pressure is called a barometer.

The barometer, shown in Fig. 7.1.3, was invented by Evangelista Torricelli. It is a glass tube that is more than 760 mm long and closed at one end. The glass tube is filled with mercury and inverted to dip its open end in a dish that contains a layer of mercury. The mercury falls from the tube due to its weight but stops falling when the column of mercury is 760 mm in height at sea level due to the atmospheric pressure pushing it back into the tube. Remember 760 mmHg = 1 atm. Above 760 mm is a vacuum in the tube.

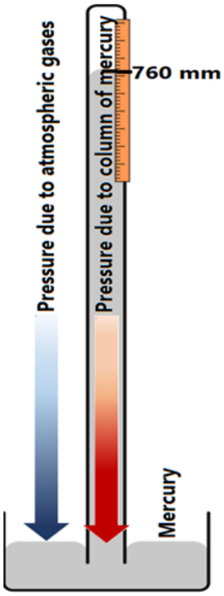


Figure 7.1.3: A mercury barometer. Modified from: Danomagnum / Public domain

> The pressure of gases in a laboratory is usually measured using an instrument called a manometer.

A manometer is a U-shaped glass tube partially filled with mercury, as shown in Fig. 7.1.4. One end of the U-tube is connected to a gas chamber in which pressure is being measured, and the other end is either closed (with a vacuum on the closed end), called a closed-ended manometer, or it is open to the atmosphere, called an open-ended manometer.

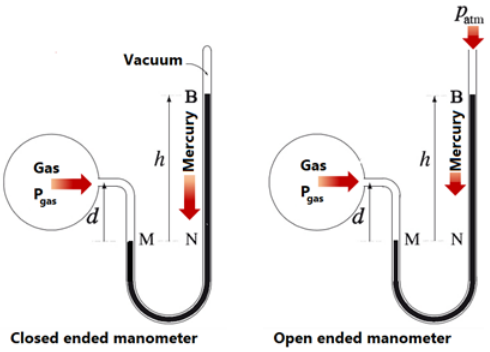


Figure 7.1.4: Manometers. Source: Modified from Algarabia / Public domain

> In the case of a closed-ended manometer, the gas pressure is equal to the difference in the height of mercury in the two arms of the U-tube in mmHg, i.e., height (*h*) from point N to point B in mm units as shown in Fig. 7.1.4.

Example 7.1.3

Calculate the pressure in atm for the gas shown in Fig. 7.1.4 in the closed-ended manometer if *h* = 40 mm?

Solution

In a closed-ended manometer, the gas pressure is equal to the height *h* in mm Hg: P = 40 mm Hg.

Pressure in atm:

$$40\ \cancel{\text{mmHg}} \times \frac{1\ \text{atm}}{760\ \cancel{\text{mmHg}}} = 5.3 \times 10^{-2}\ \text{atm}$$

In the case of an open-ended manometer, the gas pressure is equal to the difference in the height of mercury in the two arms of the U-tube in mm of Hg plus the atmospheric pressure outside expressed in mm of Hg.

Variation of air pressure with altitude

The air pressure decreases, and the gas concentration decreases as the altitude increases, as illustrated in Fig. 7.1.5. The oxygen concentration in the air also decreases as the altitude increases. That is why mountain climbers experience an inadequate supply of oxygen to the body at high altitudes -a medical condition called hypoxia.

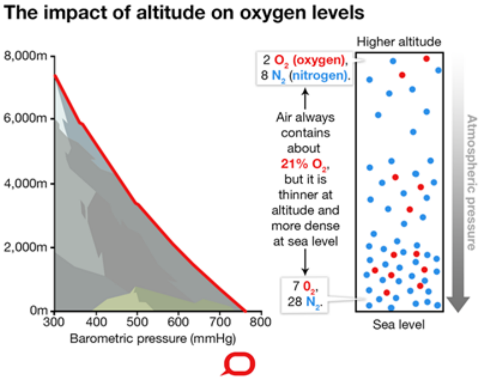


Figure 7.1.5: Air pressure decreases and the air concentration and oxygen concentration in it decreases as the altitude increases. Source: Brendan Scott/The Conversation, CC BY-ND https://images.theconversation.com/f....png?ixlib=rb-

Blood pressure

The heart pumps the blood into the circulatory system. When the heart contracts, it applies the pressure on the blood in it, and the blood pumps out of the heart into the circulatory system, as illustrated in Fig. 7.1.6. The blood pressure in the circulatory system is highest at this point, and it is called **systolic** pressure. It can be in the range of 100 to 200 mm Hg. A desirable systolic pressure range is 100 to 120 mm Hg. When heart muscles relax, the cavity in the heart expands and more blood fills in the heart. The blood pressure in the circulatory system is minimum at this point, and it is called **diastolic** pressure. The diastolic pressure may vary in the range of 60 to 110 mm Hg. A desirable diastolic pressure is less than 80 mm Hg.

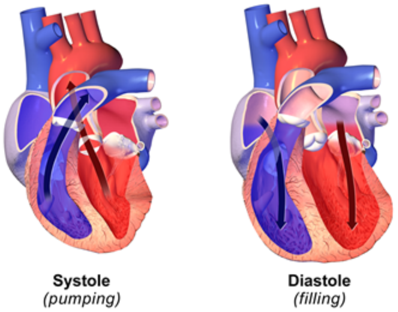


Figure 7.1.6: Diagram of heart illustrating systole, i.e., blood pumping out of heart vs Diastole i.e., blood filling into the heart. Source: BruceBlaus / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

The device used to measure blood pressure is called a **sphygmometer**. It consists of a cuff that wraps around the upper arm, a pump to inflate air in the cuff, and a stethoscope to hear the sound of blood flow, as illustrated in Fig. 7.1.7. The cuff is inflated with air to a pressure above the systolic pressure and it results in cutting off the blood flow through the brachial artery in the upper arm. A stethoscope is used to hear the sound of blood flow. No sound is heard at this point. The pressure in the cuff is slowly reduced. When the pressure in the cuff is equal to systolic pressure, the blood begins to spurt into the artery, and a tapping sound is heard through the stethoscope. At the point when the pressure is equal to the diastolic pressure, the blood flows freely through the artery, and the tapping sound disappears. The blood pressure reading is reported as a set of two numbers, e.g., 120/80, where the higher number is systolic, and the lower number is the diastolic pressure.

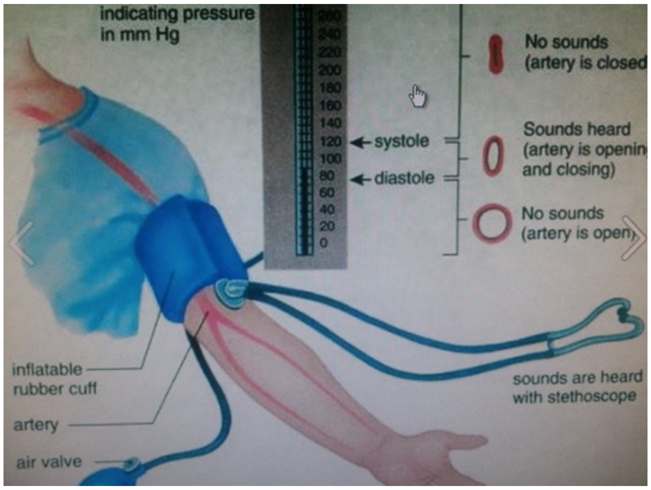


Figure 7.1.7: A healthcare professional performing blood pressure monitoring on a patient. Source: Roa'a najim / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Kinetic molecular theory of gases

The physical characteristics of the gases are explainable by a model called the **kinetic molecular theory of gases**, illustrated in Fig. 7.1.8.

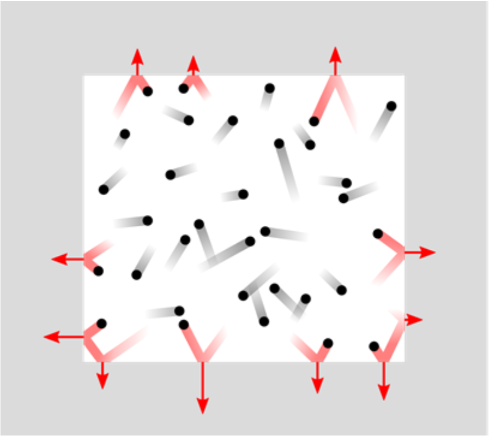


Figure 7.1.8: A model of a gas that is based on kinetic molecular theory of gases. The molecules are the spheres and the tails attached to the molecules represent the trajectories of molecular motion. The red tails represent molecules bouncing back from the wall resulting in the pressure exerted by the gas on the wall of the container. Source: Becarlson / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Postulates of kinetic molecular theory of gases

1. Gases consist of particles called molecules that are far apart from each other. As a consequence of the vast distances, the intermolecular forces are negligible, and the volume occupied by the gas molecules is negligible.
2. The gas molecules are moving in straight lines in random directions until they collide with another molecule or the wall of the container.
3. The collisions are elastic, i.e., the total energy is conserved, but the molecules change direction and change speed after the collision. It results in the distribution of molecular speeds over a wide range.
4. The average kinetic energy of the gas molecules is directly proportional to the absolute temperature. The average kinetic energy of the molecules of different gases is the same at the same temperature.

Explanation of the characteristics of the gases based on the kinetic molecular theory of gases

1. Upon exposing gas to a vacuum, the gas molecules keep moving in a straight path in the vacuum until they collide with a container boundary and bounce back. It explains gases are expandable. Collisions of gas molecules with the wall exert outward pressure on the wall and, as a reaction, the wall exerts an equal inward pressure on the gas. Applying more pressure to the gas through any portion of the gas boundary disturbs the above-mentioned balance of action and reaction forces, resulting in an inward movement of the portion of the boundary surface. In other words, the gases are compressible.
2. If a boundary separating two gases is removed, the random molecular motions ultimately mix the two gases making a homogeneous mixture, i.e., gases are entirely miscible with other gases.
3. When temperature increases the gas molecules move faster and colloid more frequently, which explains the fact that gases exert more pressure upon heating and expand if the boundary is not rigid. The more frequent bursting of tires in summer is due to the pressure increase due to heating.
4. When more gas fills in the tire, the pressure increases due to more frequent collisions. Compressing the gas into smaller volume have the same effect, i.e., the molecular collisions increase increasing the pressure.

The physical characteristics of the gases are independent of the nature of the gas molecules due to negligible intermolecular interactions but depend on four physical properties, i.e., pressure, volume, temperature, and amount of gas. The following sections describe the relationships between the physical properties of the gases.

7.2: The pressure-volume relationship

Pressure-volume relationship

Consider a gas in a cylinder with a piston pushing it down due to massive objects placed on it and due to outside air pressure, as illustrated in Fig. 7.2.1, The gas molecules strike the piston surface, applying pressure upward equal to the downward pressure applied by the piston that keeps the piston stationary. Increasing the pressure on the piston, e.g., by adding more weight to it, causes the piston to move down, reducing the gas volume. The gas molecules have less distance to travel before striking the piston surface which increases the collision frequency and causes the gas pressure to increase until becomes equal to the outside pressure.

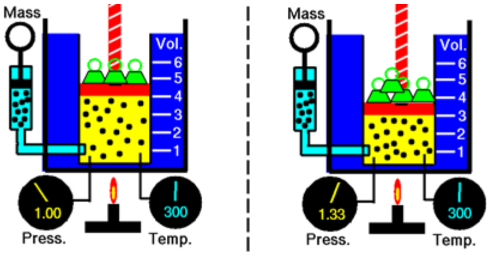


Figure 7.2.1: Illustration of Boyle's law: for a given amount of gas at a constant temperature, the volume is inversely proportional to the pressure. Source: NASA's Glenn Research Center / Public domain.

When a change in one parameter causes a change in another, the parameters are related. When an increase in one parameter causes a decrease in another, the two are inversely proportional to each other. Robert Boyle studied the quantitative relationship between the volume and pressure of the gas, keeping the quantity of gas and the temperature constant. The research concluded in a law called Boyle's law, which states that:

Boyle's law

The volume of a gas is inversely proportional to the pressure of the gas provided the temperature and the amount of the gas remain constant.

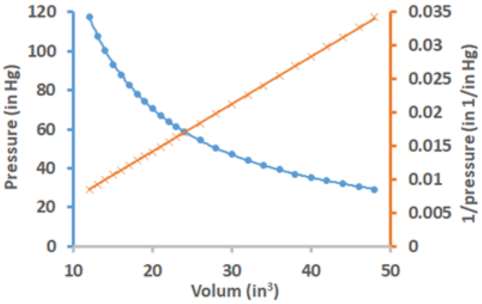


Figure 7.2.2: Boyles law: the volume of the gas is inversely proportional to the pressure of the gas. Source: Robert Boyle, *A Defence of the Doctrine Touching the Spring And Weight of the Air* (1662)

Fig. 7.2.2 illustrates the results of Boyle's experiment. The mathematical form of Boyle's law is:

$$V \propto \frac{1}{P}$$

, or

$$V = \frac{\mathrm{k}}{P}$$

, or

$$PV = \mathrm{k}$$

, where k is a consant. The graph of volume versus pressure is curvilinear, but the graph of volume versus the reciprocal of pressure is a linear graph showing the inverse proportionality between the volume and the pressure. Since the product PV is a constant, it implies that:

$$P_1V_1 = P_2V_2 = k$$

, i.e., a product of initial pressure (P_1) and initial volume (V_1) is equal to the product of final pressure (P_2) and final volume (V_2) of gas provided the quantity of the gas and temperature does not change.

✓ Example 7.2.1

The pressure of a 1.32 L sample of SO_2 gas at 0.532 atm is increased to 1.231 atm. Calculate the new volume of the gas if the temperature and the quantity of the gas remain the same?

Solution

Given: P_1 = 0.532 atm, P_2 = 1.231 atm, V_1 = 1.32 L V_2 = ?

Formula: $P_1V_1 = P_2V_2 = k$, rearrange to isolate the desired variable: $V_2 = \frac{P_1V_1}{P_2}$.

Plug in the values in the rearranged formula and calculate: $V_2 = \frac{0.532\text{ atm}\times 1.32\text{ L}}{1.231\text{ atm}} = 0.570\text{ L}$

✓ Example 7.2.2

An oxygen tank holds 20.0 L of oxygen at a pressure of 10.0 atm. What is the final pressure when the gas is released and occupies a volume of 200 L?

Solution

Given: V_1 = 20.0 L, V_2 = 200 L, P_1 = 10.0 atm P_2 = ?

Formula: $P_1V_1 = P_2V_2 = k$, rearrange to isolate the desired variable: $P_2 = \frac{P_1V_1}{V_2}$.

Plug in the values in the rearranged formula and calculate: $P_2 = \frac{10.0\text{ atm}\times 20.0\text{ L}}{200\text{ L}} = 1.00\text{ atm}$.

Breathing process

Boyle’s law explains the mechanism of the breathing process. Lungs are elastic structures like balloons placed in the thoracic cavity, as illustrated in Fig. 7.2.3. The diaphragm muscle makes a flexible floor and ribs surround the cavity.

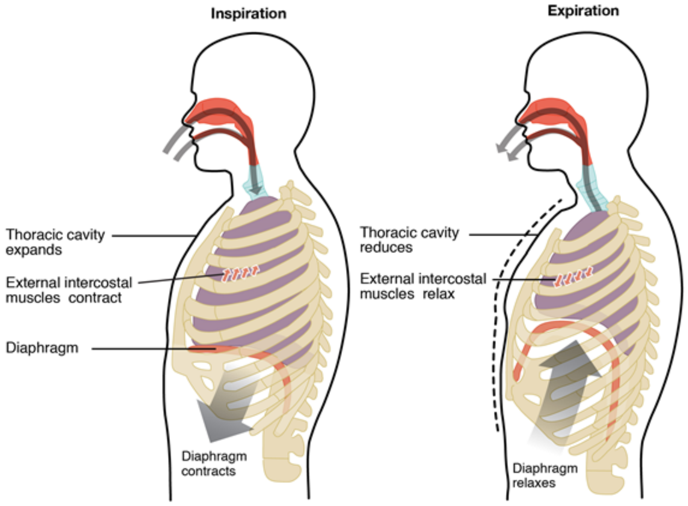


Figure 7.2.3: Illustration of breathing process –inspiration and expiration occur due to the expansion and contraction of the thoracic cavity, respectively. Source: OpenStax College / CC BY (https://creativecommons.org/licenses/by/3.0)

Inhalation

The inhalation or the inspiration process starts when the diaphragm contract and move down and the rib muscles contract, expanding the thoracic cavity. Volume increases, the air pressure decreases inside the inside thoracic cavity and the atmospheric air flows into the lungs until the pressure in the lungs is equal to the outside pressure.

Exhalation

The exhalation or the expiration process starts when the diaphragm expands and moves upwards, and the rib muscles relax, contracting the thoracic cavity. Volume decreases and the air pressure increases inside the thoracic cavity that pumps the air out of the lungs into the atmosphere.

7.3: The temperature-volume relationship

Consider a gas in a cylinder with a piston in Fig. 7.3.1. Increasing temperature increases the average kinetic energy (KE) of the gas molecules. The kinetic energy (KE) is directly proportional to the velocity of the molecules, i.e., $KE = \frac{1}{2}mv^2$, where m is the mass and v is the velocity. So, increasing temperature increases the velocity resulting in more frequent and more forceful collisions resulting in increased gas pressure inside the chamber. The gas volume starts to increase causing the pressure to decrease until the pressure inside the chamber is equal to the pressure outside. In other words, increasing temperature increases the volume of the gas if the pressure and amount of gas are not changed.

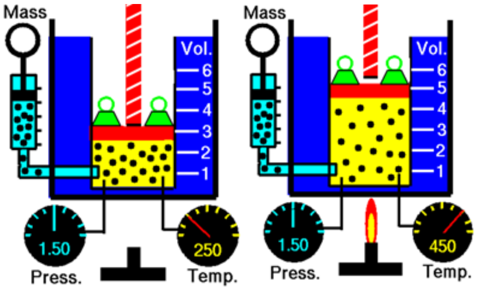


Figure 7.3.1: Increasing temperature increases the volume of the gas i.e., $\frac{V_1}{T_2} = \frac{V_2}{T_2} = \mathrm{k}$. Source: NASA's Glenn Research Center / Public domain.

If two related parameters increase or decrease together, they are directly proportional to each other.

Charles's law

Charles’s law states that the volume of a given amount of gas is directly proportional to the temperature in the Kelvin scale at constant pressure.

Fig. 7.3.2 demonstrates that the volume of a gas decreases when the gas is cooled down.

Figure 7.3.1: Air balloon (left) shrinks when its temperature is decreased by submerging in liquid nitrogen (middle) and re-expands when returned to room temperature condition (right). Source: Ryan Poling aka expictura on Flickr.https://en.Wikipedia.org/wiki/File:Nitrogen.ogv#file, CC BY 2.0

The mathematical forms of Charles’s law are the following.

$$V \propto T$$

, or

$$V = \mathrm{k}T$$

, or

$$\frac{V}{T} = \mathrm{k}$$

, where k is a constant, V is volume, and T is the temperature (in kelvin scale) of the gas. Since $\frac{V}{T}$ is a constant, it implies that

$$\frac{V_1}{T_1} = \frac{V_2}{T_2} = \mathrm{k}$$

where V_1 is the initial volume, T_1 is the initial temperature in Kelvin, V_2 is the final volume, and T_2 is the final temperature in Kelvin, provided the amount of gas and pressure do not change. Note that the kelvin scale is used in Charles’s law because the kelvin scale does not have negative numbers which means the linear curve starts from the origin without any y-intercept. If the given temperature is not in the kelvin scale, first convert the temperature to the Kelvin scale and then use the gas laws for the calculations.

✓ Example 7.3.1

A sample of CO_2 occupies 3.23 L volume at 25.0 ^oC. Calculate the volume of the gas at 50.0 ^oC if pressure and amount of gas do not change?

Solution

Given: T_1 = 25.0 ^oC + 273 = 298 K, T_2 = 50.0^oC + 273 = 323 K, V_1 = 3.23 L, V_2 = ?

Formula: $\frac{V_1}{T_1} = \frac{V_2}{T_2}$, rearrange the formula to isolate the desired variable: $V_2 = \frac{V_1 T_2}{T_1}$

Plug in the values in the rearranged formula and calculate: $V_2 = \frac{3.23\text{ L} \times 323\text{ K}}{298\text{ K}} = 3.50\text{ L}$

Charles's law explains the drifting of warm air upward in the atmosphere. As the gas is wormed, its volume increases and its density decreases which makes the gas drift upward. A hot air balloon, shown in Fig. 7.3.3 operates using hot air.

Figure 7.3.3: A hot air balloon seen from a view directly below. The burner, or flame, is firing into the envelope above. The warm air is less dense than the atmospheric air which makes the balloon rise in the air. Source: Arpingstone at English Wikipedia / Public domain.

7.4: The pressure-temperature relationship

Consider a gas in a cylinder with a piston in Figure 7.4.1. Increasing temperature increases the average kinetic energy (KE) and the average velocity of the gas molecules resulting in more frequent and more forceful collisions which result in increased gas pressure applied on the piston or the walls of the gas container.

Gay-Lussac's law

Gay-Lussac's law states that the pressure of a gas is directly proportional to the absolute temperature provided the volume and amount of gas are not changed.

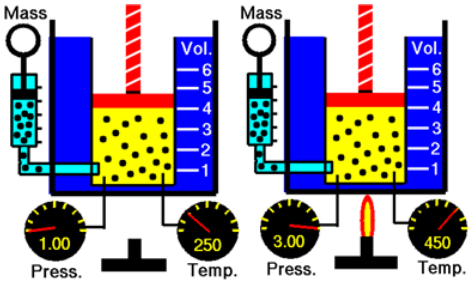


Figure 7.4.1: Increasing temperature increases pressure, i.e., $\frac{P_1}{T_1}=\frac{P_2}{T_2}$. Source: NASA's Glenn Research Center / Public domain.

The mathematical forms of Gay-Lussac's law are the following.

$$P \propto T$$

, or

$$P = \mathrm{k}T$$

, or

$$\frac{P}{T} = \mathrm{k},$$

where k is a constant, P is pressure, and T is the temperature (in kelvin scale) of the gas. Since Since $\frac{P}{T}$ is a constant, it implies that

$$\frac{P_1}{T_1} = \frac{P_2}{T_2} = \mathrm{k},$$

where P_1 is the initial pressure, T_1 is the initial temperature in Kelvin, P_2 is the final pressure, and T_2 is the final temperature in Kelvin, provided the amount of gas and volume do not change.

Example 7.4.1

The pressure of an oxygen tank containing 15.0 L oxygen is 965 Torr at 55 ^{o}C. What will be the pressure when the tank is cooled to 16 ^{o}C.

Solution

First, convert the temperatures to the Kelvin scale before applying gas laws.

Given: T_1 = 55 ^{o}C + 273.15 = 328.15 K, T_2 = 16 ^{o}C + 273.15 = 289.15 K, P_1 = 965 Torr, P_2 = ?

Formula:

$$\frac{P_1}{T_1} = \frac{P_2}{T_2},$$

rearrange the formula to isolate the desired variable:

$$P_2 = \frac{P_1 T_2}{T_1}$$

Plug in the values in the rearranged formula and calculate:

$$P_2 = \frac{965 \text{ Torr} \times 298.15 \text{ K}}{328.15 \text{ K}} = 850 \text{ Torr}$$

7.5: The combined gas law

The laws relating to pressure P, volume V, and temperature T for a constant amount n of a gas are the following:

1. If n and T are constant: $P_1V_1 = P_2V_2$, that is Boyle's law.
2. If P and n are constant: $\frac{V_1}{T_1} = \frac{V_2}{T_2}$, that is Charles's law.
3. If V and n are constant: $\frac{P_1}{T_1} = \frac{P_2}{T_2}$, that is Gay Lussac's law.

All three relationships are combined in the following law.

Combined gas law

If n is constant:

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

, that is the combined gas law.

The combined gas law allows calculating the effect of varying two parameters on the third.

Example 7.5.1

A weather balloon contains $212\ \mathrm{L}$ of helium at $25^{\circ}\mathrm{C}$ and $750\ \mathrm{mmHg}$. What is the volume of the balloon when it ascends to an altitude where the temperature is $-40^{\circ}\mathrm{C}$ and $540\ \mathrm{mmHg}$, assuming the quantity of gas remains the same?

Solution

Given and desired parameters (temperatures must be converted to Kelvin scale):

$$\begin{array}{lll} \mathrm{P_1 = 750\ mmHg}, & \mathrm{V_1 = 212\ L}, & \mathrm{T_1 = 25^{\circ}C + 273.15 = 298.15\ K} \\ \mathrm{P_2 = 540\ mmHg}, & \mathrm{V_2 = ?} & \mathrm{T_2 = -40^{\circ}C + 273.15 = 233.15\ K} \end{array}$$

Formula:

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2},$$

rearrange the formula to isolate the desired parameter:

$$V_2 = \frac{P_1V_1T_2}{T_1P_2}.$$

Calculations:

$$V_2 = \frac{750\ \cancel{\mathrm{mmHg}} \times 212\ \mathrm{L} \times 233.15\ \cancel{\mathrm{K}}}{298.15\ \cancel{\mathrm{K}} \times 540\ \cancel{\mathrm{mmHg}}} = 230\ \mathrm{L}.$$

7.6: The volume-amount relationship

Figure $7.6.1$ illustrates the effect of the amount of gas on the volume. Adding more gas molecules increases the collision frequency of the molecules with the walls increasing the gas pressure. The gas expands to reduce pressure until the pressure of gas in the chamber is equal to the outside pressure.

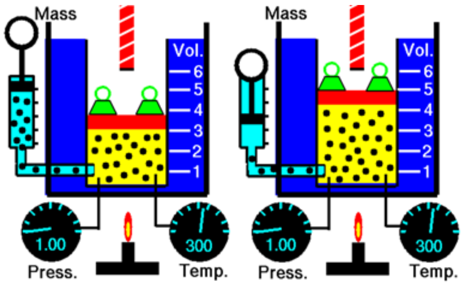


Figure $7.6.1$: When more gas is added the volume of a gas increases, i.e., $V_1/n_1 = V_2/n_2$. Source: NASA's Glenn Research Center / Public domain.

Avogadro's law

Avogadro’s law states that the volume of a gas is directly proportional to the amount of gas in moles provided the temperature and pressure of the gas are not changed.

The mathematical forms of Avogadro's law are the following.

$$V \propto n$$

or

$$V = \mathrm{k}n$$

or

$$\frac{V}{n} = \mathrm{k}$$

where V is the volume, n is the number of moles, and k is the constant for the gas under the conditions of constant temperature and pressure. Since V/n is a constant, it implies that:

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

where V_1 and n_1 is initial volume and the initial amount of gas, respectively, and V_2 and n_2 is final volume and the final amount of gas in mole, provided the temperature and pressure are not changed.

Example 7.6.1

A weather balloon containing 3.0 moles of helium has a volume of $66\ \mathrm{L}$. What is the final volume if 2.0 moles of helium is added to it. The pressure and temperature of the gas do not change?

Solution

Given $\quad V_1 = 66 L, \quad n_1 = 3.0\ \mathrm{mol}, \quad V_2 = ?, \quad n_2 = 3.0 + 2.0 = 5.0\ \mathrm{mol}$

Formula:

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

rearrange the formula to isolate the desired variable:

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

Plug in the values and calculate:

$$V_2 = \frac{66\ \text{L} \times \times 5.0\ \text{mol}}{3.0\ \text{mol}} = 110\ \text{L}.$$

7.7: Ideal gas law

Combined relationships between pressure, volume, temperature, and amount of gases

The gas laws described above give the following relationships between volume V, pressure P, the temperature in kelvin T, and the amount of gas in moles n:

$V \propto 1/P$, at constant T and n,

$V \propto T$, at constant P and n, and

$V \propto n$, at constat T and P.

The three proportionalities combine to give the following ideal gas relationship:

$$V \propto \frac{nT}{P}$$

The proportionality changes to an equation by introducing a constant of proportionality:

$$V = \frac{nRT}{P}$$

, that rearranges to

$$PV = nRT$$

where R is the proportionality constant called the **gas constant**.

Ideal gas law

The equation: $PV = nRT$ is called the ideal gas law.

The value of R can be calculated by: $R = \frac{PV}{nT}$, where n is the quantity of gas in a mole, T is the temperature in kelvin, P is the pressure that can be in various units, and V is the volume that can be in various units. The value of R in different units of P, V, and PV products are given in Table 1. If values of any three among the P, V, n, and T are known, the value of the fourth one can be calculated by using the ideal gas law.

Caution

In these calculations, the units of R should be in agreement with the units of P, V, n, and T. If they are not in agreement, the given unit of P, V, n, and T must be converted to agree with the units of R.

Table 1: The numerical values of gas constant R in various units

Value	Units
0.08206	L-atm/mol-K
8.314	J/mol-K
1.987	cal/mol-K
8.314	m^3-Pa/mol-K
62.36	L-torr/mol-K

The ideal gas equation in a rearranged form is $\frac{PV}{nT} = R$ is a constant, that implies that:

$$\frac{P_1V_1}{n_1T_1} = \frac{P_2V_2}{n_2T_2} = R$$

If one or two parameters in the ideal gas equation $\frac{P_1V_1}{n_1T_1}=\frac{P_2V_2}{n_2T_2}$ are constant; they cancel out, leaving the relationship between the remaining parameters, e.g.

if n and T are constant: $P_1V_1=P_2V_2$, that is Boyle's law,

if P and n are constant: $\frac{V_1}{T_1}=\frac{V_2}{T_2}$, that is Charles's law,

if P and T are constant: $\frac{V_1}{n_1}=\frac{V_2}{n_2}$, that is Avogadro's law,

if V and n are constant: $\frac{P_1}{T_1}=\frac{P_2}{T_2}$, that is Gay Lussac's law,

if V and T are constant: $\frac{P_1}{n_1}=\frac{P_2}{n_2}$, that is pressure-mole relationship,

and if n is constant: $\frac{P_1V_1}{T_1}=\frac{P_2V_2}{T_2}$, that is combined gas law.

Example 7.7.1

Calculate the volume of 1.000 mole of a gas in liters (L) at 0.000 ^{o}C and 1.000 atm?
Solution: Given n=1.000 mol, T= 0 ^{o}C+273.15=273.15 K, P=1.000 atm, and R=0.08206 L-atm/mol-K

Solution

Given n=1.000 mol, T= 0 ^{o}C+273.15=273.15 K, P=1.000 atm, and R=0.08206 L-atm/mol-K

Formula: $PV=nRT$, rearrange the formula to: $V=\frac{nRT}{P}$.

Plug in the values and calculate: $V=\frac{1.000\text{ mol}\times 0.08206\frac{\text{L-atm}}{\text{mol-K}}\times 273.15\text{ K}}{1.000\text{ atm}}=22.41\text{ L}$

Note

The volume of 1 mol of an ideal gas is 22.41 L at 0 ^{o}C and 1 atm pressure, as calculated in the above example

Example 7.7.2

Calculate the volume of a container that has 1.50 mol of He gas at 7.2 atm and 25 ^{o}C?

Solution

P=7.2 atm, V=? n=1.50 mol, T=25 ^{o}C}+273=298 K, R=0.08206 $\mathrm{L-atm/mol-K}$

Formula: $PV=nRT$, rearrange the formula to: $V=\frac{nRT}{P}$

Plug in the values and calculate: $V=\frac{1.50\text{ mol}\times 0.08206\frac{\text{L-atm}}{\text{mol-}K}\times 298\text{ K}}{7.2\text{ atm}}=5.1\text{ L}$

Example 7.7.3

Calculate the pressure in a 5.1 L container that has 0.60 mol of He at 25 ^{o}C?

Solution

P = ?, V=5.1 L, n = 0.60 mol, T=25 ^{o}C+273=298 K, $R=0.08206\frac{\text{L-atm}}{\text{mol-}K}$

Formula: $PV=nRT$, rearrange the formula, plug in the values and calculate: $P=\frac{nRT}{V}=\frac{0.60\text{ mol}\times 0.08206\frac{\text{L-atm}}{\text{mol-}K}\times 298\text{ K}}{5.1\text{ L}}=2.9\text{ atm}$

Example 7.7.4

Calculate the pressure of 0.60 mol of He in example 3 mixed with 1.50 mol of He in example 2 in a container of 5.1 L volume at 25 ^{o}C?**Solution**

P_{total} = ?, n_{total} = 1.5 mol + 0.60 mol = 2.1 mol, V = 5.1 L, T = 25 ^{o}C + 273 = 298 K, and $R = 0.08206\,\frac{\text{L}-\text{atm}}{\text{mol}-K}$

Formula: $P_{\text{total}}\,V = n_{\text{total}}\,RT$, rearrange, plug in the values and calculate:

$$P_{\text{total}} = \frac{n_{\text{total}}\,RT}{V} = \frac{2.1\text{ mol}\times 0.08206\,\frac{L-atm}{mol-K}\times 298\text{ K}}{5.1\text{ L}} = 10.1\text{ atm}$$

Note

The P_{total} of 2.1 mol He in example 4 is equal to P of 1.50 mole He in example 2+P of 0.6 mol He in example 3, i.e., 7.2 atm +2.9 atm =10.1 atm. This calculation demonstrates that when gases are mixed, the total pressure is the sum of the pressures that each fraction will exert if it was alone in that space. It is demonstrated by mixing the same gas, i.e., He with He, but it remains true when different gases are mixed, as long as all the gases involved obey the ideal gas law.

Molar volume of gases at standard temperature and pressure

The temperature of 0^{o}C and pressure of 1 atm is called **standard temperature and pressure (STP)** for gases.

Standard temperature and pressure

Currently accepted STP is 0^{o}C and 1 bar. The molar volume of an ideal gas at 0^{o}C and 1 bar is 22.71 L, but for most practical purposes, the older definition of STP of 0^{o}C and 1 atm is used.

The calculations in example 1 of the previous section show that the molar volume of an ideal gas is 22.41 L at STP. Fig. 7.7.1 illustrates the molar volume of an ideal gas at STP.

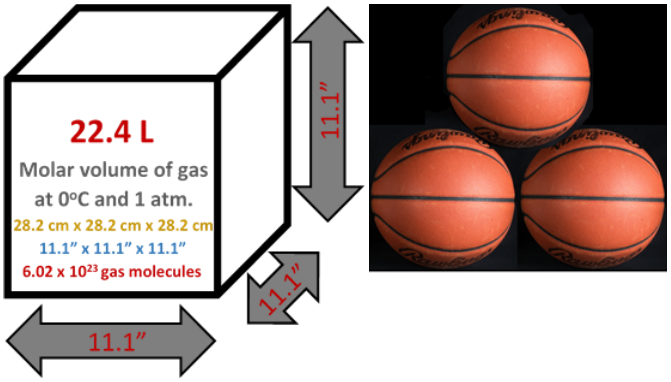


Figure 7.7.1: The molar volume of gases at STP is 22.4 L which is the volume of 11.1” x 11.1” x 11.1”, i.e., about the volume of three basketballs.

Fig. 7.7.2 shows that the molar volume of real gases is very close to that of the ideal gas. The small differences between the molar volume of real gases and the ideal gas are because ideal gas molecules are assumed to have negligible volume and negligible intermolecular interactions. The real gas molecules do have some volume and some intermolecular interactions that cause deviations of real gases from the ideal behavior. However, for practical purposes, the calculations based on ideal gas law remain applicable for the majority of real gases under ambient conditions.

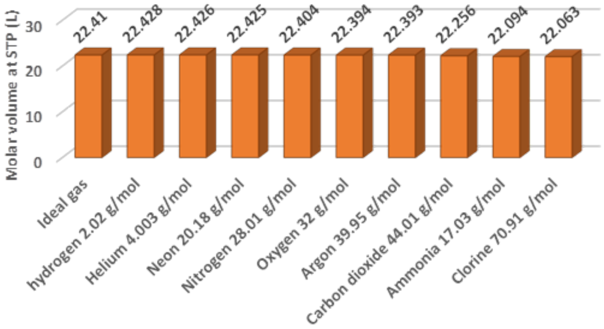


Figure 7.7.2: Comparison of molar volume of some real gases with an ideal gas at STP.

The molar volume of gases at STP is an equality between the number of moles and the volume of gas at STP, i.e.:

$$1 \text{ mol gas } = 22.4 \text{ L gas at STP}$$

The equality gives two conversion factors, i.e.,

$$\frac{1 \text{ mol gas}}{22.4 \text{ L gas}}, \text{ and } \frac{22.4 \text{ L gas}}{1 \text{ mol gas}}.$$

The conversion factors are used to convert volume to moles and mol to volume of gas, respectively, at STP.

Example 7.7.5

Calculate the volume of 64.0 g of oxygen at STP?

Solution

Given: mass of oxygen = 55.2 g. Required: volume of the oxygen =?

Strategy: 1st convert the grams of oxygen to moles of oxygen by using reciprocal of molar mass as a conversion factor and then convert the moles of oxygen to volume of oxygen by using 2nd conversion factor described above:

$$\text{volume of oxygen } = 64.0\ \cancel{\text{g oxygen}} \times \frac{1\ \text{mol}\ \cancel{\text{oxygen}}}{32\ \text{g}\ \cancel{\text{of oxygen}}} \times \frac{22.41 \text{ L}}{1\ \text{mol}\ \cancel{\text{oxygen}}} = 44.82 \text{ L oxygen}$$

7.8: Dalton’s law of partial pressure

Calculations in examples 2 and 3 of section 7.7 prove that 1.50 mol He in 5.1 L chamber exerts a pressure of 7.2 atm; 0.6 mol He in the same chamber exerts a pressure of 2.9 atm, and a mixture of the two in the same chamber at the same temperature exerts a pressure equal to the sum of the pressures that each fraction exerts if it is alone in the chamber, i.e., $P_{total} = 7.2atm + 2.9atm = 10.1atm$. What if one of the gas was hydrogen, and the other helium? The answer is: that the calculations using the ideal gas law remain the same because it is the number of molecules, not the type of molecules that are involved in the calculations. Properties of gases depend on the number of moles of gas n, and not on the nature of the gas, as illustrated in Fig. 7.8.1.

Dalton's law of partial pressure

The total pressure of a mixture of gases equals the sum of the pressure that each component gas in the mixture would exert if it was present alone.

The mathematical form of Dalton’s law is:

$$P_{\text{tatal}} = P_{\text{He}} + P_{\text{exygen}} = 9.3\text{ atm} + 2.4\text{ atm} = 11.5\text{ atm}$$

, where P_1, P_2, P_3 are partial pressures of individual gas#1, #2, #3 in the mixture.

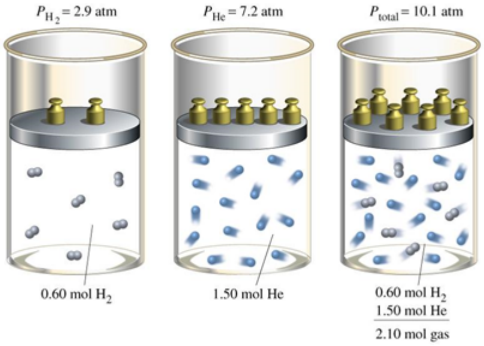


Figure 7.8.1: Illustration of Dalton’s law of partial pressures: the total pressure of a H_2+He mixture equals the sum of the pressure that of H_2 and He exert alone the same size chamber at the same temperature. Source: Dr. Blair Jesse Ellyn Reich / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Atmospheric air is a mixture of nitrogen, oxygen, argon, carbon dioxide, water vapors, and trance amount of some other gases. The atmospheric pressure is the sum of the partial pressures of components of air, as illustrated in Fig. 7.8.2.

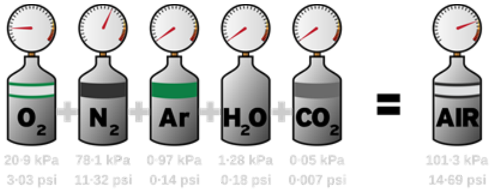


Figure 7.8.2: Partial pressures of main atmospheric constituents at sea level. Source: Andrew Jarvis / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0).

Example 7.8.1

A 46 L He and 12 L O_2 sample, both at 1.0 atm and 25 ^{o}C were pumped into a 5.0 L scuba diving tank at 25 ^{o}C. Calculate the partial pressure of each gas and the total pressure in the tank?

Solution

For He before mixing: V = 46 L, T = 25 ^{o}C + 273 = 298 K, P = 1.0 atm, n_{He}=?, $R = 0.08206\frac{L\text{–atm}}{\text{mol}-K}$

Formula and calculations: $n_{\text{He}} = \text{PV/RT} = \frac{1.0\text{ atm}\times 46\text{ L}}{0.08206\frac{\text{Latm}}{\text{mol}-\text{K}}\times 298\text{ K}} = 1.9\text{ mol}$

For O_2 before mixing: V=12 L, T =25 ^{o}C + 273 =298 K, P=1.0 atm, n_{O_2} = ?, $R = 0.08206\frac{\text{L}-\text{atm}}{\text{mol}-\text{K}}$

Formula and calculations: $n_{H_2} = \mathrm{PV/RT} = \frac{1.0\ \mathrm{atm} \times 12\ \mathrm{L}}{0.08206 \frac{\mathrm{L-atm}}{\mathrm{mol}-K} \times 298\ \mathrm{K}} = 0.49\ \mathrm{mol}$

After mixing: V=5 L, T =25 $^{\mathrm{o}}$C+273 = 298 K, n_{He}=1.9 mol, n_{O_2} =0.49 mol, $R = 0.08206 \frac{L-\mathrm{atm}}{\mathrm{mol}-K}$.
Requried: P_{He} = ?, P_{O_2}=?, and P_{total}=?

Formula: $P_{He} = \frac{n_{He}RT}{V} = \frac{1.9\ \mathrm{mol} \times 0.08206 \frac{L-atm}{\mathrm{mol}-K} \times 298\ \mathrm{K}}{5.0\ \mathrm{L}} = 9.3\ \mathrm{atm}$, $P_{O_2} = \frac{n_{\mathrm{oxygen}}\ RT}{V} = \frac{0.49\ \mathrm{mol} \times 0.08206 \frac{\mathrm{L-atm}}{\mathrm{mol}-K} \times 298\ \mathrm{K}}{5.0\ \mathrm{L}} = 2.4\ \mathrm{atm}$,

$$P_{\mathrm{total}} = P_{He} + P_{O_2} = 9.3\ \mathrm{atm} + 2.4\ \mathrm{atm} = 11.5\ \mathrm{atm}.$$

Hyperbaric chamber -a medical tool

The hyperbaric chamber is an air chamber that is at two to three atmospheric pressure, as shown in Fig. 7.8.3. The solubility of gases increases with an increase in pressure. A patient placed in a hyperbaric chamber has a higher concentration of oxygen dissolved in blood because the partial pressure of oxygen is two to three times higher than in the atmospheric air. The higher concentration of oxygen is toxic to many strains of bacteria. Therefore the hyperbaric chambers are used to treat burn patients, in surgeries, and to treat some cancers.

The hyperbaric chambers are also used to treat carbon monoxide (CO) poisoning because the higher concentration of oxygen in the chamber can displace the CO bound with hemoglobin faster than atmospheric oxygen does. Another use of hyperbaric chambers is to treat scuba divers suffering from the bends. If a diver ascends too quickly, the nitrogen dissolved in blood makes bubbles in the vessels that block the blood flow –a condition called bends. The divers suffering from the bends are placed in a hyperbaric chamber at high pressure, and then the pressure is slowly decreased to atmospheric pressure. The nitrogen dissolves in blood under higher pressure and slowly diffuses out through the lungs as the pressure is gradually decreased.

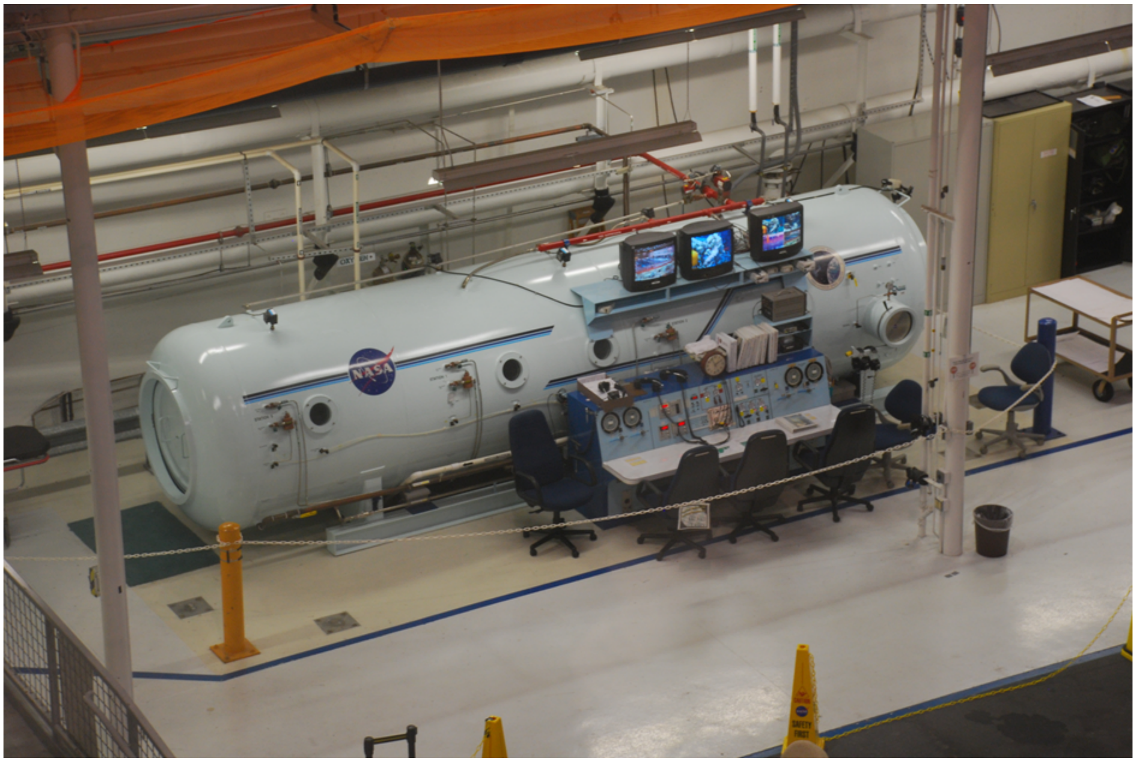


Figure 7.8.3: The hyperbaric chamber at the Neutral Buoyancy Lab. Source: Mike / CC BY (https://creativecommons.org/licenses/by/2.0)

CHAPTER OVERVIEW

8: Nuclear chemistry

8.1: Introduction to nuclear chemistry

What is a nuclear reaction?

Unlike chemical reactions that involve valence electrons, **nuclear reactions involve changes in the nucleus of an atom,** as shown in Fig. 8.1.1.

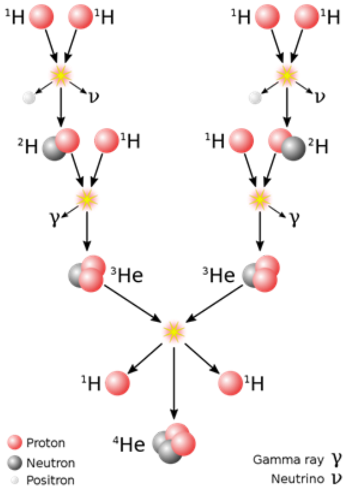


Figure 8.1.1: The proton-proton chain reaction, branch I, dominates in stars the size of the Sun or smaller. Source: Sarang, Public domain, via Wikimedia Commons

Nuclear reaction

Nuclear reactions involve changes in the nucleus of an atom. A nuclear reaction may result in one or more of the following: i) conversion of an atom to its isotope or an atom of another element, ii) conversion of mass into energy or vice versa, and iii) release of nuclear radiations.

Although nuclear reactions are less numerous than chemical reactions, they are essential in many aspects, e.g., they are the source of energy in the sun and stars and the synthesis of elements in the universe. Nuclear reactions are becoming essential in human life in the form of electricity production from nuclear power plants, a source of radioisotopes for medical imaging to visualize organs and diagnose diseases, to treat tumors, and cancerous cells, as shown in Fig. 8.1.2.

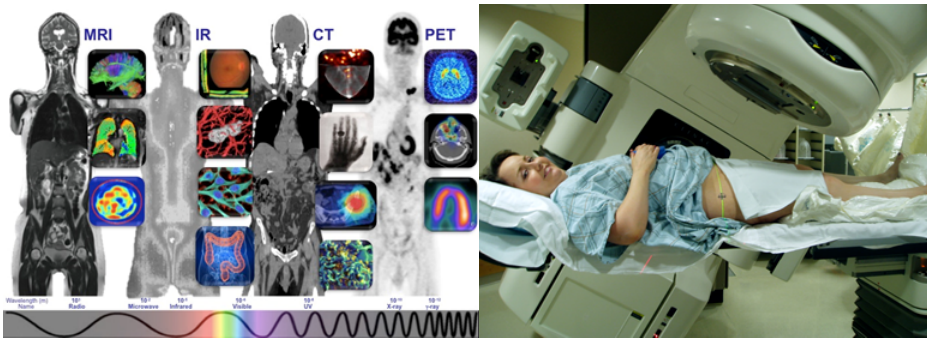


Figure 8.1.2: Spectrum of medical imaging (left) and radiation therapy of the pelvis. (right). Source: Martin Tornai, CC BY 4.0 <https://creativecommons.org/licenses/by/4.0>, via Wikimedia Commons, and Dina Wakulchik from Indianapolis, Indiana, USA / CC BY (https://creativecommons.org/licenses/by/2.0)

Nuclear nomenclature and symbols

Nucleoid

Nucleoid is another name for the nucleus of an atom, that is often used in nuclear chemistry

The composition of a nucleoid is represented by the same symbol that represents the isotopes of elements, as $^{A}_{Z}X$, where X is the element symbol, Z is the number of protons, and A is the number of protons and neutron in the nucleus. For example, carbon exists as a mixture of $^{12}_{6}C$, and $^{13}_{6}C$ isotopes. The name of the element, followed by the number of nucleons separated by a hyphen, is another way of representing a nucleoid. For example, carbon-12, carbon-13, and carbon-14 represent the carbon nucleoids having 6 protons each, but 6, 7, and 8 neutrons, respectively. Similarly, hydrogen exists as a mixture of $^{1}_{1}H$, $^{2}_{1}H$, and $^{3}_{1}H$, that can also be represented as hydrogen-1, hydrogen-2, and hydrogen-3, respectively.

Nucleons

The protons and neutrons are also called nucleons.

Nuclear reaction

> A nuclear reaction is a process in which two nuclei, or a nucleus and an external subatomic particle, collide to produce one or more new nuclides.

The nuclear reaction is a reaction that involves nucleoids. The reactant nucleoid, called the **parent nucleoid**, usually transforms into a different nucleoid called the **daughter nucleoid**. The daughter nucleoid may be an isotope of the parent nucleoid, or it may be a different element. The conversion of an isotope to another isotope of the same or a different element is a nuclear reaction that is called **transmutation** or a nuclear transformation, as shown in Fig. 8.1.3.

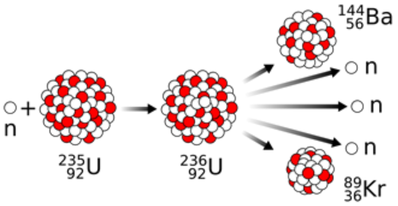


Figure 8.1.3: A nuclear fission reaction in which a partent nucleoid $^{235}_{92}U$ absorbs a neutron and transforms to a daughter nucleoid $^{236}_{92}U$, which later on transforms to two daughter nucleoids $^{144}_{56}Ba$ and $^{89}_{36}Kr$ along with emission three protons. Copy and Paste Caption here. Source: MikeRun, CC BY-SA 4.0 <https://creativecommons.org/licenses/by-sa/4.0>, via Wikimedia Commons

Nuclear radiations

> Nuclear radiation or radioactivity is the particles and energy emitted by the nucleus during a nuclear reaction.

The nuclear reaction is accompanied by the emission of nuclear radiations including high-energy electromagnetic traditions called gamma-rays (γ-rays), subatomic particles like electrons, positrons, protons, neutrons, or a small nucleus, like $^{4}_{2}He^{2+}$ called alpha-particles (α-particles). Nuclear radiations are ionizing radiations, i.e., they can knock off electrons from the atoms they come in contact with.

Radioactive

The nucleoids that are capable of spontaneous disintegration, causing the emission of nuclear radiation, are called radioactive.

> The process of emission of nuclear radiation by a spontaneous disintegration of radioactive nucleoids is called radioactivity, as illustrated in Fig. 8.1.4.

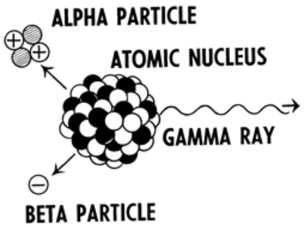


Figure 8.1.4: Illustration of radioactive decay of a nucleoid. Source: Pearson Scott Foresman, Public domain, via Wikimedia Commons

The nuclear radiations include gamma-rays (γ-rays), alpha-particles (α-particles), beta-particle (β-particles), neutrons (n), and positron ($\beta+$-particles).

Gamma-rays

The gamma-rays are electromagnetic radiations that have no mass and have energy higher than that of X-rays. The symbol γ, ${}^0_0\gamma$, or γ-ray represents a gamma-ray.

Alpha-particles

The alpha-particles (α-particles) are helium nuclei with two protons, two neutrons, and without electrons, i.e., ${}^4_2\mathrm{He}^{2+}$. The α-particles are also represented as ${}^4_2\mathrm{He}$ or Helium-4.

Beta-particles

The beta-particles (β-particles) are fast-moving electrons that have atomic number -1, charge -1, and negligible mass. The symbol β, β^-, ${}^0_{-1}\beta$, or ${}^0_{-1}\mathrm{e}$ also represents a β-particle.

Positrons

Positrons are anti-particle of electron, i.e., they have the same mass but opposite charge than that of an electron. The symbol $+\beta$, β^+, ${}^0_{+1}\beta$, or ${}^0_{+1}\mathrm{e}$ represents a positron.

8.2: Radioactivity

The cause of radioactivity

Only a particular combination of protons and neutrons forms stable nucleoids; the rest are unstable nucleoids, as illustrated in Fig. 8.2.1. The observations on the stable nucleoids are the following.

Observations on the stable nucleoids

1. Hydrogen with one proton and no neutrons is a stable nucleoid.
2. Other light nucleoids, up to atomic number 20 are usually stable when the number of protons is equal to the number of neutrons
3. The medium nucleoids from atomic numbers 20 to 82 are generally stable when the number of neutrons is more than the number of protons.
4. The heavier nucleoids with atomic number 84 or more are unstable.

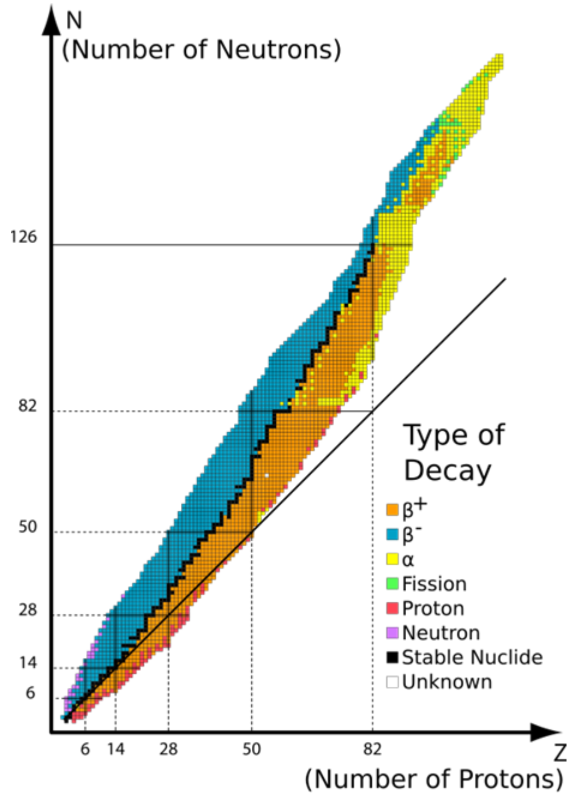


Figure 8.2.1: Graph of isotopes by type of nuclear decay. Orange and blue nuclides are unstable, with the black squares between these regions representing stable nuclides. The unbroken line passing below many of the nuclides represents the theoretical position on the graph of nuclides for which the proton number is the same as the neutron number. The graph shows that elements with more than 20 protons must have more neutrons than protons, in order to be stable. Source: Table_isotopes.svg: Napy1kenobiderivative work: Sjlegg / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

The nucleoids shown as black dots in Fig. 8.2.1 are naturally occurring stable nucleoids. All nucleoids shown in colored dots other than black are unstable.

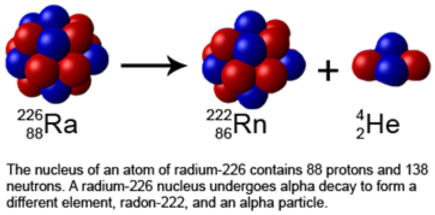
Note

The unstable nucleoids are radioactive -they spontaneously disintegrate, i.e., they tend to re-arrange the nucleon composition in the nucleus to become a more stable nucleoid.

The radioactivity releases energy and particles, i.e., nuclear radiation along with the re-arrangement of the nucleus, as explained in the following sections.

Alpha-decay

The α-emission is one of the important processes for stabilizing heavy unstable nucleoids shown with yellow dots in Fig. 8.2.1. Since the α-particle has two protons and two neutrons, the daughter nucleoid produced along with the α-decay has two fewer protons and four fewer mass numbers in it than the parent nucleoid, as illustrated in Fig. 8.2.2.



The nucleus of an atom of radium-226 contains 88 protons and 138 neutrons. A radium-226 nucleus undergoes alpha decay to form a different element, radon-222, and an alpha particle.

Figure 8.2.2: Illustration of alpha-decay process. Source: PerOX / CC0

For example:

$$^{238}_{92}\mathrm{U} \longrightarrow {}^{234}_{90}\mathrm{Th} + {}^{4}_{2}\mathrm{He}$$

Some times the α-decay is accompanied by γ-emission, e.g.:

$$^{210}_{84}\mathrm{Po} \longrightarrow {}^{206}_{82}\mathrm{Pb} + {}^{4}_{2}\mathrm{He} + \gamma$$

Note that the γ-rays have zero mass, so they do not change the atomic number and mass number of the parent nucleoid.

Steps of writing a nuclear reaction equation

1. Write the symbols of the know nucleoids, particles, and radiations in the reactants and products, separated by an arrow. Leave a question mark for the unknown pieces of information.
2. Balance the mass number on the two sides of the equation.
3. Balance the atomic number on the two sides of the equation.
4. Wright the symbols of the unknown nucleoid or particles by finding them in the periodic table, based on the atomic numbers.

α-decay in smoke detectors

Smoke detectors used in homes need α-particles for their function. Americium-241 is the α-decay-emitter used in the smoke detectors.

Example 8.2.1

Write the nuclear reaction equation for the α-decay of americium-241.

Solution

Step 1. The symbol and the atomic number of americium in the periodic table are Am and 95, respectively. So the initial equation is:

$$^{241}_{95}\mathrm{Am} \longrightarrow {}^{?}_{?}? + {}^{4}_{2}\mathrm{He}$$

Step 2. Balance the mass number on the two sides of the equation, i.e., the mass number of unknown nucleoid is 241-4 = 237:

$$^{241}_{95}\mathrm{Am} \longrightarrow {}^{237}_{?}? + {}^{4}_{2}\mathrm{He}$$

Step 3. Balance the atomic number on the two sides of the equation, i.e., the atomic number of the unknown nucleoid is 95-2 = 93:

$$^{241}_{95}\mathrm{Am} \longrightarrow {}^{237}_{93}? + {}^{4}_{2}\mathrm{He}$$

Step 4. Find the symbol of the unknown nucleoid from the periodic table of elements, i.e., the element at atomic number 93 is neptunium symbol Np:

$$^{241}_{95}\mathrm{Am} \longrightarrow {}^{237}_{93}\mathrm{Np} + {}^{4}_{2}\mathrm{He}$$

This is the balanced nuclear equation for the α-decay of americium-241 in smoke detectors.

Radium-226, present in many types of rocks and soils, is an α-emitter producing radon-226 in the process. The radon-226 is also an α-emitter that can diffuse into houses from the rocks and soil underneath the buildings. Radon is an environmental health issue in the buildings when its concentration becomes above a certain level. The nuclear equation for the α-decay of radon-222 is the following.

$$^{222}_{86}\mathrm{Rn} \longrightarrow {}^{218}_{84}\mathrm{Po} + {}^{4}_{2}\mathrm{He}$$

✓ Example 8.2.2

Write the nuclear equation for the α-decay of radium-226.

Solution

Step 1. The initial equation is:

$$^{226}_{88}\mathrm{Rn} \longrightarrow {}^{?}_{?}? + {}^{4}_{2}\mathrm{He}$$

Step 2. Balance the mass number on the two sides of the equation, i.e., is 226-4 = 222:

$$^{226}_{88}\mathrm{Rn} \longrightarrow {}^{222}_{?}? + {}^{4}_{2}\mathrm{He}$$

Step 3. Balance the atomic number on the two sides of the equation, i.e., 88-2 = 86:

$$^{226}_{88}\mathrm{Rn} \longrightarrow {}^{222}_{86}? + {}^{4}_{2}\mathrm{He}$$

Step 4. Find the symbol of the unknown nucleoid from the periodic table of elements, i.e., the element at atomic number 86 is radon symbol Rn:

$$^{226}_{88}\mathrm{Rn} \longrightarrow {}^{222}_{?}\mathrm{Rn} + {}^{4}_{2}\mathrm{He}$$

This is the balanced nuclear equation for the α-decay of radium-226 in rocks and soil.

Beta-decay

The nucleoids marked blue in Fig. 8.2.1. have more neutrons than needed for stability. They usually stabilize them by converting one of the neutrons (n) into a proton (p) and an electron (e) by the following nuclear process:

$$^{1}_{0}\mathrm{n} \longrightarrow {}^{1}_{1}\mathrm{p} + {}^{0}_{-1}\mathrm{e}$$

The proton stays in the nucleus, but the electron emits from the nucleus, as illustrated in Fig. 8.2.3. The emitted electron is called β-particle. The process of the β-particle emission is called beta-decay. Note that the neutron has zero atomic number as there is no proton in it, and the electron has a -1 atomic number to balance the +1 atomic number of the proton. Proton has +1 and electron has -1 charge, which is also balanced. The mass number of an electron is zero as it has negligible mass compared to the mass of a proton or a neutron. The electrical charges and the emission of another particle called neutrino are ignored in this equation.

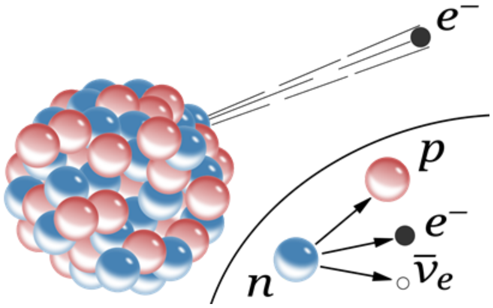


Figure 8.2.3: Illustration of beta-decay. A neutron (n) is transformed into a proton (p) in the nucleus, ejecting an electron (e⁻) and some energy as radiation. Source: Inductiveload/ Public domain

An example of β-decay is the transformation of nitrogen-16 to oxygen-17:

$$^{16}_{7}\mathrm{N} \longrightarrow {}^{16}_{8}\mathrm{O} + {}^{0}_{-1}\mathrm{e}$$

> Note that in the β-decay process, the mass number remains the same, but the atomic number increases by one in the daughter nucleus. The nuclear equation is balanced because the mass number is the same (16 = 16+0), and the atomic number is also the same (7 = 8-1) on the two sides of the equation.

Uses of some beta-emitters

Iodine-131 is used for radiation therapy of an overactive thyroid gland.

Yttrium-90 is used to treat cancer and is also injected into large joints to relieve the pain due to arthritis.

Phosphorous-32 is used to treat leukemia and other blood disorders.

Carbon-14 is used to determine the age of a fossil or an old object.

Example 8.2.3

Write the nuclear equation for the β-decay of iodine-131.

Solution

Step 1. The symbol and the atomic number of iodine in the periodic table are I and 53, respectively. So the initial equation is:

$$^{131}_{53}\mathrm{I} \longrightarrow {}^{?}_{?}? + {}^{0}_{-1}\mathrm{e}$$

Step 2. Balance the mass number on the two sides of the equation, i.e., the mass number of unknown nucleoid is 131-0 = 131:

$$^{131}_{53}\mathrm{I} \longrightarrow {}^{131}_{?}? + {}^{0}_{-1}\mathrm{e}$$

Step 3. Balance the atomic number on the two sides of the equation, i.e., the atomic number of the unknown nucleoid is 53-(-1) = 54:

$$^{131}_{53}\mathrm{I} \longrightarrow {}^{131}_{54}? + {}^{0}_{-1}\mathrm{e}$$

Step 4. Find the symbol of the unknown nucleoid from the periodic table of elements, i.e., the element at atomic number 54 is xenon symbol Xe:

$$^{131}_{53}\mathrm{I} \longrightarrow {}^{131}_{54}\mathrm{Xe} + {}^{0}_{-1}\mathrm{e}$$

This is the balanced nuclear equation for the α-decay of iodine-131 that is used to treat over-active thyroid glands.

Example 8.2.4

Write the nuclear equation for the β-decay of yttrium-90.

Solution

Step 1. The symbol and the atomic number of yttrium in the periodic table are Y and 39, respectively. So the initial equation is:

$$^{90}_{39}\mathrm{Y} \longrightarrow {}^{?}_{?}? + {}^{0}_{-1}\mathrm{e}$$

Step 2. Balance the mass number on the two sides of the equation, i.e., the mass number of unknown nucleoid is 90-0 = 90:

$$^{90}_{39}\mathrm{Y} \longrightarrow {}^{90}_{?}? + {}^{0}_{-1}\mathrm{e}$$

Step 3. Balance the atomic number on the two sides of the equation, i.e., the atomic number of the unknown nucleoid is 39-(-1) = 40:

$$^{90}_{39}\mathrm{Y} \longrightarrow {}^{90}_{40}? + {}^{0}_{-1}\mathrm{e}$$

Step 4. Find the symbol of the unknown nucleoid from the periodic table of elements, i.e., the element at atomic number 40 is zirconium symbol Z:

$$^{90}_{39}\mathrm{Y} \longrightarrow {}^{90}_{40}\mathrm{Z} + {}^{0}_{-1}\mathrm{e}$$

This is the balanced nuclear equation for the β-decay of yttrium-90.

Positron emission

The nucleoids marked orange in Fig. 8.2.1. have more protons than needed for stability. They usually stabilize them by converting one of the protons (p) into a neutron (n) and a positron $\beta+$ by the following nuclear process:

$$^{1}_{1}\mathrm{p} \longrightarrow {}^{1}_{0}\mathrm{n} + {}^{0}_{1}\mathrm{e}$$

The neutron stays in the nucleus, but the positron emits from the nucleus, as illustrated in Fig. 8.2.4. Note that the positron has a +1 mass number that balances the +1 atomic number of the proton on the other side of the equation. The positron has a +1 charge that also balances the +1 charge of the proton on the other side of the equation. The mass number of a positron is zero as it has negligible mass compared to the mass of a proton or a neutron. The electrical charges are not shown in the nuclear equation.

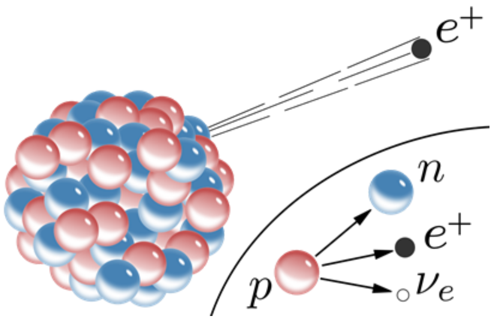


Figure 8.2.4: Illustration of positron-emission. A proton (p) is transformed into a neutron (n) in the nucleus, ejecting a positron (e^+) and some energy as radiation. Source: Master-m1000 / Public domain

Carbon-11 is an example of positron-emitter:

$$^{11}_{6}\mathrm{I} \longrightarrow {}^{11}_{5}\mathrm{B} + {}^{0}_{1}\mathrm{e}$$

> Note that in the positron-emission process, the mass number remains the same, but the atomic number decreases by one in the daughter nucleus. The nuclear equation is balanced because the mass number is the same (11 = 11+0), and the atomic number is also the same (7 = 5+1) on the two sides of the equation.

Uses of some positron emittors

Positron emission is used in positron emission tomography (PET) which is a medical imaging technique. Short-lived positron-emitting isotopes ${}^{11}C$, ${}^{13}N$, ${}^{15}O$, and ${}^{18}F$ used for positron emission tomography are typically produced by proton irradiation of natural or enriched targets described in a later section.

Fluorine-18 in fluorodeoxyglucose, abbreviated as $[{}^{18}F]$FDG is a positron emitter commonly used to detect cancer, and in $[{}^{18}F]$NaF is widely used for detecting bone formation. Other examples are oxygen-15 in $[{}^{15}O]H_2O$ used to measure blood flow and nitrogen-13 used to tag ammonia molecules for myocardial perfusion imaging.

$${}^{15}_{8}\mathrm{O} \longrightarrow {}^{15}_{7}\mathrm{N} + {}^{0}_{1}\mathrm{e}$$

$${}^{13}_{7}\mathrm{N} \longrightarrow {}^{13}_{6}\mathrm{C} + {}^{0}_{1}\mathrm{e}$$

Example 8.2.5

Write the nuclear equation for the positron-emission of fluorine-18?

Solution

Step 1. The symbol and the atomic number of fluorine in the periodic table are F and 9, respectively. So the initial equation is:

$${}^{18}_{9}\mathrm{F} \longrightarrow {}^{?}_{?}? + {}^{0}_{1}\mathrm{e}$$

Step 2. Balance the mass number on the two sides of the equation, i.e., the mass number of unknown nucleoid is 18-0 = 131:

$${}^{18}_{9}\mathrm{F} \longrightarrow {}^{131}_{?}? + {}^{0}_{1}\mathrm{e}$$

Step 3. Balance the atomic number on the two sides of the equation, i.e., the atomic number of the unknown nucleoid is 9-(+1) = 8:

$${}^{18}_{9}\mathrm{F} \longrightarrow {}^{131}_{8}? + {}^{0}_{1}\mathrm{e}$$

Step 4. Find the symbol of the unknown nucleoid from the periodic table of elements, i.e., the element at atomic number 8 is oxygen symbol O:

$${}^{18}_{9}\mathrm{F} \longrightarrow {}^{18}_{8}? + {}^{0}_{1}\mathrm{e}$$

This is the balanced nuclear equation for the positron-emission of fluorine-18.

Gamma-emission

The gamma-rays are high-energy electromagnetic radiations that do not have mass or charge. So, pure γ-emission happens from the nucleus, but it does not result in transmutation, simply the nucleoid changes from a more unstable state, called a **metastable state**, to a relatively stable state, as illustrated in Fig. 8.2.5.

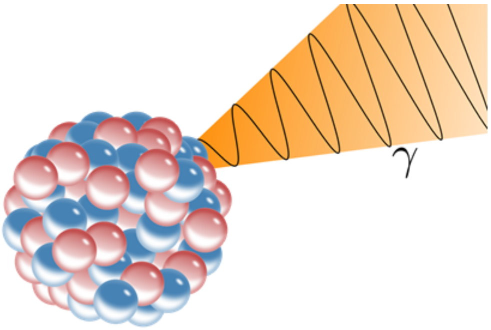


Figure 8.2.5: An illustration of gamma-emission, the γ-ray originates from the radioactive nucleus, changes the energy state but does not change the identity of the nucleoid. Source: Inductiveload / Public domain

A symbol *m* or * next to the mass number as a superscript to the right indicates the metastable state of the parent nucleoid. For example, technetium-99m is a γ-emitter widely used in medical imaging:

$${}^{99\,\mathrm{m}}_{43}\mathrm{Tc} \longrightarrow {}^{199}_{43}\mathrm{Tc} + \gamma$$

Similarly, boron-11m is a γ-emitter:

$${}^{11\,\mathrm{m}}_{5}\mathrm{B} \longrightarrow {}^{11}_{5}\mathrm{B} + \gamma$$

Note that the nucleoid remains the same after γ-emission, except for the change form metastable to a more stable state indicated by m.

Often, the γ-emission accompanies α-emission or β-emission. For example, polonium-210 decays by a simultaneous α-emission and γ-emissions.

$${}^{210}_{84}\mathrm{Po} \longrightarrow {}^{206}_{82}\mathrm{Pb} + {}^{4}_{2}\mathrm{He} + \gamma$$

Similarly, iridium-192 used in implants to treat breast cancer, and cobalt-60 used as an external radiation source for cancer treatment, simultaneously emit β and γ-rays.

$${}^{192}_{77}\mathrm{Ir} \longrightarrow {}^{192}_{78}\mathrm{Pt} + {}^{0}_{-1}\mathrm{e} + \gamma$$

$${}^{60}_{27}\mathrm{Co} \longrightarrow {}^{60}_{28}\mathrm{Ni} + {}^{0}_{-1}\mathrm{e} + \gamma$$

Iodine-131 decays to β-particle and xenon-131m that is rapidly followed by a γ-decay of xenon-131m.

$${}^{131}_{53}\mathrm{I} \longrightarrow {}^{131\,\mathrm{m}}_{54}\mathrm{Xe} + {}^{0}_{-1}\mathrm{e}$$

$${}^{131\,\mathrm{m}}_{54}\mathrm{Xe} \longrightarrow {}^{131}_{54}\mathrm{Xe} + \gamma$$

Less common forms of radioactivity

Several relatively less common forms of radioactivity are known. Some examples are the following.

1. Neutron-emission is a mode of radioactive decay in which one or more neutrons are ejected from a nucleus.
2. Proton-emission is a rare form of radioactivity in which a proton emits from a nucleoid.
3. Spontaneous fission is a radioactive process in which a more massive nucleoid breaks into smaller nucleoids, often along with the emission of smaller nuclear particles.
4. In electron-capture, an external electron is captured to react with proton and produce a neutron in the nucleus.

For example, beryllium-7 decays by electron capture, as shown in the following equation.

$${}^{7}_{4}\mathrm{Be} + {}^{0}_{-1}\mathrm{e} \longrightarrow {}^{7}_{3}\mathrm{Li} + \gamma$$

Note that the mass number remains the same, but the atomic number decreases by one in the electron-capture process.

Chromium-51, which is used for imaging the spleen, decays by the electron capture and γ-emission.

$${}^{51}_{24}\mathrm{Cr} + {}^{0}_{-1}\mathrm{e} \longrightarrow {}^{51}_{23}\mathrm{V} + \gamma$$

Summary of decay mode of radioactive nucleoids

Fig. 8.2.6 summarizes the changes in the nucleoid composition upon different radioactive events described above.

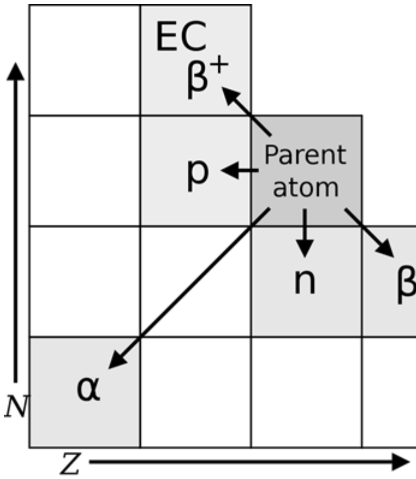


Figure 8.2.6: Transition diagram for decay modes of a radionuclide, with neutron number N and atomic number Z (shown are α, , β± are beta-particle, and positron,p+is proton, and n0 is neutron missions, EC denotes electron capture). Source: MarsRover / GFDL (http://www.gnu.org/copyleft/fdl.html)

8.3: Half-life of radioisotopes

The half-life ($t_{1/2}$) of a radioisotope is the time it takes for half of the sample to decay.

It tells the rate of decay of the radioisotope – the faster the rate of decay, the shorter the half-life.

General features of the half-life

1. The half-life is different for different nucleoids, as shown in Fig. 8.3.1, and Table 1. It varies from a fraction of a second to more than 10^{20} s, i.e., more than 3 trillion years.
2. The farther a nucleoid is away from the stable nucleoid (shown by black dots in Fig. 8.3.1), the less stable it is, and the faster it decays.
3. The half-life is independent of concentration, temperature, and pressure, i.e., the $t_{1/2}$ is a characteristic constant of a radioisotope.
4. Natural radioactive isotopes usually have a longer half-life, e.g., $t_{1/2}$ carbon-14 is 5730 years and uranium-235 is 7.0 x 10^8 years.
5. The radioisotopes used for imaging and treatment in medical sciences are usually synthesized and have a short half-life so that they may not persist in the body for an unnecessarily long time. For example, phosphorous-32, iodine-131, and technetium-99m have half-lives of 14.3 days, 8.1 days, and 6.0 hours, respectively.

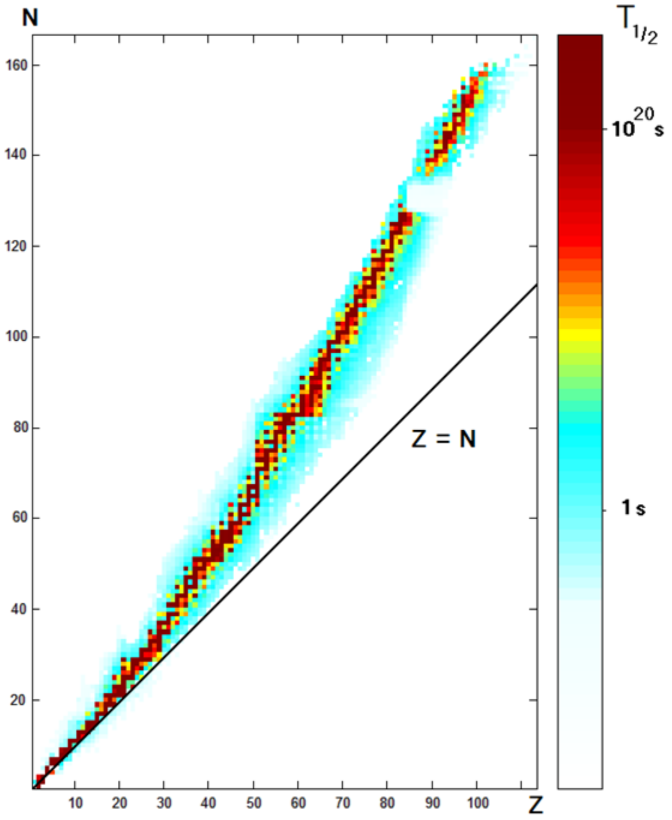


Figure 8.3.1: Graph of the stability of every known nucleoid. Plotted as Z (number of protons) versus N (number of neutrons). The color corresponds to the value of the half-life $t_{½}$ with a strong log scale, as it varies between 10^{-20} and 10^{20} seconds. Source: Fffred~commonswiki/ Public domain

Table 1: Half-lives ($t_{1/2}$) of some common radioisotopes

Radioisotope	Symbol	Half-life	Use
Carbon-14	$^{14}_{6}C$	5730 years	Radioisotope dating

Radioisotope	Symbol	Half-life	Use
Hydrogen-3	${}^{3}_{1}\mathrm{H}$	12.3 years	Radioisotope dating
Potassium-40	${}^{40}_{19}\mathrm{K}$	1.3 x 10^{9} years	Radioisotope dating
Rhenium-187	${}^{187}_{75}\mathrm{Re}$	4.3 x 10^{10} years	Radioisotope dating
Uranium-238	${}^{238}_{92}\mathrm{U}$	4.5 x 10^{9} years	Radioisotope dating
Uranium-235	${}^{235}_{92}\mathrm{U}$	7.0 x 10^{8} years	Nuclear reactor fuel
Cobalt-60	${}^{60}_{27}\mathrm{Co}$	5.3 years	Medical (external radiation source)
Iodine-131	${}^{131}_{53}\mathrm{I}$	8.1 days	Medical
Iron-59	${}^{59}_{26}\mathrm{Fe}$	45 days	Medical
Molybdenum-99	${}^{99}_{42}\mathrm{Mo}$	67 hours	Medical
Sodium-24	${}^{24}_{11}\mathrm{Na}$	15 hours	Medical
Technetium-99m	${}^{99\,\mathrm{m}}_{43}\mathrm{Te}$	6 hours	Medical
Phosphoros-32	${}^{32}_{15}\mathrm{P}$	14.3 dsys	Medical

Decay curve of radioisotopes

During each successive half-life, half of the initial amount will radioactively decay, as illustrated in Fig. 8.3.2. for the case of phosphorous-32 that decays with a half-life of 14.3 days by the following nuclear reaction

$$ {}^{32}_{15}\mathrm{P} \longrightarrow {}^{32}_{16}\mathrm{S} + {}^{0}_{-1}\mathrm{e} $$

Suppose there is 100 mg of the phosphorous-32 in the beginning; 50 mg will be left behind after 14.3 days, i.e., after 1 half-life; and 25 mg will be left after 28.6 days, i.e., after 2 half-lives. A negligible amount of the parent isotope phosphorous-32 is left after 9 half-lives.

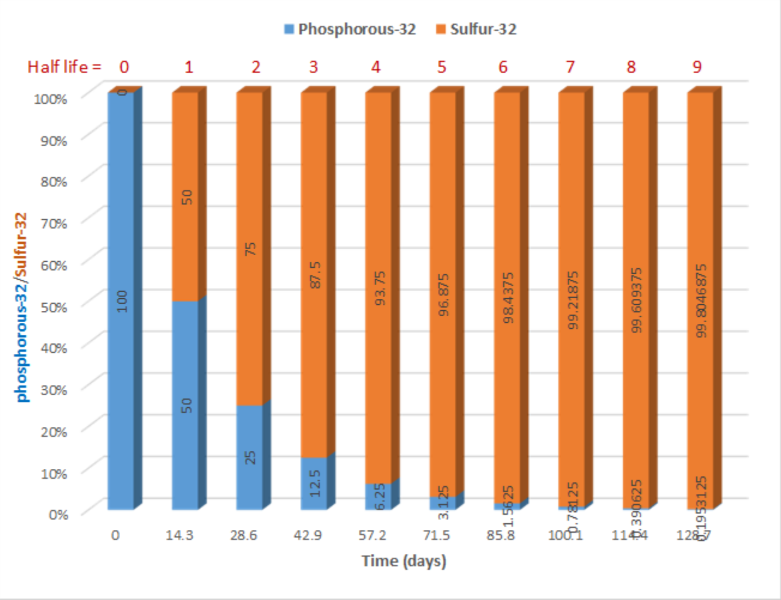


Figure 8.3.2: Decay of phosphorous-32 (blue color) and accumulation of sulfur-32 (orange color) after each half-life.

The amount of a radioisotope remaining after the given time can be calculated from the known initial amount and time spent, by the following formula:

$$ m_f = m_i (0.5)^n $$

where m_i is the initial amount, m_f is the final amount, and n is the number of half-lives passed. The formula works even if the number of half-lives is not a whole number.

✓ Example 8.3.1

If 50.0 mg of iodine-131 was injected for medical treatment, how many milligrams will be left after 40.5 days? (Half-life of iodine-131 is 8.1 days)

Solution

Given: m_i = 50.0 mg, Time = 40.5 days, Desired ? m_f

The equality: 1 half-live = 8.1 days, gives the following conversion factors.

$$\frac{1 \text{ half-life}}{8.1 \text{ days}} \quad \text{and} \quad \frac{8.1 \text{ days}}{1 \text{ half-life}}$$

For calculating the half-lives, multiple the given time with the conversion factor that cancels the time:

$$n = 40.5 \ \cancel{\text{days}} \times \frac{1 \text{ half-life}}{8.1 \ \cancel{\text{days}}} = 5 \text{ half-lives}$$

For calculating the amount left, plug in the values in the formula:

$$m_f = m_i(0.5)^n = 50.0\text{mg}(0.5)^5 = 1.56 \text{ mg}$$

Radioisotope dating

Natural radioactivity is used to establish the age of objects of archeological, anthropological, or historic interest. All living objects have carbon in their composition. Carbon-14 is a radioactive isotope of carbon with a half-life of 5730 years. Carbon-14 is produced by the transmutation of nitrogen-14 upon neutron bombardment by cosmic rays, as illustrated in Fig. 8.3.3. Its concentration in a carbon source for the living organism remains almost constant because its decay counterbalances its production by cosmic rays. Living organisms continuously replenish carbon, so the carbon-14 concentration remains almost constant as long as the object is alive. After the object dies, the carbon-14 decreases with time, reducing to half after one half-life. The carbon-12 isotope is not radioactive, so its concentration remains constant. Measurement of the carbon-14/carbon-12 ratio allows calculating the age of the object after its death. The age of early civilizations, like the Indus valley civilization examples shown in Fig. 8.3.4 were determined by the carbon-14 dating method.

Figure 8.3.4: Excavated ruins of Mohenjo-daro, Sind province of Pakistan, showing the Great Bath in the foreground. Mohenjo-daro, on the right bank of the Indus River, is a UNESCO World Heritage Site. Dated 3300 BCE to 1300 BCE. Source: Saqib Qayyum / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Because the carbon-14 decreases with time, the object older than 20,000 years of age does not have sufficient carbon-14 left to determine their age accurately. Other radioisotopes with a longer half-life, e.g., uranium-238 with a half-life of 4.5 x 10^9 years, are used to determine the age of ancient objects. For example, the age of rock samples from the moon, as shown in Fig. 8.3.5 was determined by uranium-238 radioisotope dating.

Figure 8.3.5: Lunar Olivine Basalt sample collected from the moon by the Apollo 15 mission, at station 9A on the rim of Hadley Rille. It was formed around 3.3 billion years ago. On display in the National Museum of Natural History. Source: Wknight94 talk / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

8.4: Radiation measurements

Radioactivity measurement

Radioactivity is measured in terms of the rate of radioactive events. Nuclear radiations are ionizing radiations, i.e., they knock off electrons from atoms or molecules that come in their path, leaving behind cations. Geiger Muller counter is one of the radiations measuring instruments that counts the disintegration of radionucleotide per second by registering the current produced by the ionization action of the radiation, as illustrated in Fig. 8.4.1. It is not just one ionization event; the nuclear particle keeps ionizing the atoms in its track until its energy is exhausted, as illustrated in Fig. 8.4.2. The instrument records the flash of electric current produced by the ionization of each radioactive disintegration.

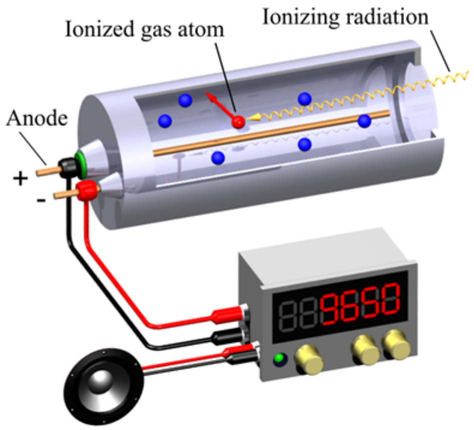


Figure 8.4.1: Geiger-Mueller counter. Source source Svjo-2 / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

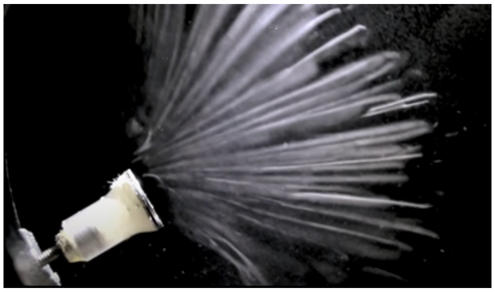


Figure 8.4.2: Tracks of α-particles from americium-241 made visible in a cloud chamber. Source: https://youtu.be/noP7HT-Uins

Becquerel (Bq)

The SI unit of radioactivity is Becquerel (Bq), i.e., the number of nuclei that disintegrate per second.

The common unit of radiation intensity is Curie (Ci), i.e., 3.7 x 10^{10} disintegrations per second. The relationship between Becquerel and Curie is the following.

$$1 \mathrm{Ci}=3.7 \times 10^{10} \mathrm{~Bq}=3.7 \times 10^{10} \text { disintegrations }$$

Often the radioisotope for medical use has the information of millicurie per milliliter (mCi/mL) from which the volume for the desired dose can be calculated.

Example 8.4.1

A patient must be given a 5.0 mCi dose of iodine-131 that is available as $Na^{131}I$ solution containing 3.8 mCi/mL. What volume of the solution should be administered?

Solution

Use the reciprocal of 3.8 mCi/mL as a conversion factor:

$$5.0 \ \cancel{\text{mCi}} \times \frac{1 \text{ mL}}{3.8 \ \cancel{\text{mCi}}} = 1.3 \text{ mL dose}$$

Radiation exposure measurements

Absorbed dose

The ionizing radiation dose or called the absorbed dose is measured in terms of energy deposited by ionizing radiation in a unit mass of matter being irradiated, as illustrated in Fig. 8.4.3

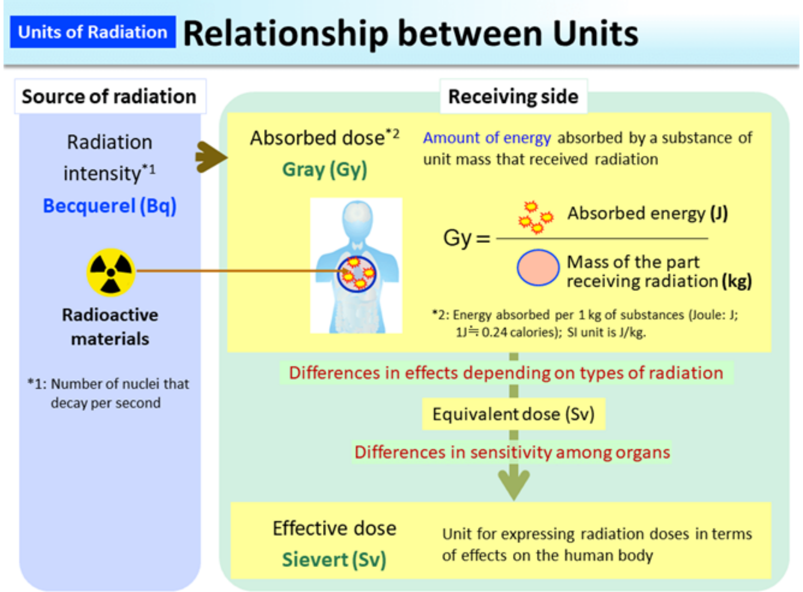


Figure 8.4.3: Source: Ministry of the Environment of Japan website, https://www.env.go.jp/en/chemi/rhm/b...g-02-03-03.png

Gray (Gy)

The SI unit of absorbed dose is gray (Gy) which is defined as the absorption of one joule of radiation energy per kilogram of matter (J/kg).

The common unit of absorbed dose is rad, which stands for radiation absorbed dose. The rad is one-hundredth of a gray, i.e.:

$$1 \text{ Gy} = 100 \text{ rad}$$

Equivalent dose

The same amount of energy deposited in tissues by different types of radiation carries different levels of health risks in terms of causing cancer and genetic damage, expressed as a radiation weighting factor (W_R), as illustrated in Fig. 8.4.4, and listed in Fig. 8.4.5. For example, 1 Gy of beta-particles carries a risk of 5.5% chances of eventually developing cancer, while 1 Gy of alpha-particles has 20 times more risk compared to the β-particle (ref.: https://en.Wikipedia.org/wiki/Sievert, accessed on 07/15/2020). The health risk of the ionizing radiation is measured in the units of equivalent dose. Sievert (Sv) is an SI unit of an equivalent dose of ionizing radiation that measures the health effects of low levels of ionizing radiation on the human body.

Sievert (Sv)

The equivalent doze in Sievert (Sv) is equal to the product of absorbed dose in grays (Gy) multiplied the radiation weighting factor (W_R), i.e., $\text{The equivalent dose in Sv} = \text{ Absorbed dose in Gy} \times W_R$

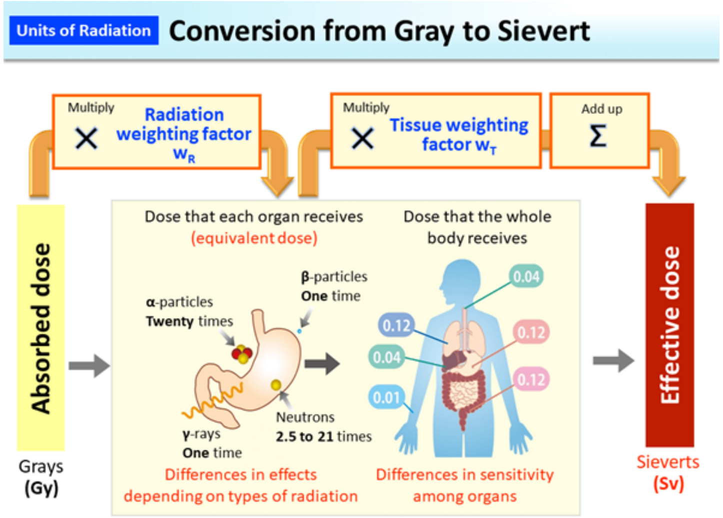
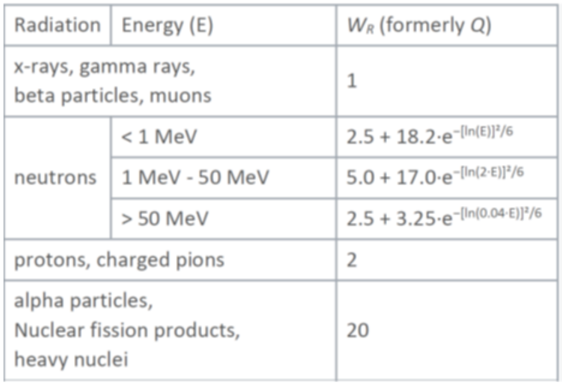


Figure 8.4.4: Illustration of radiation equivalent dose, effective dose, radiation weight factors (W_R), and tissue weighting factors (W_T). Source: Ministry of the Environment of Japan website, https://www.env.go.jp/en/chemi/rhm/b...g-02-03-04.png



Radiation	Energy (E)	W_R (formerly Q)
x-rays, gamma rays, beta particles, muons		1
neutrons	< 1 MeV	$2.5 + 18.2 \cdot e^{-[\ln(E)]^2/6}$
	1 MeV - 50 MeV	$5.0 + 17.0 \cdot e^{-[\ln(2 \cdot E)]^2/6}$
	> 50 MeV	$2.5 + 3.25 \cdot e^{-[\ln(0.04 \cdot E)]^2/6}$
protons, charged pions		2
alpha particles, Nuclear fission products, heavy nuclei		20

Figure 8.4.5: Radiation weighting factors W_R used to represent relative biological effectiveness according to ICRP report 103, Source of data: https://en.Wikipedia.org/wiki/Sievert, accessed on 07/16/2020

The common unit of equivalent dose is rem (rem stands for roentgen equivalent man), which is:

$$1 \text{ Sv} = 100 \text{rem}$$

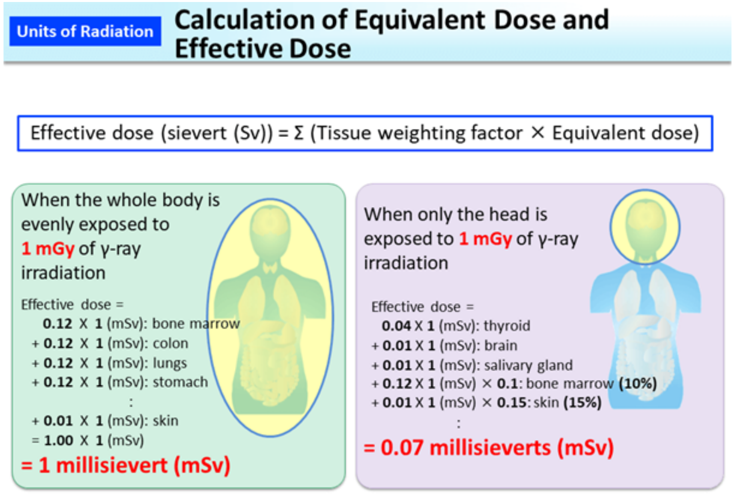
The personnel working in a radiation environment are required to wear film badges or electronic personal dosimeters, as shown in Fig. 8.4.6, that record the dose received. A record of each person's dose is usually maintained by the radiation facilities to comply with the allowed radiation exposure limits.

Figure 8.4.6: View of readout on an electronic personal dosimeter. The clip is used to attach it to the wearer's clothing. Source: Rama / CC BY-SA 2.0 FR (https://creativecommons.org/licenses...2.0/fr/deed.en)

Effective dose

The equivalent dose is equal to the effective dose in sievert (Sv) when the whole human body is exposed equally to the radiation. If part of the body is exposed, then an effective dose in sievert (Sv) is calculated by the summation of the product of equivalent dose in Sv with tissue weighting factor (W_T) for each tissue exposed to the radiation, as illustrated in Fig. 8.4.4 and calculated with example in Fig. 8.4.7. The reason for this calculation is that the effect of the same equivalent dose is different in different tissues. The tissue weighting factors (W_T) are listed in Table 1.

> An effective dose takes the absorbed dose and adjusts it for radiation type and organ sensitivity, i.e.,:
>
> $$\text{The effective dose in Sv} = \text{ Equivalent dose in Sv} \times \mathrm{W_T}$$



Units of Radiation

Calculation of Equivalent Dose and Effective Dose

Effective dose (sievert (Sv)) = Σ (Tissue weighting factor × Equivalent dose)

When the whole body is evenly exposed to **1 mGy** of γ-ray irradiation

Effective dose =
0.12 X **1** (mSv): bone marrow
\+ **0.12** X **1** (mSv): colon
\+ **0.12** X **1** (mSv): lungs
\+ **0.12** X **1** (mSv): stomach
:
\+ **0.01** X **1** (mSv): skin
= **1.00** X **1** (mSv)

= 1 millisievert (mSv)

When only the head is exposed to **1 mGy** of γ-ray irradiation

Effective dose =
0.04 X **1** (mSv): thyroid
\+ **0.01** X **1** (mSv): brain
\+ **0.01** X **1** (mSv): salivary gland
\+ **0.12** X **1** (mSv) × **0.1**: bone marrow **(10%)**
\+ **0.01** X **1** (mSv) × **0.15**: skin **(15%)**
:

= 0.07 millisieverts (mSv)

Figure 8.4.7: Example calculations of effective dose. Source: Ministry of the Environment of Japan website, https://www.env.go.jp/en/chemi/rhm/b...g-02-03-06.png

Table 1: Tissue weighting factors (W_T) ICRP103 (2007), source of data: Source: https://en.Wikipedia.org/wiki/Sievert, accessed on 07/16/2020

Organs	$\mathbf{W_T}$
Gonads	0.08
Red bone marrow	0.12
Colon	0.12
Lung	0.12
Stomach	0.12
Breasts	0.12
Bladder	0.04
Liver	0.04
Oesophagus	0.04
Thyroid	0.04
Skin	0.01
Bone surface	0.01
Salivary glands	0.01
Brain	0.01
Remainder of body	0.12
Total	1.00

8.5: Ionizing radiation exposures

Interaction of radiation with matter

The ionizing radiations knock off electrons from atoms and molecules. Water composes about 60% of the human body. The oxygen atom in water has eight valence electrons, four in the two bonding pairs, and four in the two lone pairs, as shown in Fig. 8.5.1. If one of them is knocked off by radiation, the result is a radical-cation. It is radical because it has one unpair electron and its octet is incomplete, and cation because an electron has been lost. The radical cation can then release a proton to become a hydroxyl radical. The radicals are very reactive species due to the incomplete octet. The radicals tend to react with any material around that causes damage to the tissues. Notably, the damage to DNA is the most dangerous, causing mutation, cancer, and hereditary problems.

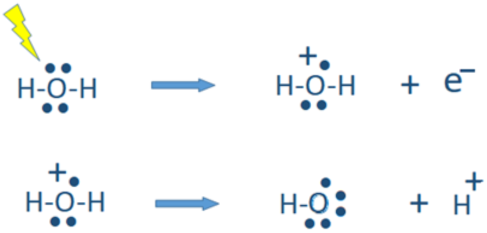


Figure 8.5.1: Ionization radiations knock off an electron from molecules like water, producing very reactive radical cations that lead to the production of very reactive radicals like hydroxyl radical in this case.

The cells that are proliferating are more susceptible to the harmful effects of radiation exposure, including bone marrow, skin, reproductive organs, and intestinal lining, as well as all the cells of growing children. If the bone marrow cells are damaged, the red blood cells may not be produced. Damage to the reproductive cells or the cells of a fetus may cause congenital disabilities. Fortunately, the cancer cells are multiplying and affected by the radiation exposure much more than the surrounding healthy cells, which allows for selectively killing the cancerous cells by radiation treatment. The use of ionizing radiations in cancer treatment is described in a later section.

Effects of radiation exposure on humans

Exposure of humans to less than 0.25 Sv usually does not have any noticeable effect. Whole-body exposure of 1 Sv results in a temporary decrease in the white blood cell counts. More than 1 Sv exposure may cause nausea, vomiting, fatigue, and a reduction in white blood cell count. More than 3 Sv doses to the whole body can decrease the white blood cell count to zero and cause diarrhea, hair loss, and infection. Exposure to 5 Sv can cause death in 50% of the people receiving the dose –it is called a lethal dose for one-half of the population (LD_{50}). Whole-body exposure of 6 Sv or higher is fatal to all humans within a few weeks. Fig. 8.5.2 illustrates the effects.

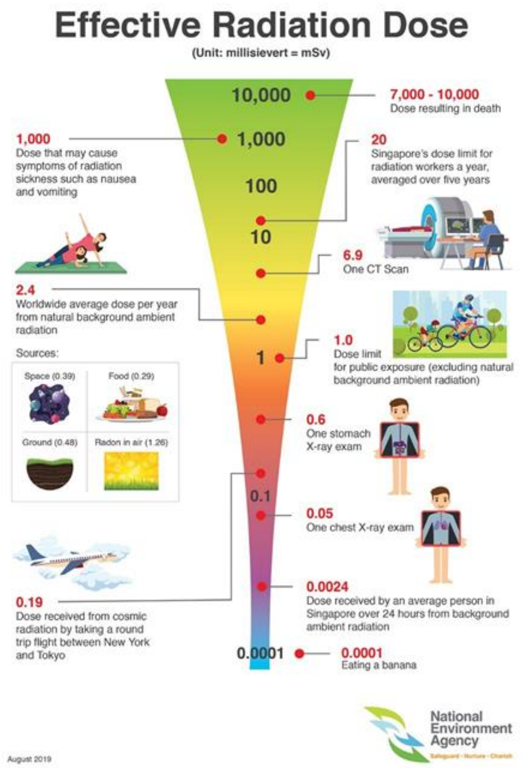


Figure 8.5.2: Health Effects of Ionising Radiation on People. Source: National Environment Agency, Open Data Licence, https://www.nea.gov.sg/our-services/...tion-on-people

Background radiation exposures

Humans are exposed to radiation in the cases of nuclear accidents, during nuclear radiation treatments, particularly for treating different forms of cancers, and during medical imaging for medical diagnostic purposes. Besides these human-made radiation exposures, humans are regularly exposed to natural sources of radiation, called background radiation. The background radiation can be in foods, e.g., potassium-40 is a naturally occurring radioactive isotope present in potassium-containing foods. Carbon-14, radon-222, strontium-90, and iodine-131 are other radioisotopes present in the air and foods around us. Radioactive isotopes of uranium and thorium and their decay products are the source of radiation in soil. The extraterrestrial sources of radiation are cosmic rays that are stopped in the upper atmosphere, but some may reach the ground and expose the people. The average annual radiation dose per person in the U.S. is 6.2 millisieverts (620 millirem).

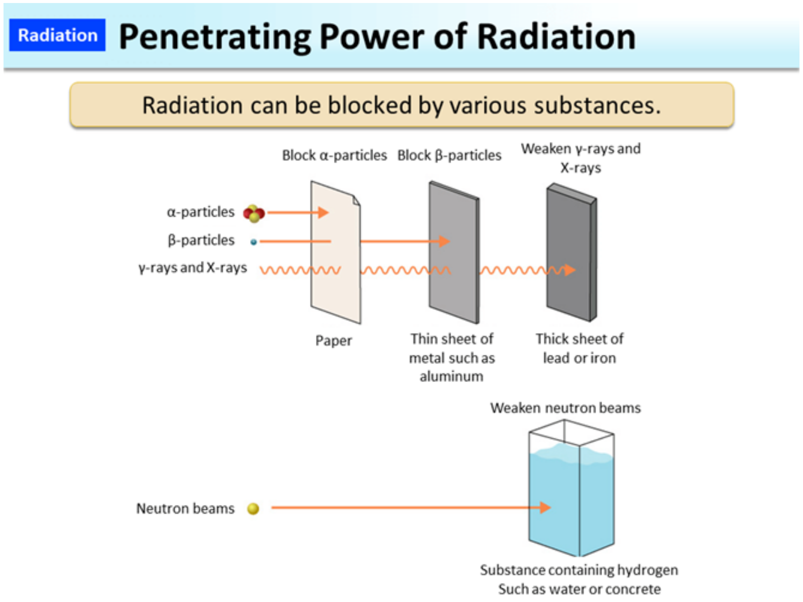


Figure 8.5.3: Source: Ministry of the Environment of Japan website, https://www.env.go.jp/en/chemi/rhm/b...g-01-03-08.png

Radiation protection

Different types of radiation have different penetration depths in the air and the human body. The α-particles are heavy with two protons and two neutrons; they cause much ionization but travel a few centimeters in air. A sheet of paper can stop the α-particles, as illustrated in Fig. 8.5.3. Exposure to α-particles from an external source affects only the outer layer of the skin. However, an internal source can cause significant damage to the nearby tissues, as illustrated in Fig. 8.5.4

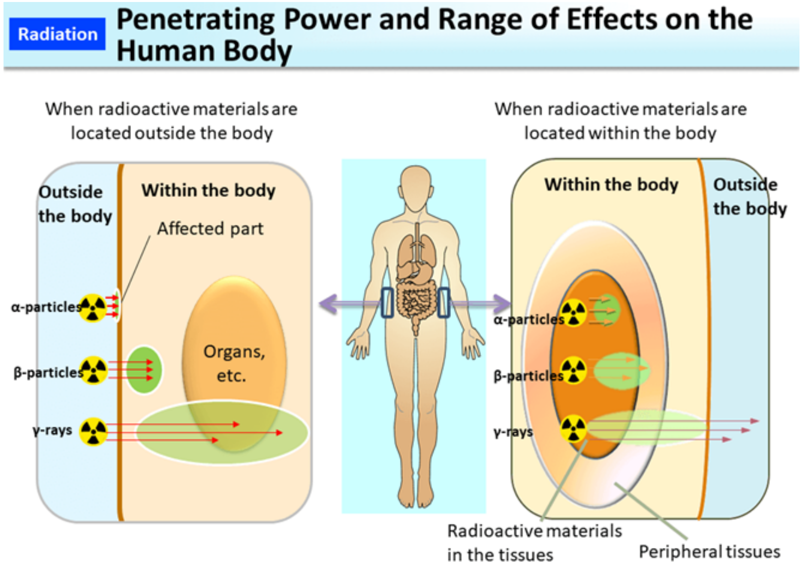


Figure 8.5.4: Source: Ministry of the Environment of Japan website, https://www.env.go.jp/en/chemi/rhm/b...g-01-03-10.png

The β-particles are fast-moving electrons that can travel several meters in the air. A 2-4 mm thick aluminum plate can stop them. The β-particles can penetrate 4 to 5 centimeters into the tissue. External exposure to the β-particles can burn the skin, but internal organs remain safe. Internal exposure to the β-particle is more dangerous than external exposure.

The γ-rays and X-rays can travel long distances in air, up to half a kilometer, and are not easily stopped by common material. A thick layer of lead or concrete shield is required to stop the γ-rays and X-rays. External exposure to the γ-rays and X-rays is the most dangerous because these rays can penetrate deep and damage the organs.

Neutrons are high-energy neutral particles that also have high penetrating power. They lose energy by colliding with atoms of substances. The most effective shielding is the water or concrete that has moisture in it to stop the neutrons effectively.

The workers in a radiation environment wear heavy clothes, gloves, and lab coats to provide additional protection. The radioactive materials are usually stored in shielded containers, even the syringes containing radioactive materials for injection are shielded. The general rules for protection against the radiation are:

Radiation protection measures

1. keep minimum possible time in the radiation environment -less the time means less exposure,
2. keep as much distance from the radiation source as possible -the radiation intensity drops inversely proportional to the square of the distance, and
3. keep shielding between you and the source of radiation as much as possible -the more the shielding the less the exposure.

8.6: Medical uses of radioisotopes

The use of nuclear chemistry in medical technologies is increasing over time. The medical uses can be divided into two categories :

1. medical imaging of organs or diagnosing any malfunction and
2. therapeutic use, mainly for killing cancerous cells.

Radioisotopes in medical imaging

Criteria of radioisotope selection for medical imaging

1. those that emit γ-rays, directly or indirectly, during their decay,
2. can be delivered to the organ of interest in pure form or tagged in a compound,
3. are short-lived or can be excreted from the body after use.

Table 8.6.1 lists some radioisotopes commonly used in medical imaging. A low dose of the radioisotope is administered to a patient. The γ-rays cross over the body and are recorded like X-rays. A computer finally converts the recording into a useful image. The image is compared with an image of a healthy organ to diagnose any malfunction.

Table 8.6.1: Some of the commonly used radioisotopes in medical imaging

Radioisotope	Symbol	Mode of decay	Half-life	Use in medical imaging
Carbon-11	${}^{11}_{6}\text{C}$	β^+, g	20.3 m	Brain scan to trace glucose
Fluorine-19	${}^{18}_{9}\text{F}$	β^+, g	109m	Brain scan to trace glucose
Chromium-51	${}^{51}_{24}\text{Cr}$	E.C., g	27.3 d	Diagnose albinism; image the spleen and gastrointestinal track
Gallium-67	${}^{67}_{31}\text{Ga}$	E.C., g	78.3 h	Whole-body scan for tumors
Selenium-75	${}^{75}_{34}\text{Se}$	E.C., g	118 d	Pancreas scan
Krypton-81m	${}^{81m}_{36}\text{Kr}$	g	13.3 s	Lung ventilation scan
Xenon-133	${}^{133}_{54}\text{Xe}$	β	5.24 d	Lung ventilation scan
Strontium-81	${}^{81}_{38}\text{Sr}$	β	22.2 m	Scan for bone cancer and bone diseases
Mercury-197	${}^{197}_{80}\text{Hg}$	E.C., g	64.1 h	Kidney scan
Iron-59	${}^{59}_{26}\text{Fe}$	β, g	44.5 d	Bone marrow function and anemias
Iodine-131	${}^{131}_{53}\text{I}$	β, g	8.04 d	Diagnosis of thyroid malfunction
Iodine-123	${}^{123}_{53}\text{I}$	E.C., g	13.2 h	Diagnosis of thyroid malfunction
Technetium-99m	${}^{99m}_{43}\text{Te}$	g	6.01 h	Brain, liver, kidney, bone scans, and diagnosis of the damaged heart muscle
Phosphorous-32	${}^{32}_{15}\text{P}$	β	14.3 d	Detect eye tumors

Radioisotope	Symbol	Mode of decay	Half-life	Use in medical imaging
Thallium-201	$^{201}_{81}\text{Tl}$	E.C., g	3.05 d	Heart scan and exercise stress test

An example of medical imaging is the thyroid gland in the neck that produces the hormone thyroxin, which controls the overall rate of metabolism in the body. Each thyroxin molecule contains four iodine atoms. Administration of radioactive Na^{131}I or Na^{123}I salt accumulates the iodine in the thyroid gland in a few hours. Decay of ^{131}I and ^{123}I involves γ-emission.

$$^{131}_{53}\text{I} \longrightarrow {}^{131}_{54}\text{Xe} + {}^{0}_{-1}\text{e} + \gamma$$

$$^{123}_{53}\text{I} + {}^{0}_{-1}\text{e} \longrightarrow {}^{123}_{52}\text{Xe} + \gamma$$

The γ-emission from the iodine localized in the thyroid gland is recorded, as shown in Fig. 8.6.1. An overactive thyroid (hyperthyroidism) cumulates more and underactive thyroid (hypothyroidism) cumulates less iodine than a healthy thyroid.

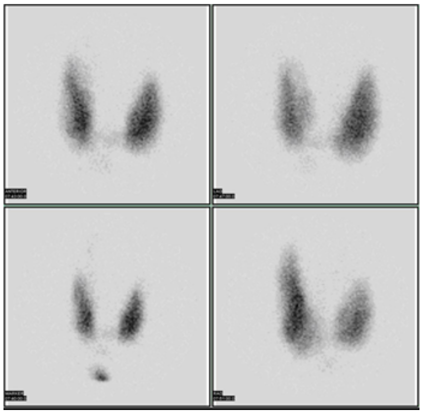


Figure 8.6.1: Thyroid scan with iodine-123 for evaluation of hyperthyroidism. Source: Myohan at en.Wikipedia / CC BY (https://creativecommons.org/licenses/by/3.0)

Another example is positron emission tomography (PET). Positron emitters like carbon-11 and fluorine-18 incorporated in a suitable compound like glucose allow following the metabolic path of the compound. For example, 18-fluorodeoxyglucose)18-FDG) is a glucose molecule in which one of the oxygen is replaced with ^{18}F. Intravenous injection of the 18-FDG ultimately results in the cumulation of 18-FDG in the brain and other body organs where glucose is used in the metabolic process. The ^{18}F emits a positron, which, being an anti-particle of the electron, reacts with the electron and produces two g γ-rays.

$$^{18}_{9}\text{F} \longrightarrow {}^{18}_{8}\text{O} + {}^{0}_{1}\text{e} + \gamma$$

$$^{0}_{1}\text{e} + {}^{0}_{1}\text{e} \longrightarrow 2\gamma$$

The γ-rays are used to obtain an image of the organ. The image reveals problem areas in the form of an abnormal concentration of glucose in the part of the organ. For example, Fig. 8.6.2 compares the PET image of a healthy brain versus a brain with Alzheimer's disease.

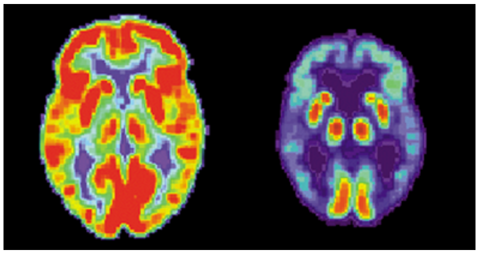


Figure 8.6.2: PET scan of brain: healthy (left) and Alzheimer's disease (right). Source: US National Institute on Aging, Alzheimer's Disease Education and Referral Center / Public domain

Since glucose metabolism happens in all organs, whole-body PET scans can be used to diagnose lung, colorectal, head and neck, and esophageal cancers as well as other diseases that involve abnormal glucose metabolism. For example, tumors have high metabolic rates; the PET scans using 18-FDG are used to detect them, as shown in Fig. 8.6.3.

File:PET-MIPS-anim.gif

Figure 8.6.3: Whole-body PET scan using ^{18}F-FDG. The normal brain and kidneys are labeled, and radioactive urine from breakdown of the FDG is seen in the bladder. In addition, a large metastatic tumor mass from colon cancer is seen in the liver. Source: Jens Maus (http://jens-maus.de/) / Public domain

Medical imaging without using radioisotopes

Major examples of medical imaging using external radiation sources include the following.

1. X-rays, which are external radiation source, is commonly used for medical imaging of organs and bones.
2. Computed tomography (CT) scan uses computer processing of many X-ray measurements, from different angles, to produce a cross-sectional view (virtual slices) of the organ.
3. Magnetic resonance image (MRI) is another powerful medical imaging technique that is based on the fact that hydrogen atoms splint into two two energy states when placed in a strong magnetic field. When illuminated with infrared (IR) radiation of the energy matching with the energy gap between the two groups, the hydrogen atoms are excited from the lower to higher energy state. The decay of the excited state emits the IR radiations that are recorded to obtain the image of soft tissues that contain many hydrogen atoms in the form of water molecules. Fig. 8.6.4 shows some examples.

Figure 8.6.4: Spectrum of medical imaging. Source: Martin Tornai, CC BY 4.0 <https://creativecommons.org/licenses/by/4.0>, via Wikimedia Commons

Radiation therapy

The purpose of radiation therapy is to selective kill the diseased cells or tissues by exposing them to radiation. Higher radiation doses are required for therapy than for imaging. The radiation source can be external or internal.

External radiation therapy

In the external irradiation, the radiation from the source, such as coba which are often used, other radiation sources are being developed, such as proton beam from the cyclotron, which have been used to kill inoperable tumors near or in the eye, skull base, or spine. Proton therapy uses a beam of proton to deliver radiation directly to the tumor.

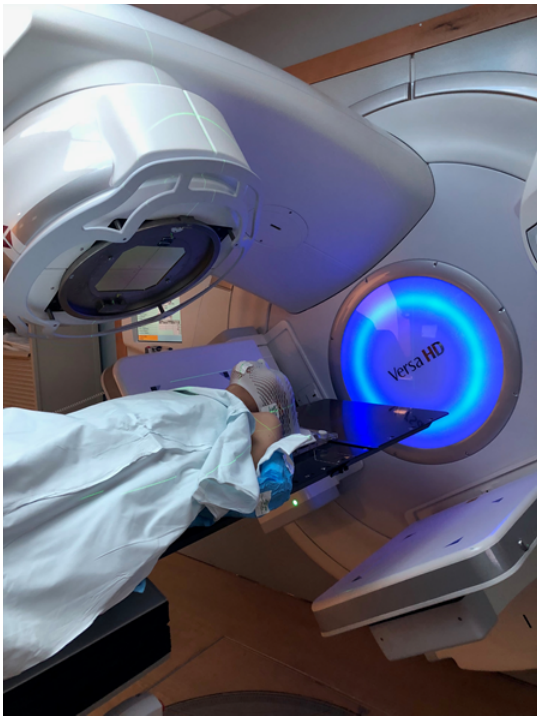


Figure 8.6.5: Radiation therapy for Hodgkin's Lymphoma in a Versa HD.. Souce: Jakembradford, CC BY-SA 4.0 <https://creativecommons.org/licenses/by-sa/4.0>, via Wikimedia Commons

Internal radiation therapy

Internal radiation therapy is used when a short-lived radioisotope can be made to selectively concentrate in the organ or tissue of interest. For example, iodine-131 is β and γ-emitter, is administered to a patient, is picked up by the thyroid gland, and is used to treat hyperthyroidism. Another example is actinium-225, which is an α-emitter with a half-life of 10 days. Actinium-225 installs in a monoclonal antibody that is attached to a prostate-specific antigen and delivered selectively to treat prostate tumors.

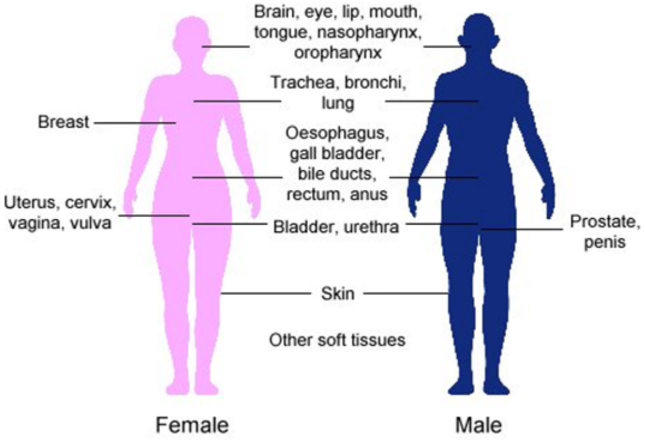


Figure 8.6.6: Body sites in which brachytherapy can be used to treat cancer. Source: Rock mc1 / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

Brachytherapy

Brachytherapy or seed implantation is a form of internal radiation treatment that delivers a high dose for a short period compared to the external radiation treatment. Fig. 8.6.6 shows the sites in the body where brachytherapy can be used to treat cancer. For example, 40 or more titanium capsules, about the size of a rice grain (Fig. 8.6.7), are implanted to treat prostate cancer. The seed contains γ-emitter like iodine-125 (half-life 60 days), palladium-103 (half-life 17 days), or cesium-131 (half-life 10 days). The seed may be left in the body because, due to the short half-life, they are no more significantly radioactive after the treatment.

Figure 8.6.7: Photo of radioactive seeds. These implants are a form of radiation therapy for prostate cancer. Source: Nuclear Regulatory Commission from US / Public domain

Another option is temporary brachytherapy, e.g., iridium-192 needles that deliver higher radiation doses are inserted to treat prostate cancer and removed after 5 to 10 min. The iridium-192 wires are also used as a follow-up treatment after breast cancer surgery to kill any residual or recurring cancer cells. The iridium-192 wires are inserted through a catheter implanted in the space from where the tumor was removed. The wires are removed after delivering the required radiation dose. The process is repeated twice a day for five days. The catheter is removed, and no radioactive material is left in the body after the treatment.

8.7: Making radioisotopes for medical uses

Natural radioisotopes usually have a long half-life and are not best suited for medical applications. The medical application usually requires short-lived radioisotopes. The radioisotopes are usually produced in nuclear reactors where particles, like α-particles, β-particles, and neutrons, are abundant. Particle accelerators, such as the one shown in Fig. 8.7.1 also accelerate and direct the nuclear particles at the targets. The high-energy nuclear particles may be absorbed by and transmute the target nuclei to radioisotopes in a nuclear reaction.

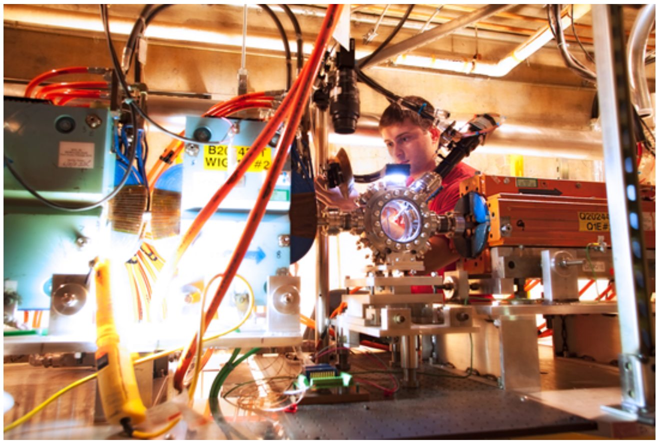


Figure 8.7.1: SLAC's particle accelerator may be two miles long, but researchers at FACET are working to develop more compact versions that could be widely used in medicine and industry -- particle accelerators are used for cancer research, processing computer chips, and even producing the shrink wrap used to keep your Thanksgiving turkey fresh. Source: ENERGY.GOV / Public domain

Radioisotopes in medical applications are usually produced by the particle bombardment method. One reaction that happens naturally by neutron bombardment from cosmic rays on nitrogen-14 is the following.

$$^{14}_{7}\mathrm{N} + ^{1}_{0}\mathrm{n} \longrightarrow ^{14}_{6}\mathrm{C} + ^{1}_{1}\mathrm{p}$$

An example of an artificial nuclear reaction initiated by α-particle bombardment on nitrogen, observed by Rutherford that lead to the discovery of proton, is illustrated in Fig. 8.7.2.

$$^{4}_{2}\mathrm{He} + ^{14}_{7}\mathrm{N} \longrightarrow ^{17}_{8}\mathrm{O} + ^{1}_{1}\mathrm{p}$$

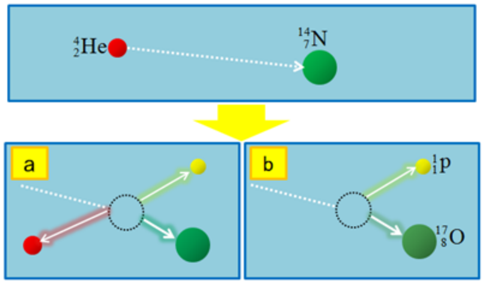


Figure 8.7.2: A nuclear reaction observed by Rutherford using a cloud chamber. When an alpha ray strikes nitrogen, reaction "a" (proton knock-off) does not occur; reaction "b" (α-p) occurs.). Source: アリオト / Public domain

Another example is the nuclear reaction initiated by α-particles on beryllium, observed by James Chadwick, which lead to the discovery of the neutron.

$$^{4}_{2}\mathrm{He} + ^{9}_{4}\mathrm{Be} \longrightarrow ^{12}_{6}\mathrm{C} + ^{1}_{0}\mathrm{n}$$

An example of radioisotope production for medical uses is the following. Gold-198, used as a tracer in the liver, is produced by neutron bombardment on gold-197.

$$^{197}_{79}\mathrm{Au} + ^{1}_{0}\mathrm{n} \longrightarrow ^{198}_{79}\mathrm{Au}$$

Similarly, gallium-67 used in medical diagnostics is produced by proton bombardment on zinc-66.

$$ {}_{30}^{66}\mathrm{Zn} + {}_{1}^{1}\mathrm{p} \longrightarrow {}_{31}^{67}\mathrm{Ga} $$

Molybdenum-99 is a radioactive isotope produced in a nuclear reactor by neutron bombardment of molybdenum-98.

$$ {}_{42}^{98}\mathrm{Mo} + {}_{0}^{1}\mathrm{n} \longrightarrow {}_{42}^{99}\mathrm{Mo} + \gamma $$

Molybdenum-99 is also produced as a fission product of uranium-235. Molybdenum-99 decays to technetium-99m that has several uses in nuclear medical imaging and treatment.

$$ {}_{42}^{99}\mathrm{Mo} \longrightarrow {}_{43}^{99\,\mathrm{m}}\mathrm{Tc} + {}_{-1}^{0}\mathrm{e} $$

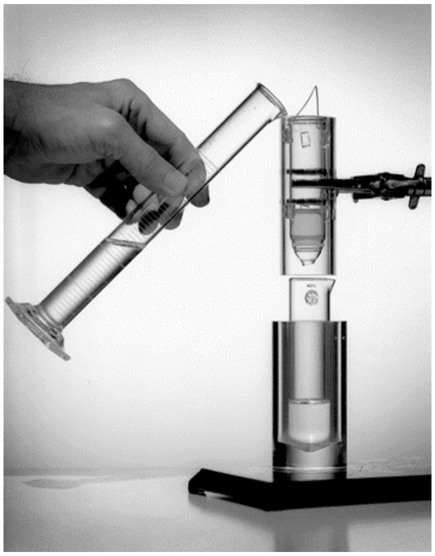


Figure 8.7.1: The first technetium-99m generator developed at Brookhaven National Laboratory, circa 1958, shown without shielding. A Tc-99m pertechnetate solution is being eluted from Mo-99 molybdate bound to a chromatographic substrate. Source: Brookhaven National Laboratory. / Public domain

Technetium-99m is short-lived (half-life 6 h), and needs to be produced in the hospital to minimize its decay during the transport. Its parent molybdenum-99 has a half-life of 66h and can be transported without significant decay during the transport. Molybdenum-99/technetium-99m generators are supplied to the hospitals in a shielded container. Fig. 8.7.3 illustrates the first Molybdenum-99/technetium-99m generator developed at Brookhaven National Laboratory. Molybdate (MoO_4^{2}) ion is adsorbed onto alumina adsorbent in a column. When molybdenum-99 decays to technetium-99m, the ion change to pertechnetate (TcO_4^{-}), which is less tightly bound to the alumina. Pouring a saline solution through the column elutes the technetium-99m as TcO_4^{-} ion, which is then used for medical purposes in the hospitals.

Destruction of an inoperable tumor has also been tested by α-emission from boron-10 upon neutron bombardment.

$$ {}_{0}^{1}\mathrm{n} + {}_{5}^{10}\mathrm{B} \longrightarrow {}_{4}^{7}\mathrm{Li} + {}_{2}^{4}\mathrm{He} $$

8.8: Nuclear fusion and fission

Conversion of matter into energy in nuclear reactions

When free nucleons come together to make a nucleoid, they release energy equal to the nuclear binding energy. The energy is produced at the expense of the mass of the nucleons following the famous Einstein equation:

$$E = mc^2$$

, where E is the energy, m is the mass, and c is the speed of light. In other words, the mass of nucleons in nucleoids is slightly less than the mass of the free nucleons, as some of their mass is released as nuclear binding energy.

The nuclear binding energy per nucleon is different for different nucleoids, as shown in Fig. 8.8.1. The composition of nucleoids changes during the nuclear reaction, and the difference in the nuclear binding energy is released as energy during the process, which is the source of energy in the sun, stars, nuclear power plants, and nuclear weapons.

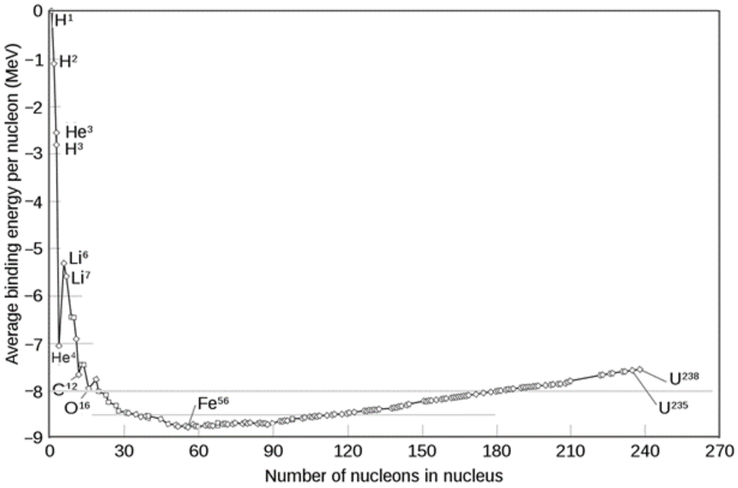


Figure 8.8.1: Graph of the binding energy released by an atom as a function of its nucleons, the energy is in megaelectron volts (MeV) where 1 Mev = 1.60218 10^{-13} J. Source: Modified from Fastfission/ Public domain

The most stable nucleoid with the highest average binding energy per nucleon is iron-56.

Nuclear fusion

The lighter nucleoids tend to combine and make heavier nucleoids that are more stable and lease a tremendous amount of energy –a process called nuclear fusions.

Nuclear fission

The heavier nucleoids, particularly those having a mass number higher than 92, tend to split into two smaller nucleoids that are more stable and lease a large amount of energy –a process called nuclear fission.

Both the fusion and fission processes release a tremendous amount of energy, called nuclear energy or atomic energy, which is the difference between the nuclear binding energy of the parent and the daughter nucleoid.

Nuclear fusion -a source of energy in the sun and stars

The universe is composed of about 98% hydrogen and helium. Sun is composed of about 74% hydrogen, 25% helium, and 1% all other elements. The light nucleoid like hydrogen and helium fuse to make heavier nucleoids and subatomic particles like neutrons in a process called nuclear fusion. Nuclear fusion releases energy that is the difference in the nuclear binding energy of their nucleons in the daughter and parent nucleoids. Fusion energy is the source of energy for the sun and stars. Some of the nuclear fusion reactions, illustrated in Fig. 8.1.1 are the following.

$${}^{1}_{1}\mathrm{H} + {}^{1}_{1}\mathrm{H} \longrightarrow {}^{2}_{2}\mathrm{H} + {}^{0}_{1}\mathrm{e}$$

$$ {}_{1}^{1}\mathrm{H} + {}_{1}^{2}\mathrm{H} \longrightarrow {}_{2}^{3}\mathrm{H} $$

$$ {}_{2}^{3}\mathrm{H} + {}_{2}^{3}\mathrm{H} \longrightarrow {}_{2}^{4}\mathrm{H} + 2\,{}_{1}^{1}\mathrm{H} $$

$$ {}_{2}^{3}\mathrm{H} + {}_{1}^{1}\mathrm{H} \longrightarrow {}_{2}^{4}\mathrm{H} + {}_{1}^{0}\mathrm{e} $$

Although hydrogen is abundant on earth and a potential source of energy, the controlled fusion reaction is not yet economically feasible. The main difficulty is that the fusion of nuclei requires extremely high temperature, greater than a hundred thousand Celsius, and extremely high pressure, greater than a hundred thousand atmospheres, to overcome the repulsive forces of the like charges of the nuclei before they can fuse. For this reason, nuclear fusion reactions are also called thermonuclear reactions. Such conditions exist in sun and stars where these reactions routinely happen, but there are many technical problems yet to overcome before the energy can be harnessed economically from the nuclear fusion reactions on earth. A nuclear explosion can create the conditions needed for the thermonuclear reactions and are used to carry out uncontrolled thermonuclear reactions to boost the explosive power of nuclear weapons. Such a nuclear weapon is called a thermonuclear or hydrogen bomb.

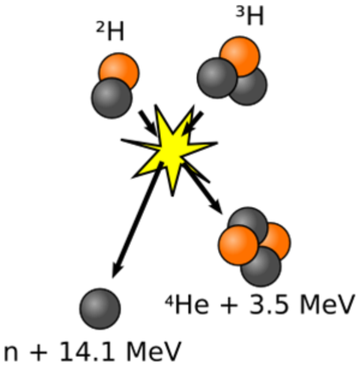


Figure 8.8.2: Fusion of deuterium with tritium creating helium-4, freeing a neutron, and releasing 17.59 MeV as kinetic energy of the products while a corresponding amount of mass disappears, in agreement with kinetic $E = \Delta mc^2$, where Δm is the decrease in the total rest mass of particles. Source: Wykis (talk · contribs), Public domain, via Wikimedia Commons

One of the potential candidate reactions for nuclear fusion reactors is the fusion of deuterium with tritium, illustrated in Fig. 8.8.2, which requires a little less harsh conditions. Most of the research is focused on the device called Tokamak, which uses strong magnetic fields to contain and heat the materials for the reaction, but so far it is not economically feasible to use it as a source of energy for commercial uses.

Nuclear fission -the source of energy in nuclear power plants and in nuclear weapons

Nuclear fission is a radioactive decay process in which a heavier nucleoid splits into two or lighter nucleoids and releases a tremendous amount of energy that is the difference in the binding energy of nucleons in the daughter and the parent nucleoids. The nucleoids that do spontaneous fission are marked green in Fig. 8.2.1.

Nuclear fuel

Induced fission is fission that occurs upon bombardment of a nucleoid with a nuclear particle, like a neutron. For example, the bombardment of uranium-235 or plutonium-239 by a neutron causes the fission and releases about three neutrons along with the smaller nucleoids, as illustrated in Fig. 8.8.3. The neutrons released by the fission cause fission of another nucleoid starting a **nuclear chain reaction**. The nuclei like uranium-235 or plutonium-239 that produce neutrons in the product that are capable of continuing the fission in a chain reaction are called **fissile**. The fissile nucleoids are nuclear fuels used in nuclear power plants to produce nuclear energy.

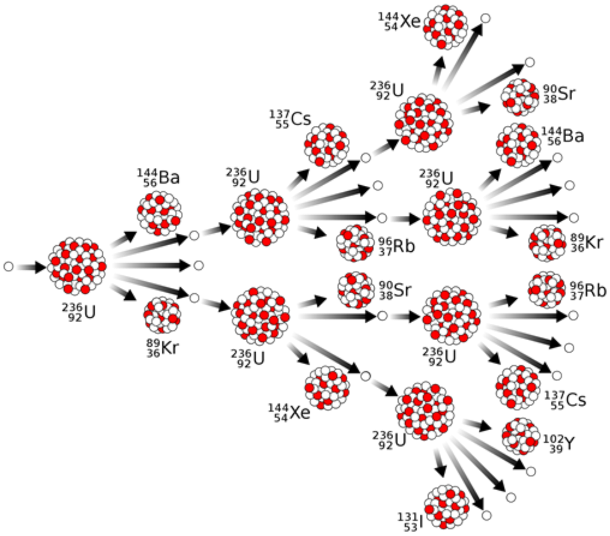


Figure 8.8.3: Illustration of a nuclear fission chain reaction. Source: MikeRun / CC BY-SA (https://creativecommons.org/licenses/by-sa/4.0)

Fate of neutron released in a fission event

The neutrons released in a fission event may be lost, absorbed by another nucleus like uranium-238 that does not fission, or may be absorbed by another fissile nucleoid and repeat the fission, as illustrated in Fig. 8.8.4. Three situations may arise, If, on the average;

1. less than one neutron released causes new fission, the process dyes,
2. one neutron released causes new fission, the fission continues in a controlled way as in nuclear power plants,
3. more than one neutron released causes new fission, the fission increases exponentially resulting in a nuclear explosion, as illustrated in Fig. 8.8.3.

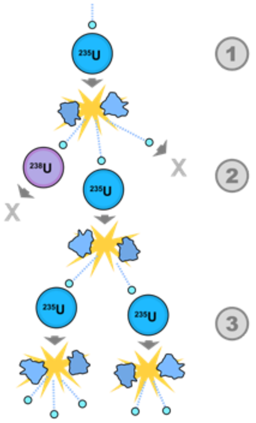


Figure 8.8.4: A schematic nuclear fission chain reaction. 1. A uranium-235 atom absorbs a neutron and fissions into two new atoms (fission fragments), releasing three new neutrons and some binding energy. 2. One of those neutrons is absorbed by an atom of uranium-238 and does not continue the reaction. Another neutron is simply lost and does not collide with anything, also not continuing the reaction. However, the one neutron does collide with an atom of uranium-235, which then fissions and releases two neutrons and some binding energy. 3. Both of those neutrons collide with uranium-235 atoms, each of which fissions and releases between one and three neutrons, which can then continue the reaction. Source: Fastfission/ Public domain

Note that each fission event does not necessarily split the parent nucleoid into exact same daughter nucleoids, it can split into different combinations of daughter nucleoids resulting in a mixture of products that are usually radioactive, as illustrated in Fig. 8.8.4.

Atomic bomb

A certain minimum mass of the fissile material, called **critical mass**, is necessary for a fission event to grow exponentially and cause a nuclear explosion. The critical mass is less for a more enriched fissile material. Therefore, usually enriched uranium-235 or plutonium 239 is used as an explosive in an atomic bomb. The mass more than the critical mass, called supercritical mass, is split into sub-critical portions which are kept separate in the weapon to avoid a nuclear explosion. When needed, the conventional chemical explosion is used to force the sub-critical portions to combine and make a supercritical mass for a nuclear explosion to happen, as illustrated in Fig. 8.8.5.

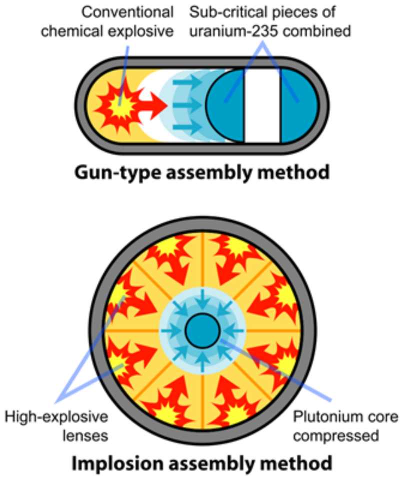


Figure 8.8.5: Schematic representation of the two methods with which to assemble a fission bomb. Source: Fastfission/ Public domain

Nuclear power plant

Nuclear power plants, like the one illustrated in Fig. 8.8.6, harness the energy released during fission for electricity production. The fissile material is assembled in the form of fuel rods in the core of a nuclear reactor. It is important to sustain the nuclear chain reaction but it is critical to keep it under control so that the chain reaction may not grow exponentially and cause a nuclear explosion. Rods of material, like palladium or boron that are efficient neutron absorbers, are included in the design of the reactor core. The neutron absorber rods can be lowered or raised to control the neutron flux available to sustain the fission chain reaction.

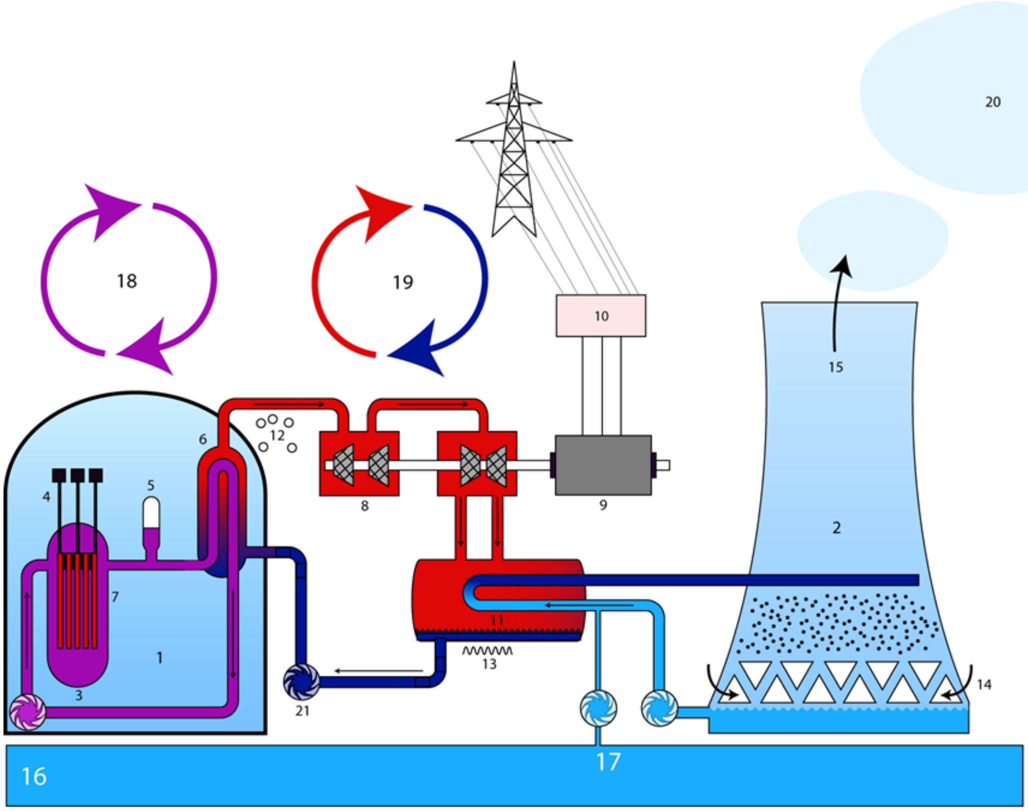


Figure 8.8.1: Design of a nuclear power plant with a pressurized water reactor (PWR).

1. reactor block, 2. cooling tower, 3. reactor, 4. control rod, 5. support for pressure, 6. steam generator, 7. fuel element, 8. turbine, 9. generator, 10. transformer, 11. condenser, 12. gaseous, 13. liquid, 14.air, 15.air (humid), 16. river, 17. cooling-water circulation, 18. primary circuit, 19. secondary circuit, 20. water vapor, 21. pump. Source: Steffen Kuntoff / CC BY-SA 2.0 DE (https://creativecommons.org/licenses...2.0/de/deed.en)

The reactor core is surrounded by a coolant and moderator, which may be regular water (H_2O) or heavy water (D_2O), or some other material. It is called coolant because it takes away the heat produced by the fission reaction and moderator because it also slows down the fast neutrons released in fission. The slow neutrons are more effective for the fission reaction. The coolant transfers its heat to a steam generator. All of these components are housed in a containment building to keep the radioactivity contained, even if a nuclear accident happens. The steam is used to drive a turbine for electricity production, and the condensed water is cooled using water from the cooling tower and returned for reuse, as illustrated in Fig. 8.8.6.

Nuclear power plants produce about 20% of the electricity in the USA. Fig. 8.8.7 shows a nuclear power plant in Arkansas. In some countries, the contribution of nuclear power to the total electricity is much higher, e.g., about 70% of electricity is produced by nuclear power plants in France. Nuclear power is considered an energy source of the future, or at least for a transition from fossil fuel to the next major energy source when the fossil fuel reserves will exhaust.

Figure 8.8.1: Russellville nuclear power plant in Arkansas, showing a cooling tower in the front with non-radioactive steam evaporating from it. Source: Edibobb, CC BY 3.0 <https://creativecommons.org/licenses/by/3.0>, via Wikimedia Commons

The fission products in the nuclear power plants become **radioactive waste** that needs to be stored for at least 10 half-lives to reach an acceptable radioactivity level. Based on the 28.8 years half-life of strontium-90 which is the long-lived and dangerous product in nuclear waste, a storage time of 300 years is needed. Handling radioactive waste is an issue of concern associated with nuclear power production. Plutonium-239 is another radioactive isotope produced from neutron absorption by uranium-238. Uranium-238 is a major constituent (99.28%) in the natural uranium along with fissile uranium-235 (0.71%). Plutonium-239 has a long half-life (24,000 Years) but it can be extracted in a fuel reprocessing plant and used as a nuclear fuel.

Index

Glossary

Element | An element is pure matter composed of only one type of atom.

Matter | Matter is anything that has mass and occupies space.

Pure matter | Pure matter has a constant and a non-variable composition of the type of atoms.

Symbol of element | One or two-letter abbreviation of the name of an element. The first letter is always capitalized, and the second, if needed, is small.

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        - 3.2: Naming binary ionic compounds — *Public Domain*
        - 3.3: Polyatomic ions and their compounds — *Public Domain*
        - 3.4: Naming acids — *Public Domain*
        - 3.5: Naming binary covalent compounds — *Public Domain*
        - 3.6: Lewis structures of molecules — *Public Domain*
        - 3.7: Molecular shapes –Valence shell electron pair repulsion (VSEPR) theory — *Public Domain*
        - 3.8: Polarity of molecules — *Public Domain*
        - 3.9: Intramolecular forces and intermolecular forces — *Public Domain*
    - 4: Stoichiometry –the quantification of chemical reactions — *Public Domain*
        - 4.1: Stoichiometry — *Public Domain*
        - 4.2: The mole — *Public Domain*
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        - 4.4: Patterns of chemical reactions — *Public Domain*
        - 4.5: Oxidation-reduction reactions — *Public Domain*
        - 4.6: Energetics of chemical reactions — *Public Domain*
        - 4.7: Stoichiometric calculations — *Public Domain*
    - 5: Solutions — *Public Domain*
        - 5.1: Introduction to solution — *Public Domain*
        - 5.2: Solubility — *Public Domain*
        - 5.3: Electrolytes — *Public Domain*
        - 5.4: Concentration of solutions — *Public Domain*
        - 5.5: Osmosis — *Public Domain*
    - 6: Acids and bases — *Public Domain*
        - 6.1: What is an acid and a base? — *Public Domain*
        - 6.2: Brønsted–Lowry acids and bases — *Public Domain*
        - 6.3: Strength of acids and bases — *Public Domain*
        - 6.4: Acid-base equilibrium — *Public Domain*
        - 6.5: Dissociation of water — *Public Domain*
        - 6.6: The pH — *Public Domain*
        - 6.7: Acid-base reactions — *Public Domain*
        - 6.8: pH Buffers — *Public Domain*
    - 7: Gases — *Public Domain*
        - 7.1: Characteristics of gases — *Public Domain*
        - 7.2: The pressure-volume relationship — *Public Domain*

    - 7.3: The temperature-volume relationship — *Public Domain*
    - 7.4: The pressure-temperature relationship — *Public Domain*
    - 7.5: The combined gas law — *Public Domain*
    - 7.6: The volume-amount relationship — *Public Domain*
    - 7.7: Ideal gas law — *Public Domain*
    - 7.8: Dalton’s law of partial pressure — *Public Domain*
- 8: Nuclear chemistry — *Public Domain*
    - 8.1: Introduction to nuclear chemistry — *Public Domain*
    - 8.2: Radioactivity — *Public Domain*
    - 8.3: Half-life of radioisotopes — *Public Domain*
    - 8.4: Radiation measurements — *Public Domain*
    - 8.5: Ionizing radiation exposures — *Public Domain*
    - 8.6: Medical uses of radioisotopes — *Public Domain*
    - 8.7: Making radioisotopes for medical uses — *Public Domain*
    - 8.8: Nuclear fusion and fission — *Public Domain*
- Back Matter — *Undeclared*
    - Index — *Undeclared*
    - Glossary — *Undeclared*
    - Detailed Licensing — *Undeclared*